Dual-Potential Finite-Difference Method for Electrodynamics With Multiphysics Solvers

Samuel W Belling, Laleh Avazpour, Irena Knezevic

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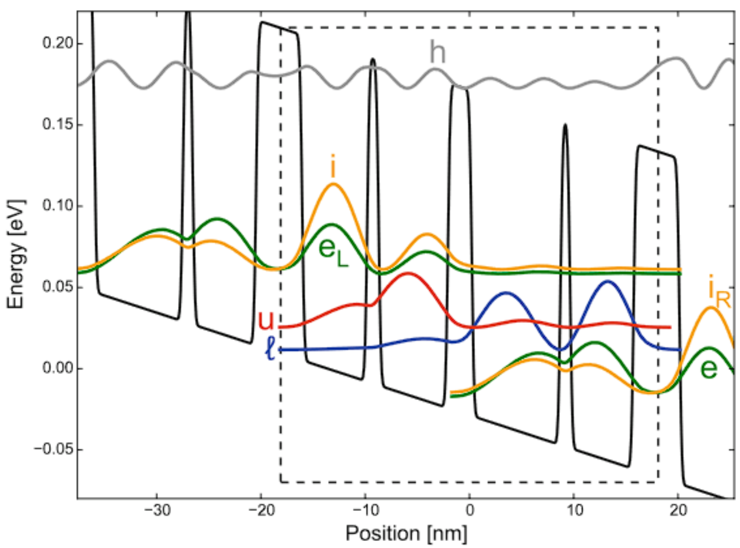
Light-Matter Coupling

- Optoelectronic device modeling requires coupling light to matter degrees of freedom



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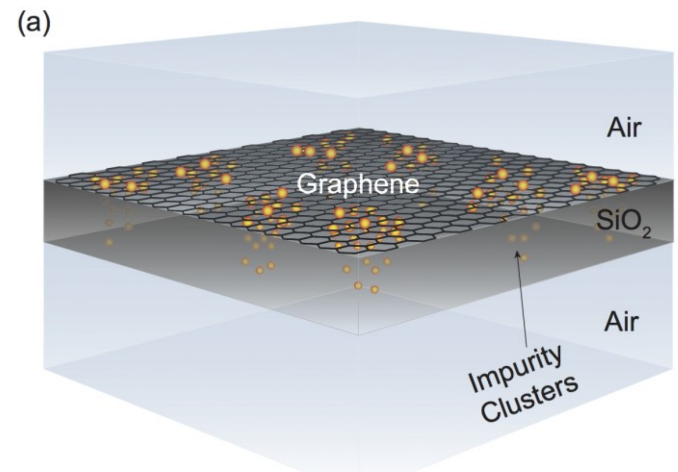

N. Sule, S. C. Hagness, and I. Knezevic, *Phys. Rev. B* **89**, 165402 (2014)

- Approaches vary in complexity: Semiclassical transport, quasistatic electromagnetic fields
- Quantum transport, dynamic electromagnetic fields
- Fully quantum light/matter

Semiclassical Transport with FDTD

- Goal is to handle time-dependent phenomena
  - AC biasing, excitation by E&M fields, terahahertz
- Approach: Self-consistently couple full-wave E&M simulation to transport

K. Tomizawa, Numerical Simulation of Submicron Semiconductor Devices (Artech House, Boston, 1993).

M. Lundstrom, Fundamentals of Carrier Transport, 2nd ed. (Cambridge University Press, Cambridge, 2000)

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M. A. Alsunaidi, S. M. Imtiaz, and S. El-Ghazaly, *IEEE Trans. Microw. Theory Tech*. **44**, 799 (1996).

