Evaluating a Lagrangian Soot Tracking Method for the Prediction of Primary Soot Particle Size under Engine-like Conditions

This paper reports the implementation and evaluation of a Lagrangian soot tracking (LST) method for the modeling of soot in diesel engines. The LST model employed here has the tracking capability of a Lagrangian method and the ability to predict primary soot particle sizing. The Moss-Brookes soot model is used here as the Eulerian method to simulate soot formation and oxidation processes. The inception, surface growth and oxidation models are adopted and modified such that the associated reaction rates can be computed using the Lagrangian approach. The soot nuclei are treated as Lagrangian particles when the mass of incipient soot exceeds a designated threshold value. Their trajectories are then computed using the particle momentum equation. The change of primary soot particle size is dependent on the modified Lagrangian surface growth and soot oxidation models. Performance of the LST model in predicting temporal soot cloud development, mean soot diameter and primary soot size distribution is evaluated using measurements of n-heptane and n-dodecane spray combustion obtained under diesel engine-like conditions. In addition, sensitivity studies are carried out to investigate the influence of soot surface ageing and oxidation rates on the primary soot particle size distribution. With the use of surface ageing, the predicted maximum primary soot particle sizes are closer to the experimentally measured maximum primary soot sizes. Also, the associated particle size distribution shows a lognormal shape. A higher rate of soot oxidation due to OH causes the soot particles to be fully oxidized downstream of the flame. In general, the LST model performs better than the Eulerian method in terms of predicting soot sizing and accessing information of individual soot particles, both of which are shortcomings of the Eulerian method.

General Information
State: Published
Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, Thermal Energy, University of Nottingham, Malaysia Campus
Authors: Cai Ong, J. (Ekstern), Pang, K. M. (Intern), Walther, J. H. (Intern), Ho, J. (Ekstern), Kiat Ng, H. (Ekstern)
Pages: 70-95
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BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.21 SJR 0.843 SNIP 1.199
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.072 SNIP 1.318 CiteScore 2.47  
BFI (2014): BFI-level 1  
Scopus rating (2014): SJR 1.068 SNIP 1.586 CiteScore 2.72  
Web of Science (2014): Indexed yes  
BFI (2013): BFI-level 1  
Scopus rating (2013): SJR 1.187 SNIP 1.858 CiteScore 2.9  
ISI indexed (2013): ISI indexed yes  
BFI (2012): BFI-level 1  
Scopus rating (2012): SJR 1.294 SNIP 1.638 CiteScore 2.64  
ISI indexed (2012): ISI indexed yes  
Web of Science (2012): Indexed yes  
BFI (2011): BFI-level 1  
Scopus rating (2011): SJR 1.137 SNIP 1.623 CiteScore 2.63  
ISI indexed (2011): ISI indexed yes  
BFI (2010): BFI-level 1  
Scopus rating (2010): SJR 1.169 SNIP 1.604  
Web of Science (2010): Indexed yes  
BFI (2009): BFI-level 1  
Scopus rating (2009): SJR 1.457 SNIP 1.782  
Web of Science (2009): Indexed yes  
BFI (2008): BFI-level 2  
Scopus rating (2008): SJR 1.375 SNIP 1.353  
Scopus rating (2007): SJR 0.999 SNIP 0.892  
Scopus rating (2006): SJR 1.044 SNIP 0.929  
Scopus rating (2005): SJR 0.812 SNIP 0.737  
Scopus rating (2004): SJR 1.278 SNIP 1.932  
Scopus rating (2003): SJR 0.616 SNIP 0.554  
Scopus rating (2002): SJR 0.666 SNIP 0.636  
Scopus rating (2001): SJR 0.455 SNIP 0.419  
Scopus rating (2000): SJR 0.457 SNIP 0.687  
Web of Science (2000): Indexed yes  
Scopus rating (1999): SJR 0.52 SNIP 0.349  
Original language: English  
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Publication: Research - peer-review › Journal article – Annual report year: 2018  

Near-wellbore modeling of a horizontal well with Computational Fluid Dynamics  
The oil production by horizontal wells is a complex phenomenon that involves flow through the porous reservoir, completion interface and the well itself. Conventional reservoir simulators can hardly resolve the flow through the completion into the wellbore. On the contrary, Computational Fluid Dynamics (CFD) is capable of modeling the complex interaction between the creeping reservoir flow and turbulent well flow for single phases, while capturing both the completion geometry and formation damage. A series of single phase steady-state simulations are undertaken, using such fully coupled three dimensional numerical models, to predict the inflow to the well. The present study considers the applicability of CFD for near-wellbore modeling through benchmark cases with available analytical solutions. Moreover, single phase steady-state numerical investigations are performed on a specific perforated horizontal well producing from the Siri field, offshore Denmark. The performance of the well is investigated with an emphasis on the inflow profile and the productivity index for different formation damage scenarios. A considerable redistribution of the inflow profile were found when the filtrate invasion extended beyond the tip of the perforations.  

General information  
State: Published  
Organisations: Department of Mechanical Engineering, Scientific Computing, Fluid Mechanics, Coastal and Maritime Engineering, Department of Chemistry, CERE – Center for Energy Ressources Engineering, Technical University of Denmark, Lloyd's Register Consulting  
Authors: Szanyi, M. L. (Ekstern), Hemmingsen, C. S. (Intern), Yan, W. (Intern), Watther, J. H. (Intern), Glimberg, S. L. (Ekstern)
Numerical simulation of condensation of sulfuric acid and water in a large two-stroke marine diesel engine

In the present study, three-dimensional (3D) computational fluid dynamics simulations are performed to examine the process of sulfuric acid (H2SO4) and water (H2O) condensation in a large two-stroke marine diesel engine. A skeletal n-heptane chemical mechanism is coupled with a sulfur (S) subset to simulate the combustion process as well as the formation of sulfuric oxides (SOx) and H2SO4. The condensation process is simulated using a fluid film model which is coupled with the in-cylinder gas phase. Prior to the engine simulations, the fluid film condensation model is validated using the experimental data of sulfuric acid condensation rate in a laminar pipe flow. Next, the engine model is validated against the experimental sulfur dioxide (SO2) to sulfur trioxide (SO3) conversion obtained from the corresponding test engine. Both of the validation studies show a good agreement with the experimental data. The engine model is then utilized to simulate condensation for different operating conditions. The engine simulation results reveal that the fluid film has a significant effect on the total mass of sulfuric acid vapor and a marginal effect on the total mass of water vapor. A close to linear correlation is found between the fuel sulfur content and the total condensed mass of sulfuric acid. The level of humidity of the scavenging air does not affect the condensation of sulfuric acid considerably, relative to the humidity increase, but it has a high impact on water condensation. The study of the scavenging pressure level reveals a counter intuitive behavior where the condensation rates decrease with higher scavenging pressures due to the flow regime and flame size. Next, increasing the cylinder liner temperature decreases significantly the water condensation contrary to the sulfuric acid condensation which is marginally affected. The increase in lubricant film thickness results in a decrease for both the sulfuric acid and water condensation with a more pronounced reduction for water. Finally, a comparison between the high and low load operating conditions reveals a small drop in the total condensed mass of sulfuric acid and water for the low load conditions.

General information
State: Published
Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, Thermal Energy, MAN B&W Diesel A/S
Authors: Karvounis, N. (Intern), Pang, K. M. (Intern), Mayer, S. (Ekstern), Walther, J. H. (Intern)
Pages: 1009-1020
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Main Research Area: Technical/natural sciences

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BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 7.78 SJR 3.058 SNIP 2.573
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.912 SNIP 2.61 CiteScore 6.4
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 3.254 SNIP 3.28 CiteScore 6.93
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 3.164 SNIP 3.377 CiteScore 6.59
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.854 SNIP 3.108 CiteScore 5.69
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
Adjoint Optimisation of the Turbulent Flow in an Annular Diffuser

In the present study, a numerical optimisation of guide vanes in an annular diffuser, is performed. The optimisation is performed for the purpose of improving the following two parameters simultaneously; the first parameter is the uniformity perpendicular to the flow direction, a 1/3 diameter downstream of the expansion. The second parameter is the pressure loss introduced by these guide vanes. The optimisation yields an improvement of the uniformity of 1.5% and a 28% reduction in the over all pressure loss.

General information

State: Published
Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, Technical University of Denmark, MAN Diesel and Turbo
Authors: Gotfredsen, E. (Intern), Agular Knudsen, C. (Ekstern), Kunoy, J. D. (Ekstern), Meyer, K. E. (Intern), Walther, J. H. (Intern)
Pages: 71-74
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BFI conference series: Nordic Seminar on Computational Mechanics (5010906)
Main Research Area: Technical/natural sciences
Conference: 30th Nordic Seminar on Computational Mechanics (NSCM-30), Copenhagen, 25/10/2017 - 25/10/2017

Publication: Research - peer-review » Conference abstract in proceedings – Annual report year: 2017
A regularization method for solving the Poisson equation for mixed unbounded-periodic domains

Abstract Regularized Green's functions for mixed unbounded-periodic domains are derived. The regularization of the Green's function removes its singularity by introducing a regularization radius which is related to the discretization length and hence imposes a minimum resolved scale. In this way the regularized unbounded-periodic Green's functions can be implemented in an FFT-based Poisson solver to obtain a convergence rate corresponding to the regularization order of the Green's function. The high order is achieved without any additional computational cost from the conventional FFT-based Poisson solver and enables the calculation of the derivative of the solution to the same high order by direct spectral differentiation. We illustrate an application of the FFT-based Poisson solver by using it with a vortex particle mesh method for the approximation of incompressible flow for a problem with a single periodic and two unbounded directions.

General information
State: Accepted/In press
Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering
Authors: Juul Spietz, H. (Intern), Mølholm Hejlesen, M. (Intern), Walther, J. H. (Intern)
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Journal: Journal of Computational Physics
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Ratings:
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BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.12 SJR 2.034 SNIP 1.822
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.098 SNIP 1.988 CiteScore 2.92
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.166 SNIP 2.193 CiteScore 3.12
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 2.227 SNIP 2.45 CiteScore 3.3
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.161 SNIP 2.052 CiteScore 2.69
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.06 SNIP 2.194 CiteScore 2.99
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 2.185 SNIP 2.096
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 2.439 SNIP 2.219
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 2.247 SNIP 2.03
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 2.377 SNIP 2.379
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 2.182 SNIP 2.285
A regularized vortex-particle mesh method for large eddy simulation
We present recent developments of the remeshed vortex particle-mesh method for simulating incompressible fluid flow. The presented method relies on a parallel higher-order FFT based solver for the Poisson equation. Arbitrary high order is achieved through regularization of singular Green’s function solutions to the Poisson equation and recently we have derived novel high order solutions for a mixture of open and periodic domains. With this approach the simulated variables may formally be viewed as the approximate solution to the filtered Navier Stokes equations, hence we use the method for Large Eddy Simulation by including a dynamic subfilter-scale model based on test-filters compatible with the aforementioned regularization functions. Further the subfilter-scale model uses Lagrangian averaging, which is a natural candidate in light of the Lagrangian nature of vortex particle methods. A multiresolution variation of the method is applied to simulate the benchmark problem of the flow past a square cylinder at Re = 22000 and the obtained results are compared to results from the literature.

General information
State: Published
Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering
Authors: Spietz, H. J. (Intern), Walther, J. H. (Intern), Hejlesen, M. M. (Intern)
Number of pages: 1
Publication date: 2017
Event: Abstract from 70th Annual Meeting of the American Physical Society Division of Fluid Dynamics (DFD17), Denver, United States.
Main Research Area: Technical/natural sciences
Electronic versions:
abstract_hejusp.pdf
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2017

Carbon Nanotubes as Thermally Induced Water Pumps
Thermal Brownian motors (TBMs) are nanoscale machines that exploit thermal fluctuations to provide useful work. We introduce a TBM-based nanopump which enables continuous water flow through a carbon nanotube (CNT) by imposing an axial thermal gradient along its surface. We impose spatial asymmetry along the CNT by immobilizing certain points on its surface. We study the performance of this molecular motor using molecular dynamics (MD) simulations. From the MD trajectories, we compute the net water flow and the induced velocity profiles for various imposed thermal gradients. We find that spatial asymmetry modifies the vibrational modes of the CNT induced by the thermal gradient, resulting in a net water flow against the thermal gradient. Moreover, the kinetic energy associated with the thermal oscillations rectifies the Brownian motion of the water molecules, driving the flow in a preferred direction. For imposed thermal gradients of 0.5-3.3 K/nm, we observe continuous net flow with average velocities up to 5 m/s inside CNTs with diameters of 0.94, 1.4, and 2.0 nm. The results indicate that the CNT-based asymmetric thermal motor can provide a controllable and robust system for delivery of continuous water flow with potential applications in integrated nanofluidic devices.

General information
State: Published
Cavity prediction in sand mould production applying the DISAMATIC process

The sand shot in the DISAMATIC process is simulated by the discrete element method (DEM) taking into account the influence and coupling of the airflow with computational fluid dynamics (CFD). The DEM model is calibrated by a ring shear test, a sand pile experiment and a slump test. Subsequently, the DEM model is used to model the propagation of the green sand inside the mold chamber and the results are compared to experimental video footage. The chamber contains two cavities designed to quantify the deposited mass of green sand. The deposition of green sand in these two cavities is investigated with three cases of different air vent settings which control the ventilation of the chamber. These settings resulted in different air- and particle-velocities as well as different accumulated masses in the cavities, which were
successfully simulated by the model.

**General information**

State: Published  
Organisations: Department of Mechanical Engineering, Manufacturing Engineering, Fluid Mechanics, Coastal and Maritime Engineering, DISA Industries A/S  
Authors: Hovad, E. (Intern), Larsen, P. (Ekstern), Spangenberg, J. (Intern), Walther, J. H. (Intern), Thorborg, J. (Intern), Hattel, J. H. (Intern)  
Pages: 204-217  
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Main Research Area: Technical/natural sciences

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BFI (2018): BFI-level 1  
BFI (2017): BFI-level 1  
Web of Science (2017): Indexed yes  
BFI (2016): BFI-level 1  
Scopus rating (2016): CiteScore 3.16 SJR 0.983 SNIP 1.482  
Web of Science (2016): Indexed yes  
BFI (2015): BFI-level 1  
Scopus rating (2015): SJR 0.965 SNIP 1.598 CiteScore 2.99  
Web of Science (2015): Indexed yes  
BFI (2014): BFI-level 1  
Scopus rating (2014): SJR 0.89 SNIP 1.649 CiteScore 2.67  
Web of Science (2014): Indexed yes  
BFI (2013): BFI-level 1  
Scopus rating (2013): SJR 0.901 SNIP 1.875 CiteScore 2.64  
ISI indexed (2013): ISI indexed yes  
BFI (2012): BFI-level 1  
Scopus rating (2012): SJR 0.854 SNIP 1.826 CiteScore 2.36  
ISI indexed (2012): ISI indexed yes  
BFI (2011): BFI-level 1  
Scopus rating (2011): SJR 0.921 SNIP 1.86 CiteScore 2.45  
ISI indexed (2011): ISI indexed yes  
Web of Science (2011): Indexed yes  
BFI (2010): BFI-level 1  
Scopus rating (2010): SJR 0.94 SNIP 1.547  
BFI (2009): BFI-level 1  
Scopus rating (2009): SJR 0.98 SNIP 1.65  
BFI (2008): BFI-level 1  
Scopus rating (2008): SJR 0.911 SNIP 1.597  
Web of Science (2008): Indexed yes  
Scopus rating (2007): SJR 0.854 SNIP 1.316  
Web of Science (2007): Indexed yes  
Scopus rating (2006): SJR 1.118 SNIP 1.324  
Web of Science (2006): Indexed yes  
Scopus rating (2005): SJR 1.253 SNIP 1.399  
Web of Science (2005): Indexed yes  
Scopus rating (2004): SJR 0.867 SNIP 1.341  
Scopus rating (2003): SJR 1.348 SNIP 1.489  
Scopus rating (2002): SJR 1.285 SNIP 1.369  
Scopus rating (2001): SJR 1.11 SNIP 1.292
CFD modeling of condensation process of water vapor in supersonic flows

The condensation phenomenon of vapor plays an important role in various industries, such as the steam flow in turbines and refrigeration systems. A mathematical model is developed to predict the spontaneous condensing phenomenon in the supersonic flows using the nucleation and droplet growth theories. The numerical approach is validated with the experimental data, which shows a good agreement between them. The condensation characteristics of water vapor in the Laval nozzle are described in detail. The results show that the condensation process is a rapid variation of the vapor-liquid phase change both in the space and in time. The spontaneous condensation of water vapor will not appear immediately when the steam reaches the saturation state. Instead, it occurs further downstream the nozzle throat, where the steam is in the state of supersaturation.
Characterization and Erosion Modeling of a Nozzle-Based Inflow-Control Device
In the petroleum industry, water-and-gas breakthrough in hydrocarbon reservoirs is a common issue that eventually leads to uneconomic production. To extend the economic production lifetime, inflow-control devices (ICDs) are designed to delay the water-and-gas breakthrough. Because the lifetime of a hydrocarbon reservoir commonly exceeds 20 years and it is a harsh environment, the reliability of the ICDs is vital.

General information
State: Accepted/In press
Organisations: Department of Chemistry, Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, Welltec, Lloyd’s Register Consulting
Authors: Olsen, J. J. (Intern), Hemmingsen, C. S. (Intern), Bergmann, L. (Ekstern), Nielsen, K. K. (Ekstern), Glimberg, S. L. (Ekstern), Walther, J. H. (Intern)
Number of pages: 10
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Main Research Area: Technical/natural sciences

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Journal: SPE Journal
ISSN (Print): 1086-055X
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BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.95 SNIP 2.003 CiteScore 3.01
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.976 SNIP 1.838 CiteScore 2.37
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.185 SNIP 2.152 CiteScore 2.43
Choanoflagellates are unicellular aquatic organisms with a single flagellum that drives a feeding current through a funnel-shaped collar filter on which bacteria-sized prey are caught. Using computational fluid dynamics (CFD) we model the beating flagellum and the complex filter flow of the choanoflagellate Diaphanoeca grandis. Our CFD simulations based on the current understanding of the morphology underestimate the experimentally observed clearance rate by more than an order of magnitude: The beating flagellum is simply unable to draw enough water through the fine filter. Our observations motivate us to suggest a radically different filtration mechanism that requires a flagellar vane (sheet), and addition of a wide vane in our CFD model allows us to correctly predict the observed clearance rate.

Computational Fluid Dynamics of Choanoflagellate Filter-Feeding
Choanoflagellates are unicellular aquatic organisms with a single flagellum that drives a feeding current through a funnel-shaped collar filter on which bacteria-sized prey are caught. Using computational fluid dynamics (CFD) we model the beating flagellum and the complex filter flow of the choanoflagellate Diaphanoeca grandis. Our CFD simulations based on the current understanding of the morphology underestimate the experimentally observed clearance rate by more than an order of magnitude: The beating flagellum is simply unable to draw enough water through the fine filter. Our observations motivate us to suggest a radically different filtration mechanism that requires a flagellar vane (sheet), and addition of a wide vane in our CFD model allows us to correctly predict the observed clearance rate.

General information
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Organizations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, National Institute of Aquatic Resources, Centre for Ocean Life, Department of Physics, Biophysics and Fluids
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Event: Abstract from 70th Annual Meeting of the American Physical Society Division of Fluid Dynamics (DFD17), Denver, United States.
Main Research Area: Technical/natural sciences
Drag reduction in silica nanochannels induced by graphitic wall coatings

Transport of water in hydrophilic nanopores is of significant technological and scientific interest. Water flow through hydrophilic nanochannels is known to experience enormous hydraulic resistance. Therefore, drag reduction is essential for the development of highly efficient nanofluidic devices. In this work, we propose the use of graphitic materials as wall coatings in hydrophilic silica nanopores. Specifically, by conducting atomistic simulations, we investigate the flow inside slit and cylindrical silica channels with walls coated with graphene (GE) layers and carbon nanotubes (CNTs), respectively. We develop realistic force fields to simulate the systems of interest and systematically compare flow rates in coated and uncoated nanochannels under different pressure gradients. Moreover, we assess the effect that GE and CNT translucencies to wettability have on water hydrodynamics in the nanochannels. The influence of channel size is investigated by systematically varying channel heights and nanopore diameters. In particular, we present the computed water density and velocity profiles, volumetric flow rates, slip lengths and flow enhancements, to clearly demonstrate the drag reduction capabilities of graphitic wall coatings.

Effects of Nozzle Diameter on Diesel Spray Flames: A numerical study using an Eulerian Stochastic Field Method

The present numerical study aims to assess the performance of an Eulerian Stochastic Field (ESF) model in simulating spray flames produced by three fuel injectors with different nozzle diameters of 100 μm, 180 μm and 363 μm. A comparison to the measurements shows that although the simulated ignition delay times are consistently overestimated, the relative differences remain below 28%. Furthermore, the change of the averaged pressure rise with respect to the variation of nozzle diameter is captured by the model. The simulated flame lift-off lengths also agree with the measurements, with a maximum relative difference of 13%. The spray flame produced by a larger nozzle diameter has a fuel-richer premixed core region despite the longer lift-off length, indicating that the higher fueling rate used with the larger nozzle diameter is a more dominating factor than the lift-off length is in influencing the air entrainment into the upstream of the spray flames. In addition, the simulated normalised flame lengths are found to decrease when the nozzle diameters increase. These predictions are in good qualitative agreement with the experimental observation. This work proves that the ESF model can serve as an important tool for the simulation of spray flames in marine diesel engines, where fuel injectors with different nozzle diameters are applied for pilot and main injections.
Hybrid vortex simulations of wind turbines using a three-dimensional viscous-inviscid panel method

A hybrid filament-mesh vortex method is proposed and validated to predict the aerodynamic performance of wind turbines and to simulate the resulting wake. Its novelty consists of using a hybrid method to accurately simulate the wakedownstream of the wind turbine while reducing the computational time used by the method. The proposed method uses a hybrid approach, where the near wake is resolved by using vortex filaments, which carry the vorticity shed by the trailing edge of the blades. The interaction of the vortex filaments in the near vicinity of the wind turbine is evaluated using a direct calculation, whereas the contribution from the large downstream wake is calculated using a mesh-based method. The hybrid method is first validated in detail against the well-known MEXICO experiment, using the direct filament method as a comparison. The second part of the validation includes a study of the influence of the time-integration scheme used for evolving the wake in time, aeroelastic simulations of the National Renewable Energy Laboratory 5 MW wind turbine and an analysis of the central processing unit time showing the gains of using the hybrid filament-mesh method.

General information
State: Published
Organisations: Department of Wind Energy, Fluid Mechanics, Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering
Authors: Ramos García, N. (Intern), Hejlesen, M. M. (Intern), Sørensen, J. N. (Intern), Walther, J. H. (Intern)
Pages: 1871-1889
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Main Research Area: Technical/natural sciences

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BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.37 SJR 1.104 SNIP 2.306
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.196 SNIP 2.086 CiteScore 3.06
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Hydrodynamics of microbial filter feeding

Microbial filter feeders are an important group of grazers, significant to the microbial loop, aquatic food webs, and biogeochemical cycling. Our understanding of microbial filter feeding is poor, and, importantly, it is unknown what force microbial filter feeders must generate to process adequate amounts of water. Also, the trade-off in the filter spacing remains unexplored, despite its simple formulation: A filter too coarse will allow suitably sized prey to pass unintercepted, whereas a filter too fine will cause strong flow resistance. We quantify the feeding flow of the filter-feeding choanoflagellate Diaphanoeca grandis using particle tracking, and demonstrate that the current understanding of microbial filter feeding is inconsistent with computational fluid dynamics (CFD) and analytical estimates. Both approaches underestimate observed filtration rates by more than an order of magnitude; the beating flagellum is simply unable to draw enough water through the fine filter. We find similar discrepancies for other choanoflagellate species, highlighting an apparent paradox. Our observations motivate us to suggest a radically different filtration mechanism that requires a flagellar vane (sheet), something notoriously difficult to visualize but sporadically observed in the related choanocytes (sponges). A CFD model with a flagellar vane correctly predicts the filtration rate of D. grandis, and using a simple model we can account for the filtration rates of other microbial filter feeders. We finally predict how optimum filter mesh size increases with cell size in
microbial filter feeders, a prediction that accords very well with observations. We expect our results to be of significance for small-scale biophysics and trait-based ecological modeling.

**General information**

State: Published

Organisations: National Institute of Aquatic Resources, Centre for Ocean Life, Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, Department of Physics, Biophysics and Fluids


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Main Research Area: Technical/natural sciences

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BFI (2018): BFI-level 2

BFI (2017): BFI-level 2

Web of Science (2017): Indexed yes

BFI (2016): BFI-level 2

Scopus rating (2016): CiteScore 8.56 SJR 6.321 SNIP 2.629

Web of Science (2016): Indexed yes

BFI (2015): BFI-level 2

Scopus rating (2015): SJR 6.767 SNIP 2.682 CiteScore 8.84

Web of Science (2015): Indexed yes

BFI (2014): BFI-level 2

Scopus rating (2014): SJR 6.853 SNIP 2.725 CiteScore 8.86

Web of Science (2014): Indexed yes

BFI (2013): BFI-level 2

Scopus rating (2013): SJR 6.989 SNIP 2.73 CiteScore 9.5

ISI indexed (2013): ISI indexed yes

Web of Science (2013): Indexed yes

BFI (2012): BFI-level 2

Scopus rating (2012): SJR 6.792 SNIP 2.682 CiteScore 9.49

ISI indexed (2012): ISI indexed yes

Web of Science (2012): Indexed yes

BFI (2011): BFI-level 2

Scopus rating (2011): SJR 6.771 SNIP 2.636 CiteScore 9.31

ISI indexed (2011): ISI indexed yes

Web of Science (2011): Indexed yes

BFI (2010): BFI-level 2

Scopus rating (2010): SJR 6.769 SNIP 2.529

Web of Science (2010): Indexed yes

BFI (2009): BFI-level 2

Scopus rating (2009): SJR 6.913 SNIP 2.544

Web of Science (2009): Indexed yes

BFI (2008): BFI-level 2

Scopus rating (2008): SJR 6.899 SNIP 2.445

Web of Science (2008): Indexed yes

Scopus rating (2007): SJR 6.766 SNIP 2.441

Web of Science (2007): Indexed yes

Scopus rating (2006): SJR 6.734 SNIP 2.434

Web of Science (2006): Indexed yes

Scopus rating (2005): SJR 6.784 SNIP 2.551
Investigation of journal orbit and flow pattern in a dynamically loaded journal bearing

A hydrodynamic journal bearing has been investigated using both the traditional two-dimensional (2D) Reynolds equation, and the full solution being the three-dimensional (3D) Navier-Stokes equations. The two approaches are compared by performing an investigation of two inlet groove designs: the axial and the circumferential groove, respectively, on a bearing with length-to-diameter ratio of 0.5 exposed to a sinusoidal load pattern. Pressure distributions, journal orbits and frictional losses are compared. The modelling of grooves by pressure boundary conditions versus geometric conditions is examined. It is investigated if the presence of a groove increases frictional losses and the increase relates to groove dimensions. Furthermore, the influence of the groove design on the flow field is studied using the 3D solution.

General information
State: Published
Organisations: Center for Bachelor of Engineering Studies, Afdelingen for Maskin og Design, Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, Solid Mechanics, MAN Diesel & Turbo
Authors: Christiansen, C. K. (Intern), Walther, J. H. (Intern), Klit, P. (Intern), Vølund, A. (Ekstern)
Pages: 450-457
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Tribology International
Volume: 114
ISSN (Print): 0301-679X
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.16 SJR 1.382 SNIP 2.094
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.437 SNIP 2.04 CiteScore 2.61
BFI (2014): BFI-level 1
Iterative Brinkman penalization for simulation of impulsively started flow past a sphere and a circular disc

We present a Brinkman penalization method for three-dimensional (3D) flows using particle vortex methods, improving the existing technique by means of an iterative process. We perform simulations to study the impulsively started flow past a sphere at Re=1000 and normal to a circular disc at Re=500. The simulation results obtained for the flow past a sphere are found in qualitative good agreement with previously published results obtained using respectively a 3D vortex penalization method and a 3D vortex method combined with an accurate boundary element method. From the results obtained for the flow normal to a circular disc it is found that the iterative method enables the use of a time step that is one order of magnitude larger than required by the standard non-iterative Brinkman penalization method.

State: Published
Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering
Authors: Spietz, H. J. (Intern), Hejlesen, M. M. (Intern), Walther, J. H. (Intern)
Pages: 261–274
Modelling of temporal and spatial evolution of sulphur oxides and sulphuric acid under large, two-stroke marine engine-like conditions using integrated CFD-chemical kinetics

In this work, three-dimensional computational fluid dynamics (CFD) studies of sulphur oxides (SOx) and sulphuric acid (H2SO4) formation processes in a large, low speed two-stroke marine diesel engine are carried out. The current numerical study aims to investigate the conversion of sulphuric dioxide (SO2) to sulphur trioxide (SO3) and the possibility of H2SO4 condensation which are the prerequisites to better understand the corrosion-induced wear phenomenon. This is achieved with the aid of the implementation of a multicomponent surrogate model, which comprises a skeletal n-heptane mechanism and a reduced sulphur subset mechanism. In the present work, performance of the coupled CFD-chemical kinetic model is evaluated using both qualitative and quantitative methods. The modelling results show that the temporal and spatial evolutions of SOx predicted by the skeletal model are similar to those by the base mechanism. Predictions of the variations of SOx and the associated SO2 to SO3 conversion in response to the change of fuel sulphur content, swirl velocity, start of injection, scavenge pressure and humidity qualitatively agree with numerical and experimental results from the literature. The model is further evaluated using the measured SO2 to SO3 conversion levels in a low load, low scavenge pressure case and a low load, high scavenge pressure case. The absolute values of simulated and measured conversion levels are close, although the former appear to be higher. The current results show that the flame impinges at the cylinder liner near top dead centre. The gas is cooled rapidly by the wall temperature and H2SO4 is produced in the region where the local temperature is less than 600 K. Based on the fluegas correlation, the acid dew point temperature is higher than the wall temperature, suggesting that acid condensation may begin early at the top part of the cylinder liner. The predicted distribution corresponds well with the distribution of corroded parts observed in service engines. The model is expected to serve as an important tool to simulate the rates of SO2 absorption into lubricating oil film and H2SO4 condensation in this combustion system.

