Abstract: We introduce a 3-dimensional electromagnetic eigenmodal algorithm for the theoretical analysis of resonating nano-optical structures. The method, a variant of the Jacobi–Davidson algorithm, solves the electric field vector wave, or \textit{curl-curl}, equation for the electromagnetic eigenmodes of resonant optical structures with a finite element method. In particular, the method includes transparent boundary conditions that enable the analysis of resonating structures in unbounded space. We demonstrate the performance of the method. First, we calculate the modes of several dielectric resonator antennas and compare them to theoretically determined results. Second, we calculate the modes of a nano-cuboid and compare them to theoretically determined results. Third, we numerically analyze spherical nanoparticles and compare the result to the theoretical Mie solution. Fourth, we analyze optical dipole antenna configurations in order to assess the method’s capability for solving technologically relevant problems.

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1. Introduction

The interaction of nano-meter structured, metallic, aka. plasmonic, devices with light, especially from lasers, has attracted considerable interest during the last few years. Consequentially, a significant body of literature exists, see e.g. [1–4]. The concept of the antenna, in particular, transferred from the microwave to the optical region, has attracted enormous interest since the conversion of propagating light into localized, electromagnetic energy, and vice-versa, holds the promise of novel technological applications in many fields, such as in sensing, detection manipulation and communication [5–8]. Certainly, it is well beyond the scope of this study to give a comprehensive overview. Simultaneously, fabrication technology has advanced impressively and is now capable of producing ultra-smooth structures with justifiable effort [9].

Since the behavior of nano-optical devices is sometimes counter-intuitive and the fabrication processes are often time-consuming, the theoretical analysis of these devices has become indispensable in order to identify promising candidates and to assess their performance before resources are committed in the clean room.

Generally speaking, theoretical methods are classified into analytical [10], semi-analytical [11] and numerical approaches [12–14]. While analytical methods can provide detailed insight into the behavior of devices and allow for relatively simple parameter sweeps, quite often their applicability is limited to simplified geometries and, thus, their predictions are of limited validity when technologically relevant problems are studied. Numerical methods on the other hand allow for the detailed modeling of delicate geometrical details, almost fully preserving the reality of the device. Thus, they are the methods of choice for detailed performance analysis. We note however that such detailed wealth of prediction comes at a price in the form of significantly increased computational effort and substantial pre- and post-processing work. In between these methods is the class of semi-analytical methods that are usually more flexible with respect to geometry, but on the other hand still provide analytical insight. Among the many semi-analytical methods we particularly mention the multiple multipole (MMP) method, originated by Hafner [11] in the 1980s. The MMP method subdivides geometry into subdomains for which the analytical solutions are available. It then matches the superposition of these scaled analytical solutions on the interfaces between the subdomains by formulating the mismatch as an error energy. The resulting, overdetermined linear system is then solved and the mismatch on the subdomain interfaces is a direct measure for accuracy.

Here, we use the finite element method (FEM) [12] in the time-harmonic regime to calculate electromagnetic modes associated with resonant nano-optical devices. We derive and solve the corresponding electromagnetic eigenmodal problem. The resonance wavelength, the decay rate and the quality factor (Q factor) are derived from the (complex) eigenvalue, and the electromagnetic fields are derived from the calculated eigenvector. The radiated power, dissipated energy and stored energy of the system can be computed as well. We demonstrate the performance of the method by solving four different problems, namely:

(i) The dielectric resonator antenna (DRA) [15,16]: the problem is solved in the microwave region. A theoretical model, applicable under specific conditions, is available to benchmark the method.
(ii) The single nano-cuboid: the problem is solved in the optical region. We compare the numerical solution with the theoretical model proposed in (i).

(iii) The single spherical nanoparticle: we compare the numerical solution with the Mie solution [17].

(iv) The optical dipole antenna of finite lateral dimensions: we realistically model the dipole antenna with two smoothly rounded arms. This geometry has traditionally been studied via the thin wire approximation [18]. The FDTD method [19] experiences intrinsic difficulties when modeling rounded objects. Other work [20–22] is restricted to 2-dimensional geometries. In [23, 24], the 3-D FEM is restricted to relatively small-scale problems due to the huge memory consumption and excessive computation time, further suffering from relatively low accuracy. In [25, 26], the surface integral equation (SIE) method experiences difficulties when modeling the substrate. Here, we study a technologically relevant geometrical discretization of the optical dipole antenna, free of the aforementioned limitations. Both bright and dark modes [27] are investigated.

2. Formulation of the problem

The electromagnetic background of our simulations originates in the Maxwell equations combined with proper boundary conditions. In the time-harmonic regime, after eliminating the magnetic field \( \mathbf{H}(x) \), the electric field \( \mathbf{E}(x) \) satisfies

\[
\nabla \times (\mu_r^{-1} \nabla \times \mathbf{E}(x)) + i k_0 \sigma Z_0 \mathbf{E}(x) - k_0^2 \varepsilon_r \mathbf{E}(x) = 0, \quad \nabla \cdot (\varepsilon_r \mathbf{E}(x)) = 0, \quad x \in \Omega. \quad (1)
\]

Here, \( \Omega \subset \mathbb{R}^3 \) is a bounded domain, \( k_0(=\omega \sqrt{\mu_0 / \varepsilon_0}) \) is the complex wavenumber in free space; \( \omega(=\omega + i\alpha) \) is the complex angular frequency, \( \omega \) is the angular frequency and \( \alpha \) is the exponential decay rate; \( \mu_r, \varepsilon_r \) are relative magnetic permeability and relative electric permittivity, respectively; \( \sigma \) is the ohmic loss of the material; \( Z_0(=\sqrt{\mu_0 / \varepsilon_0}) \) is the characteristic impedance of free space.

We model the material loss of the nano metallic structure through the complex permittivity \( \varepsilon_r \), normally with negative real part, instead of ohmic loss \( \sigma \). The dielectric function is not generally constant, but \( \varepsilon_r \) depends on the frequency \( \omega \), or, equivalently, the real part of \( k_0 \) [28]. In this paper, we use experimental data from Johnson and Christy [28] and employ a piecewise linear interpolation. We obtain the dielectric function within the spectral range from 0.64 eV to 6.60 eV [28]. The substrate’s, e.g., glass, or the environment’s, e.g. a covering layer of water, dielectric functions are not constant either [29]. However, since the variation is usually small within a certain optical spectral range, we assume that the dielectric properties of the substrate and the environment are constant.

The formulation of the nano-optical device simulation uses a bounded domain \( \Omega = \Omega_1 \cup \Omega_2 \cup \Omega_3 \). It encloses the nano-optical device \( \Omega_1 \), its substrate \( \Omega_2 \), and the environment \( \Omega_3 \), cf. Fig. 1. We solve the eigenproblem Eq. (1), where

\[
\varepsilon_r = \begin{cases} 
\varepsilon_i(\text{Re}(k_0)), & x \in \Omega_1, \\
\varepsilon_{\text{sub}}, & x \in \Omega_2, \\
\varepsilon_{\text{env}}, & x \in \Omega_3.
\end{cases} \quad (2)
\]

\( \varepsilon_{\text{sub}} \) and \( \varepsilon_{\text{env}} \) are the constant relative permittivity for the substrate and the environment, respectively. \( \varepsilon_r \) depends on \( \text{Re}(k_0) \) in the subdomain \( \Omega_1 \).

