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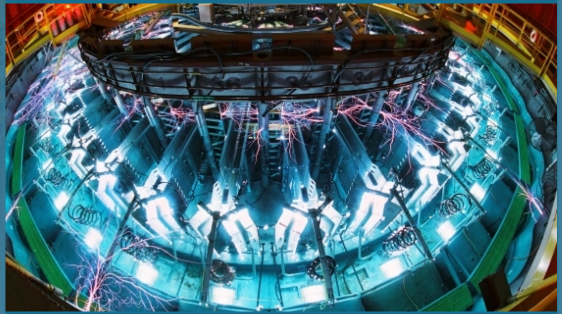
Deriving consistent surface fields for compatible FETD discretizations of Maxwell's equations



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Collaborators: Nicholas Roberds, Caleb Logemann, Ed Love, Eric C. Cyr**,** The Empire Team

Recent work
N. Roberds, D. McGregor, *"A transient near to far field transformation method and verification benchmarking procedure."* Submitted.

Initial idea
D. McGregor, et al. "*Variational, stable, and self-consistent coupling of 3D electromagnetics to 1D transmission lines in the time domain*," J. Comput. Phys., 2022**.**

Empire is a massively parallel, performance portable, plasma simulation code.

Electromagnetics: Unstructured, compatible FETD
Plasmas: PIC+DSMC (production), multi fluid-kinetic hybrid (research)

M. Bettencourt, et al. "*EMPIRE-PIC: A Performance Portable Unstructured Particle-In-Cell Code,*" Communications in Computational Physics, 2021.

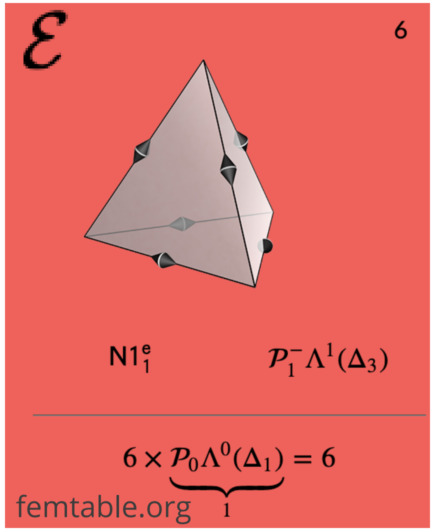
Discretization

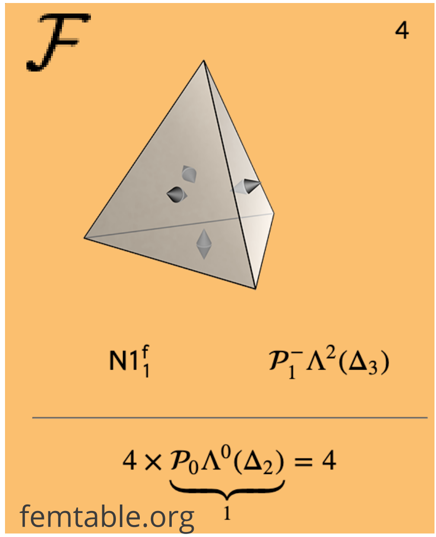
$$(\mathbf{E},\mathbf{B}) \in \mathcal{E} \times \mathcal{F}:$$

$$\begin{cases} \int_\Omega \epsilon \frac{\partial}{\partial t}\mathbf{E}\cdot\mathbf{\Psi} + \mathbf{J}\cdot\mathbf{\Psi} - \mu^{-1}\mathbf{B}\cdot\mathbf{curl}\ \mathbf{\Psi}\ dv = -\int_{\partial\Omega} \mathbf{H}\times\mathbf{n}\cdot\mathbf{\Psi}\ da, \\ \int_\Omega \frac{\partial}{\partial t}\mathbf{B}\cdot\mathbf{\Phi} + \mathbf{curl}\ \mathbf{E}\cdot\mathbf{\Phi}\ dv = 0 \end{cases}$$

$$\forall(\mathbf{\Psi},\mathbf{\Phi}) \in \mathcal{E}\times\mathcal{F}.$$

Temporal discretization for fields is a DIRK scheme





Lagrangian Kinematics for each particle

Accelerate uses the Boris Push (semi-implicit vxB)

