RF computations: Needs in performance, capability, and optimization

(John Cary
Acknowledgments: Greg Werner, Ilya Zilberter, Slava Yakovlev,
Frank Marhauser, Gennady Morozov, Haipeng Wang)
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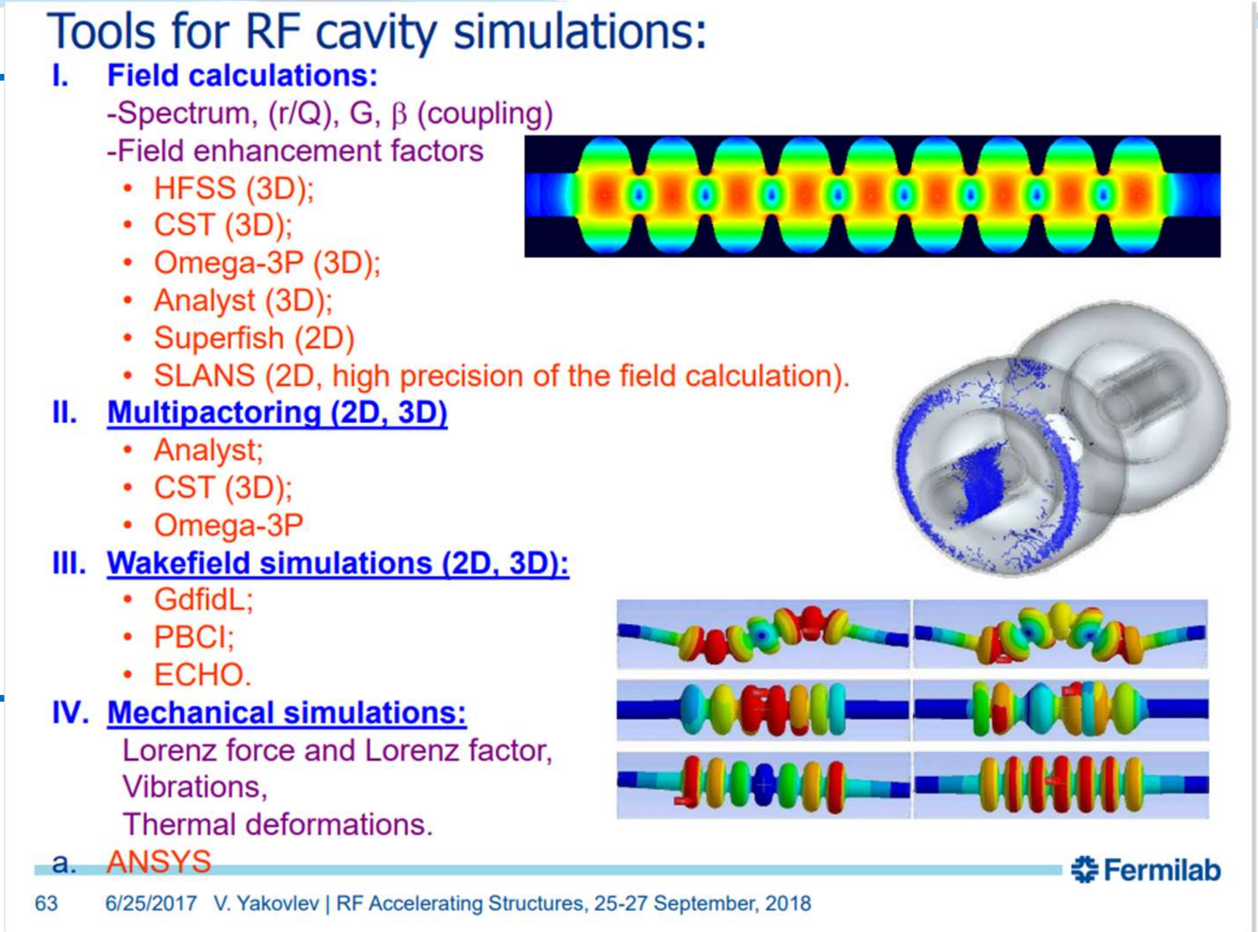
Existing capabilities
Performance Needs
Capability Needs
Optimization Needs

V. Yakovlev, “RF accelerating structures”, PHY863, MSU, 2018092[5-7]
Gennady Romanov, “Multipactor simulations at FNAL with CST Particle Studio”, PIP-II Workshop, 20201203

Many tools for SRF cavity modeling. Why?