On the interface \( \Gamma_{13} \) the tangential component of \( \mathbf{E}(x) \) must be continuous. On the artificial surface \( \Gamma \) we use the 1st order absorbing, aka. transparent, boundary condition (ABC) [12]

\[
\mathbf{n} \times \nabla \times \mathbf{E}(x) = -ik \mathbf{n} \times (\mathbf{n} \times \mathbf{E}(x)), \quad (3)
\]
where \( k = k_0 \sqrt{\mu \varepsilon} \) is the wavenumber of the surrounding medium. We let \( \Omega \) be a sphere of radius \( R_b \). \( R_b \) should be as large as possible to minimize the artificial reflections on \( \Gamma \) introduced by the ABC, which arise in the case of non-orthogonal incidence of out-going wave. On the other hand, \( R_b \) should be small to limit the size of the discretized system. By numerical experiment we fix \( R_b \) such that a change of \( R_b \) does not result in a significant deviation of the computed resonant wavelength, cf. the discussion in Sections 4.3. Following this rule, we observe that the minimum distance between \( \Gamma \) and the device \( \Omega_1 \) is at least (and usually larger than) \( 1/3 \) of the resonance wavelength.

We solve Eqs. (1)–(3) to determine the electric field \( E(x) \) and the wavenumber \( k_0 \). The corresponding magnetic field is obtained by

\[
H(x) = \frac{1}{-i\theta \mu_0 \mu_r} \nabla \times E(x) = \frac{i}{k_0 \mu_0 \mu_r} \nabla \times E(x).
\] (4)

The resonant frequency is \( f = \omega / 2\pi \) (\( \omega = \text{Re}(\tilde{\omega}) \)). The decay rate \( \alpha (= \text{Im}(\tilde{\omega})) \) is directly connected to the loss. In analogy to an oscillating system with damping, the quality factor is defined as

\[
Q_1 = |\omega / 2\alpha|.
\] (5)

We compute the system’s total energy \( U \), stored energy \( U_s \), dissipated energy \( U_d \), and the radiated power \( P_r \) of the dispersive metallic nano-structure, respectively. Under the condition of no magnetic dispersion (\( \mu_r = 1 \)), the total energy is [30,31]

\[
U = \frac{\varepsilon_0}{4} \int_{\Omega} \left( \text{Re}(\varepsilon_r) + \frac{2 \omega \text{Im}(\varepsilon_r)}{\gamma} \right) |E(x)|^2 dx + \frac{\mu_0}{4} \int_{\Omega} |H(x)|^2 dx.
\] (6)

where \( \gamma \) is the damping frequency of the dispersive metal with \( \gamma = \tau^{-1} \) where \( \tau \) is the relaxation time. \( \tau \approx 31 \text{fs} \) for silver and \( \tau \approx 9.3 \text{fs} \) for gold [28].

If (i) the metal dielectric function can be described by the Drude model [17], and (ii) \( \omega \tau \gg 1 \), we obtain the stored energy [32,33] in Eq. (7), equivalent to the Brillouin formula [34],

\[
U_s = \frac{\varepsilon_0}{4} \int_{\Omega} \left( \text{Re}(\varepsilon_r) + \omega \frac{d(\text{Re}(\varepsilon_r))}{d\omega} \right) |E(x)|^2 dx + \frac{\mu_0}{4} \int_{\Omega} |H(x)|^2 dx.
\] (7)

We note that computing the stored energy for nano-metallic structures is still a matter of intense, scientific debate [32,33]. We emphasize that Eq. (7) holds only if both assumptions (i)
and (ii) are satisfied. The second assumption, i.e., \( \omega \tau \gg 1 \), holds for all eigenmodes computed in this paper, e.g., \( \omega \tau > 100 \) for silver spheres, Section 4.3, and \( \omega \tau > 20 \) for gold dipole antennas, Section 4.4. While the Drude model is a good fit for dispersive silver, still, there is a difference between the analytical model and the experimental data from [28], particularly noticeable in the range of 2.5 eV to 3.5 eV [33], cf. Section 4.3. For the optical dispersion of gold, the Drude model is a rough fit. In particular, the difference between the analytical model’s imaginary part of \( \varepsilon_r \) and the experimental data is considerable for the photon energy above 2 eV [35]. Therefore, in the spectral range above 2 eV the calculation of the stored energy via Eq. (7) is invalid for gold, cf. discussion in Section 4.4.2. However, we employ Eq. (7) in order to assess its accuracy by comparing it to results derived via an alternative route. Dissipated energy [33] is then computed as

\[
U_d = \frac{\varepsilon_0}{2} \int_{\Omega_1} \text{Im}(\varepsilon_r)|\mathbf{E}(x)|^2 \, dx. \tag{8}
\]

Radiated power is calculated via the Poynting theorem [18],

\[
P_r = \frac{1}{2} \int_{\Gamma} \text{Re}(\mathbf{E}(x) \times \mathbf{H}(x)^\ast) \cdot d\mathbf{x}. \tag{9}
\]

Therefore the system’s quality factor can also be defined by

\[
Q_2 = \frac{\omega U_s}{\omega U_d + P_r}. \tag{10}
\]

We comment that \( Q_2 \) will appear to be a less reliable definition than \( Q_1 \), since \( U_s \) in (7) may not be accurate enough for nano-metallic structures. Therefore, in our numerical examples, we list both \( Q_1 \) and \( Q_2 \) for comparison purposes. The radiative quantum yield \( \eta \) is evaluated as the ratio of radiation loss and total loss, i.e.,

\[
\eta = \frac{P_r}{P_r + \omega U_d}. \tag{11}
\]

In the special case of a non-dispersive medium that has no dissipative loss, e.g., the dielectric resonator antenna (DRA) with constant \( \text{Re}(\varepsilon_r) \) and \( \text{Im}(\varepsilon_r) = 0 \), (7) and (8) lead to

\[
U_s = \frac{\varepsilon_0}{2} \int_{\Omega} \text{Re}(\varepsilon_r)|\mathbf{E}(x)|^2 \, dx, \quad U_d = 0, \tag{12}
\]

such that \( Q_2 = \omega U_s/P_r \) and \( Q_1 \equiv Q_2 \).