General information
State: Published
Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, Thermal Energy, Department of Chemical and Biochemical Engineering, CHEC Research Centre, MAN Diesel & Turbo SE
Authors: Pang, K. M. (Intern), Karvounis, N. (Intern), Walther, J. H. (Intern), Schramm, J. (Intern), Glarborg, P. (Intern), Mayer, S. (Ekstern)
Pages: 60-73
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Applied Energy
Volume: 193
ISSN (Print): 0306-2619
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 7.78 SJR 3.058 SNIP 2.573
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.912 SNIP 2.61 CiteScore 6.4
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 3.254 SNIP 3.28 CiteScore 6.93
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 3.164 SNIP 3.377 CiteScore 6.59
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
On phonons and water flow enhancement in carbon nanotubes

The intriguing physics of water transport through carbon nanotubes (CNTs) has motivated numerous studies, reporting flow rates higher than those estimated by continuum models. The quantification of water transport in CNTs remains unresolved, however, with flow rates reported by different experiments and simulations having discrepancies of over three orders of magnitude. Reports of ultrafast and more modest rates conflict with each other. Molecular dynamics (MD) simulations have been used to resolve this puzzle by helping to decipher how the CNT walls interact with water molecules.

**General information**

State: Published
Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, Swiss Federal Institute of Technology, National Institute of Chemistry
Authors: Cruz-Chu, E. R. (Ekstern), Papadopoulou, E. (Ekstern), Walther, J. H. (Intern), Popadić, A. (Ekstern), Li, G. (Ekstern), Praprotnik, M. (Ekstern), Koumoutsakos, P. (Ekstern)
Pages: 1106-1107
Publication date: 2017
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Nature Nanotechnology
Volume: 12
ISSN (Print): 1748-3387
Slip divergence of water flow in graphene nanochannels: the role of chirality

Graphene has attracted considerable attention due to its characteristics as a 2D material and its fascinating properties, providing a potential building block for nanofabrication. In nanochannels the solid-liquid interface plays a non-negligible role in determining the fluid dynamics. Therefore, for an optimal design of nanofluidic devices, a comprehensive understanding of the slippage in a water flow confined between graphene walls is important. In nanofluidic systems, experimental and computational studies have found the slip length to increase nonlinearly when the shear rate is larger than a critical value. Here, by conducting molecular dynamics simulations, we study the influence of the graphene crystallographic orientation on the slip boundary conditions inside a nanoslit channel. The flow in channels with heights of 2.0, 2.4 and 2.8 nm is driven parallel to the zig-zag and arm-chair crystallographic directions. We extract flow rates, velocity profiles, slip velocities and slip lengths. The slip velocity displays a linear relationship to the shear stress up to a critical value, which is not size dependent. Moreover, the slip length is found to be shear stress dependent above a critical shear stress value of 0.4 MPa. Furthermore, our results indicate that after this critical shear stress is reached, the flow rates are significantly influenced (up to 10%) by the particular orientation of the graphene topology.

General information
State: Published
Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, Universidad de Concepcion
Suspended particle transport through constriction channel with Brownian motion

It is well known that translocation events of a polymer or rod through pores or narrower parts of micro- and nanochannels have a stochastic nature due to the Brownian motion. However, it is not clear whether the objects of interest need to have a larger size than the entrance to exhibit the deviation from the dynamics of the surrounding fluid. We show by numerical analysis that the particle injection into the narrower part of the channel is affected by thermal fluctuation, where the particles have spherical symmetry and are smaller than the height of the constriction. The Péclet number (Pe) is the order parameter that governs the phenomena, which clarifies the spatio-temporal significance of Brownian motion compared to hydrodynamics. Furthermore, we find that there exists an optimal condition of Pe to attain the highest flow rate of particles relative to the dispersant fluid flow. Our finding is important in science and technology from nanopore DNA sequencers and lab-on-a-chip devices to filtration by porous materials and chromatography.

General information
State: Published
Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, Tokyo University of Agriculture and Technology
Authors: Hanasaki, I. (Ekstern), Walther, J. H. (Intern)
Number of pages: 8
Publication date: 2017
Main Research Area: Technical/natural sciences

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Volume: 96
Article number: 023109
ISSN (Print): 1539-3755
Ratings:
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.95 SJR 0.993 SNIP 0.896
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.047 SNIP 0.978 CiteScore 1.89
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.22 SNIP 1.123 CiteScore 2.05
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.311 SNIP 1.239 CiteScore 2.28
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.42 SNIP 1.226 CiteScore 2.28
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.485 SNIP 1.225 CiteScore 2.28
ISI indexed (2011): ISI indexed yes
The collapse of Tacoma Narrows Bridge: a piece to the puzzle

On Nov. 7th 1940 the newly constructed Tacoma Narrows Bridge collapsed due to excessive torsional oscillations caused by the formation and shedding of large coherent vortices. The subsequent wind tunnel tests conducted on both section- and full bridge models concluded that the bridge should have collapsed at a wind speed corresponding to approximately half of the wind speed at the day of the collapse. This discrepancy questions our understanding of the phenomena responsible for the failure of the bridge. The present study aims at clarifying this "mystery" by considering historical records made available by the US coast guards, and by performing wind tunnel tests and detailed numerical ow simulations. Our findings indicate that the discrepancy is caused by an until now unnoticed yawed wind direction relative to the bridge, which was present at the day of the collapse.

General information
State: Published
Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, Technical University of Denmark, COWI A/S, FORCE Technology
Authors: Walther, J. H. (Intern), Christensen, D. S. (Ekstern), Maltte, M. G. (Ekstern), Roenne, M. (Ekstern), Spietz, H. J. (Intern), Larsen, A. (Ekstern), Larsen, S. V. (Ekstern)
Number of pages: 1
Publication date: 2017
Event: Abstract from 70th Annual Meeting of the American Physical Society Division of Fluid Dynamics (DFD17), Denver, United States.
Main Research Area: Technical/natural sciences
Electronic versions: 266213.pdf
DOI: 10.1103/PhysRevE.96.023109
Thermophoretic transport of water nanodroplets confined in carbon nanotubes: the role of friction

The development of efficient nanofluidic devices requires driving mechanisms that provide controlled transport of fluids through nanoconduits. Temperature gradients have been proposed as a mechanism to drive particles, fullerenes and nanodroplets inside carbon nanotubes (CNTs). In this work, molecular dynamics (MD) simulations are conducted to study thermophoresis of water nanodroplets inside CNTs. To gain insight into the interplay between the thermophoretic force acting on the droplet and the retarding liquid-solid friction, sets of constrained and unconstrained MD simulations are conducted. The results indicate that the thermophoretic motion of a nanodroplet displays two kinetic regimes: an initial regime characterized by a decreasing acceleration and afterwards a terminal regime with constant velocity. During the initial regime, the magnitude of the friction force increases linearly with the droplet velocity whereas the thermophoretic force has a constant magnitude defined by the magnitude of the thermal gradient and the droplet size. Subsequently, in the terminal regime, the droplet moves at constant velocity due to a dynamic balance between the thermophoretic force and the retarding friction force.

General information
State: Published
Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, Universidad de Concepcion
Authors: Oyarzua, E. (Ekstern), Walther, J. H. (Intern), Zambrano, H. (Ekstern)
Number of pages: 1
Publication date: 2017
Event: Abstract from 70th Annual Meeting of the American Physical Society Division of Fluid Dynamics (DFD17), Denver, United States.
Main Research Area: Technical/natural sciences

Wake structure and thrust generation of a flapping foil in two-dimensional flow

We present a combined numerical (particle vortex method) and experimental (soap film tunnel) study of a symmetric foil undergoing prescribed oscillations in a two-dimensional free stream. We explore pure pitching and pure heaving, and contrast these two generic types of kinematics. We compare measurements and simulations when the foil is forced with pitching oscillations, and we find a close correspondence between flow visualisations using thickness variations in the soap film and the numerically determined vortex structures. Numerically, we determine wake maps spanned by oscillation frequency and amplitude, and we find qualitatively similar maps for pitching and heaving. We determine the drag–thrust transition for both pitching and heaving numerically, and we discuss it in relation to changes in wake structure. For heaving with low oscillation frequency and high amplitude, we find that the drag–thrust transition occurs in a parameter region with wakes in which two vortex pairs are formed per oscillation period, in contrast to the common transition scenario in regions with inverted von Kármán wakes.

General information
State: Published
Organisations: Department of Physics, Biophysics and Fluids, Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering
Authors: Andersen, A. P. (Intern), Bohr, T. (Intern), Schnipper, T. (Intern), Walther, J. H. (Intern)
Number of pages: 12
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Fluid Mechanics
Volume: 812
Article number: R4
ISSN (Print): 0022-1120
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.82 SJR 1.671 SNIP 1.636
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
3D Lagrangian VPM: simulations of the near-wake of an actuator disc and horizontal axis wind turbine

The application of a 3-dimensional Lagrangian vortex particle method has been assessed for modelling the near-wake of an axisymmetrical actuator disc and 3-bladed horizontal axis wind turbine with prescribed circulation from the MEXICO (Model EXperiments InControlled conditions) experiment. The method was developed in the framework of the open-source Parallel Particle-Mesh library for handling the efficient data-parallelism on a CPU (Central Processing Unit) cluster,
and utilized a O(N log N)-type fast multipole method for computational acceleration. Simulations with the actuator disc resulted in a wake expansion, velocity deficit profile, and induction factor that showed a close agreement with theoretical, numerical, and experimental results from literature. Also the shear layer expansion was present; the Kelvin-Helmholtz instability in the shear layer was triggered due to the round-off limitations of a numerical method, but this instability was delayed to beyond 1 diameter downstream due to the particle smoothing. Simulations with the 3-bladed turbine demonstrated that a purely 3-dimensional flow representation is challenging to model with particles. The manifestation of local complex flow structures of highly stretched vortices made the simulation unstable, but this was successfully counteracted by the application of a particle strength exchange scheme. The axial and radial velocity profile over the near wake have been compared to that of the original MEXICO experiment, which showed close agreement between results.

**General information**

State: Published  
Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, Delft University of Technology  
Authors: Berdowski, T. (Ekstern), Ferreira, C. M. D. (Ekstern), Walther, J. H. (Intern)  
Number of pages: 13  
Publication date: 2016  
Conference: The Science of Making Torque from Wind, Munich, Germany, 05/10/2016 - 05/10/2016  
BFI conference series: European Academy of Wind Energy: The Science of Making Torque from Wind (5010078)  
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Journal of Physics: Conference Series (Online)  
Volume: 753  
Article number: 032004  
ISSN (Print): 1742-6596  
Ratings:  
  BFI (2018): BFI-level 1  
  BFI (2017): BFI-level 1  
  Web of Science (2017): Indexed yes  
  BFI (2016): BFI-level 1  
  Scopus rating (2016): CiteScore 0.45 SJR 0.24 SNIP 0.383  
  Web of Science (2016): Indexed yes  
  BFI (2015): BFI-level 1  
  Scopus rating (2015): SJR 0.24 SNIP 0.373 CiteScore 0.35  
  Web of Science (2015): Indexed yes  
  BFI (2014): BFI-level 1  
  Scopus rating (2014): SJR 0.253 SNIP 0.344 CiteScore 0.32  
  Web of Science (2014): Indexed yes  
  BFI (2013): BFI-level 1  
  Scopus rating (2013): SJR 0.231 SNIP 0.272 CiteScore 0.25  
  ISI indexed (2013): ISI indexed no  
  Web of Science (2013): Indexed yes  
  BFI (2012): BFI-level 1  
  Scopus rating (2012): SJR 0.28 SNIP 0.354 CiteScore 0.33  
  ISI indexed (2012): ISI indexed no  
  BFI (2011): BFI-level 1  
  Scopus rating (2011): SJR 0.292 SNIP 0.352 CiteScore 0.43  
  ISI indexed (2011): ISI indexed no  
  BFI (2010): BFI-level 1  
  Scopus rating (2010): SJR 0.288 SNIP 0.344  
  Web of Science (2010): Indexed yes  
  BFI (2009): BFI-level 1  
  Scopus rating (2009): SJR 0.253 SNIP 0.321  
  BFI (2008): BFI-level 1  
  Scopus rating (2008): SJR 0.265 SNIP 0.294  
  Web of Science (2008): Indexed yes  
  Scopus rating (2007): SJR 0.257 SNIP 0.39
A high order regularisation method for solving the Poisson equation and selected applications using vortex methods

A regularisation method for solving the Poisson equation using Green’s functions is presented. The method is shown to obtain a convergence rate which corresponds to the design of the regularised Green’s function and a spectral-like convergence rate is obtained using a spectrally ideal regularisation. It is shown that the regularised Poisson solver can be extended to handle mixed periodic and free-space boundary conditions. This is done by solving the equation spectrally in the periodic directions which yields a modified Helmholtz equation for the free-space directions which in turn is solved by deriving the appropriate regularised Green’s functions. Using an analogy to the particle-particle particle-mesh method, a framework for calculating multi-resolution solutions using local refinement patches is presented. The regularised Poisson solver is shown to maintain a high order converging solution for different configurations of the refinement patches. The regularised Poisson solver has been implemented in a high order particle-mesh based vortex method for simulating incompressible fluid flow. A re-meshing of the vortex particles used to ensure the convergence of the method and a re-projection of the vorticity field is included to explicitly fulfil the kinematic constraints of the flow field. The high order, unbounded particle-mesh based vortex method is used to simulate the instability, transition to turbulence and eventual destruction of a single vortex ring. From the simulation data, a novel analysis on the vortex ring dynamics is presented based on the alignment of the vorticity vector with the principal axis of the strain rate tensor. A novel iterative implementation of the Brinkman penalisation method is introduced for the enforcement of a fluid-solid interface in re-meshed vortex methods. The iterative scheme is shown to improve the enforcement of the interface and also allow the simulation to perform significantly larger time steps, than what is customary for the method. The improved accuracy of the iterative implementation is demonstrated by considering challenging benchmark problems such as the impulsively started flow past a cylinder and a flat plate normal or inclined to the flow. The iterative implementation is shown to enhance the quality of the solution by Brinkman penalisation significantly for simulations of highly unsteady flows past complex geometries. A stochastic method of generating a synthetic turbulent flow field is combined with a 2D-mesh-free vortex method to simulate the effect of an oncoming turbulent flow on a bridge deck cross-section within the atmospheric boundary layer. The mesh-free vortex method is found to be capable of preserving the a priori specified statistics as well as anisotropic characteristics of the synthesized turbulent flow field. From the simulation, the aerodynamic admittance of four aerodynamically different bridge sections are compared to available wind tunnel data, showing good agreement between the two. A vorticity formulated stochastic turbulence generator is presented which improves the kinetic properties of the generated turbulent field compared to present methods. Additional measures, such as explicit high order smoothing of the flow field, is introduced to insure that the generated field can be introduced into numerical simulations without an excessive loss of energy due to numerical dissipation.

General information
State: Published
Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering
Authors: Hejlesen, M. M. (Intern), Walther, J. H. (Intern)
Number of pages: 105
Publication date: 2016

Publication information
Publisher: Technical University of Denmark (DTU)
Original language: English

Series: DCAMM Special Report
Number: S198
ISSN: 0903-1685
Main Research Area: Technical/natural sciences
Electronic versions:
A multiresolution method for solving the Poisson equation using high order regularization

We present a novel high order multiresolution Poisson solver based on regularized Green's function solutions to obtain exact free-space boundary conditions while using fast Fourier transforms for computational efficiency. Multiresolution is achieved through local refinement patches and regularized Green's functions corresponding to the difference in the spatial resolution between the patches. The full solution is obtained utilizing the linearity of the Poisson equation enabling superposition of solutions. We show that the multiresolution Poisson solver produces convergence rates that correspond to the regularization order of the derived Green's functions.
Carbon nanotube-based coatings to induce flow enhancement in hydrophilic nanopores

With the emergence of the field of nanofluidics, the transport of water in hydrophilic nanopores has attracted intensive research due to its many promising applications. Experiments and simulations have found that flow resistance in hydrophilic nanochannels is much higher than those in macrochannels. Indeed, this might be attributed to significant fluid adsorption on the channel walls and to the effect of the increased surface to volume ratio inherent to the nanoconfinement. Therefore, it is desirable to explore strategies for drag reduction in nanopores. Recently, studies have found that carbon nanotubes (CNTs) feature ultrafast waterflow rates which result in flow enhancements of 1 to 5 orders of magnitude compared to Hagen-Poiseuille predictions. In the present study, CNT-based coatings are considered to induce water flow enhancement in silica nanopores with different radius. We conduct atomistic simulations of pressurized water flow inside tubular silica nanopores with and without inner coaxial carbon nanotubes. In particular, we compute water density and velocity profiles, flow enhancement and slip lengths to understand the drag reduction capabilities of single- and multi-walled carbon nanotubes implemented as coating material in silica nanopores.
**CFD modelling of condensation process of water vapor in supersonic flows**

The condensation phenomenon of vapor plays an important role in various industries, such as the steam flow in turbines and refrigeration system. A mathematical model is developed to predict the spontaneous condensing phenomenon in the supersonic conditions using the nucleation and droplet growth theories. The numerical approach is validated with the experimental data, which shows a good agreement between them. The condensation characteristics of water vapor in the Laval nozzle are studied numerically in this paper. The results show that the condensation process is a rapid variation of the vapor-liquid phase change both in space and in time. The spontaneous condensation of water vapor will not appear immediately when the steam reaches the saturation state. Instead, it occurs further downstream the nozzle throat, where the steam is in the state of supersaturation.

**General information**

State: Published
Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, University of Nottingham, Changzhou University
Authors: Wen, C. (Intern), Walther, J. H. (Intern), Yan, Y. (Ekstern), Yang, Y. (Ekstern)
Number of pages: 8
Publication date: 2016

**Host publication information**

Title of host publication: Proceedings of the International Heat Transfer Symposium 2016
Main Research Area: Technical/natural sciences
Condensation, Water vapor, Laval nozzle

**Electronic versions:**
ATE_paper.pdf
Source: PublicationPreSubmission
Source-ID: 125067081

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**CNT based thermal Brownian motor to pump water in nanodevices**

Brownian molecular motors are nanoscale machines that exploit thermal fluctuations for directional motion by employing mechanisms such as the Feynman-Smoluchowski ratchet. In this study, using Non Equilibrium Molecular Dynamics, we propose a novel thermal Brownian motor for pumping water through Carbon Nanotubes (CNTs). To achieve this we impose a thermal gradient along the axis of a CNT filled with water and impose, in addition, a spatial asymmetry by fixing specific zones on the CNT in order to modify the vibrational modes of the CNT. We find that the temperature gradient and imposed spatial asymmetry drive the water flow in a preferential direction. We systematically modified the magnitude of the applied thermal gradient and the axial position of the fixed points. The analysis involves measurement of the vibrational modes in the CNTs using a Fast Fourier Transform (FFT) algorithm. We observed water flow in CNTs of 0.94, 1.4 and 2.0 nm in diameter, reaching a maximum velocity of 5 m/s for a thermal gradient of 3.3 K/nm. The proposed thermal motor is capable of delivering a continuous flow throughout a CNT, providing a useful tool for driving liquids in nanochannels by exploiting thermal gradients.

**General information**

State: Published
Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, Universidad de Concepcion
Authors: Oyarzua, E. (Ekstern), Zambrano, H. (Ekstern), Walther, J. H. (Intern)
Number of pages: 1
Publication date: 2016

**Host publication information**

Title of host publication: Bulletin of the American Physical Society
Volume: 61
Publisher: American Physical Society
Article number: A22.00009
Main Research Area: Technical/natural sciences

**Electronic versions:**
MWS_DFD16_2016_001066.pdf
Derivation and analysis of the analytical velocity and vortex stretching expressions for an O (N log N)-FMM

In the current paper, a method for deriving the analytical expressions for the velocity and vortex stretching terms as a function of the spherical multipole expansion approximation of the vector potential is presented. These terms are essential in the context of 3D Lagrangian vortex particle methods combined with fast summation techniques. The convergence and computational efficiency of this approach is assessed in the framework of an O (N log N)-type Fast Multipole Method (FMM), by using vorticity particles to simulate a system of coaxial vortex rings for which also the exact results are known. It is found that the current implementation converges rapidly to the exact solution with increasing expansion order and acceptance factor. An investigation into the computational efficiency demonstrated that the O(N log N)-type FMM is already viable for a particle size of only several thousands and that this speedup increases significantly with the number of particles. Finally, it is shown that the implementation of the FMM with the current analytical expressions is at least twice as fast as when opting for using even the simplest implementation of finite differences instead.

General information
State: Published
Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, Delft University of Technology, Fraunhofer Institute for Wind Energy and Energy System Technology (IWES)
Authors: Berdowski, T. (Ekstern), Walther, J. H. (Intern), Ferreira, C. M. D. (Ekstern), Meng, F. (Ekstern)
Number of pages: 11
Publication date: 2016
Conference: The Science of Making Torque from Wind, Munich, Germany, 05/10/2016 - 05/10/2016
BFI conference series: European Academy of Wind Energy: The Science of Making Torque from Wind (5010078)
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Physics: Conference Series (Online)
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ISSN (Print): 1742-6596
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BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.45 SJR 0.24 SNIP 0.383
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.24 SNIP 0.373 CiteScore 0.35
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.253 SNIP 0.344 CiteScore 0.32
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.231 SNIP 0.272 CiteScore 0.25
ISI indexed (2013): ISI indexed no
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.28 SNIP 0.354 CiteScore 0.33
ISI indexed (2012): ISI indexed no
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.292 SNIP 0.352 CiteScore 0.43
ISI indexed (2011): ISI indexed no
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.288 SNIP 0.344
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.253 SNIP 0.321
BFI (2008): BFI-level 1
Effect of delta wing on the particle flow in a novel gas supersonic separator

The present work presents numerical simulations of the complex particle motion in a supersonic separator with a delta wing located in the supersonic flow. The effect of the delta wing on the strong swirling flow is analysed using the Discrete Particle Method. The results show that the delta wings re-compress the upstream flow and the gas Mach number decreases correspondingly. However, the Mach number does not vary significantly from the small, medium and large delta wing configurations. The small delta wing generates a swirl near its surface, but has minor influences on the flow above it. On the contrary, the use of the large delta wing produces a strong swirling flow in the whole downstream region. For the large delta wing, the collection efficiency reaches 70% with 2 μm particles, indicating a good separation performance of the proposed supersonic separator.

General information
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Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, Thermal Energy, Changzhou University, CSIRO
Authors: Wen, C. (Intern), Yang, Y. (Ekstern), Walther, J. H. (Intern), Pang, K. M. (Intern), Feng, Y. (Ekstern)
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BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.16 SJR 0.983 SNIP 1.482
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.965 SNIP 1.598 CiteScore 2.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.89 SNIP 1.649 CiteScore 2.67
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.901 SNIP 1.875 CiteScore 2.64
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Effect of meniscus contact angle during early regimes of spontaneous capillarity in nanochannels

In capillary imbibition, the classical Lucas-Washburn equation predicts a singularity as the fluid enters the channel consisting in an anomalous infinite velocity of the capillary meniscus. The Bosanquet's equation overcomes this problem by taking into account fluid inertia predicting an initial imbibition regime with constant velocity. Nevertheless, the initial constant velocity predicted by Bosanquet's equation is much greater than experimentally observed. In the present study, we conduct atomistic simulations to investigate capillary imbibition of water in silica nanochannels with heights between 4 and 18 nm. We also find that the meniscus contact angle remains constant during the inertial regime and its value depends upon the height of the channel. We also find that the meniscus velocity computed at the channel entrance is related to the particular value of the meniscus contact angle. Moreover, after the inertial regime, the meniscus contact angle is found to be time dependent for all the channels under study. We propose an expression for the time evolution of the dynamic contact angle in nanochannels which, when incorporated in Bosanquet's equation, satisfactorily explains the initial capillary rise.

General information
State: Published
Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, Universidad de Concepcion
Authors: Karna, N. (Ekstern), Oyarzua, E. (Ekstern), Walther, J. H. (Intern), Zambrano, H. (Ekstern)
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Publication date: 2016

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Title of host publication: Bulletin of the American Physical Society
Volume: 61
Effect of swirling device on flow behavior in a supersonic separator for natural gas dehydration

The supersonic separator is a revolutionary device to remove the condensable components from gas mixtures. One of the key issues for this novel technology is the complex supersonic swirling flow that is not well understood. A swirling device composed of an ellipsoid and several helical blades is designed for an annular supersonic separator. The supersonic swirling separation flow of natural gas is calculated using the Reynolds Stress model. The results show that the viscous heating and strong swirling flow cause the adverse pressure in the annular channel, which may negatively affect the separation performance. When the swirling flow passes through the annular nozzle, it will damage the expansion characteristics of the annular nozzle. The blade angles and numbers are both optimized by evaluating the swirling and expansion effects for the supersonic separation.
Effect of the meniscus contact angle during early regimes of spontaneous imbibition in nanochannels

Nanoscale capillarity has been extensively investigated; nevertheless, many fundamental questions remain open. In spontaneous imbibition, the classical Lucas-Washburn equation predicts a singularity as the fluid enters the channel consisting of an anomalous infinite velocity of the capillary meniscus. Bosanquet's equation overcomes this problem by taking into account fluid inertia predicting an initial imbibition regime with constant velocity. Nevertheless, the initial constant velocity as predicted by Bosanquet's equation is much greater than those observed experimentally. In the present study, large scale atomistic simulations are conducted to investigate capillary imbibition of water in slit silica nanochannels with heights between 4 and 18 nm. We find that the meniscus contact angle remains constant during the inertial regime and its value depends on the height of the channel. We also find that the meniscus velocity computed at the channel entrance is related to the particular value of the meniscus contact angle. Moreover, during the subsequent visco-inertial regime, as the influence of viscosity increases, the meniscus contact angle is found to be time dependent for all the channels under study. Furthermore, we propose an expression for the time evolution of the dynamic contact angle in nanochannels which, when incorporated into Bosanquet's equation, satisfactorily explains the initial capillary rise.

General information
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Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, Universidad de Concepcion
Authors: Karna, N. K. (Ekstern), Oyarzua, E. (Ekstern), Walther, J. H. (Intern), Zambrano, H. A. (Ekstern)
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BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
LES And URANS simulations of the swirling flow in a dynamic model of a uniflow-scavenged cylinder

The turbulent swirling flow in a uniflow-scavenged two-stroke engine cylinder is investigated using computational fluid dynamics. The investigation is based on the flow in a scale model with a moving piston. Two numerical approaches are tested; a large eddy simulation (LES) approach with the wall-adaptive local eddy-viscosity (WALE) model and a Reynolds-Averaged Navier-Stokes approach using the k-ω Shear-Stress Transport model. Combustion and compression are neglected. The simulations are verified by a sensitivity study and the performance of the turbulence models are evaluated by comparison with experimental results. Both turbulence models produce results in good agreement with experimental data. The agreement is particularly good for the LES, immediately after the piston passes the bottom dead center. Furthermore, in the piston standstill period, the LES predicts a tangential profile in agreement with the measurements, whereas the k-ω SST model predicts a solid body rotation. Several instabilities are identified during the scavenging process. The formation of a vortex breakdown with multiple helical vortex structures are observed after the scavenge port opening, along with the shedding of vortex rings with superimposed swirl. The turbulence models predict several flow reversals in the vortex breakdown region through the scavenge process. Flow separations in the scavenge ports lead to a secondary axial flow, in the separated region. The secondary flow exits in the top of the scavenge ports, resulting in large velocity gradients near the cylinder liner above the scavenge ports.

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Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, MAN Diesel & Turbo SE
Authors: Hemmingsen, C. S. (Intern), Ingvorsen, K. M. (Intern), Mayer, S. (Ekstern), Walther, J. H. (Intern)
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Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.991 SNIP 1.691 CiteScore 2.35
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.175 SNIP 1.788 CiteScore 2.29
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.224 SNIP 2.066 CiteScore 2.3
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.17 SNIP 2.215 CiteScore 2.37
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.375 SNIP 2.174 CiteScore 2.28
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.328 SNIP 2.169 CiteScore 2.6
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.414 SNIP 2.108
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.36 SNIP 1.814
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.047 SNIP 1.411
Scopus rating (2007): SJR 1.523 SNIP 1.81
Modelling of Combustion and Pollutant Formation in a Large, Two-Stroke Marine Diesel Engine using Integrated CFD-Skeletal Chemical Mechanism

In this reported work, simulation studies of in-cylinder diesel combustion and pollutant formation processes in a two-stroke, low-speed uniflow-scavenged marine diesel engine are presented. Numerical computation is performed by integrating chemical kinetics into CFD computations. In order to minimize the computational runtime, an in-house skeletal n-heptane chemical mechanism is coupled with the CFD model. This surrogate fuel model comprises 89 reactions with 32 species essential to diesel ignition/combustion processes as well as the formation of soot precursors and nitrogen monoxide (NO). Prior to the marine engine simulation, coupling of the newly developed surrogate fuel model and a revised multi-step soot model [1] is validated on the basis of optical diagnostics measurement obtained at varying ambient pressure levels [2]. It is demonstrated that the variation of ignition delay times, liftoff lengths and averaged soot volume fraction (SVF) with respect to the change of ambient pressure captured using the model agree reasonably well with the measurement, apart from those at the low pressure condition. Numerical models are subsequently validated against experimental combustion characteristics under high load condition in a marine diesel engine. Comparisons to the measurement show that the simulated pressure rise started 1.0 crank angle degree in advance and the calculated peak pressure is 1.7 % lower. The associated flame liftoff length is negligible, yielding high local equivalence ratio and SVF values. In addition, the oxygen availability is found to affect the production of acetylene and hence soot particles. For the current test condition, the averaged NO concentration calculated when soot radiative heat loss is taken into account compared to that when only convective is considered suggests that the former is approximately 7.7 % lower. The findings here aid to gain insights of in-cylinder phenomena in this combustion system. The surrogate fuel model also allows direct couplings of sulfuric oxides formation reactions and a more comprehensive nitrogen oxides mechanism since the surrogate fuel model includes essential radicals such as O, H and OH for these pollutant formation reactions.