Concentrate on EM plus charged particles, same time scales



Tools for RF cavity simulations:

I. Field calculations:

-Spectrum, (r/Q), G, β (coupling)

-Field enhancement factors

- HFSS (3D);
- CST (3D);
- Omega-3P (3D);
- Analyst (3D);
- Superfish (2D)
- SLANS (2D, high precision of the field calculation).

II. Multipactoring (2D, 3D)

- Analyst;
- CST (3D);
- Omega-3P

III. Wakefield simulations (2D, 3D):

- GdfidL;
- PBCI;
- ECHO.

IV. Mechanical simulations:

Lorenz force and Lorenz factor,
Vibrations,
Thermal deformations.

a. ANSYS

Fermilab

63 6/25/2017 V. Yakovlev | RF Accelerating Structures, 25-27 September, 2018

Many other codes

- VSim
- Michelle
- COMSOL
- Emphasis
- CONPIC

Different codes have different strengths (not exhaustive list), but there are associated costs

- Surface fields are accurate in unstructured mesh codes
  - HFSS
  - Analyst
  - Omega-3p
- Self-consistent modeling is fast in structured mesh codes
  - CST PIC
  - VSim
- Accurate short-range wakefields need moving window (Gdfidl) or to solve for many (1000s) of modes (VSim)
- Commercial codes have ease of use
  - HFSS
  - CST
  - VSim

Costs

- Requires learning many different codes
  - Interfaces
  - How to interpret output

- Requires benchmarking the many different codes
- Requires paying for the many different codes

Recent algorithmic discoveries reduce cost and effort!

Multipacting

Wakefields

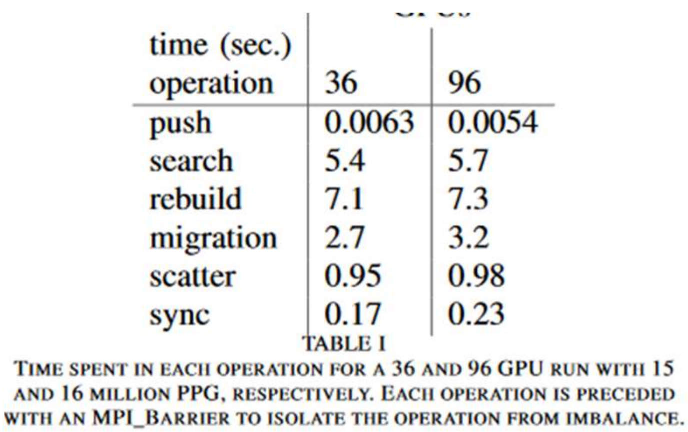
Optimization

Multipacting requires multiple solvers even when within one toolset

- G Romanov, “Fermilab … in 2009 we switched completely to (CST) Particle in Cell solver”
  - Pros: …, space-charge effects, …, user-friendly interface
  - Cons:
    - …
    - Rectangular mesh in PIC solver
    - Imported field interpolation each time amplitude changes - computationally expensive
- Space charge effects important, but
- Need unstructured mesh to get accurate fields?

Two modes of simulation

1. Import fields, track particles
2. Solve for fields in code self-consistently



time (sec.) operation	36	96
push	0.0063	0.0054
search	5.4	5.7
rebuild	7.1	7.3
migration	2.7	3.2
scatter	0.95	0.98
sync	0.17	0.23

