FEM–EM Project Plan:
Air + Spherical PML around Dielectric Microcube

Project: Validation of Pouria et al. (2025) — Figure 1

Overview

The objective of this project is to reproduce the normalized scattering cross section (σ_s/L^2) of a SiC microcube with side length $L = 1\,\mu$m, illuminated by a plane wave of unit electric field amplitude ($E_0 = 1\,$V/m), polarized along $\hat{\mathbf{x}}$ and propagating in the $-\hat{\mathbf{z}}$ direction. This setup corresponds to Figure 1 of Pouria et al. (2025). We will implement this within the our MATLAB, using Nédélec edge elements and spherical PML absorption.

The process will be divided into clear, verifiable phases.

1 Phase 0 — Repository Audit and Ground Rules

Goal: Fix conventions, units, and identify which scripts to modify.

General conventions

- Units: SI.
$$L = 1\,\mu\text{m} = 1 \times 10^{-6}\,\text{m}, \quad \lambda = 5\,\mu\text{m}, \quad k_0 = \frac{2\pi}{\lambda}, \quad \omega = ck_0.$$
- Harmonic convention: $e^{+i\omega t}$, so that $\mathbf{H} = \frac{1}{i\omega\mu_0}\nabla \times \mathbf{E}$.
- Incident field: $\mathbf{E}_{\text{inc}} = \hat{\mathbf{x}}e^{-ik_0 z}$, with $|\mathbf{E}_0| = 1\,$V/m.

Relevant files

- `Maxwell1.m`: assembly and solver of ND1 edge elements.
- `cubeMaxwell1.m`, `cubeMaxwell1final.m`: reference drivers.
- `uniformrefine3.m`, `dof3edge.m`, `gradbasis3.m`: mesh and FE utilities.
- `amg.m`, `amgMaxwell.m`: optional solvers and preconditioners.

Outcome: Only `Maxwell1.m` will be extended (new SBC + tensor-aware path). A new driver will be created for the microcube/PML case.

2 Phase 1 — Geometry and Domain Definition

Goal: Build a three-region geometry: SiC cube $\subset$ spherical air domain $\subset$ spherical PML.

Domain structure

- **SiC Cube:** centered at origin, side $L = 1\,\mu$m.
- **Air Sphere:** radius $r_{\mathrm{SBC}} \approx L + \lambda = 6\,\mu$m.
- **PML Shell:** thickness $t_{\mathrm{PML}} \approx 0.4\lambda = 2\,\mu$m, outer radius $r_{\mathrm{PML}} = 8\,\mu$m.

Meshing guidelines

- Air: $h_{\mathrm{air}} \approx \lambda/10 = 0.5\,\mu$m.
- SiC: $h_{\mathrm{SiC}} \approx 0.25\,\mu$m.
- PML: smooth grading from h_{air} to larger elements.

Implementation

- New driver: `cube_sphAir_sphPML_driver.m`.
- Tag element regions as:
  1. `REG_SiC`
  2. `REG_AIR`
  3. `REG_PML`
- Tag inner spherical boundary ($r = r_{\mathrm{SBC}}$) as **SBC boundary**.

  Checkpoints:

- Region IDs correct and nested.
- Mesh densities meet target h values.
- Visual inspection confirms geometry.

3 Phase 2 — Scattering Boundary Condition (SBC)

Goal: Implement the background-field (scattered-field) formulation on $r = r_{\mathrm{SBC}}$.

Mathematical form

The Silver–Müller boundary condition in frequency domain:

$$(\mathbf{n} \times \nabla \times \mathbf{E}) - ik_0\, \mathbf{n} \times (\mathbf{n} \times \mathbf{E}) = (\mathbf{n} \times \nabla \times \mathbf{E}_{\mathrm{inc}}) - ik_0\, \mathbf{n} \times (\mathbf{n} \times \mathbf{E}_{\mathrm{inc}}),$$

applied on the boundary with outward normal $\mathbf{n}$.

Implementation in `Maxwell1.m`

- Extend Robin/impedance BC branch to include a *nonzero* right-hand side (background injection).
- Create a helper file `incidentPlaneWave.m` providing $\mathbf{E}_{\mathrm{inc}}$ and $\nabla \times \mathbf{E}_{\mathrm{inc}}$ at quadrature points.
- Add boundary assembly routine:
  - matrix term: $-ik_0(\hat{t}_i \cdot \hat{t}_j)A_{\mathrm{face}}$,
  - vector term: SBC operator applied to $\mathbf{E}_{\mathrm{inc}}$ projected on edge tangents.

  Checks:
- Without cube: total field inside equals $\mathbf{E}_{\mathrm{inc}}$.
- With cube: smooth field continuity at SBC, no reflection.