General information

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Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, Thermal Energy
Authors: Pang, K. M. (Intern), Karvounis, N. (Intern), Schramm, J. (Intern), Walther, J. H. (Intern)
Number of pages: 1
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Modelling of diesel spray flame under engine-like conditions using an accelerated eulerian stochastic fields method: A convergence study of the number of stochastic fields

The use of transported Probability Density Function (PDF) methods allows a single model to compute the autoignition, premixed mode and diffusion flame of diesel combustion under engine-like conditions [1,2]. The Lagrangian particle based transported PDF models have been validated across a wide range of conditions [2,3]. Alternatively, the transported PDF model can also be formulated in the Eulerian framework [4]. The Eulerian PDF is commonly known as the Eulerian Stochastic Fields (ESF) model. When the same chemical mechanism and micro-mixing model were used, both ESF model and its Lagrangian counterpart generated similar results. The principal motivation for ESF compared to Lagrangian particle...
The relative ease of implementation of the former into Eulerian computational fluid dynamics (CFD) codes [5]. Several works have attempted to implement the ESF model for the simulations of diesel spray combustion under engine-like conditions. The current work aims to further evaluate the performance of the ESF model in this application, with an emphasis on examining the convergence of the number of stochastic fields, $n_{sf}$. Five test conditions, covering both the conventional diesel combustion and low temperature combustion regimes, are used. The associated ambient conditions and injection characteristics are provided in Table 1.

General information
State: Published
Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, Thermal Energy, Lund University
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Main Research Area: Technical/natural sciences

Multiphase flow in porous media using CFD

We present results from a new Navier-Stokes model for multiphase flow in porous media implemented in Ansys Fluent 16.2 [1]. The model includes the Darcy-Forchheimer source terms in the momentum equations and proper account for relative permeability and capillary pressure in the porous media. This approach is widely used for single phase flow, but not for multiphase flow in porous media. This might be due to the complexity of introducing relative permeability and capillary pressure in the CFD solver. The introduction of relative permeability and capillary pressure may cause numerical instabilities as the saturation of a grid cell approaches the residual saturation, i.e. the relative permeability goes towards zero. This means that the viscous resistance in the Darcy-Forchheimer equation approaches infinity. Furthermore, by coupling the Navier-Stokes equation and Darcy-Forchheimer equation it is possible to model both the non-porous and porous media using the same formulation.

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Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering
Authors: Hemmingsen, C. S. (Intern), Walther, J. H. (Intern)
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Event: Abstract from ECCOMAS Congress 2016, Hersonissos, Greece.
Main Research Area: Technical/natural sciences

Numerical and experimental study of pulse-jet cleaning in fabric filters

Pulse-jet cleaning and understanding of the complex physics are essential when designing fabric filters used for air pollution control. Today, low-pressure cleaning is of particular interest due to demand for reduced compressed air consumption. Pulse-jet cleaned fabric filters have been studied for many years by experimental investigation and to a limited extent by Computational Fluid Dynamics (CFD). The majority of the studies have focused on high-pressure cleaning systems, and the CFD models presented are so far two-dimensional (2D). In the work presented here, pulse-jet cleaning of low-pressure fabric filters (2 bar) is studied using a full three-dimensional (3D) CFD model. Experimental results obtained in a pilot-scale test filter with 28 bags, in length of 10 m and in general full-scale dimensions of the cleaning system are used to verify the reliability of the present CFD model. The validated CFD model reveals the strong compressible effects, a highly transient behaviour, the formation of compressible vortex rings and the shock cell phenomenon within the overexpanded supersonic jet. The cleaning nozzles and venturi design aid or oppose the pulse-pressure within the bags, and this plays an important role in the resulting efficiency of removing the dust layer from the bags. The CFD simulation shows that the traditional straight-bore nozzles provide substantial misalignment of the jet, and the add-on nozzle design offers only limited improvement. Further, the need for venturis in low-pressure filters and the importance of optimising the venturi design are demonstrated. The working principle of the venturi is to restrict backflow which is detrimental to the pressure rise in the bags. Reducing the venturi throat diameter is shown to reduce backflow and improve the pulse-pressure.

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Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering
Authors: Hemmingsen, C. S. (Intern), Walther, J. H. (Intern)
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Event: Abstract from ECCOMAS Congress 2016, Hersonissos, Greece.
Main Research Area: Technical/natural sciences

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Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering
Authors: Hemmingsen, C. S. (Intern), Walther, J. H. (Intern)
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Main Research Area: Technical/natural sciences

Numerical and experimental study of pulse-jet cleaning in fabric filters

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Numerical investigation of soot formation and oxidation processes under large two-stroke marine diesel engine-like conditions using integrated CFD-chemical kinetics

In this reported work, multi-dimensional computational fluid dynamics studies of diesel combustion and soot formation processes in a constant volume combustion chamber and a marine diesel engine are carried out. The key interest here is firstly to validate the coupling of a newly developed skeletal n-heptane mechanism and a revised multi-step soot model using laser extinction measurements of diesel soot obtained at different ambient pressure levels in an optical accessible, constant volume chamber experiment. It is revealed that ignition delay times and liftoff lengths generated using the new skeletal model are close to those produced by the larger and more comprehensive chemical mechanisms, apart from those at the low pressure condition. The current study also demonstrates that the variation of averaged soot volume fraction with respect to the change of combustion chamber pressure captured using the revised soot model agrees reasonably well with the measurements in terms of peak values. The numerical model is subsequently applied to investigate the flame development, soot/nitrogen monoxide formation and heat transfer in a two-stroke, low-speed uniflow-scavenged marine diesel engine operating at full load condition, where optical measurements are not available. Comparisons to the experimental data show that the simulated pressure rise starts 1.0 crank angle degree in advance and the calculated peak pressure is 1.7% lower. The associated flame liftoff length is negligible, yielding higher local equivalence ratio and soot volume fraction values as compared to those under similar test condition in the constant volume chamber. With the use of the revised model, the total heat transfer to the walls calculated when soot radiative heat loss is taken into account is approximately 30% higher compared to that when only convective heat loss is considered. The averaged nitrogen monoxide concentration is 7.7% lower when both convective and soot radiative heat losses are accounted for but the net soot mass production is less sensitive to soot radiation. A sensitivity study reveals that neither increasing nor decreasing the soot absorption coefficient by 30% from the baseline setup is influential to nitrogen monoxide formation, soot mass production and heat transfer. The findings here aid to gain insights and provide a better understanding of the combustion and soot processes in large, uniflow-scavenged marine engines. The numerical model developed in this work can also be applied to explore different phenomena in this combustion system.

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Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, Thermal Energy
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BFI (2016): BFI-level 2
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Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.912 SNIP 2.61 CiteScore 6.4
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 3.254 SNIP 3.28 CiteScore 6.93
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Numerical Simulation of Condensation of Sulfuric Acid and Water in a Large Two-stroke Marine Diesel Engine

We present results from computational fluid dynamics simulations of the condensation of sulfuric acid (H₂SO₄) and water (H₂O) in a large two-stroke marine diesel engine. The model uses a reduced n-heptane skeletal chemical mechanism coupled with a sulfur subset to simulate the combustion process and the formation of SOx and H₂SO₄. Condensation is modeled using a fluid film model coupled with the Eulerian in-cylinder gas phase. The fluid film condensation model is validated against both experimental and numerical results. The engine simulations reveal that the fluid film has a significant effect on the sulfuric acid gas phase. A linear correlation is found between the fuel sulfur content and the sulfuric acid condensation rate. The initial in-cylinder water content is found not to affect the sulfuric acid condensation but it has a high impact on water condensation. The scavenging pressure level shows an inverse correlation between pressure and condensation rate due to change in the flame propagation speed. Finally, increasing the cylinder liner temperature significantly decreases water condensation but has a negligible influence on the condensation of sulfuric acid.

General information
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Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, Thermal Energy
Simulating the DISAMATIC process using the discrete element method — a dynamical study of granular flow

The discrete element method (DEM) is applied to simulate the dynamics of the flow of green sand while filling a mould using the DISAMATIC process. The focus is to identify relevant physical experiments that can be used to characterize the material properties of green sand in the numerical model. The DEM parameters describing the static friction coefficients are obtained using a ring shear tester and the rolling resistance and cohesion value is subsequently calibrated with a sand pile experiment. The calibrated DEM model is used to model the sand shot in the DISAMATIC process for three different sand particle flow rates as captured on the corresponding video footage of the interior of the chamber. A mould chamber with three ribs mounted on the fixed pattern plate forming four cavities is chosen as a reference geometry to investigate the conditions found in the real moulding process. The geometry of the cast part and the casting system can make the moulding process complicated due to obstacles such as ribs that deflect the sand flow causing “shadows effects” around the cavities of the mould. These dynamic effects are investigated by the qualitative flow dynamics and quantitative mould filling times captured in the video footage and simulated by the calibrated DEM model. Both two- and three-dimensional DEM models are considered and found to produce results in good agreements with the video footage of the DISAMATIC process.
Simulation of bluff-body flows using iterative penalization in a multiresolution particle-mesh vortex method

The ability to predict aerodynamic forces, due to the interaction of a fluid flow with a solid body, is central in many fields of engineering and is necessary to identify error-prone structural designs. In bluff-body flows the aerodynamic forces oscillate due to vortex shedding and variations in the oncoming flow. This may lead to structural instability e.g. when the shedding frequency aligns with the natural frequency of the structure. Fluid structure interaction must especially be considered when designing long span bridges. A three dimensional vortex-in-cell method is applied for the direct numerical simulation of the flow past a bodies of arbitrary shape. Vortex methods use a simple formulation where only the trajectories of discrete vortex particles are simulated. The Lagrangian formulation eliminates the CFL type condition that Eulerian methods have to satisfy. This allows vortex methods to take significantly larger time steps in convection dominated flows with explicit time integration.

As vorticity is a bounded quantity and the velocity field can be calculated for freespace- or periodic boundary conditions, these method allows for a minimized domain and hence minimize computational efforts.

Pure particle-vortex methods have the disadvantage of being highly costly. The calculation of particle velocities in particle vortex methods has traditionally been done by directly applying the Biot-Savart law yielding an N2 -body problem. However the Poisson equation, that relates the vorticity- to the velocity field, can be solved efficiently using a mesh-based solver with local refinement in the boundary layer regions. We present a higher-order particle-mesh vortex method, where particle velocities are calculated by solving the Poisson equation on several uniform meshes using Fast Fourier Transforms. This we combine with an iterative penalization method, that
allows the simulation of external flows past arbitrary geometries in arbitrary motions such as bridge decks in forced heave and pitch motion

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Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering
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Event: Abstract from ECCOMAS Congress 2016, Hersonissos, Greece.
Main Research Area: Technical/natural sciences

**Simulation of impulsively started flow past a sphere and a disc using iterative brinkman penalization**

We present an iterative Brinkman penalization scheme to enforce the no-slip condition on solid boundaries in three-dimensional flow simulations. We use a high-order particle-mesh vortex method, where the velocity field is obtained from the vorticity field by solving a Poisson equation on a Cartesian mesh as a convolution of the vorticity field with a regularized Green's function [2]. By doing this we can enforce free-space boundary conditions allowing us to consider a minimal computational domain. The Brinkman penalization method [1] is an immersed body method that allows the treatment of solids having complex geometries on a Cartesian mesh. Thereby we avoid the use of unstructured meshes that conventional flow solvers rely on. In the presented iterative scheme the penalization term is only active in the solid region and in its immediate neighborhood thus the computational costs required for the solution of the penalization problem is kept at a minimum. We apply our method for the simulation of the impulsively started flow past a sphere at \( Re = 1000 \) and normal to a circular disc at \( Re = 500 \), respectively. Our results for the unsteady sphere flow are found to be in qualitative agreement with results obtained by Ploumhans et al [3] using a boundary element method. The flow is illustrated by a volume rendering of the vorticity field cf. Fig. 1. The figure shows that the flow is highly unsteady and a challenging problem for accurate analysis. Furthermore we show that the iterative scheme allows a significantly larger time step than the iterative scheme (more than a factor of 10) in the simulation of the impulsively started flow normal to a circular disc.

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Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering
Authors: Spietz, H. J. (Intern), Hejlesen, M. M. (Intern), Walther, J. H. (Intern)
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Event: Abstract from 7th International Conference on Vortex Flows and Vortex Models (ICVFM 2016), Rostock, Germany.
Main Research Area: Technical/natural sciences

**Tangential inlet supersonic separators: a novel apparatus for gas purification**

A novel supersonic separator with a tangential inlet is designed to remove the condensable components from gas mixtures. The dynamic parameters of natural gas in the supersonic separation process are numerically calculated using the Reynolds stress turbulence model with the Peng-Robinson real gas model. The results show that natural gas expands in the supersonic separator to supersonic velocities resulting in low pressures (6 bar, from about 40 bar) and temperatures (-70 °C, from 30 °C), which causes the condensation and nucleation of the condensable components. The tangential velocity can be generated by the tangential inlet, and it increases to the maximum of 200 m/s at the nozzle throat due to decrease of the nozzle area of the converging part. The tangential velocity can maintain the value of about 160 m/s at the nozzle exit, and correspondingly generates the centrifugal acceleration of 3.6×106 m/s² to remove the condensed droplets from the gas mixtures.

**General information**
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Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, Changzhou University
Authors: Wen, C. (Intern), Walther, J. H. (Intern), Yang, Y. (Ekstern)
**Thermophoresis of water droplets inside carbon nanotubes**
Carbon Nanotubes (CNTs) offer unique possibilities as fluid conduits with applications ranging from lab on a chip devices to encapsulation media for drug delivery. CNTs feature high mechanical strength, chemical and thermal stability and biocompatibility therefore they are promising candidates for nanodevice fabrication. Thermal gradients have been proposed as mechanism to drive particles, fullerenes and droplets inside CNTs. Here, by conducting Molecular Dynamics (MD) simulations, we study thermophoresis of water droplets inside CNTs. We systematically change the size of the droplets, the axial thermal gradient and CNT chirality. We find that the droplet motion in the armchair CNTs exhibits two clearly delimited stages, a regime wherein the droplet is accelerated and subsequently, a regime wherein the droplet moves with constant velocity. Inside the zigzag CNTs, the droplet accelerates during a very short time and then it moves with constant velocity. We compute the netforce during the droplet acceleration and find a correlation between the droplet acceleration and the magnitude of the thermal gradient without any dependence on the droplet size. Moreover, we conduct velocity constrained MD simulations to determine the friction and thermophoretic forces acting on the droplet.

**Ultrafast cooling by covalently bonded graphene-carbon nanotube hybrid immersed in water**
The increasing power density and the decreasing dimensions of transistors present severe thermal challenges to the design of modern microprocessors. Furthermore, new technologies such as three-dimensional chip-stack architectures require novel cooling solutions for their thermal management. Here, we demonstrate, through transient heat-dissipation simulations, that a covalently bonded graphene-carbon nanotube (G-CNT) hybrid immersed in water is a promising solution for the ultrafast cooling of such high-temperature and high heat-flux surfaces. The G-CNT hybrid offers a unique platform to integrate the superior axial heat transfer capability of individual CNTs via their parallel arrangement. The immersion of the G-CNT in water enables an additional heat dissipation path via the solid-liquid interaction, allowing for the sustainable cooling of the hot surface under a constant power input of up to 10 000 W cm$^{-2}$. 
A high order multi-resolution solver for the Poisson equation with application to vortex methods

A high order method is presented for solving the Poisson equation subject to mixed free-space and periodic boundary conditions by using fast Fourier transforms (FFT). The high order convergence is achieved by deriving mollified Green's functions from a high order regularization function which provides a correspondingly smooth solution to the Poisson equation. The high order regularization function may be obtained analogous to the approximate deconvolution method used in turbulence models and strongly relates to deblurring algorithms used in image processing. At first we show that the regularized solver can be combined with a short range particle-particle correction for evaluating discrete particle interactions in the context of a particle-particle particle-mesh (P3M) method. By a similar approach we extend the regularized solver to handle multi-resolution patches in continuum field simulations by super-positioning an inter-mesh correction. For sufficiently smooth vector fields this multi-resolution correction can be achieved without the loss of convergence rate. An implementation of the multi-resolution solver in a two-dimensional re-meshed particle-mesh based vortex method is presented and validated.

Atomistic Simulations of Fluid Flow through Graphene Channels and Carbon Nanotubes

The transport of aqueous solutions in artificial nanopores is of both fundamental and technological interest. Recently, carbon nano-structured materials (fullerenes) have attracted a great deal of attention in nanotechnology. In fact, due to their large specific surface area, high thermal conductivity, extremely low surface friction and superior mechanical properties, graphene channels and carbon nanotubes (CNTs) are promising candidates to be implemented as fluid conduits in nanosystems. Performing Non-equilibrium Molecular Dynamics simulations, we study the transport of water-electrolyte solutions inside single and multi-wall graphene channels and inside zig-zag and armchair CNTs of similar cross sectional area. In order to calibrate the force fields, we use dedicated criteria relevant to the hydrodynamics of the systems of interest. Different fluid driving mechanisms such as pressure fields, electro-osmosis and thermal gradients are evaluated. We conduct a detailed analysis of the transport efficiency of each system to impose similar volumetric flow rates. From the simulations, we extract density and velocity profiles to study the liquid structure, wall slippage and flow enhancement in order to compare the hydrodynamic performance of these two novel materials.
Atomistic study of a nanometer-scale pump based on the thermal ratchet concept

In this study, a novel concept of nanoscale pump fabricated using Carbon Nanotubes (CNTs) is presented. The development of nanofluidic systems provides unprecedented possibilities for the control of biology and chemistry at the molecular level with potential applications in low energy cost devices, novel medical tools, and a new generation of sensors. CNTs offer a number of attractive features for the fabrication of fluidic nanodevices including fast flow, useful electronic and thermal properties, high mechanical strength and biocompatibility. Therefore, the transport of liquids in CNTs is of great interest in nanofluidics. Thermophoresis is the phenomenon observed when a mixture of two or more types of motile objects experience a force induced by a thermal gradient and the different types of objects respond to it differently, inducing a motion and segregation of the objects. Using molecular dynamics simulations, we explore the possibility to design thermophoretic pumping devices fabricated of CNTs for water transport in nanoconduits. The design of the nanopumps is based on the concept of the Feynman-Smoluchowski ratchet.

General information
State: Published
Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, Universidad de Concepcion
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Main Research Area: Technical/natural sciences
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Cavitation Estimates by Orbit Prediction of a Journal Bearing - Finite Element Modelling and Experimental Studies

The paper presents a two-sided approach to establish understanding of the cavitation phenomenon in dynamically loaded journal bearings, more specifically the engine bearings of large two-stroke marine diesel engines. One disadvantage of the journal bearing is the converging-diverging geometry making it prone to cavitation which again affects the load carrying capacity of the bearing. In combustion engines the journal bearing plays a vital role especially as main and crosshead bearings transmitting the combustion forces. Those forces vary highly during one combustion cycle which is further influencing the load carrying capacity and ultimately the chances of fatal shaft-sleeve contact. By solving Reynolds equation numerically using finite elements and incorporating a cavitation algorithm, the dynamic coefficients can be used to establish the journal orbit for a given bearing and load pattern. Validation of the results is done against the Ruston and Hornsby 6VEB-X Mk III engine. Besides the numerical investigations a cavitation test rig has been developed. With this rig it is possible to generate cavitation under controlled conditions in terms of load/eccentricity and rotational speed. The development of cavitation in time in terms of position and distribution can be visually recorded.

General information
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Organisations: Department of Mechanical Engineering, Solid Mechanics, Fluid Mechanics, Coastal and Maritime Engineering, MAN Diesel & Turbo SE
Authors: Christiansen, C. K. (Intern), Klit, P. (Intern), Walther, J. H. (Intern), Vølund, A. (Ekstern)
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Main Research Area: Technical/natural sciences

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Continuum Navier-Stokes modelling of water flow past fullerene molecules

We present continuum simulations of water flow past fullerene molecules. The governing Navier-Stokes equations are complemented with the Navier slip boundary condition with a slip length that is extracted from related molecular dynamics simulations. We find that several quantities of interest as computed by the present model are in good agreement with results from atomistic and atomistic-continuum simulations at a fraction of the computational cost. We simulate the flow past a single fullerene and an array of fullerenes and demonstrate that such nanoscale flows can be computed efficiently by continuum flow solvers, allowing for investigations into spatiotemporal scales inaccessible to atomistic simulations.

General information
State: Published
Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, National Institute of Chemistry, Swiss Federal Institute of Technology
Authors: Walther, J. H. (Intern), Popadic, A. (Ekstern), Koumoutsakos, P. (Ekstern), Praprotnik, M. (Ekstern)
Number of pages: 1
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Main Research Area: Technical/natural sciences
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Continuum Navier-Stokes modelling of water ow past fullerene molecules

We present continuum simulations of water ow past fullerene molecules. The governing Navier-Stokes equations are complemented with the Navier slip boundary condition with a slip length that is extracted from related molecular dynamics simulations. We find that several quantities of interest as computed by the present model are in good agreement with
results from atomistic and atomistic-continuum simulations at a fraction of the computational cost. We simulate the flow past a single fullerene and an array of fullerenes and demonstrate that such nanoscale flows can be computed efficiently by continuum flow solvers, allowing for investigations into spatiotemporal scales inaccessible to atomistic simulations.

**General information**
State: Published
Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, National Institute of Chemistry, Swiss Federal Institute of Technology
Authors: Walther, J. H. (Intern), Popadic, A. (Ekstern), Koumoutsakos, P. (Ekstern), Praprotnik, M. (Ekstern)
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Event: Abstract from 68th Annual Meeting of the American Physical Society's Division of Fluid Dynamics (DFD), Boston, United States.
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**Continuum simulations of water flow past fullerene molecules**
We present continuum simulations of water flow past fullerene molecules. The governing Navier-Stokes equations are complemented with the Navier slip boundary condition with a slip length that is extracted from related molecular dynamics simulations. We find that several quantities of interest as computed by the present model are in good agreement with results from atomistic and atomistic-continuum simulations at a fraction of the cost. We simulate the flow past a single fullerene and an array of fullerenes and demonstrate that such nanoscale flows can be computed efficiently by continuum flow solvers, allowing for investigations into spatiotemporal scales inaccessible to atomistic simulations.

**General information**
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Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, National Institute of Chemistry, Swiss Federal Institute of Technology
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Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.939 SNIP 0.946 CiteScore 1.84
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Web of Science (2013): Indexed yes
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Scopus rating (2012): SJR 0.912 SNIP 0.745 CiteScore 1.44
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Covalently Bonded Graphene-Carbon Nanotube Hybrid for High-Performance Thermal Interfaces

The remarkable thermal properties of graphene and carbon nanotubes (CNTs) have been the subject of intensive investigations for the thermal management of integrated circuits. However, the small contact area of CNTs and the large anisotropic heat conduction of graphene have hindered their applications as effective thermal interface materials (TIMs).

Here, a covalently bonded graphene–CNT (G-CNT) hybrid is presented that multiplies the axial heat transfer capability of individual CNTs through their parallel arrangement, while at the same time it provides a large contact area for efficient heat extraction. Through computer simulations, it is demonstrated that the G-CNT outperforms few-layer graphene by more than 2 orders of magnitude for the c-axis heat transfer, while its thermal resistance is 3 orders of magnitude lower than the state-of-the-art TIMs. We show that heat can be removed from the G-CNT by immersing it in a liquid. The heat transfer characteristics of G-CNT suggest that it has the potential to revolutionize the design of high-performance TIMs.
Diesel Engine Tribology

Recent years have seen an increase in the wear rate of engine bearings, subsequently followed by bearing failure, for the large two-stroke diesel engines used for ship propulsion. Here, the engine bearings include main, big end and crosshead bearings, with the bearing type used being the journal bearing, belonging to the class of ‘hydrodynamic bearings’. This implies that the load carrying capacity is generated by a relative movement of the involved components, i.e. a velocity-driven operation. For the engine application, the velocity stems from the engine RPM. However, to comply with the latest emission requirements as well as attempting to minimise fuel expenses, the engine speed has been lowered together with an increase in the engine mean pressure which in terms lead to larger bearing loads. With worsened operating conditions from two sides, the encountered problems are understandable as the design criteria for the bearings are no longer valid, albeit still not desirable. To come up with a solution, the operating conditions of the bearings have to be understood. The main challenge is to supply sufficient with lubricant to avoid metal-metal contact under time-varying combustion load. This project has therefore revolved around the investigation of the tribological performance of the dynamically loaded journal bearing, both theoretically and experimentally. The theoretical work covers two approaches to the modelling of the bearing: a traditional finite element based solver for Reynolds equation, and a more general finite volume discretisation of the Navier-Stokes equations. In this way the influence from assumptions usually made in regards to supply grooves can be verified. A test rig has been constructed for replicating engine-like conditions. Anuridirectional load can be applied in both static and dynamic modes, while another key feature being that of a transparent polymer bearing enabling the study of film rupture and re-forming. Paper [P1] describes the development of a suitable finite volume mesh for dynamic loading, while Paper [P2] contains the perturbation implementation used for the dynamic loading. Resorting to Gümbel boundary conditions, very similar orbits are predicted for a given bearing using the two methods demonstrated in Paper [P3]. Good agreement is also obtained between the numerical and experimental results. Finally, some suggestions to improvements of the modelling as well as the experimental set-up, are made.

General information
State: Published
Organisations: Center for Bachelor of Engineering Studies, Afdelingen for Maskin og Design, Department of Mechanical Engineering, Solid Mechanics, Fluid Mechanics, Coastal and Maritime Engineering, MAN B&W Diesel A/S
Authors: Christiansen, C. K. (Intern), Klit, P. (Intern), Walther, J. H. (Intern), Vølund, A. (Ekstern)
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Early Regimes of Water Capillary Flow in Slit Silica Nanochannels

Molecular dynamics simulations are conducted to investigate the initial stages of spontaneous imbibition of water in slit silica nanochannels surrounded by air. An analysis is performed for the effects of nanoscopic confinement, initial conditions of liquid uptake and air pressurization on the dynamics of capillary filling. The results indicate that the nanoscale imbibition process is divided into three main flow regimes: an initial regime where the capillary force is balanced only by the inertial drag and characterized by a constant velocity and a plug flow profile. In this regime, the meniscus formation process plays a central role in the imbibition rate. Thereafter, a transitional regime takes place, in which, the force balance has significant contributions from both inertia and viscous friction. Subsequently, a regime wherein viscous forces dominate the capillary force balance is attained. Flow velocity profiles identify the passage from an inviscid flow to a developing Poiseuille flow. Gas density profiles ahead of the capillary front indicate a transient accumulation of air on the advancing meniscus. Furthermore, slower capillary filling rates computed for higher air pressures reveal a significant retarding effect of the gas displaced by the advancing meniscus.
Flow Dynamics of green sand in the DISAMATIC moulding process using Discrete element method (DEM)
The DISAMATIC casting process production of sand moulds is simulated with DEM (discrete element method). The main purpose is to simulate the dynamics of the flow of green sand, during the production of the sand mould with DEM. The sand shot is simulated, which is the first stage of the DISAMATIC casting process. Depending on the actual casting geometry the mould can be geometrically quite complex involving e.g. shadowing effects and this is directly reflected in the sand flow during the moulding process. In the present work a mould chamber with "ribs" at the walls is chosen as a baseline geometry to emulate some of these important conditions found in the real moulding process. The sand flow is simulated with the DEM and compared with corresponding video footages from the interior of the chamber during the moulding process. The effect of the rolling resistance and the static friction coefficient is analysed and discussed in relation to the experimental findings.

General information
State: Published
Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, Manufacturing Engineering, DISA Industries A/S, Magma Gießereitechnologie GmbH
Authors: Hovad, E. (Intern), Larsen, P. (Ekstern), Walther, J. H. (Intern), Thorborg, J. (Intern), Hattel, J. H. (Intern)
Number of pages: 9
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Main Research Area: Technical/natural sciences

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Flow enhancement of water flow through silica slit pores with graphene-coated walls

Nanofluidic devices such as Lab-On-a-Chip often are designed to transport water solutions through hydrophilic nano-conduits. In these systems with narrow confinement, the viscous forces dominate the flow and as a result, the hydrodynamic friction drag is very high. Moreover, the drag and the amount of energy required for pumping a fluid are directly related. Therefore, it is desirable to explore drag reduction strategies in nanoconfined flows. Liquids are known to slip past non-wetting surfaces. Graphene is a single-atom-thick sheet of carbon atoms arranged in a hexagonal honeycomb lattice, which features a unparalleled combination of high specific surface area, chemical stability, mechanical strength and flexibility. Recently, the wettability of water droplets on multilayer graphene sheets deposited on a silica substrate has been investigated. In this study, we investigate the role of graphene coatings to induce flow enhancement in silica channels. We conduct molecular dynamics simulations of pressurized water flow inside silica channels with and without graphene layers covering the walls. In particular, we compute density and velocity profiles, flow enhancement and slip lengths to understand the drag reduction capabilities of multilayer graphene coatings.

High order Poisson Solver for unbounded flows

This paper presents a high order method for solving the unbounded Poisson equation on a regular mesh using a Green's function solution. The high order convergence was achieved by formulating mollified integration kernels, that were derived from a filter regularisation of the solution field. The method was implemented on a rectangular domain using fast Fourier transforms (FFT) to increase computational efficiency. The Poisson solver was extended to directly solve the derivatives of the solution. This is achieved either by including the differential operator in the integration kernel or by performing the differentiation as a multiplication of the Fourier coefficients. In this way, differential operators such as the divergence or curl of the solution field could be solved to the same high order convergence without additional computational effort. The method was applied and validated using the equations of fluid mechanics as an example, but can be used in many physical problems to solve the Poisson equation on a rectangular unbounded domain. For the two-dimensional case we propose an infinitely smooth test function which allows for arbitrary high order convergence. Using Gaussian smoothing as regularisation we document an increased convergence rate up to tenth order. The method however, can easily be
extended well beyond the tenth order. To show the full extend of the method we present the special case of a spectrally ideal regularisation of the velocity formulated integration kernel, which achieves an optimal rate of convergence.