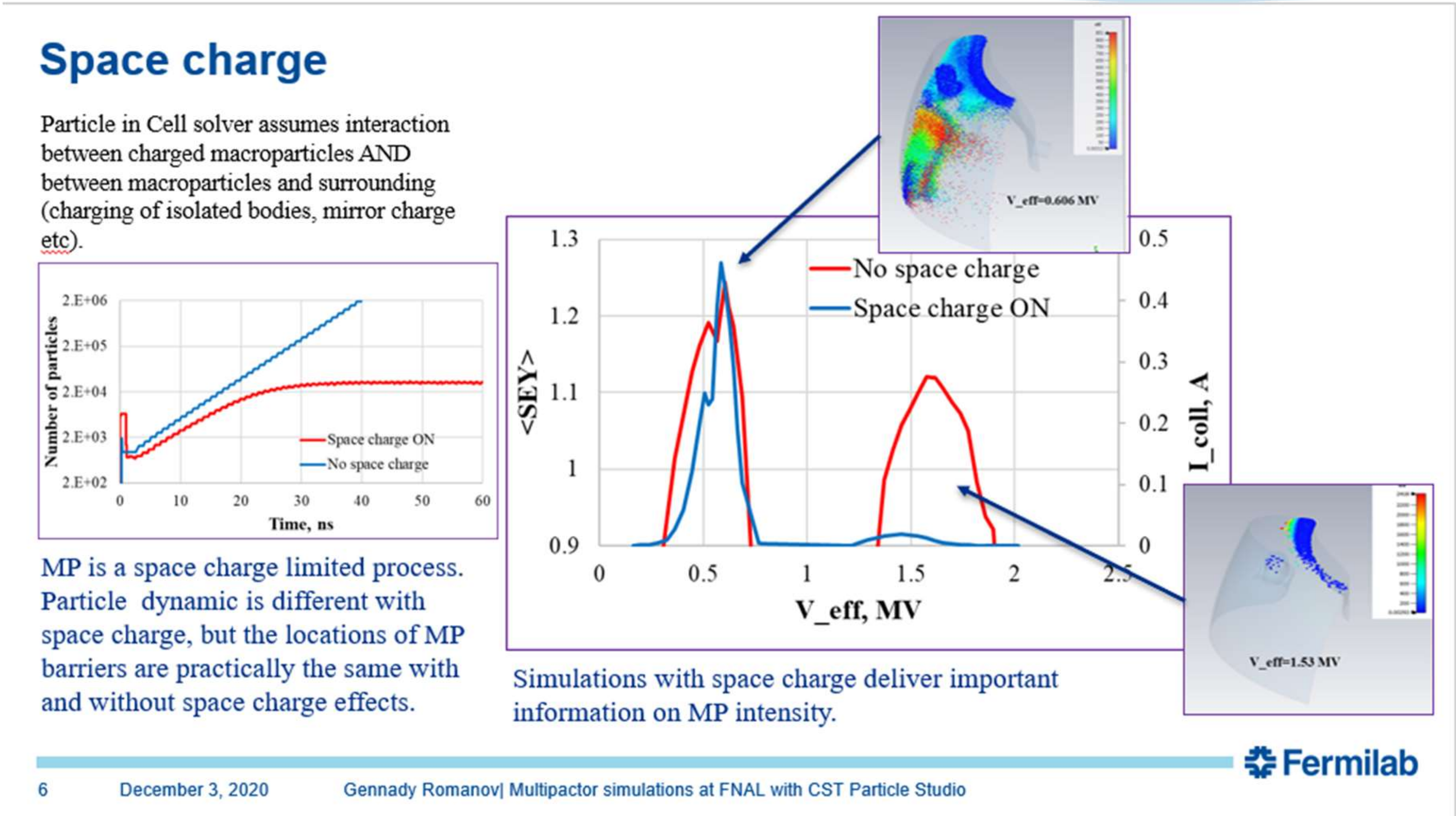
TABLE I

TIME SPENT IN EACH OPERATION FOR A 36 AND 96 GPU RUN WITH 15 AND 16 MILLION PPG, RESPECTIVELY. EACH OPERATION IS PRECEDED WITH AN MPI_BARRIER TO ISOLATE THE OPERATION FROM IMBALANCE.

Example: unstructured mesh PIC ~ 15x time for push and scatter

Given desire to use structured mesh PIC solver (for speed), how to get accuracy?

Space charge is important for Multipactor limiting



Space charge

Particle in Cell solver assumes interaction between charged macroparticles AND between macroparticles and surrounding (charging of isolated bodies, mirror charge etc).