3. Numerical solution

3.1. The finite element method

The finite element method (FEM) is a suitable method for the nano-optical devices simulation, since such devices exhibit delicate geometries with a wide span of geometrical scales. In order to apply the finite element method we need a weak form of (1). We first note that for sufficiently smooth vector functions \( \mathbf{E}(x) \) and \( \mathbf{f}(x) \) that satisfy the boundary condition (3) we have [12, 18]

\[
\int_{\Omega} \mathbf{f}(x) \cdot (\nabla \times \mu_r^{-1} \nabla \times \mathbf{E}(x)) \, dx = \int_{\Omega} \mu_r^{-1} \nabla \times \mathbf{f} \cdot \nabla \times \mathbf{E} \, dx - \int_{\Gamma} \mu_r^{-1} \mathbf{n} \cdot (\mathbf{f} \times \nabla \times \mathbf{E}) \, dx = \int_{\Omega} \mu_r^{-1} \nabla \times \mathbf{f} \cdot \nabla \times \mathbf{E} \, dx + i \int_{\Gamma} k \mu_r^{-1} \mathbf{n} \times (\mathbf{f} \times \nabla \times \mathbf{E}) \, d\mathbf{x}.
\]
Similarly, for any sufficiently smooth scalar function \( q(x) \) vanishing on \( \Gamma \) we get

\[
\int_{\Omega} \varepsilon_r (\nabla \cdot E(x)) q(x) \, dx = - \int_{\Omega} \varepsilon_r E(x) \cdot (\nabla q(x)) \, dx = 0.
\]

Therefore, a natural weak form of (1)–(3) is:

\[
\text{Find } k_0 \in \mathbb{C} \text{ and } E \in V, E \neq 0, \text{ such that for all } f \in V \text{ and all } q \in W \]
\[
\int_{\Omega} \mu_r^{-1} \nabla \times f \cdot \nabla \times E \, dx + ik_0 \left( \int_{\Gamma} \sqrt{\varepsilon_r / \mu_r} (n \times f) : (n \times E) \, dx + \int_{\Omega} \sigma Z_0 f \cdot E \, dx \right) + k_0^2 \int_{\Omega} \varepsilon_r f \cdot E \, dx = 0,
\]
\[
\int_{\Omega} \varepsilon_r E \cdot \nabla q \, dx = 0.
\]

(13)

Here, \( V \) denotes the functions in \( H(\text{curl}; \Omega) \) that satisfy the boundary condition (3) and \( W = H^1_0(\Omega) \). For details on these function spaces see, e.g., [13] or [12].

We discretize (13) by the Ritz-Galerkin method [12, 13] employing appropriate finite element subspaces of \( V \) and \( W \). To that end we triangulate \( \Omega \) by tetrahedra with Gmsh [36]. The triangulation has to respect the interfaces \( \Gamma_{13} \) and \( \Gamma_{23} \). The mesh must be fine in the vicinity of the surface of the optical device \( \Omega_1 \), but it can be coarse in the far-field zone. This strategy maintains efficiency and accuracy while, on the other hand, it reduces the computational cost.

The electric/magnetic vector functions in \( V \) are then approximated by Nédélec (edge) elements, while the scalar functions in \( W \) are approximated by Lagrange (nodal) finite elements [13]. This approach avoids the generation of spurious eigensolutions, and imposing the boundary conditions is straightforward [12].

Let the vector functions \( N_i \), \( 1 \leq i \leq n \), be the Nédélec basis functions, while the scalar functions \( N_j \), \( 1 \leq j \leq m \), denote the Lagrange basis functions. Then, Eq. (13) yield a constrained complex quadratic eigenvalue problem

\[
T(\lambda)x = Ax + \lambda Rx - \lambda^2 Mx = 0,
\]
\[
C^T x = 0,
\]

(14)

where \( \lambda (= k_0) \) is the eigenvalue and \( x \) is the eigenvector. The matrices \( A, R, M, \) and \( C \) in (14) have entries

\[
a_{ij} = \int_{\Omega} \mu_r^{-1} (\nabla \times N_i) \cdot (\nabla \times N_j) \, dx, \quad 1 \leq i, j \leq n,
\]
\[
m_{ij} = \int_{\Omega} \varepsilon_r N_i \cdot N_j \, dx, \quad 1 \leq i, j \leq n,
\]
\[
r_{ij} = i \int_{\Gamma} \sqrt{\varepsilon_r / \mu_r} (n \times N_i) \cdot (n \times N_j) \, dx + i \int_{\Omega} \sigma Z_0 N_i \cdot N_j \, dx, \quad 1 \leq i, j \leq n,
\]
\[
c_{\ell i} = \int_{\Omega} \varepsilon_r N_i(x) \cdot \nabla N_{\ell}(x) \, dx, \quad 1 \leq i \leq n, 1 \leq \ell \leq m,
\]

(15)

respectively. Since \( \varepsilon_r \) and \( \mu_r \) are element-wise constant, \( A, M, \) and \( R \) are composed of real symmetric element matrices multiplied by a complex factor. Thus, they are complex symmetric.

3.2. The eigensolver

Instead of solving the eigenvalue problem (14) we use an appropriate linearization [37]. Defining \( x_2 = \lambda x_1 \), (14) is transformed into a constrained linear eigenproblem of the form

\[
\mathcal{A} x = \begin{bmatrix} A & O \\ O & I \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \lambda \begin{bmatrix} R & M \\ I & O \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \equiv \lambda \mathcal{B} x, \quad \mathcal{B}^T x = \begin{bmatrix} C & O \\ O & C \end{bmatrix}^T x = 0.
\]

(16)
The identity matrix $I$ in (16) could be replaced by any nonsingular matrix $X$, i.e., we could write $Xx_2 = \lambda Xx_1$. Choosing $X = M$ would make both $\mathcal{A}$ and $\mathcal{M}$ complex symmetric. Since complex symmetry does not necessarily increase numerical simplicity [38] we set $X = I$.

The linearization of the quadratic eigenvalue problem allows us to use well-known eigensolvers. For solving large sparse complex eigenvalue problems the Jacobi–Davidson QZ algorithm (JDQZ) is appropriate [39, 40]. JDQZ computes a partial QZ decomposition

$$ \mathcal{A} Q = ZT_A, \quad \mathcal{B} Q = ZT_B, \quad \mathcal{C}^T Q = O, $$

where $Q$ and $Z$ are $2n \times r$ matrices, and $T_A$ and $T_B$ are upper-triangular $r \times r$ matrices. The quotients of corresponding diagonal elements of $T_A$ and $T_B$ provide the eigenvalues. We are looking for a few eigenvalues closest to a prescribed target value $\tau$. The initial target is chosen to be an estimate of the expected eigenvalue. More details on selecting the initial target are given in Section 4.1. The columns of $Q$ are the Schur vectors from which the desired eigenvectors are extracted. $Z$ is a so-called shadow space. For details on eigenvalue/eigenvector extraction and on restarting we refer to [39]. Here, we only discuss the most time consuming step of the Jacobi–Davidson algorithm, the expansion of the search space. To that end, the so-called correction equation has to be solved,

$$ (\mathcal{A} - \tilde{Z}\tilde{Z}^*)(\mathcal{A} - \tilde{\lambda}\mathcal{B})(\mathcal{A} - \tilde{Q}\tilde{Q}^*)t = r \quad \tilde{Q}^*t = 0, \quad \mathcal{C}^Tt = 0, $$

where the solution $t$ is used to span the search space. $\tilde{\lambda}$ is the actual best eigenvalue approximation, $\tilde{Q}$ is the matrix $Q$ expanded by the corresponding Schur vector $u$. $\tilde{Z}$ is the matrix $Z$ expanded by the new shadow vector $p$. So, $\tilde{Q}$ and $\tilde{Z}$ are $2n \times (r+1)$ matrices.