We use a Verlet method to tie it all together:

$$\begin{cases} \mathbf{v}^{n+1/2} = \mathbf{v}^n + \frac{Q_i\Delta t}{2M_i}(\mathbf{E}^n + \mathbf{v}^{n+1/4}\times\mathbf{B}^n)|_{\mathbf{x}^n} \\ \mathbf{x}^{n+1} = \mathbf{x}^n + \Delta t\mathbf{v}^{n+1/2} \\ (\mathbf{E}^n,\mathbf{B}^n) \to (\mathbf{E}^{n+1},\mathbf{B}^{n+1}) \text{ using } \mathbf{J}^{n+1/2} \\ \mathbf{v}^{n+1} = \mathbf{v}^{n+1/2} + \frac{Q_i\Delta t}{2M_i}(\mathbf{E}^{n+1} + \mathbf{v}^{n+3/4}\times\mathbf{B}^{n+1})|_{\mathbf{x}^{n+1}} \end{cases}$$

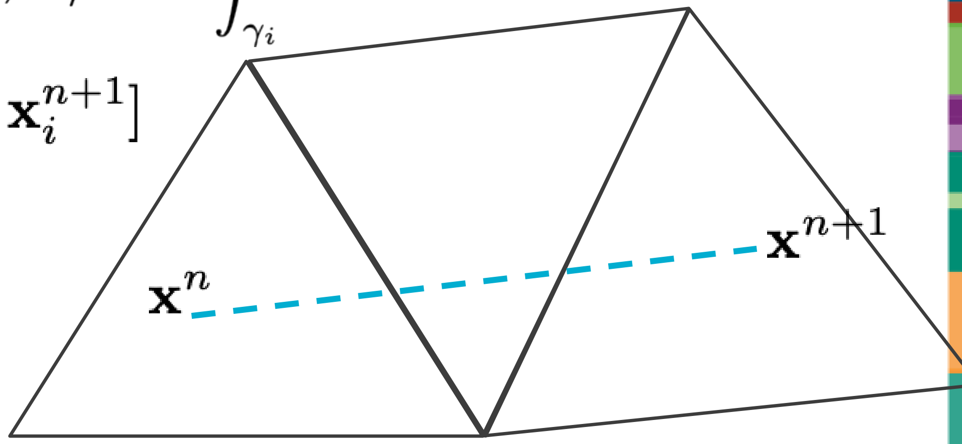
Neglecting special relativistic details which are complicated but not conceptually different

$$\mathbf{J} = \sum_i Q_i w_i \mathbf{v}_i :$$

$$\int_{t^n}^{t^{n+1}} \langle \mathbf{v}_i, \mathbf{\Psi}\rangle\ dt = \int_{\gamma_i} \mathbf{\Psi}\cdot ds$$