MP is a space charge limited process. Particle dynamic is different with space charge, but the locations of MP barriers are practically the same with and without space charge effects.

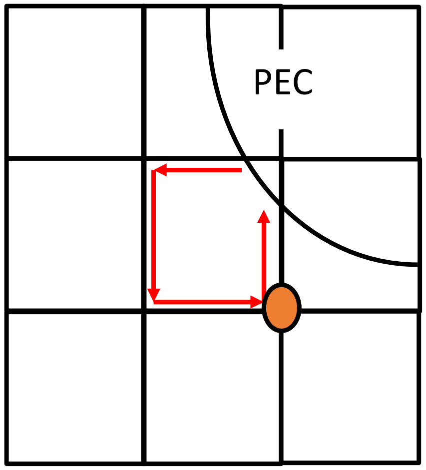
Simulations with space charge deliver important information on MP intensity.

6 December 3, 2020 Gennady Romanov| Multipactor simulations at FNAL with CST Particle Studio

Fermilab

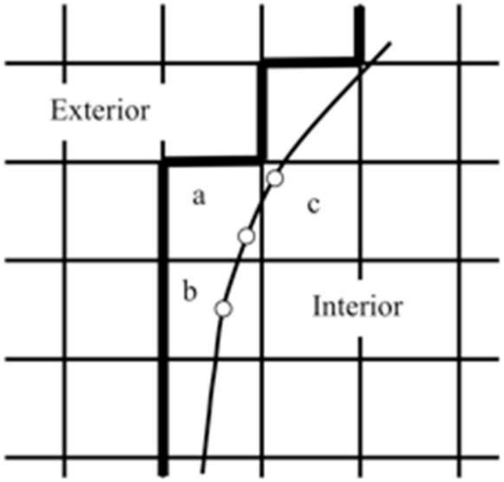
Cut-cell FDTD (VSim, CST) gives global quantities accurately

- Origin is use of cut cells



Modify magnetic update for cells cut by boundary

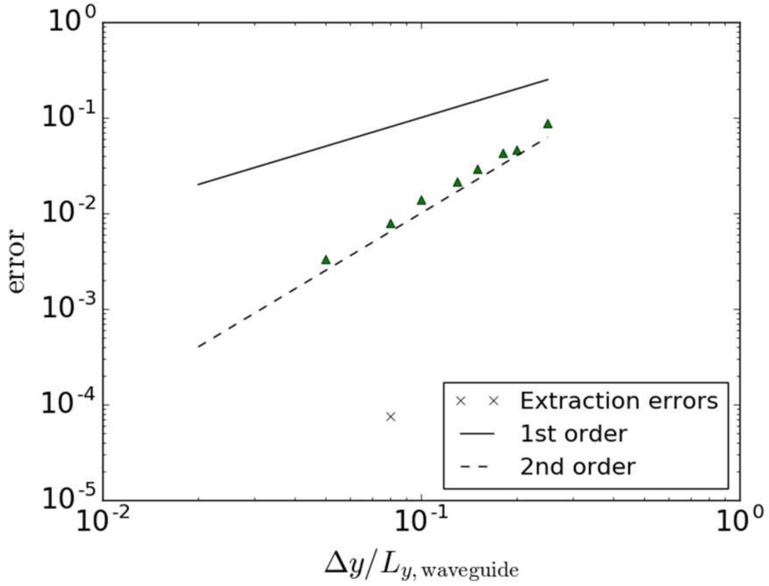
$$\frac{\Delta B}{\Delta t} = \frac{\Delta \varphi_M}{A \Delta t} = \frac{1}{A \Delta t} \sum l_i E_i$$