The solution $t$ of (18) is not needed to high accuracy. Therefore, we can approximately solve the correction equation by executing a few steps of a preconditioned Krylov space method. The Jacobi–Davidson method has the advantages of short execution time and low memory consumption, which is crucial for solving large scale eigenproblems. To impose the divergence-free condition in (14), we construct an appropriate projector to assert that each vector in the search space is in the null space of $\mathcal{C}^T$ [41–43].

The global matrix of the correction Eq. (18) has a $2 \times 2$ block structure, cf. (16). We use the block Gauss–Seidel preconditioner on the global matrix. To solve with the diagonal (1,1) block, we use the Jacobi preconditioner or a hierarchical basis preconditioner [42,43]. The diagonal (2,2) block is related to the identity matrix, so it is trivial to solve.

3.3. Implementation

We have implemented the algorithm in our software package femaxx [41] which is continuously being developed at the Swiss Federal Institute of Technology (ETH) Zurich and the Paul Scherrer Institute (PSI) in order to solve large scale electromagnetic eigenmodal problems. The code has been efficiently parallelized to profit from today’s widespread, low-cost distributed memory parallel computers. It targets solving various kinds of electromagnetic eigenmodal problems based on the finite element method in 3-dimensional space. Both linear and quadratic Nédélec elements are available. The femaxx eigensolver is based on the Trilinos software framework [44] which defines basic parallel objects such as vectors and sparse matrices. The real-symmetric Jacobi–Davidson eigensolver has been implemented with efficient multilevel preconditioning [42,43]. We have now added a complex Jacobi–Davidson eigensolver. At present, Trilinos does not support a robust complex package [44]. Thus, our complex eigensolver treats real and imaginary parts of all quantities separately. The femaxx postprocessor evaluates the electromagnetic field at any spatial location and visualizes the result with Paraview [45].
4. Validation and application of the algorithm

To validate the eigenmodal solver algorithm and, in particular, its combination with an absorbing boundary condition (ABC), we analyze three problems, namely (i) the dielectric resonator antenna (DRA), (ii) the nano-cuboid, and (iii) a spherical nanoparticle with variable radius. Eventually, in addition to the benchmark cases, we apply the algorithm to the analysis of the optical dipole antenna.

Unless otherwise specified, quadratic Nédélec elements are used with each element having 20 local degrees of freedom. We use spatially highly resolved tetrahedral meshes. In particular, for the nano-optical application examples, the size of an element in the region of the resonating structure is in the order of a few nanometers, or smaller. In combination with second order basis functions we thus employ a highly accurate field approximation. Therefore, the error caused by the spatial discretization is generally negligible.

All simulations were carried out on the Cray XT5 at the Swiss National Supercomputing Centre (CSCS) [46]. We stress that femmaxx generally operates on any reasonable distributed memory parallel computer. Naturally, given the size of the numerical problem at hand, femmaxx indeed profits from increased compute power but it does by no means enforce the use of a supercomputer.

4.1. Dielectric resonator antenna

We analyze rectangular dielectric resonator antennas (DRAs) in the microwave region. DRAs have been analyzed theoretically [15, 16]. We study DRAs with various dimensions \(a, b, d\), and dielectric function \(\varepsilon_r\). The meshes usually contain \(\approx 80'000\) tetrahedra for each DRA, so that the discretization counts \(\approx 600'000\) degrees of freedom (dof).

The radius of the computational domain \(\Omega\) is \(R_b = 30\) mm, see Fig. 2(a). Theoretical solutions from [16] and numerical results for the \(TE_{111}\) mode are given in Table 1. For all simulations, we set \(\tau\) to a real value, the equivalent of \(4.8\) GHz. Each simulation completes in \(\approx 3\) minutes using 64 cores on the Cray XT5. The normalized residual \(\frac{\|\mathcal{A}x - \lambda Bx\|_2}{\|x\|_2}\) of the converged eigenpair is in the order of \(10^{-5}\).

| \(\varepsilon_r\) (mm) | \(a\) (mm) | \(b\) (mm) | \(d\) (mm) | \(f\) (GHz) | \(f_{MI}\) (GHz) | Diff. (%) | \(Q_1\) | \(Q_2\) | \(Q_{MI}\) |
|------------------|-----------|-----------|-----------|------------|---------------|----------|--------|--------|--------|
| 79.46            | 7.45      | 7.45      | 2.98      | 4.644      | 4.346         | 6.9      | 176.8  | 174.4  | 128.7  |
| 37.84            | 8.60      | 8.60      | 2.58      | 6.221      | 5.934         | 4.8      | 31.1   | 31.3   | 37.9   |
| 37.84            | 7.45      | 7.45      | 3.51      | 5.614      | 5.337         | 5.2      | 50.8   | 51.0   | 44.0   |
| 20.0             | 10        | 10        | 4         | 6.545      | 6.409         | 2.1      | 13.3   | 13.4   | 18.1   |

We note that the theory in [16] is based on a simplified model restricted to \(\Omega_1\), i.e. the DRA, assuming perfect magnetic boundary conditions (PMC) \(\mathbf{E} \cdot \mathbf{n} = 0\) on the surface \(\Gamma_{13}\) of the DRA. In femmaxx \(\Gamma_{13}\) is treated as an interface where just the continuity of the tangential component of \(\mathbf{E}\) is enforced. \(\mathbf{E} \cdot \mathbf{n}\) need not be zero.

As expected, \(Q_1\) matches very well with \(Q_2\). However, the different treatment of the DRA walls causes a noticeable difference between \(f\) and \(f_{MI}\) and also between \(Q_1\) and \(Q_{MI}\). We note that, interestingly, our frequencies \(f\) are closer to the experimental data cited in [16] than \(f_{MI}\). Thus, the model implemented in femmaxx appears to be more realistic.

We select the last DRA as an example for the convergence behavior of the solution w.r.t. the
number $N$ of tetrahedral mesh elements. We let $N$ be $8, 28, 87$ and $645$, respectively. The computed resonant frequencies are, respectively, $6.548$ GHz, $6.545$ GHz, $6.545$ GHz and $6.545$ GHz, while the corresponding quality factors $Q_1$ are, respectively, $13.9$, $13.4$, $13.3$ and $13.3$. Thus, a tetrahedral mesh containing $\approx 80,000$ elements for each DRA in Table 1 is good enough.

The electric field distribution $|\mathbf{E}|$ of the last DRA in Table 1 ($a = b = 10$ mm, $d = 4$ mm) is shown in Fig. 2(b). Here, the number of tetrahedra of the mesh is $645$. According to the theoretical model in [16], the electric field inside the DRA along the $y$-axis satisfies $E_y = E_z = 0$.
and $E_i = Ak_i \sin(k_i y)$ where $A$ is a complex constant and $k_i = \pi/b$ is the wavenumber. We plot the three components of the electric field along the $y$-axis in Fig. 2(d). They are in good agreement with the theoretical model, except that $E_z$ varies a bit more than half a cycle inside the DRA. This, again, can be ascribed to the differing treatments of the DRA surface.