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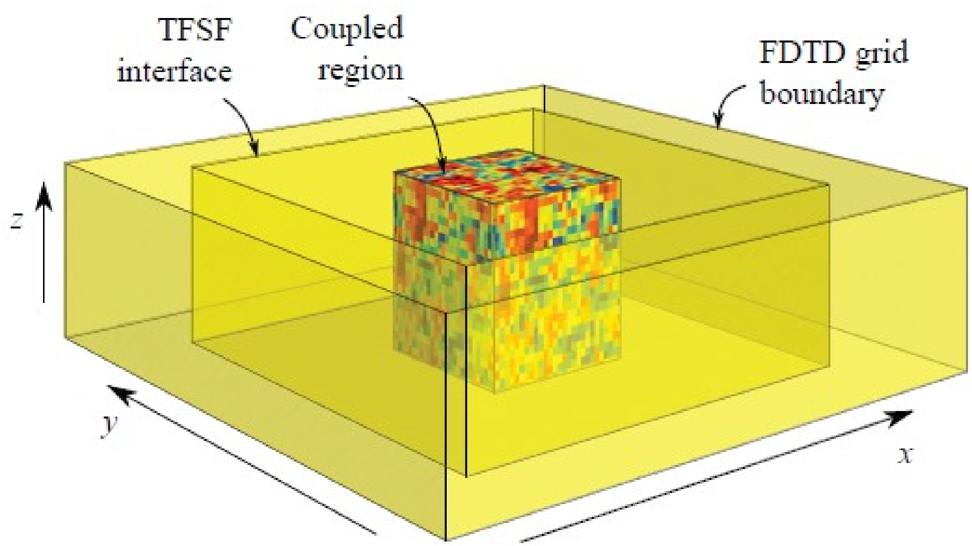


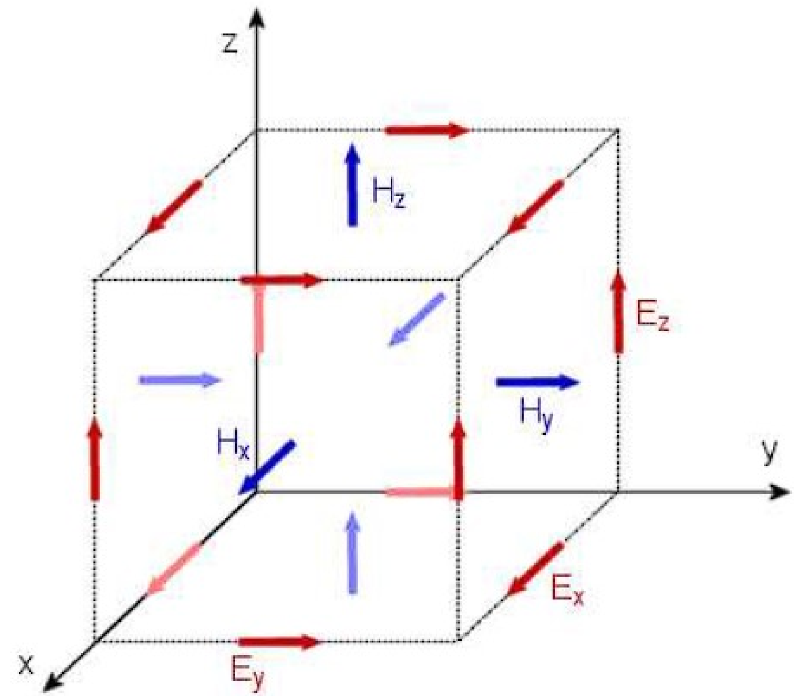
K. J. Willis, S. C. Hagness, I. Knezevic, *J. Appl. Phys.* **110**, 063714 (2011)

Classical Light

- FDTD for fields is well developed
  - Yee grid, central differences
- FDTD – time stepping routine, PML, TFSF
- Lots of work on FIELDS, we want POTENTIALS