Small area ⇒ large coefficient ⇒ unstable

Drop minimal number of faces

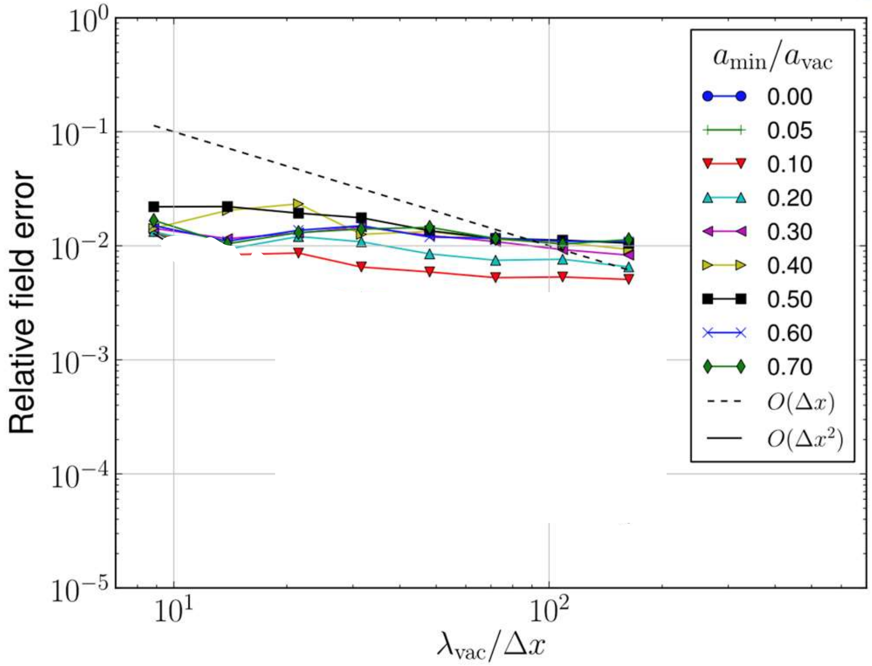
O(1) error locally:



2nd order error globally

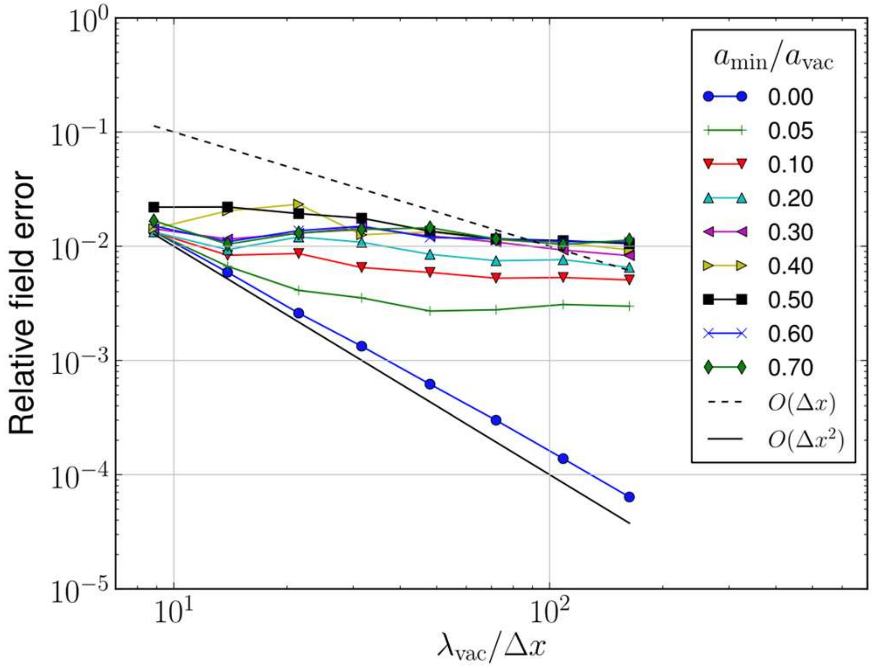
https://doi.org/10.1016/j.jcp.2009.07.025

But near-surface fields do not converge



- Fields from 3 cells in
- https://doi.org/10.1016/j.jcp.2010.12.005

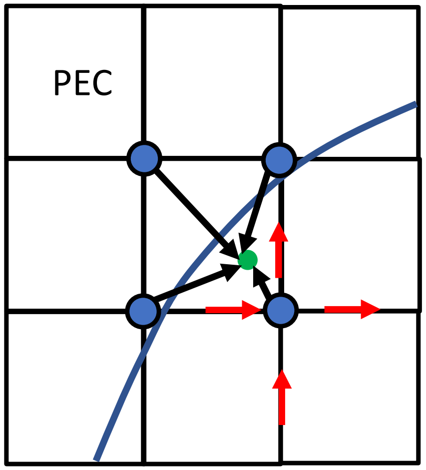
Near-surface fields found accurately with implicit solve