$$\gamma_i = [\mathbf{x}_i^n, \mathbf{x}_i^{n+1}]$$

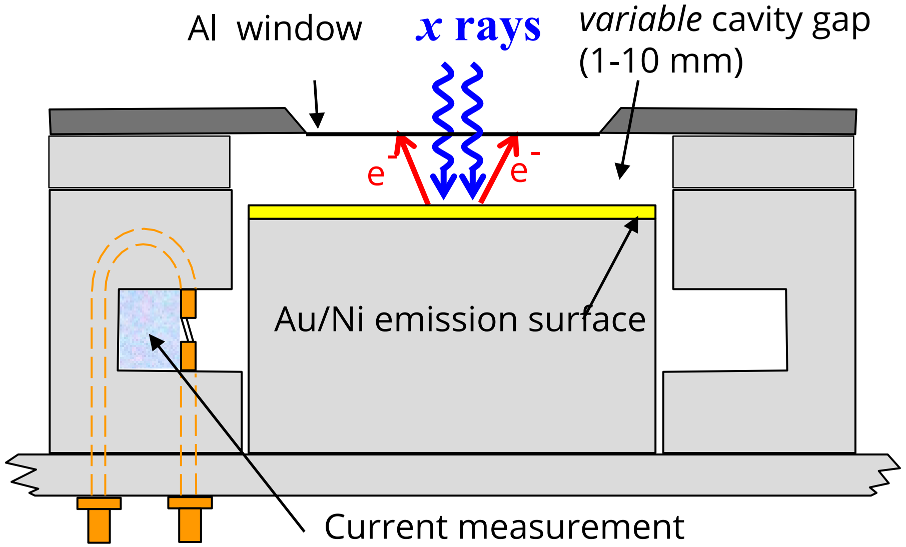
Provides Gauss' Law Involution

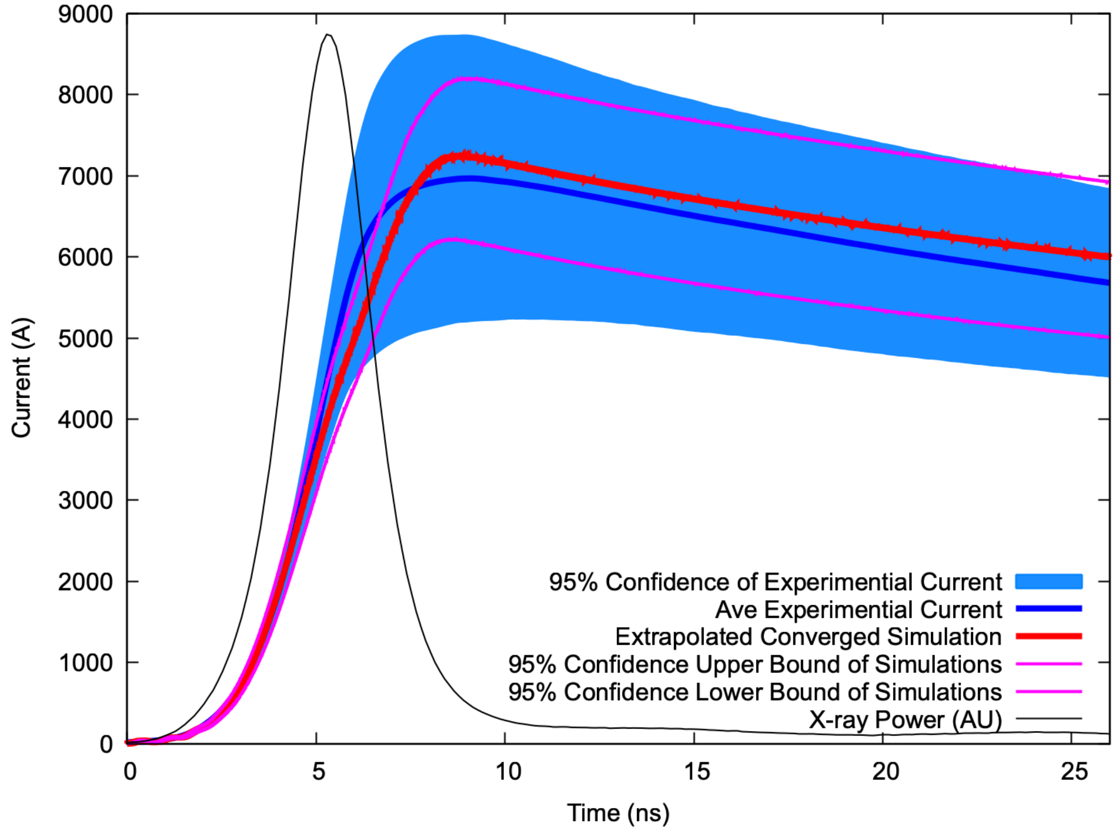


Villasenor and Buneman

Why PIC for plasmas

- Phase space is 6 –dimensional – its easier to put degrees of freedom only where you need them with particles than it is with continuum representation.
- It can agree well with experiments, even at moderate resolution.
- Plasma boundary conditions and chemistry are conceptually simple with a particle representation.





