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Benchmarking state-of-the-art optical simulation methods for analyzing large nanophotonic structures

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Five computational methods are benchmarked by computing quality factors and resonance wavelengths in photonic crystal membrane L5 and L9 line defect cavities. Careful convergence studies reveal that some methods are more suitable than others for analyzing these cavities.

**Geometry under study**

The photonic crystal (PhC) membrane represents a platform for planar integration of components, where cavities and waveguides may play a key role in realizing compact optical components. A finite-length defect waveguide forms an L\(n\) cavity, where \(n\) denotes the length of the cavity. Such L\(n\) cavities support spectrally discrete optical modes, and the fundamental cavity mode profile of an L9 cavity is shown in Fig. 1. Light may be confined to such an L\(n\) cavity for extended periods, as quantified by the quality (Q) factor. The Q factor thus represents a key parameter in the design of a PhC membrane cavity.

![Fig. 1: Optical field |Ey|² profile for the L9 cavity mode.](image)

**Table 1:** Calculated Q factors and resonance wavelengths \(\lambda\).

<table>
<thead>
<tr>
<th></th>
<th>FDTD</th>
<th>FDFD</th>
<th>FEM</th>
<th>SIE</th>
<th>FMM</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\lambda) L5 (nm)</td>
<td>1568</td>
<td>1572</td>
<td>1571</td>
<td>1572</td>
<td>1567</td>
</tr>
<tr>
<td>(\lambda) L9 (nm)</td>
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<td>1580</td>
<td>1578</td>
<td>1579</td>
<td>1570</td>
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<tr>
<td>Q L5</td>
<td>1670</td>
<td>1725</td>
<td>1705</td>
<td>1707</td>
<td>1700</td>
</tr>
<tr>
<td>Q L9</td>
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<td>108,000</td>
<td>105,000</td>
<td>104,000</td>
<td>60,000</td>
</tr>
</tbody>
</table>

**Methods and results**

The combination of the large size of the PhC L\(n\) cavity and the full 3D nature of the geometry makes the calculation of the cavity Q factor an extremely demanding numerical challenge. In this work, we focus on two structures, a low-Q L5 cavity and a high-Q L9 cavity. We employ five different computational methods, the finite-difference time-domain (FDTD) technique, the finite-difference frequency-domain (FDFD) technique, the finite-element method (FEM), the surface integral equation (SIE) approach and the Fourier modal method (FMM), to compute the cavity Q factor and the resonance wavelength for both structures. For each method, the relevant computational parameters are systematically varied to quantify the computational errors. The final results summarized in Table 1 show that the resonance wavelengths agree fairly well for the two geometries among the five methods. On the other hand, significant deviations are observed for the Q factor. Our study highlights the importance of careful convergence checks and systematic estimation of the computational error, both of which are generally missing in the literature.