For DRA’s, in the microwave region of the electromagnetic spectrum, the $\varepsilon_r$ of the employed materials is generally constant. However, in the optical region of the electromagnetic spectrum the dielectric permittivity is in general not constant but depends on the real part of eigenvalue $\text{Re}(k_0)$, cf. (2). The dispersive material property implies that the matrices $M$ and $C$ in (15) also depend on $\text{Re}(k_0)$. So, in the nano-optical region, the eigenproblem (14) becomes a ‘truly’ non-linear, i.e. not linearizable, eigenproblem. At present, femmaxx is capable of solving linear and quadratic eigenproblems. Nevertheless, we can address this non-linear eigenproblem via solving a sequence of quadratic eigenproblems. We start with an estimate $\lambda^{(0)}$ for the eigenvalue of the expected eigenmode. By means of $\text{Re}(\lambda^{(0)})$, we determine the dielectric permittivity $\varepsilon_r = \varepsilon_r(\text{Re}(\lambda^{(0)}))$, based on [28], so that the matrices $M(\text{Re}(\lambda^{(0)}))$, and $C(\text{Re}(\lambda^{(0)}))$ can be constructed. Then, we solve the quadratic eigenvalue problem (14) and consequently obtain an improved eigenvalue estimate $\lambda^{(1)}$. This procedure is repeated to yield further estimates $\lambda^{(2)}$, $\lambda^{(3)}$, etc. We terminate the iteration as soon as two consecutive estimates are close enough. In what follows, we use this iterative procedure. We first validate our method with the nano-cuboid and nano-sphere geometries. Then we use femmaxx for the analysis of specific optical devices. In the individual quadratic eigenvalue problems we use $\tau = \text{Re}(\lambda^{(j)})$ as the target.

4.2. Cuboid

We investigate the $TE_{111}$ mode of a nano-cuboid and reuse the sketch in Fig. 2(a). We let $a = b = 100 \text{ nm}$, $d = 40 \text{ nm}$, $R_b = 300 \text{ nm}$ and assume gold and silver, respectively, for the material of the nano-cuboid. We also reuse the theoretical DRA model [15,16] to compute the resonance frequency $f_{\text{MI}}$ and the electromagnetic field. The theoretically determined wavenumber $k_0$ is complex. The quality factor $Q_{\text{MI}}$ is also theoretically determined via Eq. (5). We comment that Mongia’s model was developed in the microregion of the electromagnetic spectrum. Thus, strictly speaking, it may not be used as a reference or benchmark in the optical region where the dielectric permittivity of metals is highly dispersive and exhibits considerable dielectric loss. Nevertheless, we believe that, at present, there is no better analytical model available than Mongia’s for cuboid geometries. Therefore, we use Mongia’s model as a signpost into the optical region. Fully aware that we stretch Mongia’s model beyond its original limits of applicability, we consider it useful to help acquire at least qualitative insight into the mode structure of the nano-cuboid. The results are shown in Table 2. The mesh contains $645^3$868 tetrahedra leading to $4'120'676$ degrees of freedom. For all simulations, the initial value of $\tau(=\text{Re}(\lambda^{(0)}))$ is equivalent of 1000 THz. The eigensolver calculation time for a single run is less than 10 minutes with 256 cores, while total computation time for one eigenmode is then below 40 minutes for 3–4 runs. The normalized residual of the converged eigenpair is around $10^{-5}$.

The electric field distribution $|E|$ of the gold cuboid is shown in Fig. 2(c). The three components of $E$, plotted along the $y$-axis, are displayed in Fig. 2(e). Again they are in good agreement with the fields of the theoretical model. In Fig. 2(e), $E_y \approx 0$ and $E_z \approx 0$. $E_x$ varies by a bit more than half a cycle inside the cuboid which indicates that the PMC is not strictly satisfied on the surfaces of the cuboid. We also notice that the field is strong inside the cuboid and drops to almost zero in the far-field zone, see Fig. 2(e). Therefore, the mode experiences rather high dissipative loss, but radiates only scant electromagnetic power. Thus, $\eta$ is very small.

We comment that the dielectric function $\varepsilon_r$ is not at all constant for gold and silver in the optical region of the spectrum. The dispersive material property, in combination with the different
Table 2. Numerical figures of merit for the $TE_{111}$ mode of the nano-cuboid where $\lambda$: resonant wavelength computed by $f_{\text{maxx}}$; $f$: resonant frequency computed by $f_{\text{maxx}}$; $f_{\text{MI}}$: theoretically determined resonant frequency [16]; Diff.: relative difference of $f$ and $f_{\text{MI}}$; $Q_{\text{MI}}$: theoretically determined Q factor [16].

| material | $\lambda$ (nm) | $f$ (THz) | $f_{\text{MI}}$ (THz) | Diff. (%) | $Q_1$ | $Q_2$ | $Q_{\text{MI}}$ | $\eta$ |
|----------|----------------|-----------|------------------------|----------|-------|-------|----------------|--------|
| gold     | 320.6          | 935.1     | 739.8                  | 26.4     | 0.47  | 0.82  | 0.39           | $5.9 \times 10^{-6}$ |
| silver   | 200.7          | 1494      | 1107                   | 35.0     | 0.56  | 0.79  | 0.55           | $2.5 \times 10^{-7}$ |

The treatment of the DRA wall, largely explains the noticeable difference between $f$ and $f_{\text{MI}}$. Compared to dielectric resonator antennas, the quality factors ($Q_1$, $Q_2$, or $Q_{\text{MI}}$) of the nano-cuboid are very small, significantly below 1. This is attributed to high dissipative loss. The difference between $Q_1$ and $Q_2$ is noticeable, cf. the discussion in Section 2.

4.3. Sphere

We compute the resonant, plasmonic mode of a silver sphere, hovering in vacuum, with varying radius, i.e. $R = 25, 30, 35, 40, 60$ and 70 nm. Thus, $\varepsilon_{\text{sub}} = \varepsilon_{\text{env}} = 1.0$. The radius of the computational domain is $R_b = 300$ nm. For each sphere, the mesh contains about 250,000 tetrahedra. For all simulations, the initial value of $\tau$ is equivalent to 3.00 eV. In this example we had problems with the quadratic elements. The computation of $E_{\text{res1}}$ for $R = 25$ nm and of $E_{\text{res2}}$ (see below) for $R = 60$ nm failed to converge such that we had to resort to linear elements. In general, quadratic elements deliver more accurate solutions for fewer elements but they are more demanding w.r.t. iterative solver schemes. The eigensolver calculation time for a single run is less than 10 minutes with 256 cores (or 32 cores) if quadratic (or linear) elements are used. The normalized residual of the converged eigenpair is around $5 \times 10^{-4}$. The total computation time for one eigenmode is thus below 1 hour for 5–6 runs. We study the energy range from 2 eV to 4 eV, in wavelength units, 310 nm to 620 nm. We use $\lambda$ for the numerically determined resonance wavelength and the resonance energy $E = hc/\lambda$, with $h$ the Plank constant and $c$ the speed of light in vacuum, respectively.