Conceptual Concerns

PIC currents could be very “rough”

- We should anticipate that solutions may not be smooth particularly if we are under resolving the particles.

First order accuracy in space

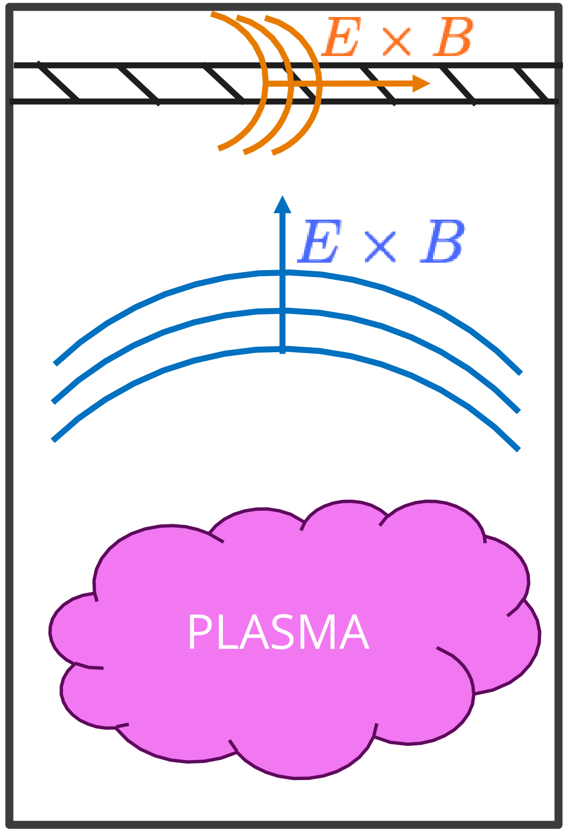
- Problems which are swept under the rug on a super-convergent cube mesh may be more obvious on unstructured tets at low resolutions.

Complex Geometry

- Primary motivation for simplex meshes. We typically mesh negative space and our geometries can have every sort pathology, e.g. reentrant corners.

I wouldn’t count on numerical solutions being “nice” in the way typically assumed in physical derivations particularly at low resolution.

An Example Problem:



You have a box containing a plasma and shielded cabling. Customer is concerned with how much energy could couple from the plasma to the cabling.

Simulate the plasma and characterize the energy coupled to the cable.

Assume we can model the plasma with adequate fidelity.

We are going to begin this problem trying the characterize current and charge on the surface of the cable.

Numerical Method Question:
Can I derive a surface current on a boundary from a numerical solution of Maxwell's equations?

Design Principals

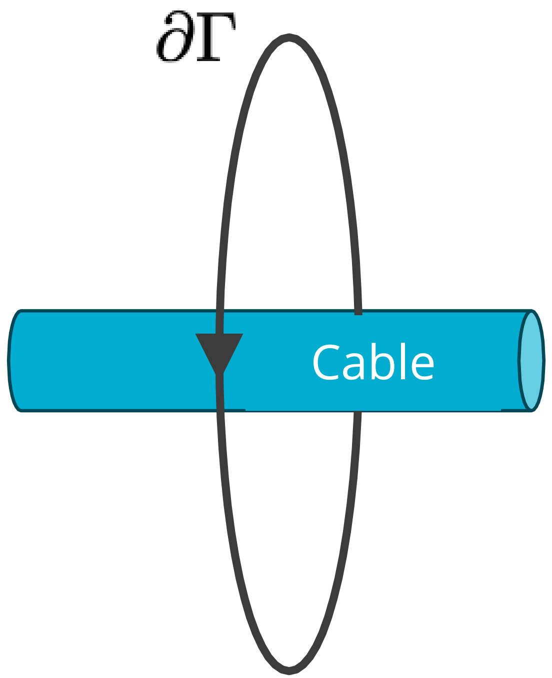
Derived variables should be

- Be robust and simple to use
  - It should work even when solutions “are not nice”
- Have a theory of convergence
  - Hard for EM-PIC so we typically relax to say “for EM only”

My qualitative design philosophy:
Methods that “fit together nicely” have a tendency to work.