- Fields from 3 cells in
- https://doi.org/10.1016/j.jcp.2010.12.005

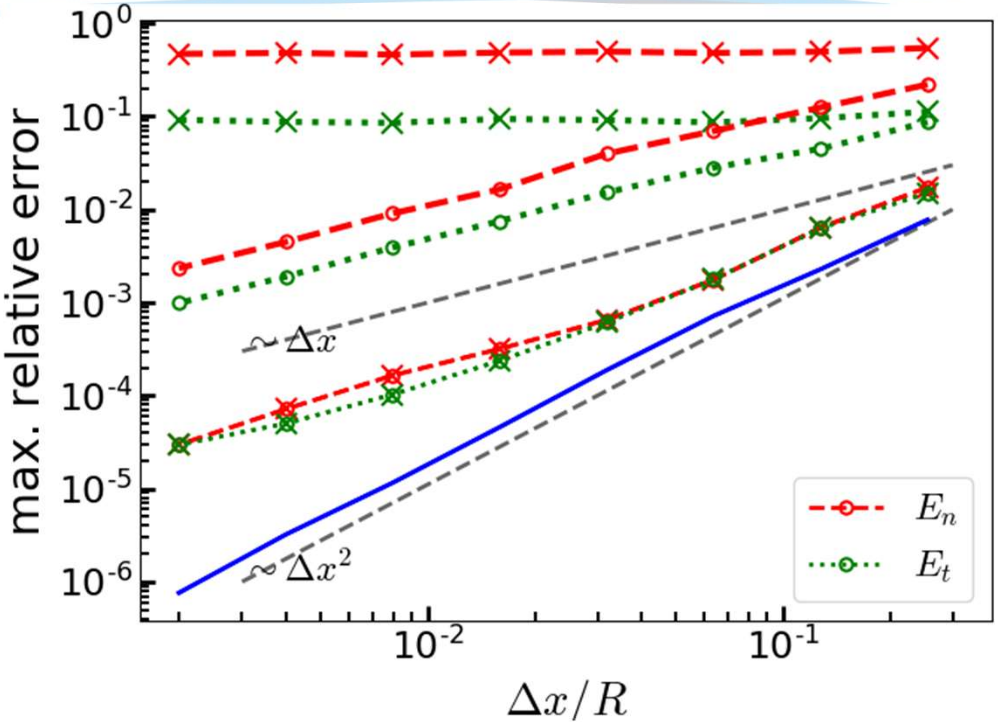
- Time step reduction removed with implicit solve - no net computational increase over explicit?
- Can one do implicit only over boundary?

Surface fields in EMPIC suffer from basic incompatibility



- Fields solved on interior edges
- Fields averaged to nodes
- Nodes interpolated to particle position
- O(1) error to neglect exterior nodes (or edges or …)
- How to get field at exterior node? (extrapolation)

Proper extrapolation gives accurate edge fields



- With extrapolated nodal fields from a cut-cell electrostatic simulation.
- Research needed for EM

