A stabilized nodal spectral solver for liquid chromatography models

Numerical methods for simulation of linear and non-linear liquid chromatography processes are compared in terms of computational cost and quality of the solution using as few as possible degrees of freedom (discrete problem size). We apply, for the first time, the p-type (order enrichment) continuous Galerkin spectral method (p-CG) for spatial discretization with exponential decay of spatial errors (spectral convergence) for smooth problems. To stabilize the method for marginally resolved or very steep shock-waves typically encountered, we use a spectral filtering approach. This effectively removes aliasing driven instabilities while retaining the high-order accuracy of the numerical method. We benchmark the stabilized p-CG method against two state-of-the-art finite element methods, namely the second-order accurate h-type (element refinement) discontinuous Galerkin method using a total-variation-diminishing limiter (h-DG-TVD) and the arbitrary-order hp-type discontinuous Galerkin spectral element method (hp-DG). Not surprisingly, the three methods provide predictions of column elution profiles that converge to the same values. However, the computational costs differ considerably. Although second-order accurate shock-capturing methods are often adopted as the default implementation, the stable arbitrary high-order methods considered in this paper are found to significantly outperform these in terms of both computational cost and discrete problem size. The p-CG method performs as well as the hp-DG method in terms of computational cost, but it has superior convergence properties, even in the presence of strong shock-waves. Further, its implementation is much simpler.