$$\mathbf{B} = \nabla \times \mathbf{A}$$

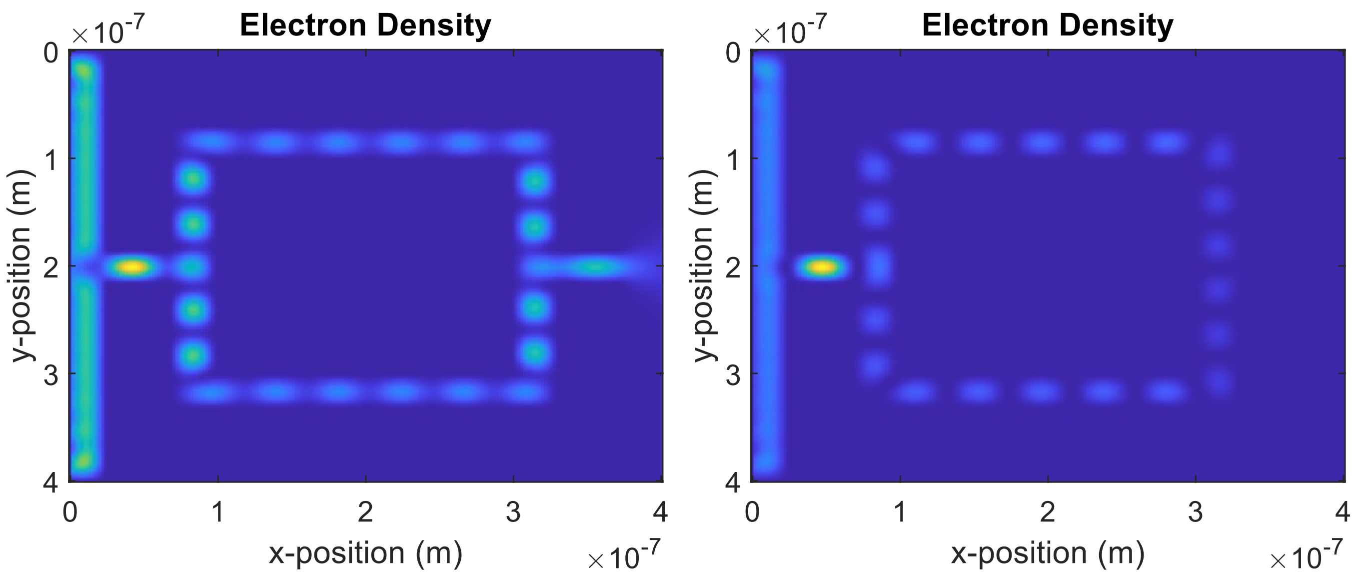
$$\mathbf{E} = -\frac{\partial \mathbf{A}}{\partial t} - \nabla \phi$$



K. J. Willis, J. S. Ayubi-Moak, S. C. Hagness, and I. Knezevic, "Global modeling of carrier-field dynamics in semiconductors using EMC-FDTD," *J. Comput. Electron.* **8**, 153-171 (2009)

Electronic Hamiltonian

- Single electron Hamiltonian is vital for pretty much any quantum transport calculation
- $\boldsymbol{A}, \phi$ enter Hamiltonian through: $\widehat{\boldsymbol{H}}_{el} = \frac{(\boldsymbol{p}-q\boldsymbol{A})^2}{2m} - q\phi(\boldsymbol{r}) + V(\boldsymbol{r})$
- Hamiltonian is NOT gauge invariant, but things like current density, charge density, **are**