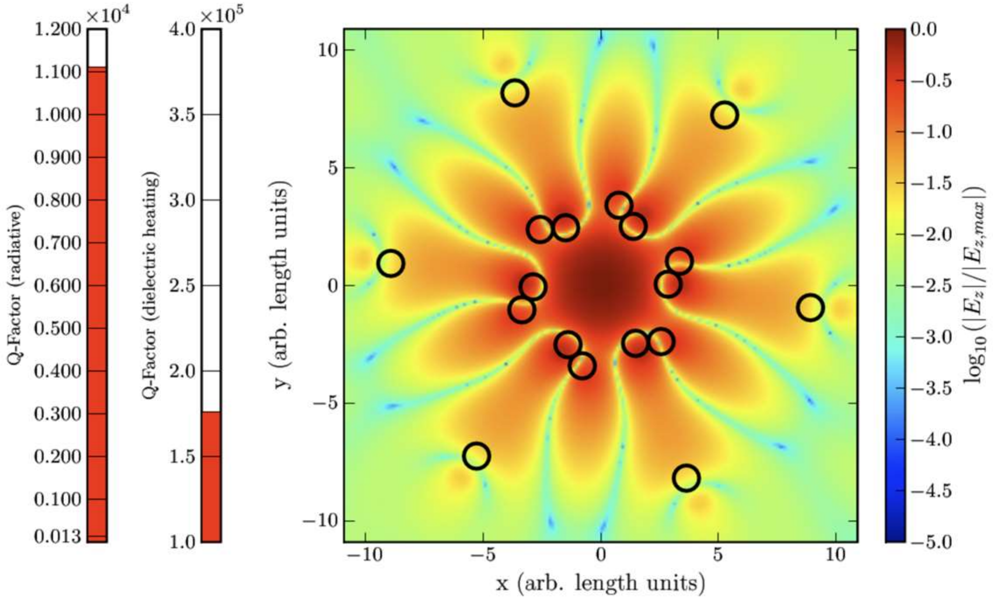
- Possible to have desired EMPIC with accurate edge fields
- Need: remove edge field error from consideration with higher-order extrapolation?

Wakefield calculations: commercial not keeping up

- Moving window – why one more piece of software?
  - Gdfidl (http://www.gdfidl.de/): used by FNAL. Accurate, but
    - no particles
    - only Linux
  - ABCI (https://abci.kek.jp/abci.htm): no MPI parallelism, no customer support
  - Echo (https://echo4d.de/): is being used for USPAS.
- Sum of modes
  - Need rapid computations of ~1000 modes.
  - Filter diagonalization? https://doi.org/10.1016/j.jcp.2008.01.040

Can we bring new tools to optimization?

- ./2018CaryICOPS/mov/PhcOptSymNoOverlapLabeled.mov
- Numerical optimization can lead to the unexpected