How do we compute the current on the surface of the cable?

The E&M Method



$$\text{PEC and } \mathbf{D} = \epsilon \mathbf{E} \text{ and } \partial\Gamma \to \partial(\text{cable}) \implies \mathbf{D} \to 0$$

$$\int_\Gamma \left(\frac{\partial}{\partial t}\mathbf{D} + \mathbf{J}\right) \cdot d\mathbf{a} = \oint_{\partial\Gamma} \mathbf{H} \cdot d\ell$$

If the loop is close enough to the boundary the HdL will recover the total current flowing along the surface of the cable.

Pro
- Analysts think this way
- Validation evidence

Con
- Convergence is not obvious.
- Can only give total current (not current density)
- Can't generalize to an interface

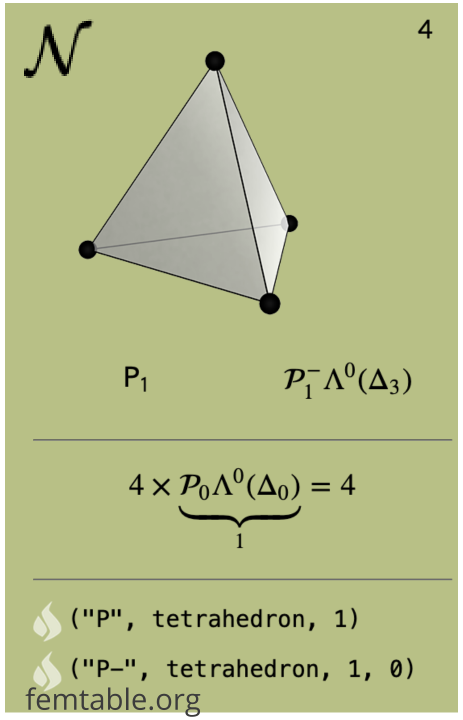
How do we compute the current on the surface of the cable?

A Projection Method

$\mathbf{H} \times \mathbf{n}$ on the surface is the surface current
$\mathbf{B} \cdot \mathbf{n}$ is the degree of freedom we current we have on the surface

$$\mathbf{H}_{\mathcal{N}} \in \mathcal{N}^3 : \int_\Omega \mathbf{H}_{\mathcal{N}} \varphi \, dV = \int_\Omega \mu^{-1} \mathbf{B} \varphi \, dV, \quad \forall \varphi \in \mathcal{N}$$

Mass lumping the projection operator recovers a nodal reconstruction operator on a structured grid which is popular in structured PIC because it cancels self force.



Pros

- Recovers the right magnetic field components on the surface of interest
- Easy to generalize to internal interfaces

Cons

- $\mathbf{H}(\text{div}) \cap \mathbf{H}(\textbf{curl}) \not< \mathbf{H}^1$
  Not clear that this will converge in general
- Noise concerns

How do we compute the current on the surface of the cable?

Dirichlet-to-Neumann Map

Consider a general Dirichlet condition
It's a linear constraint on the electric field – consider Saddle-Point system

$$(\mathbf{E}, \mathbf{B}, \mathbf{H}_\partial) \in \mathbf{H}(\mathbf{curl}) \times \mathbf{H}(\mathrm{div}) \times \mathbf{H}^{-1/2}(\mathrm{curl}, \partial\Omega) :$$

$$\begin{cases} \int_\Omega \epsilon \frac{\partial}{\partial t}\mathbf{E} \cdot \mathbf{\Psi} + \mathbf{J} \cdot \mathbf{\Psi} - \mu^{-1}\mathbf{B} \cdot \mathbf{curl}\ \mathbf{\Psi}\ dv - \langle \gamma_\tau(\mathbf{\Psi}), \mathbf{H}_\partial \rangle_\partial = 0, \\ \int_\Omega \frac{\partial}{\partial t}\mathbf{B} \cdot \mathbf{\Phi} + \mathbf{curl}\ \mathbf{E} \cdot \mathbf{\Phi}\ dv = 0 \\ \langle \gamma_\tau(\mathbf{E}), \boldsymbol{\psi} \rangle_\partial = \langle \mathbf{K}, \boldsymbol{\psi} \rangle_\partial \end{cases}$$