Our Approaches

Field-Potential

Lorenz Gauge

$\boldsymbol{E}, \boldsymbol{H}, \boldsymbol{A}, \phi$

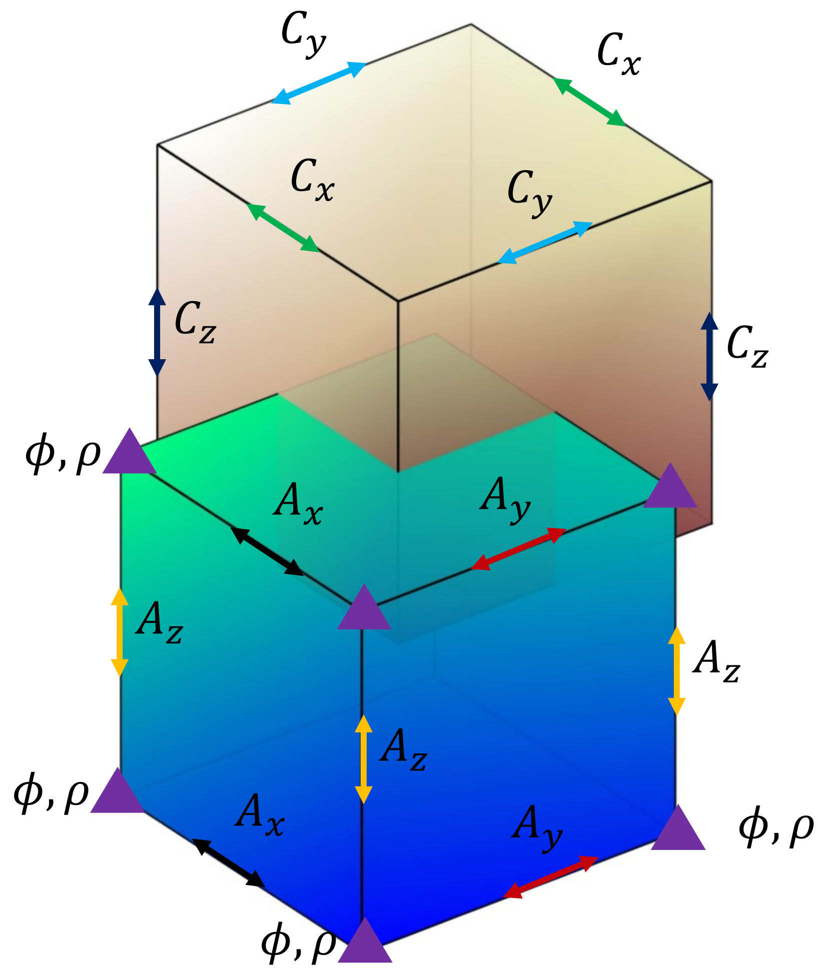
Additional equations for potentials

Dual-Potential

Coulomb Gauge

$\boldsymbol{A}, \boldsymbol{C}, \phi$

No fields, just potentials (fewer equations)



S. W. Belling, L. Avazpour, and I. Knezevic, "Coupling Classical Electrodynamics with Quantum Transport With DuPo FDTD," *In prep.* (2023)

Dual Potential FDTD

- $\mathbf{B} = \nabla \times \mathbf{A}, \ \mathbf{E} = -\frac{\partial \mathbf{A}}{\partial t} - \nabla\phi$ along with Maxwell's equations

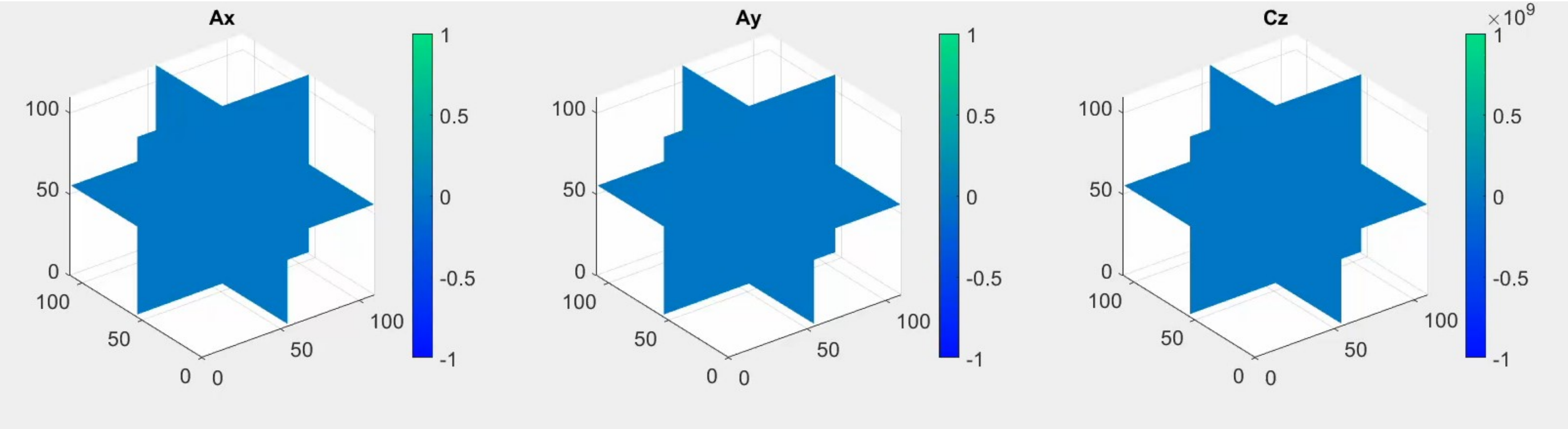
- Helmholtz decompose $\mathbf{E}$ as: $\mathbf{E} = \nabla \times \mathbf{C} + \nabla\psi$