**General information**

State: Published
Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, Université Catholique de Louvain
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**Bibliographical note**

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**Improvement in journal bearing design with application of computational fluid dynamics**

**General information**

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Organisations: Department of Mechanical Engineering, Solid Mechanics, Fluid Mechanics, Coastal and Maritime Engineering
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**Integrated Analysis of the Scavenging Process in Marine Two-Stroke Diesel Engines**

Large commercial ships such as container vessels and bulk carriers are propelled by low-speed, unison scavenged two-stroke diesel engines. An integral in-cylinder process in this type of engine is the scavenging process, where the burned gases from the combustion process are evacuated through the exhaust valve and replaced with fresh air for the subsequent compression stroke. The scavenging air enters the cylinder via inlet ports which are uncovered by the piston at bottom dead center (BDC). The exhaust gases are then displaced by the fresh air entering the cylinder. The scavenging ports are cut with an angle to introduce a swirling component to the flow. The in-cylinder swirl is beneficial for air-fuel mixture, cooling of the cylinder liner and minimizing recirculation zones where pockets of exhaust gas are trapped. However, a known characteristic of swirling flows is an adverse pressure gradient in the center of the flow, which might lead to a local deficit in axial velocity and the formation of central recirculation zones, known as vortex breakdown. Ever more
stringent emission legislations over the last 10-15 years have changed the engine lay out diagram in the pursuit of an engine which is both fuel effective and within the current emission legislations. To achieve this goal, a fundamental understanding of the in-cylinder processes, and the interactions between them are needed. This thesis aims at providing in-depth knowledge of the scavenging process and to identify the parameters that governs its performance. This thesis will present a CFD model that is tested and validated with quantitative data obtained from a dedicated test engine and during engine commissioning on location at the shipbuilder. The CFD model comprises the full geometry of a single cylinder from scavenger receiver to the exhaust receiver for a two-stroke diesel engine. Time resolved boundary conditions corresponding to measurements obtained from an operating engine as well as realistic initial conditions are used in the simulations. The CFD model provides a detailed description of the in-cylinder ow from exhaust valve opening (EVO) to exhaust valve closing (EVC). A string of studies are included in this thesis. An engine load sweep is included to evaluate the scavenging process as function of engine load. The engine load sweep follows the propeller curve, where the engine speed varies with the engine load. This implies that the pressure in the scavenge and exhaust receivers increase while the scavenge port exposure time, tscav, decrease. Further the scavenging pressure is varied while the engine speed is kept constant. From the perspective of the scavenging process this will resemble a load sweep following a generator curve. The scavenge port angle is varied to investigate the influence of in-cylinder swirl. A total of 7 port angles is applied; α = 0°, α = 10°, α = 15°, α = 18°, α = 20°, α = 25° and α = 30°. The CFD analysis shows that the bulk purity of air in the cylinder is proportional to the volumetric ow rate (mass ow rate divided by the air density) of scavenge air through the cylinder. The volumetric ow rate decreases with density for a given mass ow rate. When the engine load is increased, both the mass ow rate and the scavenging pressure is increased due to the turbo charger response. It is shown in this thesis that the increased density of the scavenge air, in conjunction with the reduced port exposure time, actually decrease the volume ow rate of air in the cylinders. This impairs the scavenging process at high engine loads. The CFD model also shows that the scavenging process consist of two sub processes. The volumetric scavenging, where the scavenge air displace the exhaust gas. And the push out process, where the piston displace the scavenge air and exhaust gas mixture between inlet port closing, IPC, and exhaust valve closing, EVC. The port angle study shows that the scavenging process is unaected by the changes in the in-cylinder swirl. Visualization of a passive scalar shows some influence of the in-cylinder distribution of scavenge air and exhaust gas, but volumetric displacement is the prime mover in the scavenging process. The CFD simulations is in good agreement with a simple perfect displacement model proposed by Sher (1990). The perfect displacement model is used as the basis for a simplified scavenging model in conjunction with a model to predict the contribution from the push out process. The model is modied to the CFD results to account for mixing between the scavenge air and the exhaustgas. The CFD model described in this Ph.D. thesis is used to investigate the response of key parameters on the scavenging process and gives detailed and profound insight to an integral in-cylinder process in the two-stroke diesel engine cycle. Further, the results from the CFD model is a valuable part of the R&D strategy of “full cycle CFD modelling” where the scavenging CFD model shall be coupled together with a combustion CFD model to simulate the complete engine cycle.

General information
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Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, MAN B&W Diesel A/S
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Projects:
Integrated Analysis of the Scavenging Process in Marine Two-Stroke Diesel Engines
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Iterative Brinkman penalization for remeshed vortex methods
We introduce an iterative Brinkman penalization method for the enforcement of the no-slip boundary condition in remeshed vortex methods. In the proposed method, the Brinkman penalization is applied iteratively only in the
neighborhood of the body. This allows for using significantly larger time steps, than what is customary in the Brinkman penalization, thus reducing its computational cost while maintaining the capability of the method to handle complex geometries. We demonstrate the accuracy of our method by considering challenging benchmark problems such as flow past an impulsively started cylinder and normal to an impulsively started and accelerated flat plate. We find that the present method enhances significantly the accuracy of the Brinkman penalization technique for the simulations of highly unsteady flows past complex geometries.

**General information**
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Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, Eidgenössische Technische Hochschule, California Institute of Technology
Authors: Hejlesen, M. M. (Intern), Koumoutsakos, P. (Ekstern), Leonard, A. (Ekstern), Walther, J. H. (Intern)
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Scopus rating (2016): CiteScore 3.12 SJR 2.034 SNIP 1.822
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.098 SNIP 1.988 CiteScore 2.92
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.166 SNIP 2.193 CiteScore 3.12
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 2.227 SNIP 2.45 CiteScore 3.3
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.161 SNIP 2.052 CiteScore 2.69
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.06 SNIP 2.194 CiteScore 2.99
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 2.185 SNIP 2.096
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 2.439 SNIP 2.219
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 2.247 SNIP 2.03
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 2.377 SNIP 2.379
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 2.182 SNIP 2.285
Web of Science (2006): Indexed yes
Kapitza Resistance between Few-Layer Graphene and Water: Liquid Layering Effects

The Kapitza resistance ($R_K$) between few-layer graphene (FLG) and water was studied using molecular dynamics simulations. The RK was found to depend on the number of the layers in the FLG though, surprisingly, not on the water block thickness. This distinct size dependence is attributed to the large difference in the phonon mean free path between the FLG and water. Remarkably, $R_K$ is strongly dependent on the layering of water adjacent to the FLG, exhibiting an inverse proportionality relationship to the peak density of the first water layer, which is consistent with better acoustic phonon matching between FLG and water. These findings suggest novel ways to engineer the thermal transport properties of solid–liquid interfaces by controlling and regulating the liquid layering at the interface.

General information
State: Published
Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, ETH Zurich, Tongji University, California Institute of Technology, Swiss Federal Institute of Technology
Authors: Alexeev, D. (Ekstern), Chen, J. (Ekstern), Walther, J. H. (Intern), Giapis, K. P. (Ekstern), Angelikopoulos, P. (Ekstern), Koumoutsakos, P. (Ekstern)
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BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 13.4
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 14.76
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 14.04
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 14.23
ISI indexed (2013): ISI indexed yes
Numerical and Experimental Investigation of Heat Flow in Permanent Magnet Brushless DC Hub Motor

This paper investigates the heat dissipation in the hub motor of an electric two-wheeler using lumped parameter (LP), finite element (FE) and computational fluid dynamic (CFD) models. The motor uses external rotor permanent magnet brushless DC topology and nearly all of its losses are generated in the stator. The hub motor construction restricts the available conductive paths for heat dissipation from the stator to the ambient only through the shaft. In contrast to an internal rotor structure, where the stator winding losses are diffused via conduction, here convection plays a major role in loss dissipation. Therefore, a LP thermal model with improved convection modelling has been proposed to calculate the temperature of the components inside the hub motor. The developed model is validated with the FE thermal model and the test data. In addition, CFD tools has been used to accurately model the internal and the external flow as well as the convective heat transfer of the hub motor. Finally, an optimization study of the hub motor has been carried out using the CFD model to improve heat transfer from the stator.

General information
State: Published
Organisations: Department of Electrical Engineering, Center for Electric Power and Energy, Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, Technical University of Denmark, University of the Faroe Islands
Number of pages: 12
Publication date: 2015
Main Research Area: Technical/natural sciences

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Journal: S A E International Journal of Alternative Powertrains
Volume: 4
Issue number: 1
Article number: V124-8EJ
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Ratings:
Scopus rating (2016): SJR 0.475 SNIP 0.893 CiteScore 1.08
On estimating the aerodynamic admittance of bridge sections by a mesh-free vortex method

A stochastic method of generating a synthetic turbulent flow field is combined with a 2D mesh-free vortex method to simulate the effect of an oncoming turbulent flow on a bridge deck cross-section within the atmospheric boundary layer. The mesh-free vortex method is found to be capable of preserving the a priori specified statistics as well as anisotropic characteristics of the synthesised turbulent flow field. From the simulation, the aerodynamic admittance is estimated and the instantaneous effect of a time varying angle of attack is briefly investigated. The obtained aerodynamic admittance of four aerodynamically different bridge sections is compared to available wind tunnel data, showing good agreement between the two.

General information
State: Published
Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, COWI A/S
Authors: Hejlesen, M. M. (Intern), Rasmussen, J. T. (Intern), Larsen, A. (Ekstern), Walther, J. H. (Intern)
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BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.61 SJR 1.002 SNIP 1.92
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.011 SNIP 1.966 CiteScore 2.51
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.929 SNIP 2.328 CiteScore 2.13
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.807 SNIP 2.636 CiteScore 2.43
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.667 SNIP 2.396 CiteScore 1.81
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.952 SNIP 3.274 CiteScore 2.3
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
Simulating external flow using vortex method in two- and three dimensions

Vortex methods are numerical methods for simulating fluid flow. They use a simple formulation where only the trajectories of discrete vortex particles are simulated. In our method, we combine a high order particle-mesh based vortex method with an iterative penalization method to simulate external flows around arbitrary geometries such as bridge decks. The method only uses a discretized geometry as input and can easily simulate an arbitrary motion of the geometry. As vorticity is a bounded quantity and the velocity field can easily be calculated for a mixture of free-space- and periodic boundary conditions, the method allows for a minimized domain and hence minimal computational resources. However, in an external flow problem, vorticity is produced in the boundary layers and transported downstream, consequently the computational domain must grow in time to encapsulate the entire vorticity field. We present a method for truncating this domain by supplementing the free-space- and periodic conditions with an outflow condition. The method is conveniently applied within the field of bridge aerodynamics as it can be used for the calculation of the aerodynamic net forces, which depend highly on the geometry and the wake forming behind it. This is demonstrated in 2D and 3D simulations.

General information
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Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, COWI A/S
Authors: Spietz, H. J. (Intern), Hejlesen, M. M. (Intern), Walther, J. H. (Intern), Larsen, A. (Ekstern)
Number of pages: 1
Publication date: 2015
Event: Abstract from 68th Annual Meeting of the American Physical Society’s Division of Fluid Dynamics (DFD), Boston, United States.
Main Research Area: Technical/natural sciences
Electronic versions:
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Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2015

Simulation of external flows using a hybrid particle mesh vortex method

The long-term goal of this project is to develop and apply state-of-the-art simulation software to enable accurate prediction of fluid structure interaction, specifically vortex-induced vibration and flutter of long-span suspension bridges to avoid error-prone structural designs. In the following a hybrid particle mesh vortex method is applied for the simulation of uniform
flow past stationary solid obstacles of arbitrary shapes.

**Sustaining dry surfaces under water**

Rough surfaces immersed under water remain practically dry if the liquid-solid contact is on roughness peaks, while the roughness valleys are filled with gas. Mechanisms that prevent water from invading the valleys are well studied. However, to remain practically dry under water, additional mechanisms need consideration. This is because trapped gas (e.g. air) in the roughness valleys can dissolve into the water pool, leading to invasion. Additionally, water vapor can also occupy the roughness valleys of immersed surfaces. If water vapor condenses, that too leads to invasion. These effects have not been investigated, and are critically important to maintain surfaces dry under water. In this work, we identify the critical roughness scale, below which it is possible to sustain the vapor phase of water and/or trapped gases in roughness valleys – thus keeping the immersed surface dry. Theoretical predictions are consistent with molecular dynamics simulations and experiments.
Water transport in graphene nano-channels

The transport of water in nanopores is of both fundamental and practical interest. Graphene Channels (GCs) are potential building blocks for nanofluidic devices due to their molecularly smooth walls and exceptional mechanical properties. Numerous studies have found a significant flow rate enhancement, defined as the ratio of the computed flow rate to that predicted from the classical Poiseuille model. Moreover, these studies point to the fact that the flow enhancement is a function of channel height and the fluid-wall physical-chemistry. In spite of the intensive research, an explicit relation between the chirality of the graphene walls and the slip length has not been established. In this study, we perform non-equilibrium molecular dynamics simulations of water flow in single- and multi-walled GCs. We examine the influence on the flow rates of dissipating the viscous heat produced by connecting the thermostat to the water molecules, the CNT wall atoms or both of them. From the atomic trajectories, we compute the fluid flow rates in GCs with zig-zag and armchair walls, heights from 1 to 4 nm and different number of graphene layers on the walls. A relation between the chirality, slip length, and flow enhancement is found.

General information
State: Published
Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, Universidad de Concepcion
Authors: Wagemann, E. (Ekstern), Oyarzua, E. (Ekstern), Walther, J. H. (Intern)
Number of pages: 1
Publication date: 2015
Event: Abstract from 68th Annual Meeting of the American Physical Society's Division of Fluid Dynamics (DFD), Boston, United States.
Main Research Area: Technical/natural sciences
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A numerical and experimental study of the scavenging process in a two-stroke marine diesel engine

General information
State: Published
Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering
Authors: Hemmingsen, C. S. (Intern), Ingvorsen, K. M. (Intern), Walther, J. H. (Intern), Meyer, K. E. (Intern)
Number of pages: 1
Publication date: 2014
Event: Abstract from 10th European Fluid Mechanics Conference (EUROMECH), KGs. Lyngby, Denmark.
Main Research Area: Technical/natural sciences
Source: PublicationPreSubmission
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Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2014

Application of finite elements and computational fluid dynamics to predict and improve the filling ratio in journal bearings under dynamic loading

General information
State: Published
Organisations: Department of Mechanical Engineering, Solid Mechanics, Fluid Mechanics, Coastal and Maritime Engineering, MAN Diesel & Turbo SE
Cavitation analysis of a journal bearing - Finite Element modelling and experimental studies

General information
State: Published
Organisations: Department of Mechanical Engineering, Solid Mechanics, Fluid Mechanics, Coastal and Maritime Engineering, MAN Diesel & Turbo SE
Authors: Christiansen, C. K. (Intern), Klit, P. (Intern), Walther, J. H. (Intern), Vølund, A. (Ekstern)
Number of pages: 1
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Publisher: Danish Technological Institute
Editors: Pleth Nielsen, L., Sivebæk, I. M., Stensig Eskildsen, S., Louring, S., Larsen, L. E.
ISBN (Print): 978-87-92765-26-0
Main Research Area: Technical/natural sciences
Conference: 16th Nordic Symposium on Tribology, Aarhus, Denmark, 10/06/2014 - 10/06/2014
Cavitation, Journal bearing, Finite Element, Filling ratio, Test Rig

Relations
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16th Nordic Symposium on Tribology
Source: PublicationPreSubmission
Source-ID: 100667431
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2014

CFD investigation of a transonic pulse-jet in a fabric filter applicaton

General information
State: Published
Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, F.L. Smidth A/S, Technical University of Denmark
Authors: Andersen, B. O. (Ekstern), Walther, J. H. (Intern), Nielsen, N. (Ekstern)
Number of pages: 2
Publication date: 2014
Event: Abstract from 10th European Fluid Mechanics Conference (EUROMECH), KGs. Lyngby, Denmark.
Main Research Area: Technical/natural sciences
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Continuum simulations of water flow in carbon nanotube membranes
We propose the use of the Navier–Stokes equations subject to partial-slip boundary conditions to simulate water flows in Carbon NanoTube (CNT) membranes. The finite volume discretizations of the Navier–Stokes equations are combined with slip lengths extracted from molecular dynamics (MD)
simulations to predict the pressure losses at the CNT entrance as well as the enhancement of the flow rate in the CNT. The flow quantities calculated from the present hybrid approach are in excellent agreement with pure MD results while they are obtained at a fraction of the computational cost. The method enables simulations of system sizes and times well beyond the present capabilities of MD simulations. Our simulations provide an asymptotic flow rate enhancement and indicate that the pressure losses at the CNT ends can be reduced by reducing their curvature. More importantly, our results suggest that flows at nanoscale channels can be described by continuum solvers with proper boundary conditions that reflect the molecular interactions of the liquid with the walls of the nanochannel.

General information
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Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, National Institute of Chemistry, Swiss Federal Institute of Technology
Authors: Popadić, A. (Ekstern), Walther, J. H. (Intern), Koumoutsakos, P. (Ekstern), Praprotnik, M. (Ekstern)
Number of pages: 11
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Scopus rating (2016): CiteScore 2.97 SJR 1.788 SNIP 1.031
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.938 SNIP 1.047 CiteScore 2.8
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.806 SNIP 1.307 CiteScore 2.89
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.871 SNIP 1.372 CiteScore 2.77
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 3.352 SNIP 1.533 CiteScore 3.4
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 3.47 SNIP 1.634 CiteScore 3.99
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 3.395 SNIP 1.421
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 3.215 SNIP 1.503
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Continuum Simulations of Water Flow in Carbon Nanotube Membranes

General information
State: Published
Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, National Institute of Chemistry, Swiss Federal Institute of Technology
Authors: Walther, J. H. (Intern), Popadic, A. (Ekstern), Koumoutsakos, P. (Ekstern), Praprotnik, M. (Ekstern)
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Event: Abstract from 67th Annual Meeting of the APS Division of Fluid Dynamics, San Francisco, CA, United States.
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Abstract
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Source-ID: 102830206
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Development of Smoothed Particle Hydrodynamics for Flow in Complex Geometries and Application of Open Source Software for the Simulation of Turbulent Flow

Turbulence modelling is a key issue in many industrial application, as the com-putational power of direct numerical simulation (DNS) is insu cient to deal with complex flow structures with high Reynolds number. Also in Industrial applications often involve turbulent flow in complex geometries. Thus de vel-oping a computational method which can deal with complex fluid structure, simulate complex geometors that change topology is particular challenging as the connectivity of the computational domain may change dynamically, and still e cient is important.
In this thesis we are presenting a remeshed particle-mesh method, the method involves three-dimensional compressible turbulent flow modelling, and coupled with an immersed boundary technique to deal with the complex solid obstacles. This dissertation is composed of three parts.
In combustion engines the scavenging process in two-stroke marine diesel engines removes combustion gases from the engine cylinder and fills up the cylinder with the fresh air charge for the next cycle. Understanding the scavenging flow is crucial for the development of such engines, since it affects fuel consumption, engine cooling and production of pollutants. We consider a state-of-the art eulerian methods to study the turbulent flow in a model diesel engine. the goals of this study include validation of large eddy simulations (LES) turbulence models.

General information
Large eddy simulations of the influence of piston position on the swirling flow in a model two-stroke diesel engine

Purpose – The purpose of this paper is to study the effect of piston position on the in-cylinder swirling flow in a simplified model of a large two-stroke marine diesel engine. Design/methodology/approach – Large eddy simulations with four different models for the turbulent flow are used: a one-equation model, a dynamic one-equation model, a localized dynamic one-equation model and a mixed-scale model. Simulations are carried out for two different geometries corresponding to 100 and 50 percent open scavenge ports. Findings – It is found that the mean tangential profile inside the cylinder changes qualitatively with port closure from a Lamb-Oseen vortex profile to a solid body rotation, while the axial velocity changes from a wake-like profile to a jet-like profile. The numerical results are compared with particle image velocimetry measurements, and in general, the authors find a good agreement. Research limitations/implications – Considering the complexity of the real engine, the authors designed the engine model using the simplest configuration possible. The setup contains no moving parts, the combustion is neglected and the exhaust valve is discarded. Originality/value – Studying the flow in a simplified engine model, the setup allows studies of fundamental aspects of swirling flow in a uniform scavenged engine. Comparing the four turbulence models, the local dynamic one-equation model is found to give the best agreement with the experimental results.
Molecular dynamics simulations of water on a hydrophilic silica surface at high air pressures

We present a force field for Molecular Dynamics (MD) simulations of water and air in contact with an amorphous silica surface. We calibrate the interactions of each species present in the system using dedicated criteria such as the contact angle of a water droplet on a silica surface, and the solubility of air in water at different pressures. Using the calibrated force field, we conduct MD simulations to study the interface between a hydrophilic silica substrate and water surrounded by air at different pressures. We find that the static water contact angle is independent of the air pressure imposed on the system. Our simulations reveal the presence of a nanometer thick layer of gas at the water–silica interface. We believe that this gas layer could promote nucleation and stabilization of surface nanobubbles at amorphous silica surfaces. © 2014 Elsevier B.V. All rights reserved.
Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, Universidad de Concepcion, NASA Ames Research Center
Authors: Zambrano, H. (Ekstern), Walther, J. H. (Intern), Jaffe, R. (Ekstern)
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Main Research Area: Technical/natural sciences

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- BFI (2017): BFI-level 1
- Web of Science (2017): Indexed Yes
- BFI (2016): BFI-level 1
- Scopus rating (2016): CiteScore 3.47 SJR 0.718 SNIP 1.212
- BFI (2015): BFI-level 1
- Scopus rating (2015): SJR 0.652 SNIP 0.997 CiteScore 2.61
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 1
- Scopus rating (2014): SJR 0.637 SNIP 1.126 CiteScore 2.34
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 1
- Scopus rating (2013): SJR 0.611 SNIP 1.082 CiteScore 2.07
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
- BFI (2012): BFI-level 1
- Scopus rating (2012): SJR 0.673 SNIP 1.041 CiteScore 1.62
- ISI indexed (2012): ISI indexed yes
- Web of Science (2012): Indexed yes
- BFI (2011): BFI-level 1
- Scopus rating (2011): SJR 0.611 SNIP 1.093 CiteScore 1.64
- ISI indexed (2011): ISI indexed yes
- Web of Science (2011): Indexed yes
- BFI (2010): BFI-level 1
- Scopus rating (2010): SJR 0.691 SNIP 1.139
- BFI (2009): BFI-level 1
- Scopus rating (2009): SJR 0.669 SNIP 0.914
- BFI (2008): BFI-level 1
- Scopus rating (2008): SJR 0.686 SNIP 0.754
- Scopus rating (2007): SJR 0.573 SNIP 0.737
- Scopus rating (2006): SJR 0.546 SNIP 0.835
- Scopus rating (2005): SJR 0.581 SNIP 0.914
- Scopus rating (2004): SJR 0.505 SNIP 0.752
- Web of Science (2004): Indexed yes
- Scopus rating (2003): SJR 0.498 SNIP 0.686
- Scopus rating (2002): SJR 0.404 SNIP 0.574
- Scopus rating (2001): SJR 0.421 SNIP 0.575
- Scopus rating (2000): SJR 0.601 SNIP 0.926
- Scopus rating (1999): SJR 0.536 SNIP 0.816

Original language: English
Molecular dynamics, Wetting, Nanodroplets, Contact angle, Solid-liquid-gas interactions
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Moving least squares simulation of free surface flows
In this paper a Moving Least Squares method (MLS) for the simulation of 2D free surface flows is presented. The emphasis is on the governing equations, the boundary conditions, and the numerical implementation. The compressible viscous isothermal Navier–Stokes equations are taken as the starting point. Then a boundary condition for pressure (or density) is developed. This condition is applicable at interfaces between different media such as fluid–solid or fluid–void. The effect of surface tension is included. The equations are discretized by a moving least squares method for the spatial derivatives and a Runge–Kutta method for the time derivatives. The computational frame is Lagrangian, which means that the computational nodes are convected with the flow. The method proposed here is benchmarked using the standard lid driven cavity problem, a rotating free surface problem, and the simulation of drop oscillations. A new exact solution to the unsteady incompressible Navier–Stokes equations is introduced for the rotating free surface problem. © 2013 Elsevier Ltd.

General information
State: Published
Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, Department of Applied Mathematics and Computer Science, Mathematics, MAN Diesel & Turbo SE
Authors: Felter, C. L. (Intern), Walther, J. H. (Intern), Henriksen, C. (Intern)
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Main Research Area: Technical/natural sciences

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Volume: 91
ISSN (Print): 0045-7930
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BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 1.022 SNIP 1.579 CiteScore 2.54
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.152 SNIP 1.665 CiteScore 2.26
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.031 SNIP 1.641 CiteScore 1.98
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.081 SNIP 1.974 CiteScore 2.17
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.135 SNIP 1.986 CiteScore 1.95
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.964 SNIP 1.845 CiteScore 1.97
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.19 SNIP 2.053
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.414 SNIP 2.124
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.326 SNIP 1.745
Scopus rating (2007): SJR 1.039 SNIP 1.649
Scopus rating (2006): SJR 1.047 SNIP 2.018
Scopus rating (2005): SJR 0.997 SNIP 1.768
Numerical analysis of the scavenge flow and convective heat transfer in large two-stroke marine diesel engines

A novel computational fluid dynamics (CFD) model is presented for the study of the scavenging process and convective heat transfer in a large two-stroke low-speed uniflow-scavenged marine diesel engine. The engine is modeled using a fully resolved 12 sector, corresponding to one scavenge port, with cyclic boundaries in the tangential direction. The CFD model is strongly coupled to experiments and effectively provides a high order "interpolation" of the engine processes through the solution of the Reynolds-Averaged Navier–Stokes (RANS) equations subject to boundary conditions obtained through experiments. The imposed experimental data includes time histories of the pressure difference across the engine and the heat release during combustion. The model is validated by a numerical sensitivity analysis and through comparison of model predictions and experimental data, which shows a good agreement. The results show an effective scavenging and a low convective heat loss in agreement with experimental data for large marine diesel engines. © 2014 Elsevier Ltd. All rights reserved.

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Authors: Sigurdsson, E. (Intern), Ingvorsen, K. M. (Intern), Jensen, M. V. (Intern), Mayer, S. (Ekstern), Matlok, S. (Ekstern), Walther, J. H. (Intern)
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Publication date: 2014
Main Research Area: Technical/natural sciences

Publication information
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BFI (2017): BFI-level 2
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Web of Science (2016): Indexed yes
Web of Science (2015): Indexed yes
Web of Science (2014): Indexed yes
Web of Science (2013): Indexed yes
Web of Science (2012): Indexed yes
Web of Science (2011): Indexed yes
Scopus rating (2016): CiteScore 7.78 SJR 3.058 SNIP 2.573
Scopus rating (2015): SJR 2.912 SNIP 2.61 CiteScore 6.4
Scopus rating (2014): SJR 3.254 SNIP 3.28 CiteScore 6.93
Scopus rating (2013): SJR 3.164 SNIP 3.377 CiteScore 6.59
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Numerical and Experimental Investigation of Heat Flow in Permanent Magnet Brushless DC Hub Motor

This paper investigates the heat dissipation in the hub motor of an electric two-wheeler using lumped parameter (LP), finite element (FE) and computational fluid dynamic (CFD) models. The motor uses external rotor permanent magnet brushless DC topology and nearly all of its losses are generated in the stator. The hub motor construction restricts the available conductive paths for heat dissipation from the stator to the ambient only through the shaft. In contrast to an internal rotor structure, where the stator winding losses are diffused via conduction, here convection plays a major role in loss dissipation. Therefore, a LP thermal model with improved convection modelling has been proposed to calculate the temperature of the components inside the hub motor. The developed model is validated with the FE thermal model and the test data. In addition, CFD tools has been used to accurately model the internal and the external flow as well as the convective heat transfer of the hub motor. Finally, an optimization study of the hub motor has been carried out using the CFD model to improve heat transfer from the stator.

General information
State: Published
Organisations: Department of Electrical Engineering, Center for Electric Power and Energy, Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, Technical University of Denmark, University of the Faroe Islands
Number of pages: 12
Publication date: 2014
PIV and LDA measurements of the swirling flow in a low-speed two-stroke diesel engine

General information
State: Published
Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, MAN Diesel & Turbo SE
Authors: Ingvorsen, K. M. (Intern), Meyer, K. E. (Intern), Walther, J. H. (Intern), Mayer, S. (Ekstern)
Number of pages: 1
Publication date: 2014
Event: Abstract from 10th European Fluid Mechanics Conference (EUROMECH), KGs. Lyngby, Denmark.
Main Research Area: Technical/natural sciences
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   PIV_and_LDA.pdf
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Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2014

Simulations of a single turbulent vortex ring using a regularized particle-mesh based vortex method

General information
State: Published
Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, Eidgenössische Technische Hochschule
Authors: Hejlesen, M. M. (Intern), Walther, J. H. (Intern)
Publication date: 2014
Event: Poster session presented at 11th World Congress on Computational Mechanics, 5th European Conference on Computational Mechanics, 6th European Conference on Computational Fluid Dynamics, Barcelona, Spain.
Main Research Area: Technical/natural sciences
Vortex rings, Turbulence, Particle-mesh methods, Regularized vortex methods
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Simulations of a single vortex ring using an unbounded, regularized particle-mesh based vortex method

In recent work we have developed a new FFT based Poisson solver, which uses regularized Greens functions to obtain arbitrary high order convergence to the unbounded Poisson equation. The high order Poisson solver has been implemented in an unbounded particle-mesh based vortex method which uses a re-meshing of the vortex particles to ensure the convergence of the method. Furthermore, we use a re-projection of the vorticity field to include the constraint of a divergence-free stream function which is essential for the underlying Helmholtz decomposition and ensures a divergence free vorticity field. The high order, unbounded particle-mesh based vortex method is used to simulate the instability, transition to turbulence and eventual destruction of a single vortex ring. From the simulation data a novel method on analyzing the dynamics of the enstrophy is presented based on the alignment of the vorticity vector with the principal axis of the strain rate tensor. We find that the dynamics of the enstrophy density is dominated by the local flow deformation and axis of rotation, which is used to infer some concrete tendencies related to the topology of the vorticity field.

General information
State: Published
Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, Technical University of Denmark
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Simulations of vortical flow using an unbounded, regularized particle-mesh based vortex method

General information
State: Published
Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering
Authors: Hejlesen, M. M. (Intern), Walther, J. H. (Intern)
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Strain Engineering of Kapitza Resistance in Few-Layer Graphene
We demonstrate through molecular dynamics simulations that the Kapitza resistance in few-layer graphene (FLG) can be controlled by applying mechanical strain. For unstrained FLG, the Kapitza resistance decreases with the increase of thickness and reaches an asymptotic value of $6 \times 10^{-10}$ m$^2$K/W at a thickness about 16 nm. Uniaxial cross-plane strain is found to increase the Kapitza resistance in FLG monotonically, when the applied strain varies from compressive to tensile. Moreover, uniaxial strain couples the in-plane and out-of-plane strain/stress when the surface of FLG is buckled. We find that with a compressive cross-plane stress of 2 GPa, the Kapitza resistance is reduced by about 50%. On the other hand it is almost tripled with a tensile cross-plane stress of 1 GPa. Remarkably, compressive in-plane strain can either increase or reduce the Kapitza resistance, depending on the specific way it is applied. Our study suggests that graphene can be exploited for both heat dissipation and insulation through strain engineering.