$$\forall (\mathbf{\Psi}, \mathbf{\Phi}, \boldsymbol{\psi}) \in \mathbf{H}(\mathbf{curl}) \times \mathbf{H}(\mathrm{div}) \times \mathbf{H}^{-1/2}(\mathrm{curl}, \partial\Omega).$$

Using notions of Buffa (2002)

Tangent Trace

$$\gamma_\tau : \mathbf{H}(\mathbf{curl}, \Omega) \to \mathbf{H}^{-1/2}(\mathrm{div}, \partial\Omega)$$

Boundary Duality Pairing

$$\langle \cdot, \cdot \rangle_\partial : \mathbf{H}^{-1/2}(\mathrm{div}, \partial\Omega) \times \mathbf{H}^{-1/2}(\mathrm{curl}, \partial\Omega) \to \mathbb{R}$$

Surface currents relax the Dirichlet constraint

How do we solve this system?

Dirichlet-to-Neumann Map: Null-Space Method

γ_τ has a well characterized null-space $\mathbf{H}_0(\mathbf{curl})$

Apply the null-space method!

$$\mathbf{E} = \mathbf{E}_0 + \mathbf{E}_\partial, \mathbf{E}_0 \in \mathbf{H}_0(\mathbf{curl}), \mathbf{E}_\partial \in \mathbf{H}(\mathbf{curl}) \cap (\mathbf{H}_0(\mathbf{curl}))^\perp$$

Solve for the lift:

$$\mathbf{E}_\partial \in \mathbf{H}(\mathbf{curl}) \cap (\mathbf{H}_0(\mathbf{curl}))^\perp : \langle \gamma_\tau(\mathbf{E}_\partial), \boldsymbol{\psi} \rangle_\partial = \langle \mathbf{K}, \boldsymbol{\psi} \rangle_\partial, \forall \boldsymbol{\psi} \in \mathbf{H}^{-1/2}(\text{curl}, \partial\Omega)$$

Solve for the volumetric response:

$$(\mathbf{E}_0, \mathbf{B}) \in \mathbf{H}_0(\mathbf{curl}) \times \mathbf{H}(\text{div}) :$$

$$\begin{cases} \int_\Omega \epsilon \frac{\partial}{\partial t}(\mathbf{E}_\partial + \mathbf{E}_0) \cdot \boldsymbol{\Psi} + \mathbf{J} \cdot \boldsymbol{\Psi} - \mu^{-1} \mathbf{B} \cdot \mathbf{curl}\ \boldsymbol{\Psi}\ dv = 0, \\ \int_\Omega \frac{\partial}{\partial t} \mathbf{B} \cdot \boldsymbol{\Phi} + \mathbf{curl}\ (\mathbf{E}_0 + \mathbf{E}_\partial) \cdot \boldsymbol{\Phi}\ dv = 0 \end{cases}$$

$$\forall (\boldsymbol{\Psi}, \boldsymbol{\Phi}, \boldsymbol{\psi}) \in \mathbf{H}_0(\mathbf{curl}) \times \mathbf{H}(\text{div}).$$

Perform Lagrange multiplier recovery:

$$\mathbf{H}_\partial \in \mathbf{H}^{-1/2}(\text{curl}, \partial\Omega) :$$

$$\langle \gamma_\tau(\boldsymbol{\Psi}), \mathbf{H}_\partial \rangle_\partial = \int_\Omega \epsilon \frac{\partial}{\partial t} \mathbf{E} \cdot \boldsymbol{\Psi} + \mathbf{J} \cdot \boldsymbol{\Psi} - \mu^{-1} \mathbf{B} \cdot \mathbf{curl} \boldsymbol{\Psi}\ dV,$$

$$\forall \boldsymbol{\Psi} \in \mathbf{H}(\mathbf{curl}) \cap (\mathbf{H}_0(\mathbf{curl}))^\perp$$