4 Phase 3 — Perfectly Matched Layer (PML)

Goal: Add a spherical PML shell absorbing outgoing waves.

Theory

Complex radial stretch:

$$s(r) = 1 + i\frac{\sigma(r)}{\omega\varepsilon_0}, \quad \sigma(r) = \sigma_0 \left(\frac{r - r_{\mathrm{SBC}}}{t_{\mathrm{PML}}}\right)^m,$$

with polynomial order $m = 3$.

Effective tensors:

$$\tilde{\varepsilon} = \varepsilon_{\mathrm{bg}}\big(s\,\mathbf{P}_r + s^{-1}(\mathbf{I} - \mathbf{P}_r)\big), \qquad \tilde{\mu} = \mu_0\big(s\,\mathbf{P}_r + s^{-1}(\mathbf{I} - \mathbf{P}_r)\big),$$

where $\mathbf{P}_r = \hat{\mathbf{r}}\hat{\mathbf{r}}^T$ is the radial projector.

Implementation

- Modify `Maxwell1.m` element assembly to handle 3×3 tensor ε and μ by quadrature.
- Preserve the scalar path for non-PML regions.
- Create helper `pmlSphericalTensors.m` returning flattened 3×3 tensors for given coordinates.

  Checks:

- No-scatterer: reflection $< 1\%$ at the SBC.
- Field decays smoothly in PML.

5 Phase 4 — Post-Processing: Scattering Cross Section

Goal: Compute σ_s/L^2 at $\lambda = 5\,\mu$m with a constant test permittivity.

Definitions

$$\begin{aligned}
I_0 &= \frac{|E_0|^2}{2\eta_0}, \\
\mathbf{H}_s &= \frac{1}{i\omega\mu_0}\nabla \times \mathbf{E}_s, \\
P_{\text{scat}} &= \oint_S \frac{1}{2}\Re[(\mathbf{E}_s \times \mathbf{H}_s^*) \cdot \mathbf{n}]\, dS, \\
\sigma_s &= \frac{P_{\text{scat}}}{I_0}, \qquad \frac{\sigma_s}{L^2} = \text{normalized scattering cross section.}
\end{aligned}$$

Implementation

- Create utility `sigma_s_post.m`:
  1. Build evaluation sphere at $r_{\text{eval}} \approx 0.8 r_{\text{SBC}}$.
  2. Interpolate $\mathbf{E}$, subtract $\mathbf{E}_{\text{inc}}$.
  3. Compute $\mathbf{H}_s$ and the Poynting flux integral.
- Optional: `power_balance.m` verifying $\sigma_{\text{ext}} = \sigma_s + \sigma_{\text{abs}}$.

  Checks:

- σ_s/L^2 insensitive to probe radius and mesh refinement.
- Field continuity across interfaces.

6 Phase 5 — Mesh and Domain Convergence

Goal: Verify numerical stability before wavelength sweep.

- Vary mesh density: coarse → fine, record DOFs.
- Change PML thickness: 0.3λ, 0.4λ, 0.5λ.
- Change SBC radius: adjust air thickness 0.8λ–1.2λ.

  Acceptance:
- $\Delta(\sigma_s/L^2) < 2\%$ for last two refinements.
- PML reflection $\ll 1\%$.

7 Phase 6 — Real Material Data and Comparison

Goal: Replace the test permittivity by real $\varepsilon_r(\lambda, 400°\mathrm{C})$ for 6H–SiC.

- Insert dataset via function `eps_SiC_6H_400C.m` with interpolation.
- Sweep over wavelength range used in COMSOL (2–16 μm).
- Plot σ_s/L^2 versus λ and overlay COMSOL results.

  Acceptance:
- Peak positions and magnitudes agree with COMSOL within a few percent.

8 Implementation Summary

Files to revise

- `Maxwell1.m`:
  1. Add SBC with background injection.
  2. Add tensor-aware (anisotropic) ε, μ path.

Files to add

- `cube_sphAir_sphPML_driver.m`
- `incidentPlaneWave.m`
- `pmlSphericalTensors.m`
- `sigma_s_post.m`
- `power_balance.m` (optional)
- `eps_SiC_6H_400C.m`

9 Milestones

1. **M0:** Geometry validated.
2. **M1:** SBC injects plane wave correctly.
3. **M2:** PML reflection $< 1\%$.
4. **M3:** Stable σ_s/L^2 for test permittivity.
5. **M4:** Mesh/PML convergence achieved.
6. **M5:** Real $\varepsilon_r(\lambda)$ sweep matches COMSOL.

10 Notes

- Start with constant $\varepsilon_r = 4 + 0.1i$ for the cube.
- Once validated, substitute the real 6H–SiC permittivity dataset.
- Always verify energy conservation and PML absorption.
- All lengths are expressed in micrometers for convenience, but simulations use SI meters.