- Gauge condition on **A** and **C**: $\nabla \cdot \mathbf{A} = 0, \nabla \cdot \mathbf{C} = 0$

$$\mathbf{E} = -\frac{\partial \mathbf{A}}{\partial t} - \nabla\phi \qquad \mathbf{E} = \nabla \times \mathbf{C} + \nabla\psi$$

$$\boldsymbol{E}_{sol} = -\frac{\partial \mathbf{A}}{\partial t} \longleftrightarrow \boldsymbol{E}_{sol} = \nabla \times \mathbf{C}$$

$$\boldsymbol{E}_{con} = -\nabla\phi \qquad \boldsymbol{E}_{con} = \nabla\psi$$



Dual Potential FDTD

- Replace **E/B** with potentials expressions in Ampere's law

$$\nabla \times \nabla \times \mathbf{A} = \mu\mathbf{J} + \mu\epsilon\frac{\partial}{\partial t}[\nabla \times \mathbf{C} + \nabla\phi]$$

$$\nabla \times \nabla \times \mathbf{A} = \mu(\mathbf{J_{rot}} + \mathbf{J_{con}}) + \mu\epsilon\frac{\partial}{\partial t}[\nabla \times \mathbf{C} + \nabla\phi]$$

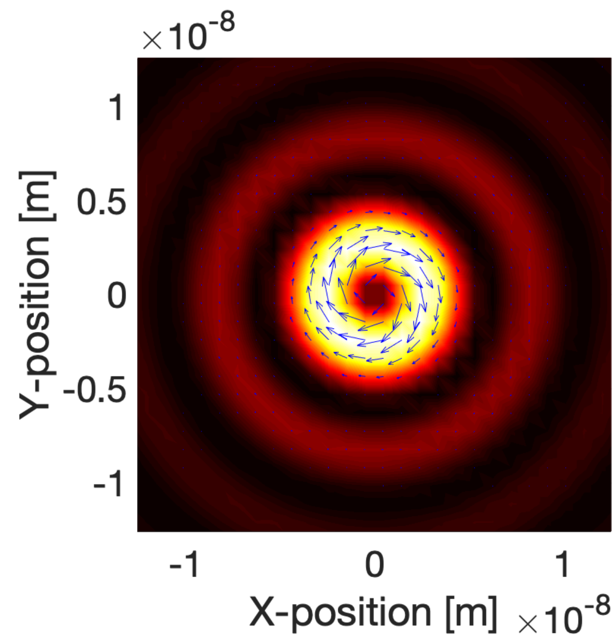
- Introduce **F** that satisfies: $\nabla \times \mathbf{F} = \mathbf{J}_{\text{rot}}$ where $\mathbf{J}_{\text{rot}}$ is the solenoidal part of current density

$$\nabla \times \nabla \times \mathbf{A} = \mu(\nabla \times \mathbf{F} + \mathbf{J_{con}}) + \mu\epsilon\frac{\partial}{\partial t}[\nabla \times \mathbf{C} + \nabla\phi$$

$$\nabla \times [\nabla \times \mathbf{A} - \mu\mathbf{F} - \mu\epsilon\frac{\partial}{\partial t}\mathbf{C}] = \mu\epsilon\nabla\phi + \mu\mathbf{J_{con}} = 0$$

$$\nabla \cdot \mathbf{A} = 0, \nabla \cdot \mathbf{C} = 0, \nabla \cdot \mathbf{F} = 0$$

$$\mu\epsilon\frac{\partial \mathbf{C}}{\partial t} = \nabla \times \mathbf{A} - \mu\mathbf{F}$$



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Dual Potential FDTD

- Final equation, take Div of:

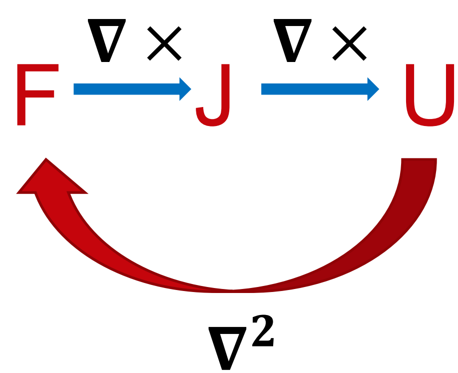
$$\nabla \times \nabla \times \mathbf{A} = \mu \mathbf{J} + \mu\epsilon \frac{\partial}{\partial t}[\nabla \times \mathbf{C} + \nabla \phi]$$