![Fig. 3. Mie solutions of silver spheres with radii of (a) 30 nm and (b) 60 nm.](image-url)
Table 3. Results of the numerical analysis and the semi-analytical Mie solutions of the silver sphere hovering in vacuum, where: $E_{\text{res1}}$: resonant energy computed by $\text{femaxx}$; $E_{\text{diff}}$: the relative difference between $E_{\text{res1}}$ and $E_{\text{mie res1}}$. $Q_{\text{diff}}$: the relative difference between $Q_{1}$ and $Q_{\text{mie res1}}$. $\lambda$: resonance wavelength in nm.

| $R$ (nm) | $\lambda$ (nm) | $E_{\text{res1}}$ (eV) | $E_{\text{mie res1}}$ (eV) | $E_{\text{diff}}$ (%) | $\eta$ | $\eta_{\text{mie}}$ | $Q_{1}$ | $Q_{2}$ | $Q_{\text{mie res1}}$ | $Q_{\text{diff}}$ (%) |
|----------|----------------|------------------------|--------------------------|-----------------------|-------|----------------------|-------|-------|----------------------|----------------------|
| 25       | 368.7          | 3.36                   | 3.41                     | 1.5                   | 0.57  | 0.48                 | 21.5  | 23.2  | 22.7                 | 5.3                  |
| 30       | 373.4          | 3.32                   | 3.37                     | 1.5                   | 0.64  | 0.63                 | 17.0  | 20.7  | 16.9                 | 0.6                  |
| 35       | 381.0          | 3.25                   | 3.33                     | 2.4                   | 0.78  | 0.75                 | 10.1  | 19.3  | 12.3                 | 17.9                 |
| 40       | 388.4          | 3.19                   | 3.25                     | 1.9                   | 0.81  | 0.86                 | 9.6   | 17.1  | 8.8                  | 9.1                  |
| 60       | 408.9          | 3.03                   | 3.02                     | 0.3                   | 0.88  | 0.95                 | 6.0   | 12.3  | 3.0                  | 100                  |
| 70       | 440.6          | 2.81                   | 2.81                     | 0                    | 0.95  | 0.98                 | 5.3   | 8.6   | 2.1                  | 152                  |

Absorption efficiency ($Q_{\text{abs}}$) occur at almost the same position, $E_{\text{mie res1}}$. In Fig. 3(a) we show the Mie solution for $R=30$ nm. The full-linewidth-at-half-maximum (FWHM) energy width $\Delta E_{\text{ext}}$ of the extinction efficiency, $Q_{\text{ext}}=Q_{\text{sca}}+Q_{\text{abs}}$, can be evaluated. The quality factor is computed as $Q_{\text{res1}}=E_{\text{res1}}/\Delta E_{\text{ext}}$ [47].

When $R=60$ or 70 nm, the peaks of $Q_{\text{sca}}$ and $Q_{\text{abs}}$ are separated from each other, such that there are two distinct resonances close together. Figure 3(b) shows the Mie solution for $R=60$ nm. We first study the resonance $E_{\text{res1}}$ where $Q_{\text{sca}}$ reaches maximum. Let $\Delta E_{\text{sca}}$ be the FWHM of $Q_{\text{sca}}$, and the quality factor of this resonance $Q_{\text{res1}}=E_{\text{res1}}/\Delta E_{\text{sca}}$. However, in such cases where two peaks overlap, $Q_{\text{sca}}$ deviates from a Lorentzian shape [48], so that evaluating $Q_{\text{res1}}$ by FWHM $\Delta E_{\text{sca}}$ is not accurate.

The radiative quantum yield $\eta_{\text{mie}}$, computed with the Mie solution, is defined as the ratio between scattering and extinction efficiency, i.e., $\eta_{\text{mie}}=Q_{\text{sca}}/Q_{\text{ext}}$.

In Table 3 and Fig. 4, we show the numerical results, compared with Mie solutions. In general, the resonance ($E_{\text{res1}}$ and $E_{\text{mie res1}}$) and radiative quantum yield ($\eta$ and $\eta_{\text{mie}}$) show good agreements. The differences are mainly attributed to the 1st order ABC employed by $\text{femaxx}$, while

![Fig. 4. Numerical and Mie solutions of Q factors and radiative quantum yield (subfigure) of silver spheres with varying radius $R$.](image-url)
the Mie model is unbounded. Quality factors ($Q_1$ and $Q_{\text{mie}}^{\text{res}}$) also match when $R = 25, 30, 35$ or 40 nm. When $R = 60$ or 70 nm, two peaks of resonances ($E_{\text{res1}}^{\text{mie}}$ and $E_{\text{res2}}^{\text{mie}}$) exist and are close together, $Q_{\text{res1}}^{\text{mie}}$ is not accurate, see discussion above, and $Q_1$ is more reliable. As noted in Section 2, in the range of 2.5 eV to 3.5 eV, the difference of silver $\varepsilon_r$ between the Drude model and the experimental data is noticeable. Therefore $Q_2$ is not accurate either. Note that $E_{\text{res1}}^{\text{mie}}$ approximates a 3-fold degenerate resonance. The corresponding computed mode splits in three simple modes since the mesh does not respect the spherical symmetry of the problem. For $R = 60$ nm, the relative differences among the three computed resonances are below 1%.

We use $R = 60$ nm as an example (see Fig. 3(b)), and study the resonance $E_{\text{res2}}^{\text{mie}}$ where $Q_{\text{abs}}$ reaches the maximum. (Our computations indicate that $E_{\text{res2}}^{\text{mie}}$ is 5-fold degenerate.) The numerical value of this mode is $E_{\text{res2}}^{\text{mie}} = 3.48$ eV and $Q_1 = 8.1$. Let the angular frequency, dissipated energy and radiated powers of resonance $E_{\text{res2}}$ be $\omega_{\text{res2}}, U_{\text{res2}}^d$ and $P_{\text{res2}}^r$, respectively. Further, let the corresponding quantities for resonance $E_{\text{res1}}$ be $\omega_{\text{res1}}, U_{\text{res1}}^d$ and $P_{\text{res1}}^r$. The electric fields are scaled so that $\int_\Omega \Re(e_r) |E(x)|^2 dx$ are equal. We define $r_d = (\omega_{\text{res2}} U_{\text{res2}}^d)/(\omega_{\text{res1}} U_{\text{res1}}^d)$ and $r_r = P_{\text{res2}}^r / P_{\text{res1}}^r$. Then $r_d = 8.9$ and $r_r = 0.21$. Resonance $E_{\text{res2}}$ has higher dissipative loss since $Q_{\text{abs}}$ reaches maximum while resonance $E_{\text{res1}}$ has higher radiation loss since $Q_{\text{sca}}$ reaches maximum. The Mie solution of this mode is $E_{\text{res2}}^{\text{mie}} = 3.45$ eV. Again, evaluating $Q_{\text{res2}}^{\text{mie}} (= 17.2)$ by FWHM $\Delta E_{\text{abs}}$ is not accurate. The electric field plots of the two modes, when $R = 60$ nm, are shown in Figures 5(a) and 5(b).

![Fig. 5.](image)

We study the electromagnetic near-field of the gold nano-optical dipole antenna investigated in [25]. The geometry is shown in Fig. 6(a) and a 3-D sketch is in 6(b). The antenna has two...
arms, each of which has dimensions $a = b = 40$ nm, $l = 100$ nm. The corners of each arm are rounded, with a radius of curvature $= 5$ nm. The gap $g$ between the two arms is 20 nm wide but will be varied in order to study the electromagnetic field enhancement as a function of the gap width. The radius $R_b$ of the spherical computational domain is 400 nm.