General Information
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Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, Swiss Federal Institute of Technology
Authors: Chen, J. (Ekstern), Walther, J. H. (Intern), Koumoutsakos, P. (Ekstern)
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Theoretical and experimental investigation of cavitation in main bearings for large two-stroke marine diesel engines

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Organisations: Department of Mechanical Engineering, Solid Mechanics, Fluid Mechanics, Coastal and Maritime Engineering, MAN Diesel & Turbo SE
Authors: Christiansen, C. K. (Intern), Klit, P. (Intern), Walther, J. H. (Intern), Vølund, A. (Ekstern)
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Turbulent swirling flow in a dynamic model of a uniflow-scavenged two-stroke engine

It is desirable to use computational fluid dynamics for optimization of the in-cylinder processes in low-speed two-stroke uniflow-scavenged marine diesel engines. However, the complex nature of the turbulent swirling in-cylinder flow necessitates experimental data for validation of the used turbulence models. In the present work, the flow in a dynamic scale model of a uniflow-scavenged cylinder is investigated experimentally. The model has a transparent cylinder and a moving piston driven by a linear motor. The flow is investigated using phase-locked stereoscopic particle image velocimetry (PIV) and time-resolved laser Doppler anemometry (LDA). Radial profiles of the phase-locked mean and rms velocities are computed from the velocity fields recorded with PIV, and the accuracy of the obtained profiles is demonstrated by comparison with reference LDA measurements. Measurements are carried out at five axial positions for 15 different times during the engine cycle and show the temporal and spatial development of the swirling in-cylinder flow. The tangential velocity profiles in the bottom of the cylinder near the end of the scavenge process are characterized by a concentrated swirl resulting in wake-like axial velocity profiles and the occurrence of a vortex breakdown. After scavenge port closing, the axial velocity profiles indicate that large transient swirl-induced structures exist in the cylinder. Comparison with profiles obtained under steady-flow conditions shows that the scavenge flow cannot be assumed to be quasi-steady. The temporal development of the swirl strength is investigated by computing the angular momentum. The swirl strength shows an exponential decay from scavenge port closing to scavenge port opening corresponding to a reduction of 34 %, which is in good agreement with theoretical predictions.

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Authors: Ingvorsen, K. M. (Intern), Meyer, K. E. (Intern), Walther, J. H. (Intern), Mayer, S. (Intern)
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Scopus rating (2015): SJR 1.193 SNIP 1.592 CiteScore 2.04
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ISI indexed (2013): ISI indexed yes
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Scopus rating (2011): SJR 1.167 SNIP 1.938 CiteScore 1.93
ISI indexed (2011): ISI indexed yes
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Scopus rating (2009): SJR 1.531 SNIP 1.881
A high order solver for the unbounded Poisson equation

In mesh-free particle methods a high order solution to the unbounded Poisson equation is usually achieved by constructing regularised integration kernels for the Biot-Savart law. Here the singular, point particles are regularised using smoothed particles to obtain an accurate solution with an order of convergence consistent with the moments conserved by the applied smoothing function. In the hybrid particle-mesh method of Hockney and Eastwood (HE) the particles are interpolated onto a regular mesh where the unbounded Poisson equation is solved by a discrete non-cyclic convolution of the mesh values and the integration kernel. In this work we show an implementation of high order regularised integration kernels in the HE algorithm for the unbounded Poisson equation to formally achieve an arbitrary high order convergence. We further present a quantitative study of the convergence rate to give further insight in the convergence of particle methods.

General information
State: Published
Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, Université Catholique de Louvain
Authors: Hejlesen, M. M. (Intern), Rasmussen, J. T. (Intern), Chatelain, P. (Ekstern), Walther, J. H. (Intern)
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A high order solver for the unbounded Poisson equation

A high order converging Poisson solver is presented, based on the Green’s function solution to Poisson’s equation subject to free-space boundary conditions. The high order convergence is achieved by formulating regularised integration kernels, analogous to a smoothing of the solution field. The method is extended to directly solve the derivatives of the solution to Poisson’s equation. In this way differential operators such as the divergence or curl of the solution field can be solved to the same high order convergence without additional computational effort. The method, is applied and validated, however not restricted, to the equations of fluid mechanics, and can be used in many applications to solve Poisson’s equation on a rectangular unbounded domain.

General information
State: Published
An improved interface penalisation for vortex methods

General information
State: Published
Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, Swiss Federal Institute of Technology, California Institute of Technology
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An Iterative Brinkman penalization for particle vortex methods

We present an iterative Brinkman penalization method for the enforcement of the no-slip boundary condition in vortex particle methods. This is achieved by implementing a penalization of the velocity field using iteration of the penalized vorticity. We show that using the conventional Brinkman penalization method can result in an insufficient enforcement of solid boundaries. The specific problems of the conventional penalization method is discussed and three examples are presented by which the method in its current form has shown to be insufficient to consistently enforce the no-slip boundary condition. These are: the impulsively started flow past a cylinder, the impulsively started flow normal to a flat plate, and the uniformly accelerated flow normal to a flat plate. The iterative penalization algorithm is shown to give significantly improved results compared to the conventional penalization method for each of the presented flow cases.
Carbon nanotube (CNT) membranes hold the promise of extraordinary fast water transport for applications such as energy efficient filtration and molecular level drug delivery. However, experiments and computations have reported flow rate enhancements over continuum hydrodynamics that contradict each other by orders of magnitude. We perform large scale molecular dynamics simulations emulating for the first time the micrometer thick CNTs membranes used in experiments. We find transport enhancement rates that are length dependent due to entrance and exit losses but asymptote to 2 orders of magnitude over the continuum predictions. These rates are far below those reported experimentally. The results suggest that the reported superfast water transport rates cannot be attributed to interactions of water with pristine CNTs alone.
Effect of air on water capillary flow in silica nanochannels

Capillarity is a classical topic in fluid dynamics. The fundamental relationship between capillarity and surface tension is solidly established. Nevertheless, capillarity is an active research area especially as the miniaturization of devices is reaching the molecular scale. Currently, with the fabrication of microsystems integrated by nanochannels, a thorough understanding of the transport of fluids in nanoconfinement is required for a successful operation of the functional parts of such devices. In this work, Molecular Dynamics simulations are conducted to study the spontaneous imbibition of water in sub 10 nm silica channels. The capillary filling speed is computed in channels subjected to different air pressures. In order to describe the interactions between the species, an effective force field is developed, which is calibrated by reproducing the water contact angle. The results show that the capillary filling speed qualitatively follows the classical Washburn model, however, quantitatively it is lower than expected. Furthermore, it is observed that the deviations increase as air pressure is higher. We attribute the deviations to amounts of air trapped at the silica-water interface which leads to changes in the dynamics contact angle of the water meniscus.

General information
State: Published
Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, Universidad de Concepcion
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Main Research Area: Technical/natural sciences

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Heat Transfer in Large Two-Stroke Marine Diesel Engines

Heat transfer between the cylinder gas and the piston surface during combustion in large two-stroke uniflow scavenged marine diesel engines has been investigated in the present work. The piston surface experiences a severe thermal load during combustion due to the close proximity of the combustion zone to the surface. At the same time, cooling of the piston crown is relatively complicated. This can cause large thermal stresses in the piston crown and weakening of the material strength, which may be critical as it can lead to formation of cracks. Information about the piston surface heat transfer is thus important for the engine manufacturers.

The piston surface heat transfer was studied in the event of impingement of hot combustion products on the piston during combustion, and an estimate was obtained of the peak heat flux level experienced on the piston surface. The investigation was carried out numerically by performing simulations with a CFD code of the heat transfer between gas and wall in a jet impingement configuration where a hot round turbulent gas jet impinged normally onto a wall under conditions approximating the in-cylinder conditions in the engine during combustion.

A jet impingement reference case was first established based on estimations of the incylinder conditions during combustion. Subsequently, variations of different jet impingement parameters were performed and the influence on the wall heat transfer was observed. In all the cases, the ratio between the jet inlet to wall distance, $H$, and the jet diameter at the inlet, $D$, was $H/D = 2$. The jet Reynolds number, $Re$, varied between $1.10 \times 10^5$ and $6.64 \times 10^5$. The resulting Nusselt numbers along the wall were calculated for dimensionless radial distances from the stagnation point, $r/D$, between 0 and 6. The maximum Nusselt number was located in the stagnation point in most of the investigated cases, and an analysis was performed of the variation of the stagnation point Nusselt number, $Nu_0$, with the jet Reynolds number and the jet turbulence intensity at the jet inlet, $TI$. Based on the observed relations, a correlation between $Nu_0$, $Re$ and $TI$ is suggested for high jet Reynolds number cases. A satisfactory validation of the correlation was not possible to perform due to insufficient available experimental data. A comparison of the correlation predictions to existing experimental data indicated however an overprediction of $Nu_0$ in the magnitude of 50% – 100%. The overprediction is considered to be caused primarily by incorrect numerical model predictions. Based on the performed jet impingement heat transfer investigations, an estimate is provided of the peak convective piston surface heat flux level experienced in the considered large marine diesel engines. The contribution from thermal radiation to the piston surface heat flux was not investigated in the present work, but a coarse estimation of the magnitude was performed. The obtained estimations indicate a peak piston surface heat flux level in the interval from about 1 MW/m² and up to 9.5 MW/m² with the actual value probably being in the lower part of this interval. This is about the same magnitude as that previously reported for automotive size diesel engines. The obtained interval is relatively large, but a more accurate prediction is difficult to achieve with the applied method due to limited knowledge about the actual local in-cylinder conditions during combustion. Therefore, further research in this area is encouraged.

**General information**

State: Published
Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, Thermal Energy
Authors: Jensen, M. V. (Intern), Walther, J. H. (Intern), Carlsen, H. (Intern), Schramm, J. (Intern)
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Multiscale Simulation of Breaking Wave Impacts

The purpose of this project is to make an accurate, robust, geometric flexible and efficient model for calculation of forces on structures from nonlinear ocean waves and breaking wave impacts. Accurate prediction of the extreme forces on wind turbine foundations, breakwaters and tidal or wave power devices are important for enhancement structural designs.

The proposed model is based on an incompressible and inviscid flow approximation and the governing equations are applied in an arbitrary Lagrangian-Eulerian moving frame of reference (ALE). The Runge-Kutta method (RK) is used for time integration and mass conservation is satisfied through a pressure-corrector type calculation of the pressure. The weighted least squares method (WLS) is combined with approximate Riemann solvers to introduce numerical smoothing of the solution around steep gradients in the velocity and pressure fields. The Poisson equation is solved and the pressure boundary conditions are satisfied by a generalized finite pointset method (GFPM); This provides a geometrically flexible and stable solution for the fluid pressure. The numerical approximations of these equations are performed on unstructured point distributions and the solutions for velocity and pressure are represented by WLS approximation of multivariate polynomials. The stencils for the ALE-WLS and GFPM methods are found through a breadth first search (BFS) in a modified Delaunay graph. This graph is the discrete representation of the fluid domain and the connectivity between the calculation points. The graph is updated according to the evolving topology of the fluid domain caused by the fluid reaching or leaving a solid boundary or the free surface colliding with it or another free-surface. After each time step the fluid domain is checked for any of these intersections and the topology is updated accordingly in its graph representation. The calculation points move in a Lagrangian way and this can cause ill-conditioning of the generalized Vandermonde matrix in the WLS and GFPM methods. To prevent this the point set is refined and coarsened by a distance based adaptivity method and redistributed via a point position filtering method. The incompressible and inviscid ALE-WLS model is applied to the following standard validation test cases: deforming elliptical drop, small amplitude standing waves and the dam break problem. The deforming elliptical drop test show that the model can calculate the kinematics and dynamics of this free surface flow accurately and robustly. The small amplitude standing wave gives the same conclusions. Long time integration of this small amplitude periodic motion is possible due to accurate free surface evolution and small errors in the fluid volume. The dam break test case shows that the incompressible and inviscid ALE-WLS model can calculate nonlinear fluid motion, fluid structure impacts and overturning waves. The propagation speed of the wetting front and impact pressures are compared to experiments and the results compare reasonably well. The incompressible and inviscid ALE-WLS model is coupled with the potential flow model of Engsig-Karup et al. [2009], to perform multiscale calculation of breaking wave impacts on a vertical breakwater. The potential flow model provides accurate calculation of the wave transformation from offshore to the vicinity of the breakwater. The wave breaking close to the breakwater and the wave impact are calculated by the incompressible ALE-WLS model. The forces calculated with the incompressible and inviscid ALE-WLS model are 1 - 2 times the corresponding compressible calculations in Bredmose et al. [2009] for the calculations without trapped air.

Among the contributions of this project are the ALE-WLS method combined with approximate Riemann solvers and the generalization of the FPM method to arbitrary order of accuracy. The WLS and GFPM stencils found using the BFS data structure, which is updated due to topology changes of the evolving fluid domain. This extension combined with ALE-WLS and approximate Riemann solvers gives a numerical model capable of calculation of forces due to breaking wave impacts. The incompressible and inviscid ALE-WLS model has been coupled with a potential flow model to provide multiscale calculation of forces from breaking wave impacts on structures.

Numerical analysis of jet impingement heat transfer at high jet Reynolds number and large temperature difference

Jet impingement heat transfer from a round gas jet to a flat wall was investigated numerically for a ratio of 2 between the jet inlet to wall distance and the jet inlet diameter. The influence of turbulence intensity at the jet inlet and choice of turbulence model on the wall heat transfer was investigated at a jet Reynolds number of 1.66 × 105 and a temperature difference between jet inlet and wall of 1600 K. The focus was on the convective heat transfer contribution as thermal radiation was not included in the investigation. A considerable influence of the turbulence intensity at the jet inlet was observed in the stagnation region, where the wall heat flux increased by a factor of almost 3 when increasing the turbulence intensity from 1.5% to 10%. The choice of turbulence model also influenced the heat transfer predictions significantly, especially in the stagnation region, where differences of up to about 100% were observed. Furthermore, the
variation in stagnation point heat transfer was examined for jet Reynolds numbers in the range from $1.10 \times 10^5$ to $6.64 \times 10^5$. Based on the investigations, a correlation is suggested between the stagnation point Nusselt number, the jet Reynolds number, and the turbulence intensity at the jet inlet for impinging jet flows at high jet Reynolds numbers. Copyright © 2013 Taylor and Francis Group, LLC.
Phase-locked stereoscopic PIV measurements of the turbulent swirling flow in a dynamic model of a uniflow-scavenged two-stroke engine cylinder

It is desirable to use computational fluid dynamics for the optimization of in-cylinder processes in large two-stroke low-speed uniflow-scavenged marine diesel engines. However, the complex nature of the turbulent swirling in-cylinder flow necessitates experimental data for validation of the used turbulence models. In the present work, the flow in a dynamic scale model of a uniflow-scavenged cylinder is investigated experimentally. The model has a transparent cylinder and a movable piston driven by a linear motor. The flow is investigated using phase-locked stereoscopic particle image velocimetry (PIV) and time resolved laser Doppler anemometry (LDA). Radial profiles of the phase-averaged mean velocities are computed from the velocity fields recorded with PIV and the validity of the obtained profiles is demonstrated by comparison with reference LDA measurements. Radial profiles are measured at five axial positions for 15 different times during the engine cycle and shows the temporal and spatial development of the swirling in-cylinder flow. The tangential velocity profiles in the bottom of the cylinder near the end of the scavenging process are characterized by a concentrated swirl resulting in wake-like axial velocity profiles and the occurrence of a vortex breakdown. After scavenge port closing the axial velocity profiles indicate that large transient swirl-induced structures exists in the cylinder. Comparison with profiles obtained under steady-flow conditions shows that the steady profiles in general will not be representative for the dynamic conditions. The temporal development of the swirl strength is investigated by computing the angular momentum. The swirl strength shows an exponential decay from scavenge port closing to scavenge port opening corresponding to a reduction of 34%.

PIV study of the effect of piston position on the in-cylinder swirling flow during the scavenging process in large two-stroke marine diesel engines

A simplified model of a low speed large twostroke marine diesel engine cylinder is developed. The effect of piston position on the in-cylinder swirling flow during the scavenging process is studied using the stereoscopic particle image velocimetry technique. The measurements are conducted at different cross-sectional planes along the cylinder length and at piston positions covering the air intake port by 0, 25, 50 and 75 %. When the intake port is fully open, the tangential velocity profile is similar to a Burgers vortex, whereas the axial velocity has a wake-like profile. Due to internal wall friction, the swirl decays downstream, and the size of the vortex core increases. For increasing port closures, the tangential velocity profile changes from a Burgers vortex to a forced vortex, and the axial velocity changes correspondingly from a wake-like profile to a jet-like profile. For piston position with 75 % intake port closure, the jet-like axial velocity profile at a cross-sectional plane close to the intake port changes back to a wake-like profile at the adjacent downstream cross-sectional plane. This is characteristic of a vortex breakdown. The non-dimensional velocity profiles show no significant variation with the variation in Reynolds number.
Simulation of the Initial 3-D Instability of an Impacting Drop Vortex Ring

Computational vortex particle method simulations of a perturbed vortex ring are performed to recreate and understand the instability seen in impacting water drop experiments. Three fundamentally different initial vorticity distributions are used to attempt to trigger a Widnall instability, a Rayleigh centrifugal instability, or a vortex breakdown-type instability. Simulations which simply have a perturbed solitary ring result in an instability similar to that seen experimentally. Waviness of the core which would be expected from a Widnall instability is not visible. Adding an opposite-signed secondary vortex ring or an image vortex ring to the initial conditions, to trigger a Rayleigh or breakdown respectively, does not appear to significantly change the instability from what is seen with a solitary ring. This suggests that a Rayleigh or vortex breakdown-type instability are not likely at work, though tests are not conclusive. Perhaps the opposite-signed secondary vortex was not strong enough or placed appropriately. Elliptical streamlines, as expected, are visible in the core of the solitary ring at early times. Support from the Canadian Natural Sciences and Engineering Research Council grant 41747 is gratefully acknowledged.

Swirling flow in a two-stroke marine diesel engine

Computational fluid dynamic simulations are performed for the turbulent swirling flow in a scale model of a low-speed two-stroke diesel engine with a moving piston. The purpose of the work is to investigate the accuracy of different turbulence models including two-equation Reynolds-Averaged Navier-Stokes models and large eddy simulations. The numerical model represent the full three-dimensional geometry and the piston motion is modeled by compressing cells in the axial direction. The CFD predictions are compared to experimental results and a reasonable agreement is found.
Turbulent swirling flow in a model of a uniflow-scavenged two-stroke engine

The turbulent and swirling flow of a uniflow-scavenged two-stroke engine cylinder is investigated using a scale model with a static geometry and a transparent cylinder. The swirl is generated by 30 equally spaced ports with angles of 0°, 10°, 20°, and 30°. A detailed characterization of the flow field is performed using stereoscopic particle image velocimetry. Mean fields are calculated using both a fixed coordinate system and a coordinate system based on the instantaneous flow topology. Time-resolved measurements of axial velocity are performed with laser Doppler anemometry, and power spectra are calculated in order to determine vortex core precession frequencies. The results show a very different flow dynamics for cases with weak and strong swirl. In the strongly swirling cases, a vortex breakdown is observed. Downstream of the breakdown, the vortex becomes highly concentrated and the vortex core precesses around the exhaust valve, resulting in an axial suction effect at the vortex center. Mean fields based on the instantaneous flow topology are shown to be more representative than mean fields based on a fixed coordinate system in cases with significant variations in the swirl center location.

General information

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Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, MAN Diesel & Turbo SE
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Web of Science (2015): Indexed yes
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Scopus rating (2014): SJR 1.235 SNIP 1.721 CiteScore 2.21
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ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.167 SNIP 1.938 CiteScore 1.93
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.016 SNIP 1.635
A high order solver for the unbounded Poisson equation

This work improves upon Hockney and Eastwood's Fourier-based algorithm for the unbounded Poisson equation to formally achieve arbitrary high order of convergence without any additional computational cost. We assess the methodology on the kinematic relations between the velocity and vorticity fields.

General information
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Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, Université Catholique de Louvain
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A high order solver for the unbounded Poisson equation with specific application to the equations of fluid kinematics

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Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, Université Catholique de Louvain
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A numerical study of the aerodynamic admittance of bridge deck sections by a two-dimensional mesh-free vortex method

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Authors: Hejlesen, M. M. (Intern), Rasmussen, J. T. (Intern), Larsen, A. (Ekstern), Walther, J. H. (Intern)
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Publication: Research › Conference abstract in journal – Annual report year: 2012

CFD modelling of combined blast and contact cooling for whole fish

General information
State: Published
Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, Icelandic Food Research, University of Iceland
Authors: Walther, J. H. (Intern), Bjarnason, V. O. (Ekstern), Margeirsson, B. (Ekstern), Arason, S. (Ekstern), Bergsson, A. (Ekstern)
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Bibliographical note
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High Order Poisson Solver for Unbounded Flows

General information
State: Published
Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering
Authors: Walther, J. H. (Intern), Hejlesen, M. M. (Intern), Rasmussen, J. T. (Intern), Chatelai, P. (Ekstern)
Implementation of the Spalart-Almaras turbulence model in the two-dimensional vortex-in-cell method

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State: Published
Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, COWI Consultants A/S
Authors: Hejlesen, M. M. (Intern), Rasmussen, J. T. (Intern), Larsen, A. (Ekstern), Walther, J. H. (Intern)
Publication date: 2012

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Title of host publication: Proceedings of the 6th European Congress on Computational Methods in Applied Sciences and Engineering
Publisher: Vienna University of Technology
Editors: Eberhardsteiner, J., Böhm, H., Rammerstorfer, F.
Main Research Area: Technical/natural sciences
Electronic versions:
eccomas2012.pdf
Source: dtu
Source-ID: u::5691
Publication: Research › Article in proceedings – Annual report year: 2012

Influence of piston displacement on the scavenging and swirling flow in two-stroke diesel engines
We study the effect of piston motion on the in-cylinder swirling flow in a low speed, large two-stroke marine diesel engine. The work involves experimental, and numerical simulation using OpenFOAM platform. Large Eddy Simulation was used with three different models, One equation Eddy, Dynamic One equation Eddy, and Ta Phouc Loc model, to study the transient phenomena of the flow. The results are conducted at six cross sectional planes along the axis of the cylinder and with the piston displaced at four fixed piston positions covering the air intake ports by 0%, 25%, 50%, and 75% respectively, for the fully opened case LES model with 8/12 million mesh points were used. We find that the flow inside the cylinder changes as the ports are closing, from a Rankine/Burger vortex profile to a solid body rotation while the axial velocity profiles change from a wake-like to a jet-like profile.

General information
State: Published
Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, Thermal Energy
Authors: Obeidat, A. (Intern), Haider, S. (Intern), Ingvorsen, K. M. (Intern), Meyer, K. E. (Intern), Walther, J. H. (Intern)
Number of pages: 5
Publication date: 2012
Main Research Area: Technical/natural sciences
Diesel engine, Swirl, Scavenging, LES simulation
Electronic versions:
Obeidat:2010.pdf
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Publication: Research › Conference abstract for conference – Annual report year: 2012

Multiscale simulation of water flow past a C_{540} fullerene
We present a novel, three-dimensional, multiscale algorithm for simulations of water flow past a fullerene. We employ the Schwarz alternating overlapping domain method to couple molecular dynamics (MD) of liquid water around the C_{540} buckyball with a Lattice–Boltzmann (LB) description for the Navier–Stokes equations. The proposed method links the MD and LB domains using a fully three-dimensional interface and coupling of velocity gradients. The present overlapping domain method implicitly preserves the flux of mass and momentum and bridges flux-based and Schwarz domain decomposition algorithms. We use this method to determine the slip length and hydrodynamic radius for water flow past a buckyball.

General information
Staying dry under water

General information
State: Published
Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, Northwestern University, Swiss Federal Institute of Technology, University of Illinois
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Pages: Paper DFD12-2012-001193
Publication date: 2012
Conference: 65th Annual Meeting of the APS Division of Fluid Dynamics, San Diego, CA, United States, 18/11/2012 - 18/11/2012
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Publication: Research › Conference abstract in journal – Annual report year: 2012

Swirling flow in model of large two-stroke diesel engine

General information
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Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, MAN Diesel & Turbo SE
Authors: Meyer, K. E. (Intern), Ingvorsen, K. M. (Intern), Mayer, S. (Ekstern), Walther, J. H. (Intern)
Pages: Paper DFD12-2012-001017
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Swirling flow in model of large two-stroke diesel engine
A scale model of a simplified cylinder in a uniflow scavenged large two-stroke marine diesel engine is constructed to investigate the scavenging process. Angled ports near the bottom of the cylinder liner are uncovered as the piston reaches the bottom dead center. Fresh air enters through the ports forcing the gas in the cylinder to leave through an exhaust valve located in the cylinder head. The scavenging flow is a transient (opening/closing ports) confined port-generated turbulent swirl flow, with complex phenomena such as central recirculation zones, vortex breakdown and vortex precession. The model has a transparent cylinder five diameters long and is fitted with a static valve with a simplified geometry. The piston motion is controlled by a linear motor. The flow in the experiment has a Reynolds number of 50000 based on cylinder diameter and bulk velocity. Stereoscopic Particle Image Velocimetry (PIV) is used to investigate the scavenging flow for cases with both static and moving piston. Measurements are carried out for several cross-sectional planes covering the majority of the cylinder length. The effect of swirl intensity is investigated using four different port angles going from 0 – 30 degree. Although the flow has a relatively low swirl number of around 0.4, a central recirculation zone is observed indicating a vortex breakdown. The steady flow is also analyzed with Proper Orthogonal Decomposition (POD). The analysis reveals systematic variations in the shape and location of the vortex core. Transient measurements using phase-locked PIV are carried out with moving piston. The transient measurements reveal a violent change in flow topology as a central recirculation zone is rapidly formed, resulting in a change from large positive to negative velocities of the axial component.

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Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, MAN Diesel & Turbo SE
Authors: Ingvorsen, K. M. (Intern), Meyer, K. E. (Intern), Schnipper, T. (Intern), Walther, J. H. (Intern), Mayer, S. (Ekstern)
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Conference: 16th International Symposium on Applications of Laser Techniques to Fluid Mechanics, Lisbon, Portugal, 09/07/2012 - 09/07/2012
Electronic versions:
FullPaper.pdf
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Publication: Research - peer-review › Article in proceedings – Annual report year: 2012

Three dimensional remeshed smoothed particle hydrodynamics for the simulation of turbulent flow in complex geometries

General information
State: Published
Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering
Authors: Obeidat, A. (Intern), Walther, J. H. (Intern)
Publication date: 2012
Main Research Area: Technical/natural sciences
Remesh smoothed particle hydrodynamics, Turbulent flow, Brinkman penalization, Thres dimensional isotropic decaying turbulence
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Turbulence modelling in the two-dimensional vortex-in-cell method

General information
State: Published
Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, COWI Consultants A/S
Authors: Hejlesen, M. M. (Intern), Rasmussen, J. T. (Intern), Larsen, A. (Ekstern), Walther, J. H. (Intern)
Publication date: 2012
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CFD, Unsteady flow computation, Vortex-in-cell method, Turbulence modelling
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Source-ID: u::5693

A multiresolution remeshed Vortex-In-Cell algorithm using patches
We present a novel multiresolution Vortex-In-Cell algorithm using patches of varying resolution. The Poisson equation relating the fluid vorticity and velocity is solved using Fast Fourier Transforms subject to free space boundary conditions. Solid boundaries are implemented using the semi-implicit formulation of Brinkman penalization and we show that the penalization can be carried out as a simple interpolation. We validate the implementation against the analytic solution to the Perlman test case and by free-space simulations of the onset flow around fixed and rotating circular cylinders and bluff body flows around bridge sections.

General information
State: Published
Organisations: Fluid Mechanics, Department of Mechanical Engineering, Université Joseph Fourier - Grenoble 1
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Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.098 SNIP 1.988 CiteScore 2.92
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.166 SNIP 2.193 CiteScore 3.12
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 2.227 SNIP 2.45 CiteScore 3.3
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Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.161 SNIP 2.052 CiteScore 2.69
Fast Water Transport in CNTs: length dependence and entrance/exit effects
Superfast water transport in carbon nanotube (CNT) membranes has been reported in experimental studies. We use Molecular Dynamics simulations to elucidate the mechanisms of water entry, exit and transport in 2nm-diameter hydrophobic CNTs embedded in a hydrophilic membrane matrix. We demonstrate, for the first time, that under imposed pressures of the order of 1 bar, water entry into the CNT cavity and exit from the CNT end, can occur only on pre-wetted membranes. We conduct large scale simulations for up to 500nm long CNTs and observe a previously unseen dependence of the flow enhancement rates on the CNT length. We relate the present findings to past computational and experimental studies, we discuss previous continuum assessments for this flow and propose underlying physical mechanisms.

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Organisations: Fluid Mechanics, Department of Mechanical Engineering, Eidgenössische Technische Hochschule
Authors: Walther, J. H. (Intern), Koumoutsakos, P. (Ekstern)
Publication date: 2011
Event: Abstract from 64th Annual Meeting of the American Physical Society's Division of Fluid Dynamics, Baltimore, MD, United States.
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Vortex-In-Cell algorithm, Bridge aerodynamics, Multiresolution, Brinkman penalization, Patches, Fixed and rotating cylinder

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Influence of outlet geometry on the swirling flow in a simplified model of a large two-stroke marine diesel engine
We present Stereoscopic particle image velocimetry measurements of the effect of a dummy-valve on the in-cylinder swirling flow in a simplified scale model of a large two-stroke marine diesel engine cylinder using air at room temperature and pressure as the working fluid and Reynolds number 19500. The static model has stroke-to-bore ratio of 4, is rotationally symmetric and the in-cylinder swirling flow is enforced by angled ports at the inlet. We consider a case analogous to engine when the piston is at bottom-dead-center. In absence of an exhaust valve the overall axial velocity profile is wake-like and flow reversal is observed on the cylinder axis, close to the inlet. Downstream, the flow reversal disappears and instead a localized jet develops. The corresponding tangential velocity profiles show a concentrated vortex with decreasing width along the downstream direction. By placing a concentric dummy-valve at the cylinder outlet, the magnitude of reverse flow at the inlet increases, the strong swirl is diminished and the axial jet disappears. We compare these findings with previous measurements in vortex chambers and discuss the relevance of these results with respect to development of marine engines.