- We arrive at: $\nabla \cdot \mu \boldsymbol{J} = \frac{\partial}{\partial t} \nabla^2 \phi = \frac{\partial}{\partial t} \rho / \epsilon$

- Calculate $\boxed{\nabla \cdot \mu \boldsymbol{J} = \frac{\partial}{\partial t} \rho / \epsilon}$ and use a Poisson equation solver whenever ϕ is needed

- Poisson solver also used on $\mathbf{F}$ to solve (recall $\nabla \cdot \boldsymbol{F} = 0$):

$$\nabla \times \nabla \times \boldsymbol{F} = \nabla^2 \boldsymbol{F} = \nabla \times \boldsymbol{J} = \boldsymbol{U}$$

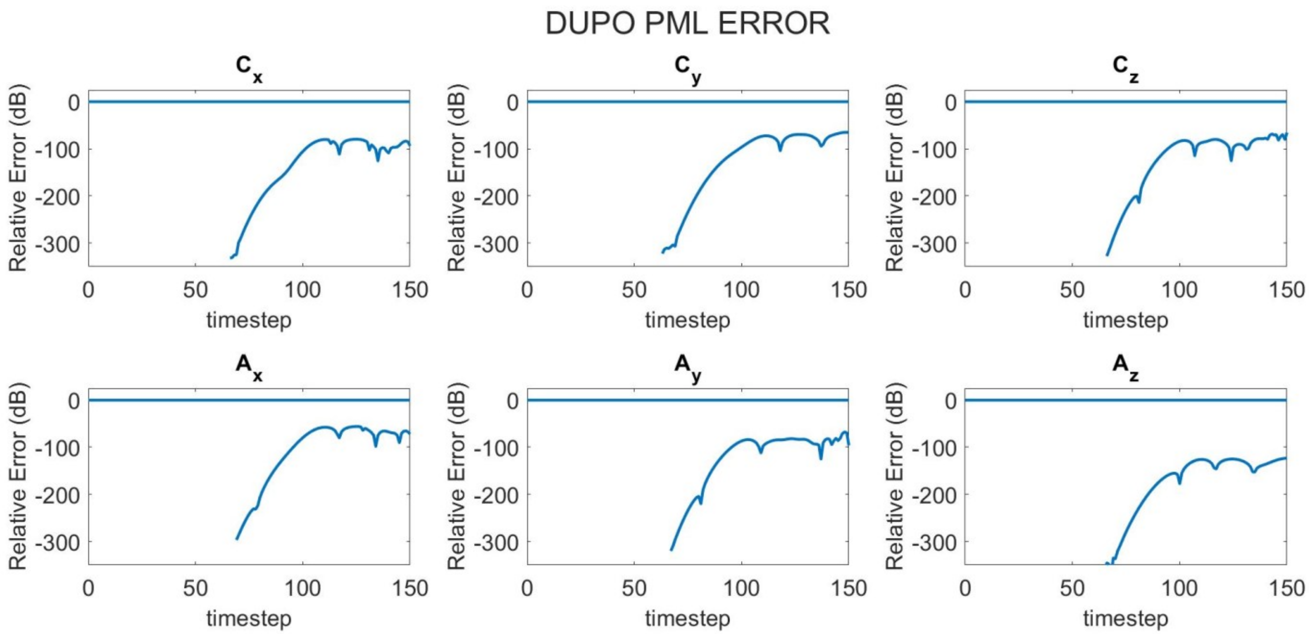


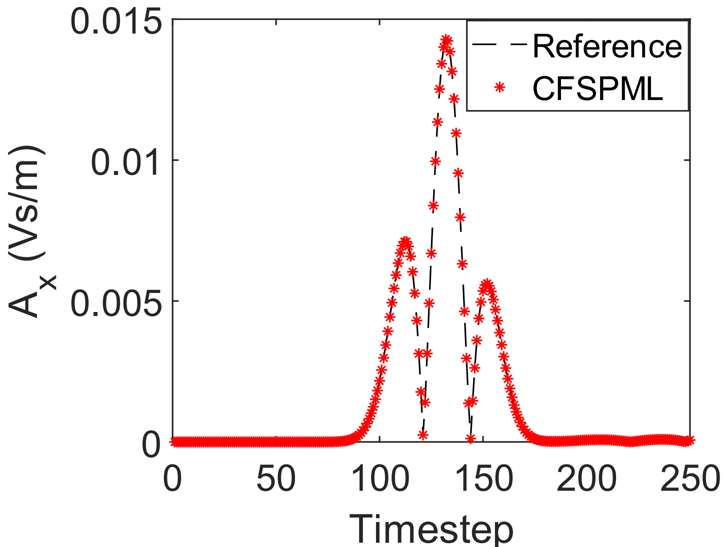
$$-\frac{\partial \mathbf{A}}{\partial t} = \nabla \times \mathbf{C}$$