Dirichlet-to-Neumann Map: Discretization

- We don't have to change anything about our time-stepping or discretization of space for solving for **E** and **B**.
- Each timestep we recover the surface current:

$$\text{Given } (\mathbf{E}, \mathbf{B}, \mathbf{J}) :$$

$$\mathbf{H}_\partial \times \mathbf{n} \in \mathcal{E}_\partial : \int \mathbf{H}_\partial \times \mathbf{n} \cdot \mathbf{\Psi} \; da = -\int_\Omega \epsilon \frac{\partial}{\partial t}\mathbf{E} \cdot \mathbf{\Psi} + \mathbf{J} \cdot \mathbf{\Psi} - \mu^{-1}\mathbf{B} \cdot \mathbf{curl}\mathbf{\Psi} \; dV, \qquad \forall \mathbf{\Psi} \in \mathcal{E}_\partial$$

$\mathcal{E}_\partial$ is the set of edge functions which have non-zero degrees of freedom only on the boundary.

Pros

- Derived from the variational theory
- Recovers the surface current density
- Easy to generalize to non-homogeneous or more general BCs and internal interfaces

Cons

- We haven't formally proven convergence just devised something that looks plausible.
  - **Is it really appropriate to discretize the surface current density on boundary edges?**

Application: Time Domain Near-to-Far-Field Transformation

N. Roberds (SNL) formulated NtF in time domain.
His request: Surface fields on an interface

Far Fields in terms of vector potentials

$$\boldsymbol{E}(\boldsymbol{x},t) = \hat{\boldsymbol{r}} \times \left(\hat{\boldsymbol{r}} \times \dot{\boldsymbol{A}}(\boldsymbol{x},t)\right) + \eta \hat{\boldsymbol{r}} \times \dot{\boldsymbol{F}}(\boldsymbol{x},t)$$

$$\boldsymbol{H}(\boldsymbol{x},t) = \hat{\boldsymbol{r}} \times \left(\hat{\boldsymbol{r}} \times \dot{\boldsymbol{F}}(\boldsymbol{x},t)\right) - \frac{1}{\eta} \hat{\boldsymbol{r}} \times \dot{\boldsymbol{A}}(\boldsymbol{x},t)$$

Potentials in terms of surface fields

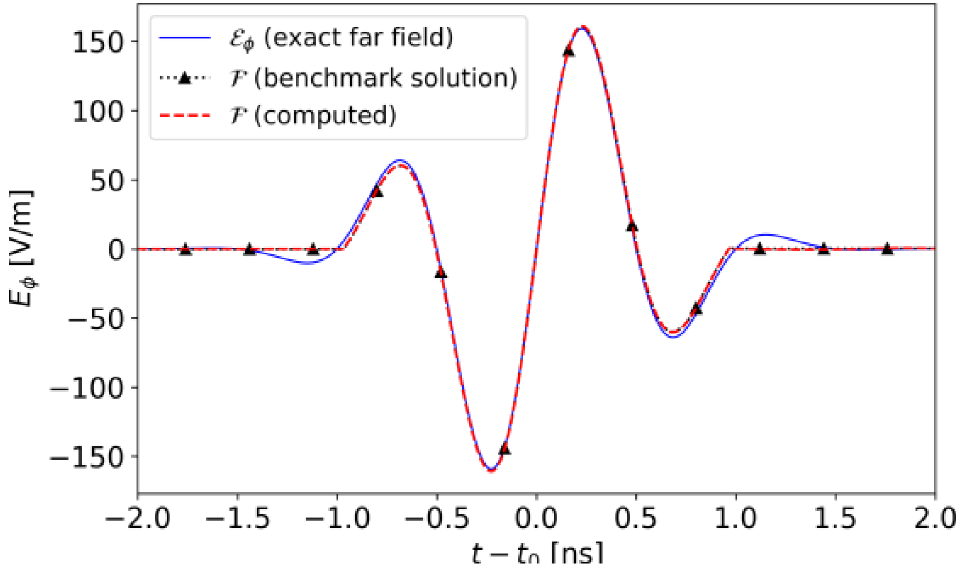
$$\mathbf{A}(\mathbf{x},t) = \frac{\mu}{4\pi r} \int_{\partial\Omega} \mathbf{n} \times \mathbf{H}(\mathbf{x}', s(\mathbf{x}',\mathbf{x},t))\ d\mathbf{x}',$$