Influence of piston position on the scavenging and swirling flow in two-stroke diesel engines
We study the effect of piston position on the in-cylinder swirling flow in a low speed large two-stroke marine diesel engine model. We are using Large Eddy Simulations in OpenFOAM, with three different models for the turbulent flow: a one equation model (OEM), a dynamic one equation model (DOEM) and Ta Phuoc Loc's model (TPLM). The simulated flows are grid-independent and they are computed in situations analogous to two different piston positions where the air intake ports are uncovered 100% and 50%, respectively. We find that the average flow inside the cylinder changes qualitatively with port closure from a Burgers vortex profile to a solid body rotation while the axial velocity changes from a wake-like profile to a jet-like profile. The numerical results are compared with measurements in a similar geometry [3] and we find a good agreement between simulations and measurements. Furthermore, we consider the unsteady flow and identify a dominant frequency in a power spectrum based on velocity which we show is due to precession of the vortex core, and compare with measurements of the unsteady flow obtained with Laser Doppler Anemometry.
Molecular Dynamics Studies of Nanofluidic Devices

Nanotechnology and fluid mechanics are two scientific areas where recent progress has disclosed a variety of new possibilities. The advances in both fields established the grounds for interdisciplinary approaches and recent findings promise novel applications that are leading to a technological revolution. Novel nanofabrication techniques have opened up possibilities for the development of small-scale integrated devices, such as lab-on-a-chip for biochemical synthesis and analysis, the integration is achieved by miniaturization of the functional elements e.g., of the channels transporting the fluid and of the sensors performing the analysis, and as the size of these devices reaches the sub-micron range we enter the field of nanofluidics. Nanofluidics is defined as the study of flows in and around nanosized objects. Modeling of transport in nanofluidic systems differs from microfluidic systems because changes in transport caused by the walls become more dominant and the fluid consists of fewer molecules. Carbon nanotubes are tubular graphite molecules which can be imagined to function as nanoscale pipes or conduits. Another important material for nanofluidics applications is silica. Nowadays, silica nanochannels are produced in nanometer scale using different nanofabrication techniques. Silica nanochannels are being implemented in several nanotechnology applications such as nanosensor devices, nano separators, nanofilters and a plethora of devices for nanobiological and biochemical applications. Experiments at the nanoscale are expensive and time consuming moreover the time scale associated to several nanoscale phenomena requires a very high time resolution of the devices performing nanoscale measurements. Computational nanofluidics is the enabling technology for fundamental studies, development, and design of such devices. Computational nanofluidics complements experimental studies by providing detailed spatial and temporal information of the nanosystem. In this thesis, we conduct molecular dynamics simulations to study basic nanoscale devices. We focus our studies on the understanding of transport mechanism to drive fluids and solids at the nanoscale. Specifically, we present the results of three different research projects. Throughout the first part of this thesis, we include a comprehensive introduction to computational nanofluidics and to molecular simulations, and describe the molecular dynamics methodology. In the second part of this thesis, we present the results of three different research projects. Firstly, we present a computational study of thermophoresis as a suitable mechanism to drive water droplets confined in different types of carbon nanotubes. We observe a motion of the water droplet in opposite direction to the imposed thermal gradient also we measure higher velocities as higher thermal gradients are imposed. Secondly, we present an atomistic analysis of a molecular linear motor fabricated of coaxial carbon nanotubes and powered by thermal gradients. The MD simulation results indicate that the motion of the capsule (inner carbon nanotube) can be controlled by thermophoretic forces induced by thermal gradients. The simulations find large terminal velocities of 100 to 400 nms−1 for imposed thermal gradients in the range of 1 to 3 Knm−1. Moreover, the results indicate that the thermophoretic force is velocity dependent and its magnitude decreases for increasing velocity. Finally, we present an extensive computational study of nanoscale systems including silica substrates and channels, water and air. This study includes the calibration of a force field to describe the silica-water-air interactions. Moreover, In this study we perform very long simulations of nanoscale systems containing silica, water and air. We investigate the solubility of air at different pressures in silica-water systems. From our simulations we infer a layer with high air density close to silica surface. Furthermore, we conduct simulations to analyze the earlier stage of the capillary filling process of silica nanochannels, we focus this study on the roll of air in this system. We find that air at high pressures can affect the capillarity in silica channels below 10 nm height.

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Authors: Zambrano Rodriguez, H. A. (Intern), Walther, J. H. (Intern)
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Particle Methods in Bluff Body Aerodynamics

Fluid-structure interaction is studied numerically in academics and the industry. Shear computational power alone is insufficient to accurately resolve the complex dynamics of high Reynolds number fluid flow. Therefore the development of more efficient and applicable computational algorithms is important. This dissertation focuses on the use of vortex particle methods and computational efficiency. The work is divided into three parts.

A novel method for the simulation of the aerodynamic admittance in bluff body aerodynamics is presented. The method involves a model for describing oncoming turbulence in two-dimensional discrete vortex method simulations by seeding the upstream flow with vortex particles. The turbulence is generated prior to the simulations and is based on analytic spectral densities of the atmospheric turbulence and a coherence function defining the spatial correlation of the flow. The method is validated by simulating the turbulent flow past a flat plate and past the Great Belt East bridge, the Øresund bridge and the Busan-Geoje bridge.

The dissertation introduces a novel multiresolution vortex-in-cell algorithm using patches of varying resolution. The Poisson equation relating the fluid vorticity and velocity is solved using fast Fourier transforms subject to free-space boundary conditions. Solid boundaries are implemented using the semi-implicit formulation of Brinkman penalization and it is shown that the penalization can be carried out as a simple interpolation. The implementation is validated against the analytic solution to the Perlman test case and by free-space simulations of the onset flow around fixed and rotating circular cylinders and bluff body flows around bridge sections.

Finally a three-dimensional vortex-in-cell algorithm is implemented into an existing open source library that enables large scale, three-dimensional particle-vortex simulations. A high order Fourier based Poisson solver is presented using novel use of regularization in the vortex-in-cell algorithm which formally enables arbitrarily high order convergence. The implementation is prepared for multiresolution though it is currently not supported by the parallel framework. The simulation of deformable and moving objects is demonstrated using Brinkman penalization and the vortex-in-cell algorithm. The model is applied to flow around spheres, a bridge section during the construction phase and the swimming motion of the medusa Aurelia aurita.
The exhalant jet of mussels Mytilus edulis

The exhalant jet flow of mussels in conjunction with currents and/or other mussels may strongly influence the mussels' grazing impact. Literature values of mussel exhalant jet velocity vary considerably and the detailed fluid mechanics of the near-mussel flow generated by the exhalant jet has hitherto been uncertain. Computational modelling of this phenomenon depends on knowledge of the velocity distribution near the exhalant siphon aperture of mussels to provide appropriate boundary conditions for numerical flow models. To be useful such information should be available for a range of mussel shell lengths. Here, we present results of a detailed study of fully open mussels Mytilus edulis in terms of filtration rate, exhalant siphon aperture area, jet velocity, gill area and body dry weight, all as a function of shell length (mean +/- SD) over the range 16.0 +/- 0.4 to 82.6 +/- 2.9 mm, with the corresponding scaling laws also presented. The exhalant jet velocity was determined by 3 methods: (1) measured clearance rate divided by exhalant aperture area, (2) manual particle tracking velocimetry (PTV) using video-microscope recordings, and (3) particle image velocimetry (PIV). The latter provides detailed 2-component velocity distributions near the exhalant siphon in 5 planes parallel to the axis of the jet and the major axis of the oval aperture, and hence estimates of momentum and kinetic energy flows in addition to mean velocity. Data obtained on particles inside the exhalant jet of filtered water was verified by the use of titanium dioxide seeding particles which were de-agglomerated by ultrasound to a size range of 0.7 to 2 μm prior to addition, to avoid retention by the gill filter of the mussels. We found that exhalant jet velocity was essentially constant at similar to 8 cm s(-1), and independent of shell length. Based on geometric similarity and scaling of mussel pump-system characteristics we found that these characteristics coincide approximately for all sizes when expressed as pressure head versus volume flow divided by shell length squared.
A multiresolution remeshed particle vortex method using patches

We present a novel multi-resolution Vortex-In-Cell (VIC) algorithm using overlapping mesh patches of different resolution. The approach is based on the method of Bergdorff et al. 2005 and the free-space solution obtained using fast Fourier transforms (FFT) by Hockney and Eastwood 1988. The hybrid vortex particle-mesh VIC algorithm interpolates particle vorticity to a mesh, solves a Poisson equation for the stream function using FFTs and calculates velocities as the curl of the stream function. With both vorticity and velocity available on the mesh, values of the substantial derivative of particle strengths is calculated on the mesh and interpolated back to the particles. This allows particle strengths and positions to be updated without expensive direct particle-particle interaction. The no-slip condition of complex solid bodies is imposed with Brinkman penalization. In the work presented, a VIC implementation with patches of varying resolution, is applied to the two-dimensional flow past a cylinder. The vorticity field can be divided into two regions, an arbitrary patch of vorticity and the remaining exterior vorticity field. Due to the linearity of the Poisson equation the velocity field corresponding to the total vorticity field is the sum of the free space solutions to the Poisson equation to each region. Hereby the flow on the patch can be simulated at a higher resolution, while including the influence from the coarser exterior region. Particles are remeshed and interpolated only to the region from which they are formed and each region is extended by a buffer1 to ensure full interpolation support in its interior. Patches of varying resolutions may be nested and can contain multiple patches.

General information
State: Published
Organisations: Fluid Mechanics, Department of Mechanical Engineering, Université Joseph Fourier - Grenoble 1
Authors: Rasmussen, J. T. (Intern), Cottet, G. (Ekstern), Walther, J. H. (Intern)
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Event: Abstract from Euromech Fluid Mechanics Conference, .
Main Research Area: Technical/natural sciences
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Atomistic simulations of flow at the nanoscale

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Organisations: Department of Mechanical Engineering
Authors: Walther, J. H. (Intern)
Publication date: 2010

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Main Research Area: Technical/natural sciences
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Coarse Grained Molecular Dynamics Simulations of Shear-Induced Instabilities of Lipid Bilayer Membranes in Water

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Organisations: Fluid Mechanics, Department of Mechanical Engineering, Center for Fluid Dynamics, Osaka University, Swiss Federal Institute of Technology
Authors: Hanasaki, I. (Ekstern), Walther, J. H. (Intern), Kawano, S. (Ekstern), Koumoutsakos, P. (Ekstern)
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Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.047 SNIP 0.978 CiteScore 1.89
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.22 SNIP 1.123 CiteScore 2.05
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.311 SNIP 1.239 CiteScore 2.28
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.42 SNIP 1.226 CiteScore 2.28
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
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Discrete vortex method simulations of a turbulent flow past bridge decks with application to aerodynamic admittance

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Organisations: Department of Mechanical Engineering, Fluid Mechanics, COWI Consultants A/S
Authors: Hejlesen, M. M. (Intern), Rasmussen, J. T. (Intern), Larsen, A. (Ekstern), Walther, J. H. (Intern)
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Discrete vortex method simulations of the aerodynamic admittance in bridge aerodynamics
We present a novel method for the simulation of the aerodynamic admittance in bluff body aerodynamics. The method introduces a model for describing oncoming turbulence in two-dimensional discrete vortex method simulations by seeding the upstream flow with vortex particles. The turbulence is generated prior to the simulations and is based on analytic spectral densities of the atmospheric turbulence and a coherence function defining the spatial correlation of the flow. The method is validated by simulating the turbulent flow past a flat plate and past the Great Belt East bridge. The results are generally found in good agreement with the potential flow solution due to Liepmann.

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State: Published
Organisations: Fluid Mechanics, Department of Mechanical Engineering, COWI A/S
Authors: Rasmussen, J. T. (Intern), Hejlesen, M. M. (Intern), Larsen, A. (Ekstern), Walther, J. H. (Intern)
Jet Impingement Heat Transfer at High Reynolds Numbers and Large Density Variations

Jet impingement heat transfer from a round gas jet to a flat wall has been investigated numerically in a configuration with \( H/D = 2 \), where \( H \) is the distance from the jet inlet to the wall and \( D \) is the jet diameter. The jet Reynolds number was 36,100 and the density ratio across the wall boundary layer was 3.3 due to a substantial temperature difference of 1600\(^\circ\)K between jet and wall. Results are presented which indicate very high heat flux levels and it is demonstrated that the jet inlet turbulence intensity significantly influences the heat transfer results, especially in the stagnation region. The results also show a noticeable difference in the heat transfer predictions when applying different turbulence models. Furthermore, calculations were performed to study the effect of applying temperature dependent thermophysical properties versus constant properties and the effect of calculating the gas density from the ideal gas law versus real gas data. In both cases the effect was found to be negligible.

Molecular Dynamics Simulation of Water Nanodroplets on Silica Surfaces at High Air Pressures

Silicon dioxide-water systems are abundant in nature and play fundamental roles in a diversity of novel science and engineering applications. Although extensive research has been devoted to study the nature of the interaction between silica and water a complete understanding of the system has not been reached. Contact angle measurements of droplets on solid surfaces offer useful quantitative measurements of the physiochemical properties of the solid-liquid interface. For hydrophobic systems the properties the solid-liquid interface are now known to be strongly influenced by the presence of air e.g., nanobubbles. In the present work we study the role of air on the wetting of hydrophilic systems. We conduct molecular dynamics simulations of a water nanodroplet on an amorphous silica surface at different air pressures. The interaction potentials describing the silica, water, and air are obtained from the literature. The silica surface is modeled by a large 32 \( \times 32 \times 2 \) nm amorphous SiO\(_2\) structure consisting of 180,000 atoms. The water consists of 1800 water molecules surrounded by N\(_2\) and O\(_2\) air molecules corresponding to air pressures of 0 bar (vacuum), 50 bar, 100 bar and 200 bar. We perform extensive simulations of the water-air equilibria and calibrate the water-air interaction to match the experimental solubility of N\(_2\) and O\(_2\) in water. For the silica-water system we calibrate the water-silica interaction to match the experimental contact angle of 27\(^\circ\). We subsequently study the effect of air and find a consistent increase in the water contact angle reaching 53\(^\circ\) at 200 bar air pressure. These results are important for the creation and stability of nanobubbles at hydrophilic interfaces.
Multiscale flow simulation of water past a fullerene

General information
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Non-periodic molecular dynamics simulations of coarse grained lipid bilayer in water

We present a multiscale algorithm that couples coarse grained molecular dynamics (CGMD) with continuum solver. The coupling requires the imposition of non-periodic boundary conditions on the coarse grained Molecular Dynamics which, when not properly enforced, may result in spurious fluctuations of the material properties of the system represented by CGMD. In this paper we extend a control algorithm originally developed for atomistic simulations [3], to conduct simulations involving coarse grained water molecules without periodic boundary conditions. We demonstrate the applicability of our method in simulating more complex systems by performing a non-periodic Molecular Dynamics simulation of a DPPC lipid in liquid coarse grained water.

General information
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Organisations: Fluid Mechanics, Department of Mechanical Engineering, Swiss Federal Institute of Technology, Osaka University
Authors: Kotsalis, E. M. (Ekstern), Hanasaki, I. (Ekstern), Walther, J. H. (Intern), Koumoutsakos, P. (Ekstern)
Pages: 2370-2373
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Particle Methods in Fluid Mechanics

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Organisations: Department of Mechanical Engineering, Fluid Mechanics
Authors: Walther, J. H. (Intern), Zambrano, H. A. (Intern), Rasmussen, J. T. (Intern)
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Piston surface heat transfer during combustion in large marine diesel engines

In the design process of large marine diesel engines, information on the maximum heat load on the piston surface experienced during the engine cycle is an important parameter. The peak heat load occurs during combustion when hot combustion products impinge on the piston surface. Although the maximum heat load is only present for a short time of the total engine cycle, it is a severe thermal load on the piston surface. At the same time, cooling of the piston crown is generally more complicated than cooling of the other components of the combustion chamber. This can occasionally cause problems with burning off piston surface material. In this work, the peak heat load on the piston surface of large marine diesel engines during combustion was investigated. Measurements of the instantaneous surface temperature and surface heat flux on pistons in large marine engines are difficult due to expensive instrumentation and high engine running costs compared to automotive engines. Therefore, the investigation in this work was carried out numerically with the use of a computational fluid dynamics (CFD) code. At the same time, numerical work on detailed in-cylinder wall heat transfer in engines has been quite limited. The numerical investigation focused on the simulation of a hot turbulent gas jet impinging on a wall under very high pressure, thus approximating the process of the actual impingement of hot combustion gasses on the piston surface during combustion. The surface heat flux at the wall was calculated under different conditions in the numerical setup in order to obtain information of the actual peak heat flux experienced at the piston in large marine diesel engines during combustion. The variation of physical parameters influencing the heat transfer during combustion included a variation of pressure, temperatures, jet velocity and jet turbulence intensity. The variation in heat flux predictions resulting from application of different turbulence models was also investigated by performing calculations with three different models: the V2F model, a k-ε RNG model and a low-Re k-ε model. The obtained results indicate peak heat fluxes in the order of 5–10 MW/m² on the piston surface during the combustion phase of the engine cycle.

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This article was originally published online on 29 December 2009 with an incorrect journal title in Ref. 22; the correct journal title should have been "Small." AIP apologizes for this error. All online versions of the article were corrected on 5 January 2010; the article was correct as it appeared in the printed version of the journal. Reference 22 appears correctly below: 22T. A. Hilder and J. M. Hill, Small 5, 300, 2009.
A numerical study of the aerodynamic admittance of bridge sections

General information
State: Published
Organisations: Department of Mechanical Engineering, Fluid Mechanics, COWI Consultants A/S
Authors: Hejlesen, M. M. (Intern), Rasmussen, J. T. (Intern), Walther, J. H. (Intern), Larsen, A. (Ekstern)
Pages: 79-82
Publication date: 2009

Control algorithm for multiscale flow simulations of water
We present a multiscale algorithm to couple atomistic water models with continuum incompressible flow simulations via a Schwarz domain decomposition approach. The coupling introduces an inhomogeneity in the description of the atomistic domain and prevents the use of periodic boundary conditions. The use of a mass conserving specular wall results in turn to spurious oscillations in the density profile of the atomistic description of water. These oscillations can be eliminated by using an external boundary force that effectively accounts for the virial component of the pressure. In this Rapid Communication, we extend a control algorithm, previously introduced for monatomic molecules, to the case of atomistic water and demonstrate the effectiveness of this approach. The proposed computational method is validated for the cases of equilibrium and Couette flow of water.

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Organisations: Fluid Mechanics, Department of Mechanical Engineering, Swiss Federal Institute of Technology, Harvard University
Authors: Kotsalis, E. M. (Ekstern), Walther, J. H. (Intern), Kaxiras, E. (Ekstern), Koumoutsakos, P. (Ekstern)
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Coupling Atomostic and Continuum Descriptions Using Dynamic Control

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Organisations: Fluid Mechanics, Department of Mechanical Engineering, Swiss Federal Institute of Technology
Authors: Kotsalis, E. M. (Ekstern), Walther, J. H. (Intern), Koumoutsakos, P. (Ekstern)
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Source: orbit
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Discrete vortex method simulations of aerodynamic admittance in bridge aerodynamics
The meshless and remeshed Discrete Vortex Method (DVM) has been widely used in academia and by the industry to model two-dimensional flow around bluff bodies. The implementation “DVMFLOW” [1] is used by the bridge design company COWI to determine and visualise the flow field around bridge sections, and to determine aerodynamic forces and the corresponding flutter limit. A simulation of the three-dimensional bridge response to turbulent wind is carried out by quasi steady theory by modelling the bridge girder as a line like structure [2], applying the aerodynamic load coefficients found from the current version of DVMFLOW in a strip wise fashion. Neglecting the aerodynamic admittance, i.e. the correlation of the instantaneous lift force to the turbulent fluctuations in the vertical velocities, leads to higher response to high frequency atmospheric turbulence than would be obtained from wind tunnel tests. In the present work we have extended the laminar oncoming flow in DVMFLOW to a turbulent one, modelled by seeding the upstream flow with vortex particles synthesized from prescribed atmospheric turbulence velocity spectra [3]. The discrete spectrum is sampled from the continuous spectrum subject to a lower cutoff imposed by the discretisation of the simulation time, to an upper limit that is chosen sufficiently high for the discrete spectrum to reproduce the standard deviation of the continuous spectrum. A time series of velocities is generated at two discrete rows of points perpendicular to the flow, forming quadratic cells over which circulation is integrated and associated with particles centered in the corresponding cells. The cell size is equal the distance traveled by a particle in the free stream during a finite number of time steps. The velocity is sampled downstream of the release area and the measured velocity spectra are found in good agreement with the target spectra. The aerodynamic admittance of the structure is measured by sampling vertical velocities immediately upstream of the structure and the lift forces on the structure. The method is validated against the analytic solution for the admittance of a turbulent flow past a flat plate [4] and two types of bridge girder sections. A fair agreement is observed for sufficiently low turbulence intensities and sufficient spatial and temporal resolutions.

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Organisations: Fluid Mechanics, Department of Mechanical Engineering, COWI Consultants A/S
Authors: Rasmussen, J. T. (Intern), Hejlesen, M. M. (Intern), Larsen, A. (Ekstern), Walther, J. H. (Intern)
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Publication: Research › Conference abstract for conference – Annual report year: 2009

Discrete vortex method simulations of aerodynamic admittance in bridge aerodynamics
The meshless and remeshed Discrete Vortex Method (DVM) has been widely used in academia and by the industry to model two-dimensional flow around bluff bodies. The implementation “DVMFLOW” [1] is used by the bridge design company COWI to determine and visualise the flow field around bridge sections, and to determine aerodynamic forces and the corresponding flutter limit. A simulation of the three-dimensional bridge response to turbulent wind is carried out by quasi steady theory by modelling the bridge girder as a line like structure [2], applying the aerodynamic load coefficients found from the current version of DVMFLOW in a strip wise fashion. Neglecting the aerodynamic admittance, i.e. the correlation of the instantaneous lift force to the turbulent fluctuations in the vertical velocities, leads to higher response to
high frequency atmospheric turbulence than would be obtained from wind tunnel tests.

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**Authors:** Rasmussen, J. T. (Intern), Hejlesen, M. M. (Intern), Larsen, A. (Ekstern), Walther, J. H. (Intern)
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**Main Research Area:** Technical/natural sciences
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**Fluid Forces and Vortex Wakes of a Flapping Foil**

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**Large-scale parallel discrete element simulations of granular flow**

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**Organisations:** Fluid Mechanics, Department of Mechanical Engineering, Swiss Federal Institute of Technology
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- ISI indexed (2012): ISI indexed yes
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Molecular Dynamics Simulations of a Linear Nanomotor Driven by Thermophoretic Forces

Molecular Dynamics of a Linear Nanomotor Driven by Thermophoresis Harvey A. Zambrano1, Jens H. Walther1,2 and Richard L. Jaffe3 1Department of Mechanical Engineering, Fluid Mechanics, Technical University of Denmark, DK-2800 Lyngby, Denmark; 2Computational Science and Engineering Laboratory, ETH Zurich, CH-8092, Switzerland and 3 NASA Ames Research Center, Moffett Field, CA 94035, USA

ABSTRACT Thermophoresis is the motion of mass induced by thermal gradients.1,2,3,4,5 In recent investigations thermophoresis has been used for driving solid and liquids confined inside carbon nanotubes.6,7,8,9 Nanomotors are an attractive goal for nanotechnology.9-13 Such nano-scale structures capable of converting thermal energy into work will be needed in many types of nanodevices, including nanoconveyors14, memory devices15 and nano-encapsulated material delivery systems16,17. Moreover to design and manufacture future molecular machines a complete understanding of the friction forces involved on the transport process at the molecular level have to be addressed.18 In this work we perform Molecular Dynamics (MD) simulations using the MD package FASTTUBE19 to study a molecular linear motor consisting of coaxial carbon nanotubes. The system consists of an outer 42.6 nm long carbon nanotube (CNT) with a chiral vector of (22,0) corresponding to a diameter of 1.723 nm. The inner CNT is modeled as an open short 3.195 nm long carbon nanotube with a chiral vector of (12,0), and diameter 0.94 nm. We describe the valence forces within the CNT using Morse, harmonic angle and torsion potentials.19 We include a nonbonded carbon-carbon Lennard-Jones potential to describe the vdW interaction between the carbon atoms within the double wall portion of the system. We equilibrate the system at 300K for 0.1 ns, by coupling the system to a Berendsen thermostat21 with a time constant of 0.1 ps. After the equilibration we impose thermal gradients in the range of 0.0–4.2 K/nm by heating two zones at the ends of the outer CNT as illustrated in Fig. 1. FIG. 1: Schematic of the computational setup. Crosssectional view of the system, the outer CNT is a (22,0) zigzag CNT and the inner one is a (12,0) zigzag CNT.

A thermal gradient is imposed by heating the end sections (in gray) of the outer CNT. We measure the position of the center of mass (COM) of the inner CNT during the simulation. We observe, for gradients higher that 1.18K/nm, a directed motion of the capsule in the direction opposite to the imposed thermal gradient as shown in Fig. 2. FIG. 2: Center of mass position (COM) as a function of time for three different thermal gradients: blue (*), 3.16K/nm; green (×), 1.58K/nm, and red (+), 1.18K/nm. To confirm that the motion of the capsule is driven by thermophoresis we perform additional simulations in order to study the friction and thermophoretic forces acting on the inner CNT. In these simulations, we constrain the velocity of center of mass of the inner CNT and extract from the simulations the external forces required to drive the inner CNT for different constrained velocities and different imposed thermal gradients (Fig. 3). FIG. 3: External force acting on the constrained inner CNT as a function of the center of mass (COM) velocity for different thermal gradients: red (+), 0.0K/nm; green (×), 1.0K/nm; blue (*), 2.0K/nm; and fuchsia (squares), 3.0K/nm. To measure the isothermal friction of the system we impose a zero thermal gradient while we vary the constrained COM velocity. At nonzero thermal gradients we measure the combined friction and thermophoretic forces. A positive force indicates resistance to the motion, whereas a negative force is indicative of thermophoresis. We find a systematic increase of the thermophoretic force as higher thermal gradients are imposed on the system. Furthermore, the measured isothermal friction is small compared to the thermophoretic force cf. Fig. 3. We infer from the simulations that the magnitude of the thermophoretic force is reduced as...
Molecular Dynamics Simulations of Water Droplets On Hydrophilic Silica Surfaces

Wetting is essential and ubiquitous in a variety of natural and technological processes. Silicon dioxide-water systems are abundant in nature and play fundamental roles in a vast variety of novel science and engineering activities such as silicon based devices, nanoscale lab on a chip systems and DNA microarrays technologies. Although extensive experimental, theoretical and computational work has been devoted to study the nature of the interaction between silica and water, at the molecular level a complete understanding of silica-water systems has not been reached. Contact angle computations of water droplets on silica surfaces offers a useful fundamental and quantitative measurement in order to study chemical and physical properties of water-silica systems. For hydrophobic systems the static and dynamic properties of the fluid-solid interface are influenced by the presence of air. Hence, nanobubbles have been observed and proposed as the origin of long range “hydrophobic” forces even for hydrophilic silica-water interfaces unusual phenomena related to nanobubbles have been observed. In this work we study the role of air on the wetting of amorphous silica-water systems. We conduct molecular dynamics (MD) simulations of a hydrophilic air-water-silica system using the MD package FASTTUBE. We employ quantum chemistry calculation to obtain air-silica interaction parameters for the simulations. Our simulations are based in the following force fields: (i) The silica-silica interaction is based on the potential model developed by Guissani et al. (ii) The water-water interaction is simulated based on the classical rigid SPC/E water model. (iii) The air-water interaction is simulated using a Lorentz-Berthelot (LB) mixing rules with values obtained from the universal force field (UFF) and from Ghysels et al. The water-air interaction is simulated using a LJ 12-6 potential with parameters obtained using LB mixing rules and values obtained from Jiang et al. for nitrogen and air oxygen and from Werder et al. for water oxygen.