We study three different dielectric material arrangements: (1) the antenna hovers in vacuum, thus $\varepsilon_{\text{sub}} = \varepsilon_{\text{env}} = 1.0$; (2) the antenna resides on a silica substrate, thus $\varepsilon_{\text{sub}} = 2.25$, $\varepsilon_{\text{env}} = 1.0$; (3) the antenna resides on a silica substrate and is covered with water, thus $\varepsilon_{\text{sub}} = 2.25$, $\varepsilon_{\text{env}} = 1.77$ [29]. We understand this arrangement to be a relatively detailed model for an optical antenna used in biochemical sensing where many processes are studied in aqueous solutions.

![Fig. 6. The nano-optical dipole antenna. (a) geometry; (b) 3-D sketch.](image)

We start by considering a single arm in vacuum whose resonant wavelength is 623.5 nm. When bringing two such arms into close proximity, the interaction of the two fundamental eigenmodes lead to mode splitting. When these two arms come close enough to each other, the so-called bright, aka. optically active, mode and the dark mode split. The modes can then be well distinguished in the scattering spectra [27,49].

4.4.1. Bright mode

We compute the bright mode within the spectral range of 400 nm to 1000 nm. For all simulations, the initial value of $\tau$ is equivalent of 660 nm. The results are presented in Table 4. The fields of model (1), an antenna in vacuum, are evaluated in the sample domain $\Omega_{\text{sample}} = 400\text{nm} \times 200\text{nm} \times 200\text{nm}$. Both magnetic and electric fields are shown in Fig. 7(a) and 7(b), respectively. A close-up view of the electric field in the gap region is shown in

| model                | $\varepsilon_{\text{sub}}$ | $\varepsilon_{\text{env}}$ | #p  | $N$     | dofs  | $\lambda$ (nm) | $Q_1$ | $Q_2$ |
|----------------------|-----------------------------|-----------------------------|-----|---------|-------|----------------|-------|-------|
| (1) in vacuum        | 1.0                         | 1.0                         | 300 | 340’269 | 2’162’346 | 665.7          | 20.0  | 19.8  |
| (2) on substrate     | 2.25                        | 1.0                         | 600 | 597’408 | 3’791’532 | 717.5          | 12.4  | 13.6  |
| (3) on substrate, water-covered | 2.25                        | 1.77                        | 600 | 597’408 | 3’791’532 | 801.7          | 10.6  | 14.3  |

Table 4. Numerical analysis of a gold nano-optical antenna (#p: number of cores; $N$: number of tetrahedra; dofs: degrees of freedom; $\lambda$: resonant wavelength computed by femaxx; $Q_1$ and $Q_2$: quality factors by Eq. (5) and Eq. (10), respectively;
Fig. 7. (a)-(c): Numerical analysis of a gold, nano-optical dipole antenna (model (1)). The gap width is 20 nm and the resonance is at 665.7 nm; (a) magnetic and (b) electric field distribution (|H| and |E|) in the vicinity of the antenna surface; (c) electric field distribution |E| around the gap; (a), (b), and (c) are evaluated on the xy-plane through the center of the antenna arms. (d) plots the electric field amplitudes |E| along the x-axis, associated with 3 material arrangements.

Fig. 7(c). The results in Table 4 confirm the influence of the substrate onto the antenna’s resonant wavelength. With increasing permittivity ε_{sub} the antenna resonance is red-shifted; with increasing ε_{env} the resonance wavelength is also red-shifted [50]. Each single run of the quadratic eigensolver requires 10 to 15 minutes. The total computation time for one bright mode is then below 90 minutes for 5–6 runs. The normalized residual of the converged eigenpair is around 5 × 10^{-4}. The memory per core required by the eigensolver is 33.38 MB for the model (1), and 28.65 MB for models (2) and (3). Thus, the method is particularly attractive when compared to other 3-dimensional FEM approaches [22, 24]. From Figs. 7(b) and 7(c) we note that a high-intensity electric field is generated in the vicinity of the antenna surface. It is stronger in the gap (Fig. 7(d)), and it is strongest at the inner corners of the antenna.

We now investigate how the gap width g affects the resonance wavelength λ and the field intensity |E|^2 in the gap. We use the dielectric arrangement of model (2). Let the gap width g be 20 nm, 10 nm, 5 nm, and 1 nm, respectively. The corresponding resonance wavelengths are then 717.5 nm, 751.9 nm, 796.3 nm, and 913.5 nm, respectively. A red shift, i.e., increasing wavelength, of the antenna resonance occurs with decreasing gap widths. Since the gap widths are significantly smaller than the resonance wavelengths, we can approximate the gap region with an electrostatic regime. Thus, we understand the gap region, including those portions of the dipole antenna, that immediately border it, to form a plate capacitor whose capacitance is given as $C = \varepsilon_0 \varepsilon_r A/d$. Here, A, d, and $\varepsilon_r$ correspond to the plate area, the distance between the plates and the dielectric property of the medium between the plates, respectively; in particular,
Fig. 8. Numerical analysis of a gold nano-optical antenna (model (2)): (a) gap width $g = 5$ nm, resonance at 796.3 nm. It shows the electric field distribution $|E|$ (visualized on the $xy$-plane) in the vicinity of the antenna surface; (b) plots of the electric field amplitude $|E|$ along the $x$-axis with varying gap width $g$.

$\varepsilon_r = 1$ since the gap is in vacuum. Then, it becomes clear that, with decreasing gap width, capacitance increases. A capacitance increase on the other hand is roughly proportional to a higher value of the dielectric permittivity and thus, for constant length of the dipole arms, the resonance wavelength increases since the resonance frequency is reduced. We comment that adding a capacitor parallel to an antenna’s terminal contacts is a well-known technique in microwave electronics in order to geometrically shorten the antenna, thus mimicking higher dielectric permittivity in the vicinity of the antenna.

On the other hand, when decreasing the gap width $g = 10$ nm, 5 nm, and 1 nm, the corresponding field intensities $|E|^2$ increase and are 3.4, 9.6, and 56 times larger than when a gap width $g = 20$ nm is employed, see Fig. 8(b). Decreasing the gap width thus dramatically increases the field intensity in the gap. An example field distribution, for a 5 nm gap width, is shown in Fig. 8(a). Due to the substrate effect the field is not symmetric with respect to the $x$-axis.