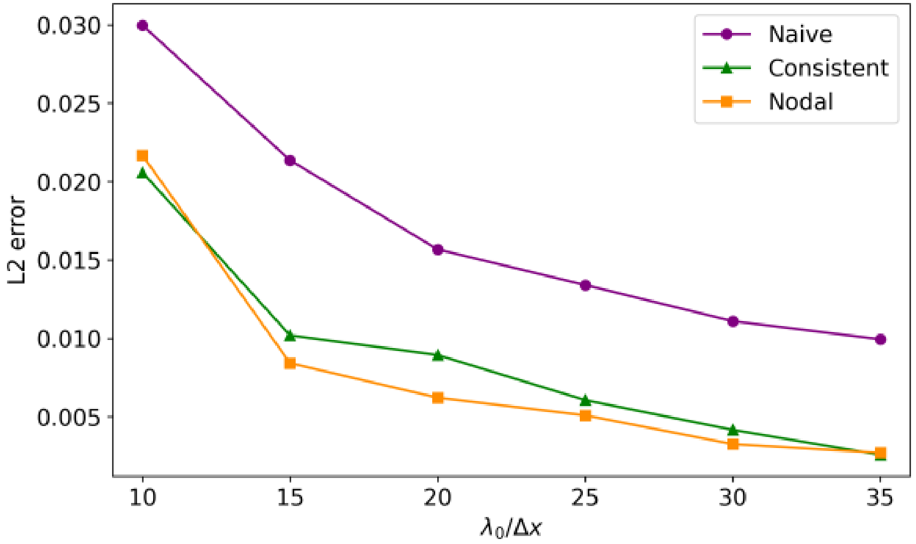
$$\mathbf{F}(\mathbf{x},t) = \frac{\epsilon}{4\pi r} \int_{\partial\Omega} \mathbf{E}(\mathbf{x}', s(\mathbf{x}',\mathbf{x},t)) \times \mathbf{n}\ d\mathbf{x}',$$

$$s = t - \frac{r - \mathbf{x}' \cdot \mathbf{r}}{c}$$

$$\mathbf{r} = \frac{\mathbf{x}}{|\mathbf{x}|}, \quad r = |\mathbf{r}|$$

DtN used method for computing Hxn





Nodal and D2N comparable **but** the test problem has a smooth solution

Closure

- Creating derived variables which "stay inside the guardrails" of convergence theory is an interesting problem with real applications and a multi-disciplinary team.
  - You have to translate questions and arguments between different disciplinary languages.
- Carrying theory over the finish line is a challenge in application setting.
  - Opportunity for academic collaborations.
- NtF test problem DtN and nodal projection performing comparably – exact solution was infinitely smooth and domain was a cube!
  - **Creating verification problems which highlight real pathologies is hard.**
- Future work
  - What to do about surface charge ($\mathbf{D} \cdot \mathbf{n}$)

References

A. Buffa, M. Costabel, D. Sheen, (2002), "*On traces for H(curl,Ω) in Lipschitz domains*", Journal of Mathematical Analysis and Applications, 2002.

N. Roberds, D. McGregor, *"A transient near to far field transformation method and verification benchmarking procedure."* Submitted.

D. McGregor, et al. "*Variational, stable, and self-consistent coupling of 3D electromagnetics to 1D transmission lines in the time domain*," J. Comput. Phys., 2022.