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Title of host publication: 13th. IACIS INTERNATIONAL CONFERENCE ON SURFACE AND COLLOID SCIENCE : 83th. ACS COLLOID AND SURFACE SCIENCE SYMPOSIUM
Molecular Dynamics Simulations of Water Nanodroplets on Silica Surfaces

Wetting is essential and ubiquitous in a variety of natural and technological processes. Silicon dioxide-water systems are abundant in nature and play fundamental roles in a vast variety of novel science and engineering activities such as silicon based devices, nanoscale lab on a chip systems and DNA microarrays technologies. Although extensive experimental, theoretical and computational work has been devoted to study the nature of the interaction between silica and water, at the molecular level a complete understanding of silica-water systems has not been reached. Contact angle computations of water droplets on silica surfaces offers a useful fundamental and quantitative measurement in order to study chemical and physical properties of water-silica systems. For hydrophobic systems the static and dynamic properties of the fluid-solid interface are influenced by the presence of air. Hence, nanobubbles have been observed and proposed as the origin of long range "hydrophobic" forces even for hydrophilic silica-water interfaces unusual phenomena related to nanobubbles have been observed. In this work we study the role of air on the wetting of amorphous silica-water systems.
Multiscale simulations of water

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Authors: Walther, J. H. (Intern), Koumoutsakos, P. (Ekstern)
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Multiscale Simulations Using Particles

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Authors: Walther, J. H. (Intern)
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Parallel Scaling of the Discrete Element Method

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Authors: Walther, J. H. (Intern)
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Phonon assisted thermophoretic motion of gold nanoparticles inside carbon nanotubes (vol 90, artn 253116, 2007)

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Main Research Area: Technical/natural sciences

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Thermally driven molecular linear motors - A molecular dynamics study

We conduct molecular dynamics simulations of a molecular linear motor consisting of coaxial carbon nanotubes with a long outer carbon nanotube confining and guiding the motion of an inner short, capsule-like nanotube. The simulations indicate that the motion of the capsule can be controlled by thermophoretic forces induced by thermal gradients. The simulations find large terminal velocities of 100-400 nm/ns for imposed thermal gradients in the range 1-3 K/nm. Moreover, the results indicate that the thermophoretic force is velocity dependent and its magnitude decreases for increasing velocity.
Thermophoretic Motion of Water Nanodroplets confined inside Carbon Nanotubes

We study the thermophoretic motion of water nanodroplets confined inside carbon nanotubes using molecular dynamics simulations. We find that the nanodroplets move in the direction opposite the imposed thermal gradient with a terminal velocity that is linearly proportional to the gradient. The translational motion is associated with a solid body rotation of the water nanodroplet coinciding with the helical symmetry of the carbon nanotube. The thermal diffusion displays a weak dependence on the wetting of the water-carbon nanotube interface. We introduce the use of the Moment Scaling Spectrum (MSS) in order to determine the characteristics of the motion of the nanoparticles inside the carbon nanotube. The MSS indicates that affinity of the nanodroplet with the walls of the carbon nanotubes is important for the isothermal diffusion, and hence for the Soret coefficient of the system.
theta-SHAKE: An extension to SHAKE for the explicit treatment of angular constraints

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Organisations: Fluid Mechanics, Department of Mechanical Engineering, Swiss Federal Institute of Technology
Authors: Gonnet, P. (Ekstern), Walther, J. H. (Intern), Koumoutsakos, P. (Ekstern)
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Main Research Area: Technical/natural sciences
A Parallel Immersed Interface Method for DPD Simulations of Complex Flow
Atomistic Simulations of Thermophoretic Motion of water Nanodroplets in Carbon Nanotubes

Open-ended nanotubes offer unique possibilities as fluid conduits with applications ranging from molecule separation devices in biocatalysis to encapsulation media for drug storage and delivery. Liquids and solids in nanochannels may be driven by electrophoresis, osmosis, gradients in the surface tension (Marangoni effect), pressure gradients, and thermophoresis. Hence, electrophoresis has been used for driving electrically charged particles in nanosystems and gradients in the surface tension have been exploited to drive flow through carbon nanotubes (CNTs) immersed into a lipid membrane. Pressure gradients imposed in nanopipes have been used to generate controlled flows for nanoscale applications, and to enhance electrophoretic motion across carbon nanotube membranes. The use of thermal gradients to induce mass transport is known as thermophoresis, the Soret effect or thermodiffusion. The first observation of thermophoresis was reported by Ludwig in 1856, who found differences in samples taken from different parts of a solution in which the temperature was not uniform. A systematic investigation of the phenomena was subsequently conducted by Soret in 1879-81, and by in 1921-1925 for thermodiffusion in gases. Ibbes found that the coefficient of thermal diffusion is more sensitive than any of the other transport coefficients to the nature of the intermolecular forces. Thus, a complete understanding of the thermal diffusion could provide a powerful means of investigation of forces between molecules. Although the theoretical explanation of thermophoresis for molecules in liquids is still under debate, the investigation of its practical usability is motivated by potential applications in nanotechnology. Hence, thermophoresis was recently used as the driving mechanism in artificially fabricated nanomotors, and thermodiffusion is expected to allow microscale manipulation and control of flow in nanofluidic devices. In a recent theoretical study, thermophoresis was shown to induce motion of solid gold nanoparticles confined inside carbon nanotubes. In the present investigation, we study thermophoretic motion of liquid water nanodroplets confined inside carbon nanotubes.
On the Water-Carbon Interaction for Use in Molecular Dynamics Simulations of Graphite and Carbon Nanotubes: Additions and corrections

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Organisations: Swiss Federal Institute of Technology, NASA Ames Research Center, Eloret Corporation
Authors: Werder, T. (Ekstern), Walther, J. H. (Intern), Jaffe, R. (Ekstern), Halicioglu, T. (Ekstern), Koumoutsakos, P. (Ekstern)
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Web of Science (2016): Indexed yes
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Web of Science (2015): Indexed yes
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Scopus rating (2014): SJR 1.44 SNIP 1.14 CiteScore 3.28
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BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.494 SNIP 1.2 CiteScore 3.53
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BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.92 SNIP 1.251 CiteScore 3.66
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Thermophoretic Motion of Water Nanodroplets confined inside Carbon Nanotubes

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Authors: Zambrano, H. A. (Intern), Walther, J. H. (Intern), Koumoutsakos, P. (Ekstern), Sbalzarini, I. F. (Ekstern)
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An immersed interface method for the Vortex-In-Cell algorithm
The paper presents a two-dimensional immersed interface for the Vortex-In-Cell (VIC) method for simulation of flows past bodies of complex geometry. The particle-mesh VIC algorithm is augmented by a local particle correction term in a Particle-Particle Particle-Mesh (P3M) context to resolve sub-grid scales incurred by the presence of the immersed interface. The particle-particle correction furthermore allows to disjoin mesh and particle resolution by explicitly resolving sub-grid scales on the particle. This P3M algorithm uses an influence matrix technique to annihilate the anisotropic sub-grid scales and ads an exact particle-particle correction term. Free-space boundary conditions are satisfied through the use of modified Green's functions in the solution of the Poisson quation for the streamfunction. The concept is extended such as to provide exact velocity predictions on the mesh with free-space boundary conditions. The random walk thecnique is employed for the diffusion in order to relax the need for a remeshing of the computational elements close to solid boundaries. A novel partial remeshing technique is introduced which only performs remeshing of the vortex elements which are located sufficiently distant from the emmersed interfaces, thus maintaining a sufficient spatial representation of the vorticity field. Convergence of the present P3M algorithm is demonstrated for a circulat patch of vorticity. The immersed interface technique is applied to the flow past a circular cylinder at a Reynolds number of 3000 and the convergence of the method is demonstrated by a systematic refinement of the spatial parameters. Finally, the flow past a cactus-like geometry considered to demonstrate the efficient handling of complex bluff body geometries. The simulations offer an insight into physically interesting flow behavior involving a temporarily negative total drag force on the section.

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Authors: Morgenthal, G. (Ekstern), Walther, J. H. (Intern)
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Web of Science (2014): Indexed yes
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BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.416 SNIP 2.256 CiteScore 2.19
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Scopus rating (2011): SJR 1.496 SNIP 2.661 CiteScore 2.54
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Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.443 SNIP 1.952
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.248 SNIP 1.7
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.817 SNIP 1.588
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.015 SNIP 1.378
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.045 SNIP 1.604
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.37 SNIP 1.214
Scopus rating (2002): SJR 1.303 SNIP 1.059
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.719 SNIP 0.964
Scopus rating (2000): SJR 0.675 SNIP 0.856
Scopus rating (1999): SJR 0.862 SNIP 0.7

Original language: English

vortex methods, Lagrangian method, immersed boundaries, particle-mesh algorithm, random walk, remeshing
A numerical study of the stability of helical vortices using vortex methods

General information
State: Published
Organisations: Fluid Mechanics, Department of Mechanical Engineering, Engineering College in Industrial Systems, Swiss Federal Institute of Technology
Authors: Walther, J. H. (Intern), Guenot, M. (Ekstern), Macheaux, E. (Intern), Rasmussen, J. T. (Intern), Chatelain, P. (Ekstern), Okulov, V. (Intern), Sørensen, J. N. (Intern), Bergdoff, M. (Ekstern), Koumoutsakos, P. (Ekstern)
Number of pages: 16
Publication date: 2007
BFI conference series: European Academy of Wind Energy : The Science of Making Torque from Wind (5010078)
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Physics: Conference Series (Online)
Volume: 75
Article number: 012034
ISSN (Print): 1742-6596
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.45 SJR 0.24 SNIP 0.383
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.24 SNIP 0.373 CiteScore 0.35
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.253 SNIP 0.344 CiteScore 0.32
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.231 SNIP 0.272 CiteScore 0.25
ISI indexed (2013): ISI indexed no
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.28 SNIP 0.354 CiteScore 0.33
ISI indexed (2012): ISI indexed no
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.292 SNIP 0.352 CiteScore 0.43
ISI indexed (2011): ISI indexed no
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.288 SNIP 0.344
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.253 SNIP 0.321
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.265 SNIP 0.294
A stochastic boundary forcing for dissipative particle dynamics

General information
State: Published
Organisations: Fluid Mechanics, Department of Mechanical Engineering, Swiss Federal Institute of Technology
Authors: Altenhoff, A. M. (Ekstern), Walther, J. H. (Intern), Koumoutsakos, P. (Ekstern)
Pages: 1125-1136
Publication date: 2007
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Computational Physics
Volume: 225
ISSN (Print): 0021-9991
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.12 SJR 2.034 SNIP 1.822
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.098 SNIP 1.988 CiteScore 2.92
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.166 SNIP 2.193 CiteScore 3.12
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 2.227 SNIP 2.45 CiteScore 3.3
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.161 SNIP 2.052 CiteScore 2.69
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.06 SNIP 2.194 CiteScore 2.99
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 2.185 SNIP 2.096
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 2.439 SNIP 2.219
Web of Science (2009): Indexed yes
Control of density fluctuations in atomistic-continuum simulations of dense liquids

We present a control algorithm to eliminate spurious density fluctuations associated with the coupling of atomistic and continuum descriptions for dense liquids. A Schwartz domain decomposition algorithm is employed to couple molecular dynamics for the simulation of the atomistic system with a continuum solver for the simulation of the Navier-Stokes equations. The lack of periodic boundary conditions in the molecular dynamics simulations hinders the proper accounting for the virial pressure leading to spurious density fluctuations at the continuum-atomistic interface. An ad hoc boundary force is usually employed to remedy this situation. We propose the calculation of this boundary force using a control algorithm that explicitly cancels the density fluctuations. The results demonstrate that the present approach outperforms state-of-the-art algorithms. The conceptual and algorithmic simplicity of the method makes it suitable for any type of coupling between atomistic and continuum descriptions of dense fluids.

General information
State: Published
Organisations: Fluid Mechanics, Department of Mechanical Engineering, Swiss Federal Institute of Technology
Authors: Kotsalis, E. (Ekstern), Walther, J. H. (Intern), Koumoutsakos, P. (Ekstern)
Pages: 016709
Publication date: 2007
Main Research Area: Technical/natural sciences

Publication Information
Volume: 76
Issue number: 1
ISSN (Print): 1539-3755
Ratings:
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.95 SJR 0.993 SNIP 0.896
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.047 SNIP 0.978 CiteScore 1.89
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Phonon assisted thermophoretic motion of gold nanoparticles inside carbon nanotubes

The authors investigate the thermally driven mass transport of gold nanoparticles confined inside carbon nanotubes using molecular dynamics simulations. The observed thermophoretic motion of the gold nanoparticles correlates with the phonon dispersion exhibited by a standard carbon nanotube and, in particular, with the breathing mode of the tube. Additionally, the results show an increased static friction for gold nanoparticles confines inside a zig-zag carbon nanotube when increasing the size length of the nanoparticles. However, an unexpected, opposite trend is observed for the same nanoparticles inside armchair tubes. © 2007 American Institute of Physics.

General information
State: Published
Organisations: Fluid Mechanics, Department of Mechanical Engineering, Swiss Federal Institute of Technology
Authors: Schoen, P. A. (Ekstern), Walther, J. H. (Intern), Poulikakos, D. (Ekstern), Koumoutsakos, P. (Ekstern)
Pages: 253116
Publication date: 2007
Main Research Area: Technical/natural sciences

Publication information
Volume: 90
Issue number: 25
ISSN (Print): 0003-6951
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.67 SJR 1.132 SNIP 0.996
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.085 SNIP 0.983 CiteScore 2.47
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.799 SNIP 1.462 CiteScore 3.25
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.149 SNIP 1.652 CiteScore 3.77
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.554 SNIP 1.754 CiteScore 3.76
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 2.805 SNIP 1.94 CiteScore 4.04
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.926 SNIP 1.789
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.857 SNIP 1.848
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 2.934 SNIP 1.83
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 3.039 SNIP 1.913
A Software framework for the Portable Parallelization of Particle-Mesh Simulation

General information
State: Published
Organisations: Fluid Mechanics, Department of Mechanical Engineering
Authors: Sbalzarini, I. (Ekstern), Walther, J. H. (Intern), Polasek, B. (Ekstern), Chatelain, P. (Ekstern), Bergdorf, M. (Ekstern), Hieber, S. (Ekstern), Kotsalis, E. (Ekstern), Koumoutsakos, P. (Ekstern)
Publication date: 2006
Event: Abstract from Euro-Par 2006, Dresden, Germany, .
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 190404
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2006

Abstract: We present a software framework for the transparent and portable parallelization of simulations using particle-mesh methods. Particles are used to transport physical properties and a mesh is required in order to reinitialize the distorted particle locations, ensuring the convergence of the method. Field quantities are computed on the particles using fast multipole methods or by discretizing and solving the governing equations on the mesh. This combination of meshes and particles presents a challenging set of parallelization issues. The present library addresses these issues for a wide range of applications, and it enables orders of magnitude increase in the number of computational elements employed in particle methods. We demonstrate the performance and scalability of the library on several problems, including the first-ever billion particle simulation of diffusion in real biological cell geometries.

General information
State: Published
Organisations: Fluid Mechanics, Department of Mechanical Engineering
Authors: Sbalzarini, I. (Ekstern), Walther, J. H. (Intern), Polasek, B. (Ekstern), Chatelain, P. (Ekstern), Bergdorf, M. (Ekstern), Hieber, S. (Ekstern), Kotsalis, E. (Ekstern), Koumoutsakos, P. (Ekstern)
Nanoparticle Traffic on Helical Tracks: Thermophoretic Mass Transport through Carbon Nanotubes

Using molecular dynamics simulations, we demonstrate and quantify thermophoretic motion of solid gold nanoparticles inside carbon nanotubes subject to wall temperature gradients ranging from 0.4 to 25 K/nm. For temperature gradients below 1 K/nm, we find that the particles move "on tracks" in a predictable fashion as they follow unique helical orbits depending on the geometry of the carbon nanotubes. These findings markedly advance our knowledge of mass transport mechanisms relevant to nanoscale applications.

General information
State: Published
Organisations: Fluid Mechanics, Department of Mechanical Engineering
Authors: Schoen, P. A. (Ekstern), Walther, J. H. (Intern), Arcidiacono, S. (Ekstern), Poulikakos, D. (Ekstern), Koumoutsakos, P. (Ekstern)
Pages: 1910-1917
Publication date: 2006
Main Research Area: Technical/natural sciences

Publication information
Journal: Nano Letters
Volume: 6
Issue number: 9
ISSN (Print): 1530-6984
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 13.4
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 14.76
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 14.04
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 14.23
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 13.78
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 13.83
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Web of Science (2008): Indexed yes
Web of Science (2007): Indexed yes
Web of Science (2006): Indexed yes
Web of Science (2005): Indexed yes
Web of Science (2003): Indexed yes
PPM – A highly efficient parallel particle-mesh library for the simulation of continuum systems

General information
State: Published
Organisations: Swiss Federal Institute of Technology
Authors: Sbalzarini, I. F. (Ekstern), Walther, J. H. (Intern), Bergdorf, M. (Ekstern), Hieber, S. E. (Ekstern), Kotsalis, E. M. (Ekstern), Koumoutsakos, P. (Ekstern)
Pages: 566-588
Publication date: 2006
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Computational Physics
Volume: 215
ISSN (Print): 0021-9991
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.12 SJR 2.034 SNIP 1.822
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.098 SNIP 1.988 CiteScore 2.92
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.166 SNIP 2.193 CiteScore 3.12
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 2.227 SNIP 2.45 CiteScore 3.3
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.161 SNIP 2.052 CiteScore 2.69
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.06 SNIP 2.194 CiteScore 2.99
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 2.185 SNIP 2.096
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 2.439 SNIP 2.219
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 2.247 SNIP 2.03
Web of Science (2008): Indexed yes
Salt transport on islands in the Okavango Delta: Numerical investigations

This study uses a numerical model to investigate the groundwater flow and salt transport mechanisms below islands in the Okavango Delta. Continuous evapotranspiration on the islands results in accumulation of solutes and the formation of a saline boundary layer, which may eventually become unstable. A novel Lagrangian method is employed in this study and compared to other numerical methods. The numerical results support the geophysical observations of density fingering on Thata Island. However, the process is slow and it takes some hundreds of years until density fingering is triggered. The results are sensitive to changes of the hydraulic gradient and the evapotranspiration rate. Small changes may lead to different plume developments. Results further demonstrate that density effects may be entirely overridden by lateral flow on islands embedded in a sufficiently high regional hydraulic gradient.

Keyword: Saline boundary layer, Density-driven groundwater flow, Particle methods, Free convection, Numerical study

General information
State: Published
Organisations: Swiss Federal Institute of Technology
Authors: Zimmermann, S. (Ekstern), Bauer, P. (Ekstern), Held, R. (Ekstern), Kinzelbach, W. (Ekstern), Walther, J. H. (Intern)
Pages: 11--29
Publication date: 2006
Main Research Area: Technical/natural sciences

Publication information
Journal: Advances in Water Resources
Volume: 29
ISSN (Print): 0309-1708
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.53 SJR 2.156 SNIP 2.056
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.303 SNIP 2.093 CiteScore 4.31
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.948 SNIP 1.964 CiteScore 3.66
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Temperature driven transport of gold nanoparticles physisorbed inside carbon nanotubes

We use molecular dynamics simulations to demonstrate the temperature driven mass transport of solid gold nanoparticles, physisorbed inside carbon nanotubes (CNTs). Our results indicate that the nanoparticle experiences a guided motion, in the direction opposite to the direction of the temperature gradient applied to the carrier CNT. The force experienced by the nanoparticle is of thermophoretic character, scaling linearly with the applied temperature gradient. The present results prove that the surface corrugation of different types of CNTs and the magnitude of the temperature gradient strongly affects the nanoparticle motion along the carbon lattice.

General information

State: Published
Organisations: Fluid Mechanics, Department of Mechanical Engineering
Authors: Schoen, P. (Ekstern), Poulikakos, D. (Ekstern), Walther, J. H. (Intern), Koumoutsakos, P. (Ekstern)
Publication date: 2006

Host publication information

Publisher: IEEE
Main Research Area: Technical/natural sciences
DOIs:
Curvature Induced L-Defects in Water Conduction in Carbon Nanotubes

General information
State: Published
Organisations: Swiss Federal Institute of Technology
Authors: Zimmerli, U. (Ekstern), Gonnet, P. G. (Ekstern), Walther, J. H. (Intern), Koumoutsakos, P. (Ekstern)
Pages: 1017-1022
Publication date: 2005
Main Research Area: Technical/natural sciences

Publication information
Journal: Nano Letters
Volume: 5
Issue number: 6
Original language: English
Source: orbit
Source-ID: 190407
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2006

Hybrid atomistic-continuum method for the simulation of dense fluid flow
We present a hybrid atomistic–continuum method for multiscale simulations of dense fluids. In this method, the atomistic part is described using a molecular dynamics description, while the continuum flow is described by a finite volume discretization of the incompressible Navier–Stokes equations. The two descriptions are combined in a domain decomposition formulation using the Schwarz alternating method. A novel method has been proposed in order to impose non-periodic velocity boundary conditions from the continuum to the atomistic domain, based on an effective boundary potential, consistent body forces, a particle insertion algorithm and specular walls. The extraction of velocity boundary conditions for the continuum from the atomistic domain is formulated by taking into account the associated statistical errors. The advantages and drawbacks of the proposed Schwarz decomposition method as compared to related flux-based schemes are discussed. The efficiency and applicability of the method is demonstrated by considering hybrid and full molecular dynamics simulations of the flow of a Lennard–Jones fluid past a carbon nanotube.
Keyword: Nanofluidics, Hybrid algorithms, Molecular dynamics, Multiscale simulation

General information
State: Published
Organisations: Swiss Federal Institute of Technology
Authors: Werder, T. (Ekstern), Walther, J. H. (Intern), Koumoutsakos, P. (Ekstern)
Pages: 373 - 390
Publication date: 2005
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Computational Physics
Volume: 205
ISSN (Print): 0021-9991
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.12 SJR 2.034 SNIP 1.822
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.098 SNIP 1.988 CiteScore 2.92
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.166 SNIP 2.193 CiteScore 3.12
Numerical Simulation of Nano-, Meso, Macro- and Multiscale Fluid Dynamics

General information
State: Published
Organisations: Fluid Mechanics, Department of Mechanical Engineering
Authors: Walther, J. H. (Intern), Koumoutsakos, P. (Ekstern)
Pages: 9-17
Publication date: 2005
Conference: 18th Nordic Seminar on Computational Mechanics, Espoo, Finland, 27/10/2005 - 27/10/2005
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Structural Mechanics
Solidification of gold nanoparticles in carbon nanotubes

The structure and the solidification of gold nanoparticles in a carbon nanotube are investigated using molecular dynamics simulations. The simulations indicate that the predicted solidification temperature of the enclosed particle is lower than its bulk counterpart, but higher than that observed for clusters placed in vacuum. A comparison with a phenomenological model indicates that, in the considered range of tube radii (RCNT) of 0.5

General information
State: Published
Organisations: Swiss Federal Institute of Technology
Authors: Arcidiacono, S. (Ekstern), Walther, J. H. (Intern), Poulikakos, D. (Ekstern), Passerone, D. (Ekstern), Koumoutsakos, P. (Ekstern)
Pages: 105502
Publication date: 2005
Main Research Area: Technical/natural sciences

Publication information
Journal: Physical Review Letters
Volume: 94
Issue number: 10
ISSN (Print): 0031-9007
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 6.33 SJR 3.56 SNIP 2.133
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 3.823 SNIP 2.205 CiteScore 5.76
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 5.027 SNIP 2.646 CiteScore 6.62
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 5.674 SNIP 2.796 CiteScore 7.46
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 6.243 SNIP 2.845 CiteScore 7.19
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 6.252 SNIP 2.886 CiteScore 7.02
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 6.418 SNIP 2.764
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Thermophoresis Between Solids: A Molecular Dynamics Study of Gold Nanoparticles Confirmed and Thermally Driven Through Carbon Nanotubes

General information
State: Published
Organisations: Fluid Mechanics, Department of Mechanical Engineering
Authors: Zimmerli, U. (Ekstern), Walther, J. H. (Intern)
Publication date: 2005
Main Research Area: Technical/natural sciences
Links:
http://echeminfo.colayer.net/COMTY_program/?11qn
Source: orbit
Source-ID: 182995
Publication: Research » Paper – Annual report year: 2005

Wetting of doped carbon nanotubes by water droplets
We study the wetting of doped single- and multi-walled carbon nanotubes by water droplets using molecular dynamics simulations. Chemisorbed hydrogen is considered as a model of surface impurities. We study systems with varying densities of surface impurities and we observe increased wetting, as compared to the pristine nanotube case, attributed to the surface dipole moment that changes the orientation of the interfacial water.

We demonstrate that the nature of the impurity is important as here hydrogen induces the formation of an extended hydrogen bond network between the water molecules and the doping sites leading to enhanced wetting. (c) 2005 Elsevier B.V. All rights reserved.

General information
State: Published
Organisations: Fluid Mechanics, Department of Mechanical Engineering, Swiss Federal Institute of Technology, University of Cyprus
Hydrodynamic properties of carbon nanotubes

We study water flowing past an array of single walled carbon nanotubes using nonequilibrium molecular dynamics simulations. For carbon nanotubes mounted with a tube spacing of 16.4 in 16.4 nm and diameters of 1.25 and 2.50 nm, respectively, we find drag coefficients in reasonable agreement with the macroscopic, Stokes-Oseen solution. The slip length is 20.11 nm for the 1.25 nm carbon nanotube, and 0.49 for the 2.50 nm tube for a flow speed of 50 m/s, respectively, and 0.28 nm for the 2.50 nm tube at 200 m/s. A slanted flow configuration with a stream- and spanwise velocity component of 100 ms⁻¹ recovers the two-dimensional results, but exhibits a significant 88 nm slip along the axis of the tube. These results indicate that slip depends on the particular flow configuration.

General information
State: Published
Organisations: Swiss Federal Institute of Technology, NASA Ames Research Center
Authors: Walther, J. H. (Intern), Werder, T. (Ekstern), Jaffe, R. (Ekstern), Koumoutsakos, P. (Ekstern)
Pages: 062201
Publication date: 2004
Main Research Area: Technical/natural sciences

Publication information
Volume: 69
ISSN (Print): 1539-3755
Ratings:
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.95 SJR 0.993 SNIP 0.896
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.047 SNIP 0.978 CiteScore 1.89
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.22 SNIP 1.123 CiteScore 2.05
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.311 SNIP 1.239 CiteScore 2.28
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.42 SNIP 1.226 CiteScore 2.28
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.485 SNIP 1.225 CiteScore 2.28
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.69 SNIP 1.215
Web of Science (2010): Indexed yes
Hydrophobic hydration of C60 and carbon nanotubes in water

We perform molecular dynamics (MD) simulations to study the hydrophobic–hydrophilic behavior of pairs of C60 fullerene molecules and single wall carbon nanotubes in water. The interaction potentials involve a fully atomistic description of the fullerenes or carbon nanotubes and the water is modeled using the flexible SPC model. Both unconstrained and constrained MD simulations are carried out. We find that these systems display drying, as evidenced by expulsion of the interstitial water, when the C60 and carbon nanotubes are separated by less than 12, and 9–10 Å, respectively. From the constrained simulations, the computed mean force between two carbon nanotubes in water exhibits a maximum at a tube spacing of 5.0 Å which corresponds to approximately one unstable layer of interstitial water molecules. The main contribution to the force stems from the van der Waals attraction between the carbon surfaces. The minimum in the potential of mean force has a value of -17 kJ mol-1 Å-1 at a tube spacing of 3.5 Å.

Keyword: Aggregation, Interfacial properties, Carbon nanotube, Fullerene, Molecular simulations

General information
State: Published
Organisations: NASA Ames Research Center, Swiss Federal Institute of Technology, Eloret Corporation
Authors: Walther, J. H. (Intern), Jaffe, R. (Ekstern), Kotsalis, E. (Ekstern), Werder, T. (Ekstern), Halicioglu, T. (Ekstern), Koumoutsakos, P. (Ekstern)
Pages: 1185-1194
Publication date: 2004
Main Research Area: Technical/natural sciences

Publication information
Journal: Carbon
Volume: 42
ISSN (Print): 0008-6223
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
Multiphase water flow inside carbon nanotubes

We present nonequilibrium molecular dynamics simulations of the flow of liquid–vapour water mixtures and mixtures of water and nitrogen inside carbon nanotubes. A new adaptive forcing scheme is proposed to impose a mean flow through the system. The flow of liquid water is characterised by a distinct layering of the water molecules in the vicinity of the boundary and a slip length that is found to increase with the radius of the carbon nanotube. Increasing the temperature and pressure of the system furthermore results in a decrease in the slip length. For the flow of mixtures of nitrogen and water we find that the slip length is reduced as compared to the slip for the pure water. The shorter slip length is attributed to the fact that nitrogen forms droplets at the carbon surface, thus partially shielding the bulk flow from the hydrophobic carbon surface.
Remeshed smoothed particle hydrodynamics simulation of the mechanical behavior of human organs
In computer aided surgery the accurate simulation of the mechanical behavior of human organs is essential for the
development of surgical simulators. In this paper we introduce particle based simulations of two different human organ
materials modeled as linear viscoelastic solids. The constitutive equations for the material behavior are discretized using a
particle approach based on the Smoothed Particle Hydrodynamics (SPH) method while the body surface is tracked using
level sets. A key aspect of this approach is its flexibility which allows the simulation of complex time varying topologies
with large deformations. The accuracy of the original formulation is significantly enhanced by using a particle
reinitialization technique resulting in remeshed Smoothed Particle Hydrodynamics (rSPH). The mechanical parameters of
the systems used in the simulations are derived from experimental measurements on human cadaver organs. We
compare the mechanical behavior of liver- and kidney-like materials based on the dynamic simulations of a tensile test
case. Moreover, we present a particle based reconstruction of the liver topology and its strain distribution under a small
local load. Finally, we demonstrate a unified formulation of fluid structure interaction based on particle methods.

General information
State: Published
Organisations: Swiss Federal Institute of Technology
Authors: Hieber, S. E. (Ekstern), Walther, J. H. (Intern), Koumoutsakos, P. (Ekstern)
Pages: 305-314
Publication date: 2004
Main Research Area: Technical/natural sciences

Publication information
Journal: Technology and Health Care
Volume: 12
ISSN (Print): 0928-7329
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.253 SNIP 0.433 CiteScore 0.81
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.288 SNIP 0.529 CiteScore 0.79
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.306 SNIP 0.513 CiteScore 0.77
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.293 SNIP 0.565 CiteScore 0.85
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.267 SNIP 0.652 CiteScore 0.9
ISI indexed (2012): ISI indexed no
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.273 SNIP 0.696 CiteScore 1.02
ISI indexed (2011): ISI indexed no
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.39 SNIP 0.824
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.302 SNIP 0.733
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.222 SNIP 0.302
Scopus rating (2007): SJR 0.16 SNIP 0.318
Scopus rating (2006): SJR 0.163 SNIP 0.193
Scopus rating (2005): SJR 0.159 SNIP 0.428
Scopus rating (2004): SJR 0.144 SNIP 0.239
Scopus rating (2003): SJR 0.143 SNIP 0.183
Scopus rating (2002): SJR 0.146 SNIP 0.466
Scopus rating (2001): SJR 0.399 SNIP 0.06
Transverse momentum micromixer optimization with evolution strategies

We conduct a numerical study of mixing in a transverse momentum micromixer. Good values for actuation frequencies can be determined using simple kinematic arguments, and evolution strategies are introduced for the optimization of mixing by adjusting the control parameters in micromixer devices. It is shown that the chosen optimization algorithm can identify, in an automated fashion, effective actuation parameters. We find that optimal frequencies for increasing number of transverse channels are superposable despite the non-linear nature of the mixing process.