$$\mu\epsilon \frac{\partial \mathbf{C}}{\partial t} = \nabla \times \mathbf{A} - \mu \mathbf{F}$$

$$\nabla \cdot \mu \boldsymbol{J} = \frac{\partial}{\partial t} \rho / \epsilon$$

PML Performance

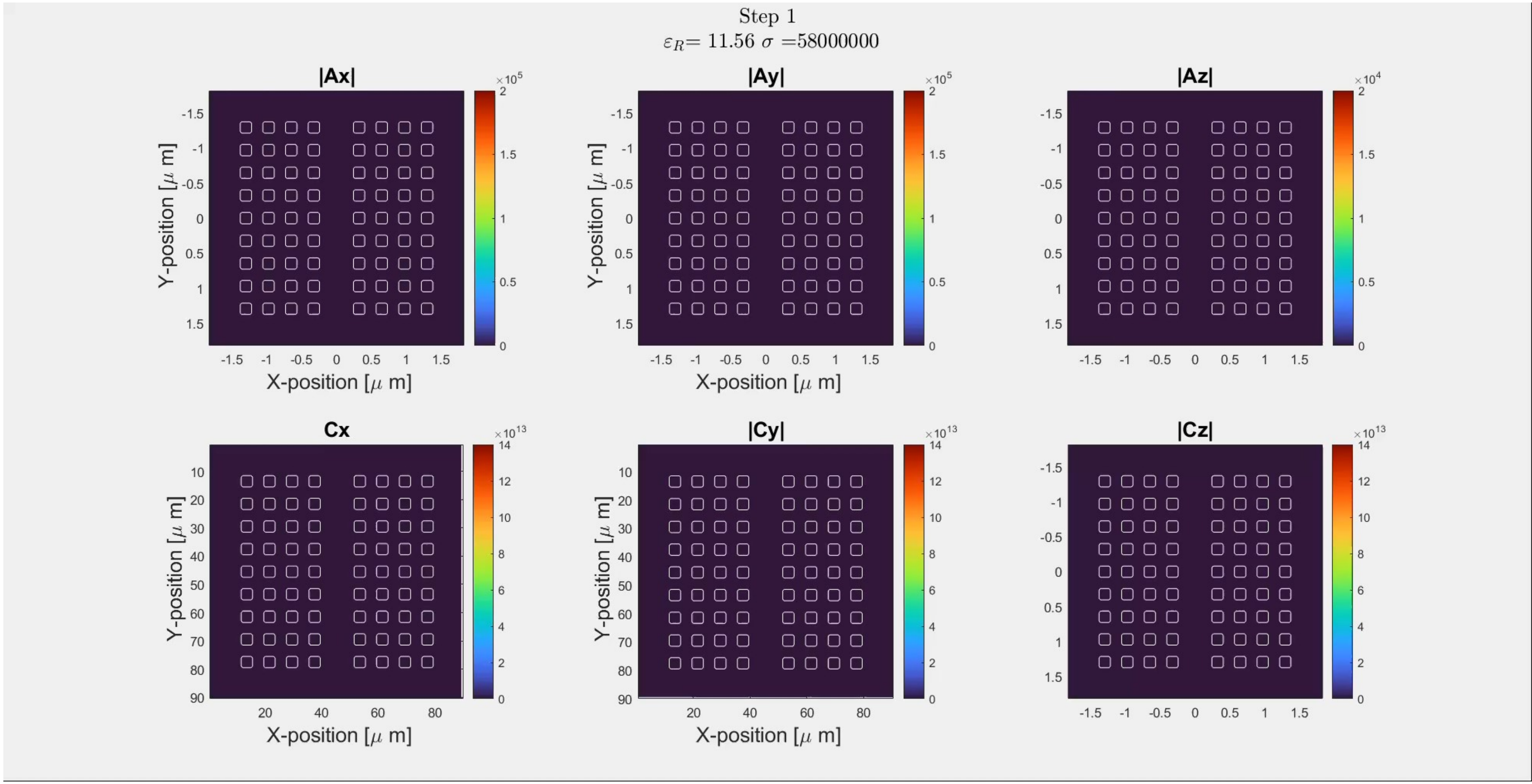




$$-\frac{\partial \mathbf{A}}{\partial t} = \nabla \times \mathbf{C}$$

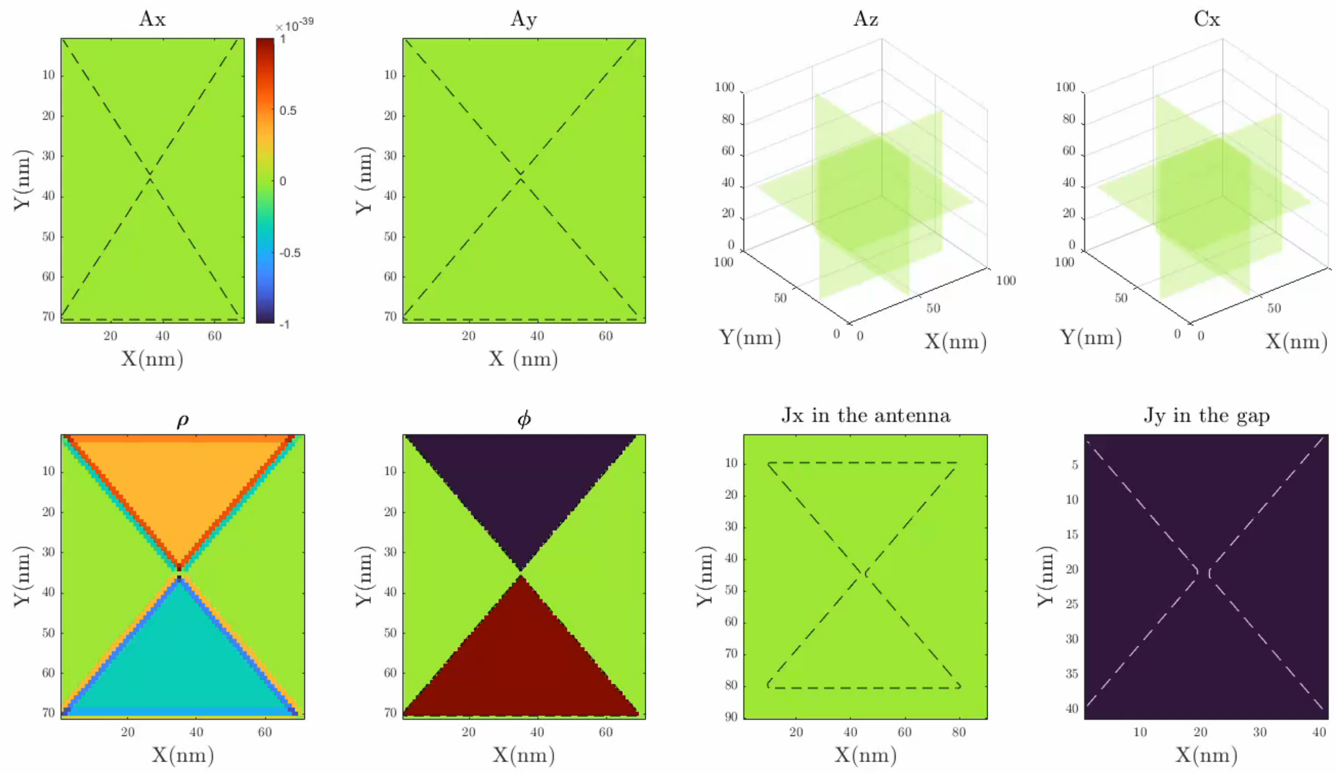
$$\mu\epsilon \frac{\partial \mathbf{C}}{\partial t} = \nabla \times \mathbf{A} - \mu \mathbf{F}$$

Example: Photonic Crystal



Coupling to Quantum Transport

- We have a unique ability to source with ϕ, calculate tunneling current, compute resulting potentials, self-consistently



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