4.4.2. Dark mode

We study the dark mode of the dipole antenna in vacuum, model (1). The respective charge profiles [27] of the bright and the dark modes are shown in Fig. 9(a). Let the angular frequency, dissipative energy and radiated powers of the dark mode be $\omega_{\text{dark}}$, $U_{\text{d}}^{\text{dark}}$ and $P_{\text{r}}^{\text{dark}}$, respectively; further, let the corresponding quantities for the bright mode be $\omega_{\text{bright}}$, $U_{\text{d}}^{\text{bright}}$ and $P_{\text{r}}^{\text{bright}}$. Again, the electric fields are scaled so that the integrals of the type $\int_{\Omega} \text{Re}(\varepsilon_r)|E(x)|^2 \, dx$ are equal. We
define $r_d = (\omega_{\text{dark}} U_{d}^{\text{dark}})/(\omega_{\text{bright}} U_{d}^{\text{bright}})$ and $r_r = P_{\text{dark}}/P_{\text{bright}}$. The radiative quantum yield $\eta$ is computed via Eq. (11). Associated results are listed in Table 5. The mesh contains about 350,000 tetrahedra which results in more than 2,000,000. For all simulations of the dark modes, the initial value of $\tau$ is equivalent of 550 nm. The eigensolver calculation time for a single run is 10 to 15 minutes with 256 cores, and the normalized residual of the converged eigenpair is around $5 \times 10^{-4}$ for the bright mode and $10^{-4}$ for the dark mode. The total computation time for one eigenmode is then below 90 minutes for 5–6 runs.

| $g$ (nm) | $\lambda$ (nm) | $\eta$ | $Q_1$ | $Q_2$ | $\lambda$ (nm) | $\eta$ | $Q_1$ | $Q_2$ | $r_d$ | $r_r$ |
|--------|----------------|--------|--------|--------|----------------|--------|--------|--------|--------|--------|
| 20     | 582.0          | 2.4 $\times$ $10^{-4}$ | 0.89   | 13.3   | 665.7          | 0.27   | 20.0   | 19.8   | 10.1   | 0.067  |
| 10     | 557.4          | 7.0 $\times$ $10^{-4}$ | 0.78   | 9.7    | 689.8          | 0.29   | 23.3   | 20.3   | 18.2   | 0.032  |
| 5      | 532.1          | 2.3 $\times$ $10^{-4}$ | 0.65   | 7.4    | 713.9          | 0.26   | 21.5   | 20.7   | 44.9   | 0.029  |

When the width $g$ of the gap between the two arms is reduced, the single arm’s degenerate fundamental mode with its resonance at 623.5 nm splits into a bright and a dark mode. With decreasing gap width, the bright mode red-shifts, due to the effect of increased capacity for smaller width, and the dark mode shifts to blue. The dark mode radiates less, i.e. $(r_r < 0.1)$, which implies that it cannot efficiently radiate energy into the far-field, thus earning its dark reputation. On the other hand, the dark mode experiences higher dissipative loss inside the two gold arms, i.e. $r_d > 10$. Its dissipative loss approximates almost 100% of the total loss, namely $\eta < 0.005$, and thus the quality factor $Q_1$ of the dark mode is smaller than the bright mode.

The resonances of all dark modes are above 2 eV, i.e. below 620 nm; on the other hand, the resonances of all bright modes are all below 2 eV, i.e. above 620 nm. Therefore, computing the stored energy with Eq. (7) is a good approximation for bright modes, but significantly less so for dark modes, cf. the discussion in section 2. As a consequence, $Q_2$ is in good agreement with $Q_1$ for bright modes, but is significantly off for dark modes.

An exemplary field distribution for the dark mode, associated with a 10 nm gap width, is shown in Fig. 9(b). In Fig. 9(c) the field plots of bright and dark modes for a 5 nm gap width are displayed. The field associated with a dark mode is not only generated in the vicinity of the antenna surface, but also inside the gold arms, corresponding to a large $U_{d}^{\text{dark}}$. The field intensity is quite low in the gap.

5. Discussion and conclusions

We have implemented a 3-dimensional finite element method for the full-wave numerical analysis of electromagnetic resonators, surrounded by free-space. Specifically, there are no cavity walls, and the resonator structures need not be enclosed within perfect electric conductor (PEC) boundary conditions. Instead, we need to apply an absorbing boundary condition (ABC) scheme. The associated quadratic eigenvalue problem is linearized so that we can employ our current implementation of the Jacobi–Davidson QZ algorithm.

We have analyzed four different electromagnetic problems. The dielectric resonator antenna (DRA), analyzed in the microwave region of the spectrum, clearly demonstrates that the proposed Jacobi–Davidson algorithm is capable of calculating the dominant mode with excellent accuracy. The differences between the theoretically determined resonance frequencies, electric field and Q factor and their numerical counterparts are attributed to the fact that, in the analytical model, the perfect magnetic conductor (PMC) condition, is imposed on all surfaces of DRA, while femaxx does not need this simplifying assumption. The theoretical model of the DRA is
Fig. 9. (a) Charge profiles; (b) the dark mode of the gold nano-optical antenna (gap width $g = 10$ nm) in vacuum: resonance at 557.4 nm. The electric field distribution $|E|$ (visualized on the $xy$-plane) in the vicinity of the antenna surface is shown; (c) the gold nano-optical antenna (gap width $g = 5$ nm) in vacuum. The electric field amplitude $|E|$ along the $x$-axis is plotted, associated with the bright mode (resonance at 713.9 nm) and the dark mode (resonance at 532.1 nm), respectively.

reused as a signpost into the optical region for simulations of a nano-cuboid. The $TE_{111}$ mode of the nano-cuboid has a field pattern similar to the DRA, but exhibits a rather small quality factor due to high dissipative loss in metals. There is a noticeable difference between the numerically determined resonance wavelength and quality factor and the analytically determined resonance wavelength and quality factor, respectively. On the other hand, the electromagnetic field solutions demonstrate amazing agreement, in particular when we consider that Mongia’s model has been stretched considerably beyond its limits of applicability. The analysis of electromagnetic scattering off spheres represents a widely used benchmark in nano-optics which a computational electrodynamics code must be able to solve. In general, we observe good agreement between the theoretically determined resonance frequency, radiative quantum yield and Q factor and their numerical counterparts.

Thus, now that femaxx has passed a series of benchmarks, we apply it to more complex geometries and configurations. One of them, the optical dipole antenna, represents an important, elementary building block in many detection and sensing devices, especially for the life and materials sciences. We observe excellent agreement with previously published results by Kern and Martin [25], who simulate a dipole antenna with 20 nm gap width. We emphasize that our algorithm allows for the simple inclusion of background media and also media covering
the antenna, e.g., an aqueous solution covering the antenna. This corresponds to a setup that is representative for many experimental arrangements. We note that the surface integral equation (SIE) method is also capable of modeling background media but at the cost of considerably increased complexity since it must include additional Green’s functions to accommodate, e.g., a substrate. Meanwhile, the finite element method ‘absorbs’ all this additional geometrical and material complexity into the corresponding mesh. On the other hand, the finite element method needs a transparent boundary condition of high-quality which should be placed as close as possible to the resonating structure, thus ensuring that precious mesh elements are not wasted but are put to good use when modeling fine geometrical details. We also note that the dark mode, with little radiated power, is another ideal test for our approach. A precise understanding of the dark modes is important for plasmonic applications [49]. Indeed, we have found the dark mode, starting from the original single arm configuration with a degenerate fundamental mode, which also strengthens the confidence into our solver. In conclusion, our approach is flexible enough to analyze nano-optical devices with almost arbitrary geometry or material arrangements. The femaxx code is therefore a useful instrument for the analysis of technologically relevant nano-optical device concepts. We continue to develop the code.

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