General information
State: Published
Organisations: Swiss Federal Institute of Technology, University of California, NASA Ames Research Center
Authors: Müller, S. D. (Ekstern), Mezic, I. (Ekstern), Walther, J. H. (Intern), Koumoutsakos, P. (Ekstern)
Pages: 521-531
Publication date: 2004
Main Research Area: Technical/natural sciences

Publication information
Journal: Computers & Fluids
Volume: 33
ISSN (Print): 0045-7930
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 1.022 SNIP 1.579 CiteScore 2.54
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.152 SNIP 1.665 CiteScore 2.26
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.031 SNIP 1.641 CiteScore 1.98
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.081 SNIP 1.974 CiteScore 2.17
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.135 SNIP 1.986 CiteScore 1.95
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.964 SNIP 1.845 CiteScore 1.97
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.19 SNIP 2.053
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.414 SNIP 2.124
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.326 SNIP 1.745
Scopus rating (2007): SJR 1.039 SNIP 1.649
Scopus rating (2006): SJR 1.047 SNIP 2.018
Scopus rating (2005): SJR 0.997 SNIP 1.768
Molecular dynamics simulations of water droplets on graphite are carried out to determine the contact angle for different water–carbon potential functions. Following the procedure of Werder et al. [J. Phys. Chem. B, 107 (2003) 1345], the C–O Lennard–Jones well depth is varied to recover the experimental value for the contact angle (84–86°) using a 2000-molecule water droplet and compensating for the line tension effect that lowers the contact angle for increasing droplet size. For the discrete graphite surface model studied by Werder et al., the effects of adding C–H Lennard–Jones interactions and changing the long-range cut-off distance are considered. In addition, a continuum graphite surface model is studied for which the water–graphite interaction energy depends only on the normal distance (z) from the water oxygen to the surface. This new model, with \( \epsilon_{210} \) repulsion and \( \epsilon_{24} \) attraction, is formulated in terms of the standard Lennard–Jones parameters, for which the recommended values are \( \sigma_{CO} = 3.19 \text{ Å} \) and \( \epsilon_{CO} = 0.365 \text{ kJ/mol} \).

Keyword: Water–carbon potential functions, Graphite, Contact angle, Molecular dynamics, Water–graphite interface
Molecular dynamics simulations are performed to study the influence of surface and fluid impurities on water–carbon interactions. In order to quantify these interactions we consider the canonical problem of wetting of a doped flat graphitic surface by a water system with impurities. As model fluid impurities we consider aqueous solutions of potassium–chloride with molar concentrations up to 1.8 M. Quantum chemistry calculations are performed to derive pair potentials for the ion–graphite interactions. The contact angle is found to decrease weakly with increasing ionic concentration, from 90° at 0 M to 81° at 1.8 M concentration. The influence of solid impurities is found to be more significant. Thus, 10, 15, and 20% coverages of chemisorbed hydrogen result in contact angles of 90°, 74° and 60°, respectively.
An influence matrix particle–particle particle-mesh algorithm with exact particle–particle correction

Keyword: Particle methods, N-body problem, Electrostatic interaction, Coulomb interaction, Particle–particle particle-mesh algorithm, Influence matrix

General information
State: Published
Organisations: Eidgenössische Technische Hochschule
Authors: Walther, J. H. (Intern)
On the Water-Carbon Interaction for Use in Molecular Dynamics Simulations of Graphite and Carbon Nanotubes

A systematic molecular dynamics study shows that the contact angle of a water droplet on graphite changes significantly as a function of the water-carbon interaction energy. Together with the observation that a linear relationship can be established between the contact angle and the water monomer binding energy on graphite, a new route to calibrate interaction potential parameters is presented. Through a variation of the droplet size in the range from 1000 to 17 500 water molecules, we determine the line tension to be positive and on the order of 2 x 10-10 J/m. To recover a macroscopic contact angle of 86°, a water monomer binding energy of -6.33 kJ mol-1 is required, which is obtained by applying a carbon-oxygen Lennard-Jones potential with the parameters CO = 0.392 kJ mol-1 and δCO = 3.19 Å. For this new water-carbon interaction potential, we present density profiles and hydrogen bond distributions for a water droplet on graphite.

General information
State: Published
Organisations: Swiss Federal Institute of Technology, NASA Ames Research Center, Eloret Corporation
Authors: Werder, T. (Ekstern), Walther, J. H. (Intern), Jaffe, R. (Ekstern), Halicioglu, T. (Ekstern), Koumoutsakos, P. (Ekstern)
Pages: 1345-1352
Publication date: 2003
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Physical Chemistry Part B: Condensed Matter, Materials, Surfaces, Interfaces & Biophysical
Volume: 107
ISSN (Print): 1520-6106
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.03 SJR 1.348 SNIP 1.02
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.367 SNIP 1.096 CiteScore 3.25
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.44 SNIP 1.14 CiteScore 3.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.494 SNIP 1.2 CiteScore 3.53
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.92 SNIP 1.251 CiteScore 3.66
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.78 SNIP 1.226 CiteScore 3.62
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.849 SNIP 1.214
An immersed interface method for the vortex-in-cell algorithm

The paper presents a two-dimensional immersed interface technique for the vortex-in-cell (VIC) method for the simulation of flows past complex geometries. The particle–mesh VIC algorithm is augmented by a local particle–particle (PP) correction term in a particle–particle particle–mesh (PPPM) context to resolve sub-grid scales incurred by the presence of the immersed interface. The PP correction furthermore allows mesh and particle resolution to be disjoined by explicitly resolving sub-grid scales on the particles. This PPPM algorithm uses an influence matrix technique to annihilate the anisotropic subgrid scales and an exact PP correction term. Free-space boundary conditions are satisfied through the use of modified Green’s functions in the solution of the Poisson equation for the stream function. The random walk technique is employed for the diffusion in order to relax the need for a remeshing of the computational elements close to solid boundaries. The immersed interface technique is applied to the flow past a circular cylinder at a Reynolds number of 3000 and the convergence of the method is demonstrated by a systematic refinement of the spatial and temporal parameters. Finally, the flow past a cactus-like geometry is considered, demonstrating the efficient handling of complex bluff body flows.

General information
State: Published
Organisations: University of Cambridge, Swiss Federal Institute of Technology
Authors: Walther, J. H. (Intern), Morgenthal, G. (Ekstern)
Pages: 039
Publication date: 2002
Conference: Selected Proceedings of the 4th International Workshop on Vortex Flows and Related Numerical Methods, Santa-Barbara, CA, 01/01/2002
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Turbulence
Volume: 3
ISSN (Print): 1468-5248
Molecular dynamics simulation of vaporization of an ultra-thin liquid argon layer on a surface

We performed molecular dynamics simulations of the vaporization phenomenon of an ultra-thin layer (2 nm) of liquid argon on a platinum surface. The simulation started from a molecular system of three phases (liquid argon, solid platinum and argon vapor) in equilibrium at 110 K. The platinum wall was then suddenly heated to a higher temperature (a moderately higher temperature of 150 K and a much higher temperature of 300 K were investigated). Features of our simulation model include a fast algorithm based on a tree data structure and a constant temperature solid wall model based on a 3-D Langevin equation. The entire vaporization process was successfully simulated. The results reveal trends that agree with our knowledge of vaporization of a similar macroscopic system. For example, for the high surface temperature the vaporization process is reminiscent of the Leidenfrost phenomenon and after the formation of a vapor region between the surface and the liquid mass, the latter deforms and tends to approximately acquire a spherical “droplet” shape, as one would have expected from macroscopic considerations. Contrary to this, a gradual evaporation process occurs at moderate wall temperatures. After complete evaporation and upon reduction of the wall temperature, condensation takes place leading to reconstruction of the initial liquid layer.

Keyword: Boiling, Nanoscale, Molecular dynamics
Carbon Nanotubes in Water: Structural Characteristics and Energetics

We study the structural properties of water surrounding a carbon nanotube using molecular dynamics simulations. The interaction potentials involve a description of the carbon nanotube using Morse, harmonic bending, torsion, and Lennard-Jones potentials. The water is described by the flexible Simple Point Charge (SPC) model by Teleman et al., and the carbon-water interactions include a carbon-oxygen Lennard-Jones potential, and an electrostatic quadrupole moment acting between the carbon atoms and the charge sites of the water. Vibration of the breathing mode of the carbon nanotube in water is inferred from the oscillations in carbon-carbon van der Waals energy, and the inverse proportionality between the radius of the carbon nanotube and the breathing frequency is in good agreement with experimental values. The results indicate, that under the present conditions, the presence of the water has a negligible influence on the breathing frequency. The water at the carbon-water interface is found to have a HOH plane nearly tangential to the interface, and the water radial density profile exhibits the characteristic layering also found in the graphite-water system. The average number of hydrogen bonds decreases from a value of 3.73 in the bulk phase to a value of 2.89 at the carbon-water interface. The inclusion of the carbon quadrupole moment is found to have a negligible influence on the structural properties of the water. Energy changes that occur by the process of introducing a carbon nanotube in water are calculated. The creation of a cavity in the bulk water to accommodate the nanotube constitutes the largest energy contribution. Results include an analysis of surface structure and energy values for planar and for concave cylindrical surfaces of water.

General information
State: Published
Organisations: NASA Ames Research Center, Eloret Corporation, ETH Zurich
Authors: Walther, J. H. (Intern), Jaffe, R. (Ekstern), Halicioglu, T. (Ekstern), Koumoutsakos, P. (Ekstern)
Pages: 9980-9987
Publication date: 2001
Main Research Area: Technical/natural sciences

Publication information
ISSN (Print): 1520-6106
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.03 SJR 1.348 SNIP 1.02
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.367 SNIP 1.096 CiteScore 3.25
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.44 SNIP 1.14 CiteScore 3.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.494 SNIP 1.2 CiteScore 3.53
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.92 SNIP 1.251 CiteScore 3.66
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.78 SNIP 1.226 CiteScore 3.62
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Molecular Dynamics Simulation of Contact Angles of Water Droplets in Carbon Nanotubes

We study the behavior of water droplets confined in a carbon nanotube by means of parallel molecular dynamics simulations. We report radial density profiles, radial hydrogen bond distributions, and contact angles for tube radii ranging from 12.5 to 37.5 Å and for droplets containing up to 4632 water molecules. Our results indicate nonwetting behavior of the pristine CNT at room temperatures.
Molecular dynamics simulation of nanodroplet evaporation

Molecular dynamics simulations are used to study the sub-critical evaporation of a nanometer-size droplet at 300 K and 3 MPa. Classical molecular dynamics techniques are combined with an adaptive tree data structure for the construction of the neighbor lists, allowing efficient simulations using hundreds of thousands of molecules. We present a systematic convergence study of the method demonstrating its convergence for heat conduction problems in submicron scales. These high resolution simulations compute values of the evaporation coefficient that are in excellent agreement with theoretical predictions.

Keyword: Nanofluidics, Molecular Dynamics Simulation, Nanodroplet

General information
State: Published
Organisations: Swiss Federal Institute of Technology
Authors: Walther, J. H. (Intern), Koumoutsakos, P. (Ekstern)
Pages: 741-748
Publication date: 2001
Main Research Area: Technical/natural sciences

Publication information

Scopus rating (2016): CiteScore 13.4
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 14.76
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 14.04
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 14.23
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 13.78
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 13.83
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Web of Science (2008): Indexed yes
Web of Science (2007): Indexed yes
Web of Science (2006): Indexed yes
Web of Science (2005): Indexed yes
Web of Science (2003): Indexed yes
Web of Science (2002): Indexed yes
Web of Science (2001): Indexed yes

Original language: English
DOIs: 10.1021/nl015640u
Source: orbit
Source-ID: 317697
Publication: Research - peer-review › Journal article – Annual report year: 2001
Three-Dimensional Vortex Methods for Particle-Laden Flows with Two-Way Coupling

This paper presents a three-dimensional viscous vortex method for the simulation of particulate flows with two-way coupling. The flow is computed using Lagrangian vortex elements advected with the local velocity, while their strength is modified to account for viscous diffusion, vortex stretching, and generating vorticity induced by the particles. The solid particles move according to viscous drag and gravity, creating vorticity, which is discretised using vortex elements. This method adaptively tracks the evolution of the vorticity field and the generation of new computational elements to account for the vorticity source term. A key aspect of the present scheme is the remeshing of the computational elements to adaptively accommodate the production of vorticity induced by the solid particles, and to ensure sufficient support for the proper resolution of the diffusion equation. High-order moment-conserving formulas are implemented to maintain the adaptive character of the method while they remain local to minimize the computational cost. These formulas are also
implemented in the particle–mesh interpolation of the field and particle quantities in the context of a Vortex-in-Cell algorithm. The method is validated against the results of a related finite-difference study for an axisymmetric swirling flow with particles. The method is then applied to the study of a three-dimensional particle blob falling under the effect of gravity. It is shown that drastically different behaviours are found depending on the presence of an initial vorticity field. Keyword: Vortex methods, Particle-laden flows, Lagrangian method

**General information**

State: Published
Organisations: NASA Ames Research Center, ETH Zurich
Authors: Walther, J. H. (Intern), Koumoutsakos, P. (Ekstern)
Pages: 39-71
Publication date: 2001
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Journal of Computational Physics
Volume: 167
ISSN (Print): 0021-9991
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.12 SJR 2.034 SNIP 1.822
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.098 SNIP 1.988 CiteScore 2.92
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.166 SNIP 2.193 CiteScore 3.12
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 2.227 SNIP 2.45 CiteScore 3.3
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.161 SNIP 2.052 CiteScore 2.69
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.06 SNIP 2.194 CiteScore 2.99
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 2.185 SNIP 2.096
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 2.439 SNIP 2.219
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 2.247 SNIP 2.03
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 2.377 SNIP 2.379
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 2.182 SNIP 2.285
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 2.491 SNIP 2.238
Web of Science (2005): Indexed yes
Simulation of Particle Laden Flows Using Particle Methods

We present simulations of an initially spherical suspension of solid particles falling due to gravity in a viscous incompressible fluid. The numerical simulations are performed using three-dimensional viscous, vortex methods\textsuperscript{1} with a two-way coupling between the fluid and the particles.

General information
State: Published
Organisations: Stanford University, NASA Ames Research Center, ETH Zurich
Authors: Walther, J. H. (Intern), Lee, S. (Ekstern), Koumoutsakos, P. (Ekstern)
Pages: S13
Publication date: 2000
Main Research Area: Technical/natural sciences

Publication information
Journal: Physics of Fluids
Volume: 12
Issue number: 9
ISSN (Print): 1070-6631
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.16 SJR 1.29 SNIP 1.291
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.366 SNIP 1.278
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.354 SNIP 1.348
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.42 SNIP 1.395
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.215 SNIP 1.356
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.445 SNIP 1.474
ISI indexed (2011): ISI indexed yes
Discrete vortex simulation of flow around five generic bridge deck sections

Two-dimensional viscous incompressible flow past five generic bridge deck cross sections are investigated by means of the discrete vortex method. The analyses yield root mean square lift coefficients and Strouhal numbers for fixed cross sections and aerodynamic derivatives for the cross sections undergoing forced oscillatory cross wind and twisting motion. Fair agreement is established between the present simulations and wind tunnel test results reported in the literature.

Keyword: Aerodynamic derivatives, Discrete vortex method, Vortex shedding, Computational bridge aerodynamics
Aeroelastic analysis of bridge girder sections based on discrete vortex simulations

Two-dimensional viscous incompressible flow past bridge girder cross-sections are simulated using the discrete vortex method. The flow around stationary cross-sections as well as cross-sections undergoing cross-wind vertical (bending) and rotary (torsional) motions are investigated for assessment of drag coefficient, Strouhal number and aerodynamic derivatives for application in aeroelastic analyses. Good to excellent agreement with wind tunnel test results is demonstrated for analyses of forced wind loading, flutter wind speed and vertical vortex-induced response of four practical girder cross-sections. The success of the simulations is attributed to the bluff nature of the cross-sections and to the two-dimensional (2-D) nature of flow around bridge girders.

Keyword: Buffeting response, Aeroelastic instability, Discrete vortex method, Computational bridge aerodynamics, Vortex-induced response
Two discrete vortex method for application to bluff body aerodynamics

Two-dimensional viscous incompressible flow past a flat plate of finite thickness and length is simulated using the discrete vortex method. Both a fixed plate and a plate undergoing a harmonic heave and pitch motion are studied. The Reynolds number is 104 and the reduced onset flow speed, $U/f_c$ is in the range 2-14. The fundamental kinematic relation between the velocity and the vorticity is used in a novel approach to determine the surface vorticity. An efficient influence matrix technique is used in a fast adaptive multipole algorithm context to obtain a mesh-free method. The numerical results are compared with the steady-state Blasius solution, and with the inviscid solution for the flow past an oscillating plate by Theodorsen.

General information
State: Published
Organisations: COWI A/S, Danish Maritime Institute
Authors: Walther, J. H. (Intern), Larsen, A. (Ekstern)
Pages: 183-193
Publication date: 1997
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Wind Engineering & Industrial Aerodynamics
Volume: 67-68
ISSN (Print): 0167-6105
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.61 SJR 1.002 SNIP 1.92
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.011 SNIP 1.966 CiteScore 2.51
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.929 SNIP 2.328 CiteScore 2.13
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.807 SNIP 2.636 CiteScore 2.43
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.667 SNIP 2.396 CiteScore 1.81
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.952 SNIP 3.274 CiteScore 2.3
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.924 SNIP 2.255
Web of Science (2010): Indexed yes
Discrete Vortex Method for Two-dimensional Flow past Bodies of Arbitrary Shape Undergoing Prescribed Rotary and Translational Motion

General information
State: Published
Organisations: Fluid Mechanics, Department of Mechanical Engineering, Department of Energy Engineering
Authors: Walther, J. H. (Intern), Jensen, J. T. (Intern), Sørensen, J. N. (Intern), Larsen, P. S. (Intern)
Publication date: Dec 1994

Publication information
Place of publication: Kgs. Lyngby, Denmark
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Projects:

Experimental and Numerical studies of water flow in choanocytes and choanoflagellates
Department of Mechanical Engineering
Period: 01/08/2016 → 31/07/2019
Number of participants: 3
Phd Student: Asadzadeh, Seyed Saeed (Ekstern)
Supervisor: Meyer, Knud Erik (Intern)
Main Supervisor:
Walther, Jens Honore (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Project: PhD

**Experimental and Numerical studies of water flow in choanocytes and choanoflagellates**
Department of Mechanical Engineering
Period: 01/08/2016 → 31/07/2019
Number of participants: 3
Phd Student:
Asadzadeh, Seyed Saeed (Intern)
Supervisor:
Meyer, Knud Erik (Intern)
Main Supervisor:
Walther, Jens Honore (Intern)

**Numerical Simulation of the Hydrodynamic Behaviour of the Lubricant Oil Film in Large Two-stoke Marine Diesel Engines**
Department of Mechanical Engineering
Period: 01/06/2015 → 31/05/2018
Number of participants: 3
Phd Student:
Karvounis, Nikolas (Intern)
Supervisor:
Vølund, Anders (Intern)
Main Supervisor:
Walther, Jens Honore (Intern)

**Two and Three Dimensional Modelling of Bridge Aerodynamics**
Department of Mechanical Engineering
Period: 01/04/2015 → 31/03/2018
Number of participants: 2
Phd Student:
Spietz, Henrik Juul (Intern)
Main Supervisor:
Walther, Jens Honore (Intern)

**Development of Improved Cavitation and Noise Radiation Prediction Methods for Marine Propellers**
Department of Mechanical Engineering
Period: 01/03/2015 → 28/02/2018
Number of participants: 4
Phd Student:
Mirsadraee, Yasaman (Ekstern)
Supervisor:
Schöön, Johannes (Ekstern)
Walther, Jens Honore (Intern)
Main Supervisor:
Andersen, Poul (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Industrial PhD
Project: PhD

Optimizing Oil Production by Novel Technology Integration - Well flow modeling

Department of Mechanical Engineering
Period: 01/09/2014 → 15/04/2018
Number of participants: 3
Phd Student:
Hemmingsen, Casper Schytte (Intern)
Supervisor:
Nielsen, Kenny Krogh (Ekstern)
Main Supervisor:
Walther, Jens Honore (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Project: PhD

Turbulence Modeling in Multiresolution Vortex Methods with Application to Bluff Body Aerodynamics

Department of Mechanical Engineering
Period: 01/11/2012 → 01/09/2016
Number of participants: 5
Phd Student:
Hejlesen, Mads Mølholm (Intern)
Main Supervisor:
Walther, Jens Honore (Intern)
Examiner:
Sørensen, Jens Nørkær (Intern)
Adams, Nikolaus Andreas (Ekstern)
Winckelmans, Grégoire (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.

Relations
Publications:
A high order regularisation method for solving the Poisson equation and selected applications using vortex methods
Project: PhD

Diesel Engine Tribology

Department of Mechanical Engineering
Period: 01/05/2012 → 28/04/2016
Number of participants: 6
Phd Student:
Christiansen, Christian Kim (Intern)
Supervisor:
Walther, Jens Honore (Intern)  
Main Supervisor:  
Klit, Peder (Intern)  
Examiner:  
Santos, Ilmar (Intern)  
Arghir, Mihai (Ekstern)  
Lethovaara, Arto (Ekstern)  

Financing sources  
Source: Internal funding (public)  
Name of research programme: Institut, samfinansiering  
Project: PhD

**integrated analysis of the scavenging process in marine two stroke diesel engines**

Department of Mechanical Engineering  
Period: 01/09/2011 → 28/01/2016  
Number of participants: 7  
Phd Student:  
Andersen, Fredrik Herland (Intern)  
Supervisor:  
Matlok, Simon (Intern)  
Mayer, Stefan (Intern)  
Main Supervisor:  
Walther, Jens Honore (Intern)  
Examiner:  
Sørensen, Jens Nørkær (Intern)  
Mihaescu, Mihai (Ekstern)  
Pedersen, Eilif (Ekstern)  

Financing sources  
Source: Internal funding (public)  
Name of research programme: ErhvervsPhD-ordningen VTU

Relations  
Publications:  
Integrated Analysis of the Scavenging Process in Marine Two-Stroke Diesel Engines  
Project: PhD

**Numerical modelling of extrusion of functionally graded ceramic materials**

Department of Mechanical Engineering  
Period: 01/01/2011 → 24/08/2015  
Number of participants: 7  
Phd Student:  
Comminal, Raphaël Benjamin (Intern)  
Supervisor:  
Pryds, Nini (Intern)  
Spangenberg, Jon (Intern)  
Main Supervisor:  
Hattel, Jesper Henri (Intern)  
Examiner:  
Walther, Jens Honore (Intern)  
Alves, Manuel Antonio Moreira (Ekstern)  
Kupferman, Raz (Ekstern)  

Financing sources  
Source: Internal funding (public)  
Name of research programme: Forskningsrådsfinansiering  
Project: PhD
Simulation and Modelling of Wakes and Wake Interaction in Offshore Wind Farms

Department of Wind Energy
Period: 01/01/2011 → 25/08/2014
Number of participants: 7
Phd Student: Sarlak Chivaee, Hamid (Intern)
Supervisor: Mikkelsen, Robert Flemming (Intern)
Shen, Wen Zhong (Intern)
Main Supervisor: Sørensen, Jens Nørkær (Intern)
Examiner: Walther, Jens Honore (Intern)
Davidson, Lars (Ekstern)
Olesen, Niels Anker (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.
Project: PhD

Scavenging and swirling flow in two-stroke diesel engines - An experimental study

Department of Mechanical Engineering
Period: 01/09/2010 → 24/03/2014
Number of participants: 6
Phd Student: Ingvorsen, Kristian Mark (Intern)
Supervisor: Walther, Jens Honore (Intern)
Main Supervisor: Meyer, Knud Erik (Intern)
Examiner: Hansen, Martin Otto Laver (Intern)
Alfredsson, Henrik (Ekstern)
Gervang, Bo Groht (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 FUU, 1/3 inst 1/3 Andet
Project: PhD

Scavenging and Swirling Flow in Two-Stroke Diesel Engines - A Numerical Study

Department of Mechanical Engineering
Period: 01/05/2010 → 29/09/2016
Number of participants: 5
Phd Student: Obeidat, Anas Hassan MohD (Intern)
Main Supervisor: Walther, Jens Honore (Intern)
Examiner: Hattel, Jesper Henri (Intern)
Ellero, Marco (Ekstern)
Rosendahl, Lasse (Ekstern)

Financing sources
Source: Internal funding (public)
**Scientific GPU Computing for PDE Solvers**

**Department of Informatics and Mathematical Modeling**
**Period:** 01/05/2010 → 12/12/2013
**Number of participants:** 6
**Phd Student:**
Glimberg, Stefan Lemvig (Intern)
**Supervisor:**
Dammann, Bernd (Intern)
**Main Supervisor:**
Engsig-Karup, Allan Peter (Intern)
**Examiner:**
Walther, Jens Honore (Intern)
Cai, Xing (Ekstern)
Olson, Luke (Ekstern)

**Financing sources**
**Source:** Internal funding (public)
**Name of research programme:** Forskningsrådsfinansiering
**Project:** PhD

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**Scavenging and Swirling Flow in Two-Stroke Diesel Engines**

**Department of Mechanical Engineering**
**Period:** 01/01/2010 → 31/12/2012
**Number of participants:** 1
**Project Manager, organisational:**
Walther, Jens Honore (Intern)

**Financing sources**
**Source:** Forskningsrådene - STVF
**Name of research programme:** Forskningsrådene - STVF
**Amount:** 4,363,000.00 Danish Kroner
**Project**

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**Hydrodynamics of Marine Animals**

**Department of Mechanical Engineering**
**Period:** 01/09/2009 → 31/03/2010
**Number of participants:** 2
**Phd Student:**
Storti, Francesca (Intern)
**Main Supervisor:**
Walther, Jens Honore (Intern)

**Financing sources**
**Source:** Internal funding (public)
**Name of research programme:** Institut stipendie (DTU) Samf.
**Project:** PhD

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**Dynamisk modellering af indvendigt rifledt fordamperrør, med henblik på øget driftsfleksibilitet af termiske kraftværker**

**Department of Mechanical Engineering**
Period: 01/02/2009 → 24/03/2014
Number of participants: 6
Phd Student:
Johansen, Axel Vodder Ohrt (Intern)
Supervisor:
Sørensen, Jens Nørkær (Intern)
Main Supervisor:
Elmegaard, Brian (Intern)
Examiner:
Walther, Jens Honore (Intern)
Dahlquist, Erik (Ekstern)
Sørensen, Kim (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: ErhvervsPhD-ordningen VTU
Project: PhD

Multiscale Simulations using Particle-Vortex Methods with Application to Bluff Body Aerodynamics
Department of Mechanical Engineering
Period: 01/09/2008 → 24/08/2012
Number of participants: 5
Phd Student:
Rasmussen, Johannes Tophøj (Intern)
Main Supervisor:
Walther, Jens Honore (Intern)
Examiner:
Sørensen, Jens Nørkær (Intern)
Chatelain, Philippe (Ekstern)
Rosendahl, Lasse (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Multiscale Simulation of Wave Forces on Ocean Energy Devices
Department of Mechanical Engineering
Period: 15/08/2008 → 28/08/2012
Number of participants: 7
Phd Student:
Lindberg, Ole (Intern)
Supervisor:
Engsig-Karup, Allan Peter (Intern)
Walther, Jens Honore (Intern)
Main Supervisor:
Bingham, Harry B. (Intern)
Examiner:
Bredmose, Henrik (Intern)
Dumbser, Michael (Ekstern)
Grue, John (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.
Project: PhD
Computational Nanofluidics. Multiscale Simulations of Flow in Nanochannels

Department of Mechanical Engineering
Period: 01/11/2007 → 23/05/2012
Number of participants: 5
Phd Student:
Zambrano Rodriguez, Harvey Alexander (Intern)
Main Supervisor:
Walther, Jens Honore (Intern)
Examiner:
Hassager, Ole (Intern)
Hansen, Jesper Schmidt (Ekstern)
Quirke, Nicholas (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Computational Nanofluidics Multiscale Simulations of Flow in Nanochannels

Department of Mechanical Engineering
Period: 01/09/2007 → 31/10/2010
Number of participants: 1
Project Manager, organisational:
Walther, Jens Honore (Intern)

Financing sources
Source: Forskningsrådene - STVF
Name of research programme: Forskningsrådene - STVF
Amount: 1,544,304.00 Danish Kroner
Project:

Heat Transfer in Large Two-Stroke Marine Diesel Engines

Department of Mechanical Engineering
Period: 01/03/2007 → 04/04/2013
Number of participants: 6
Phd Student:
Jensen, Michael Vincent (Intern)
Supervisor:
Schramm, Jesper (Intern)
Main Supervisor:
Walther, Jens Honore (Intern)
Examiner:
Sørensen, Jens Nørkær (Intern)
Davidson, Lars (Ekstern)
Rosendahl, Lasse (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 DTU-stip, 2/3 FUR/andet
Project: PhD

Aeroelsatisk analyse af vindmøllerotor

Department of Mechanical Engineering
Period: 01/08/1998 → 05/12/2002
Number of participants: 6
Phd Student:
Gaunaa, Mac (Intern)
Supervisor:
Sørensen, Jens Nørkær (Intern)
Main Supervisor:
Larsen, Poul Scheel (Intern)
Examiner:
Meyer, Stefan (Intern)
Nim, Erik (Intern)
Walther, Jens Honore (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD

Aerodynamiske strømninger med strukturiaktion
Department of Mechanical Engineering
Period: 01/10/1991 → 16/01/1995
Number of participants: 5
PhD Student:
Walther, Jens Honore (Intern)
Supervisor:
Jensen, Johannes Tejlgaard (Intern)
Sørensen, Jens Nørkær (Intern)
Main Supervisor:
Larsen, Poul Scheel (Intern)
Examiner:
Larsen, Poul Scheel (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Gammel ordning u/skema-SU
Project: PhD

Activities:

Complex Motion in Fluids Summer School
Period: 24 Sep 2017 → 29 Sep 2017
Seyed Saeed Asadzadeh (Participant)
Jens Honore Walther (Participant)
Lasse Tor Nielsen (Participant)
Julia Dölger (Participant)
Thomas Kiørboe (Participant)
Anders Peter Andersen (Participant)
Department of Mechanical Engineering
Fluid Mechanics, Coastal and Maritime Engineering
National Institute of Aquatic Resources
Centre for Ocean Life
Department of Physics
Biophysics and Fluids

Description
The school will consist of 16 lectures in total, given by 8 speakers (90'&60' each), contributed talks, poster sessions and other activities.
Degree of recognition: International
Documents:
Asadzadeh
Related event

Complex Motion In Fluids Summer School
24/09/2017 → 30/09/2017
Cambridge, United Kingdom
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.