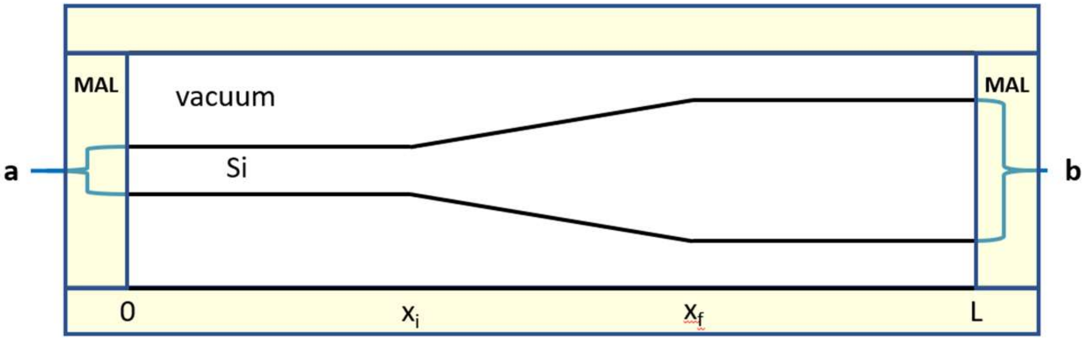


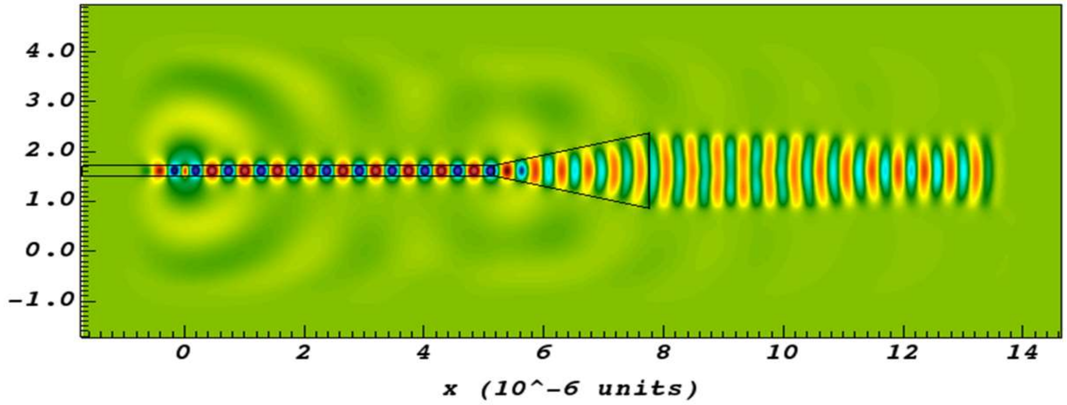
1. get close
2. converge

Adjoint computations - new approach to getting derivatives

- Forward solve gives current solution
- Backward solve with functional derivative with merit function
- Inner product gives derivatives
- Derivatives compute step change, give new system
- Rinse and repeat as necessary

Mode matching needed in photonics





- Incoming mode of small waveguide
- Couples into multiple modes of larger waveguide
- Want a single outgoing mode, g(x)h(y)
- Minimize

$$T = \int dy \left| \frac{\partial^2 D_z}{\partial x \partial y} \right|^2$$

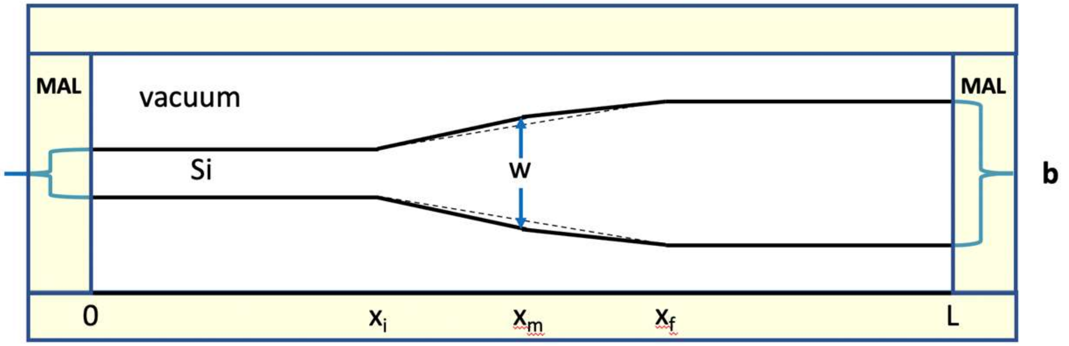
Adjoint methodology:

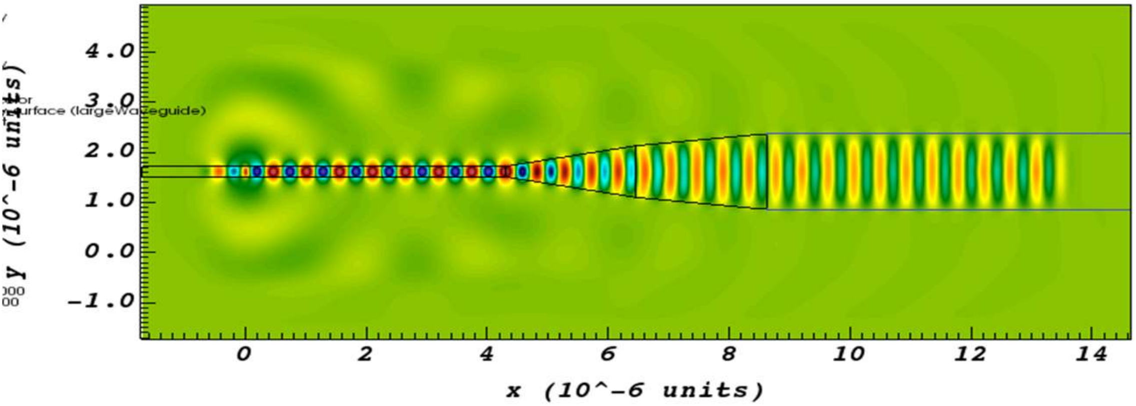
- Integrate adjoint equation (same for Maxwell)
- With source = functional derivative of goal
- Then take inner product with derivative of dynamical operator

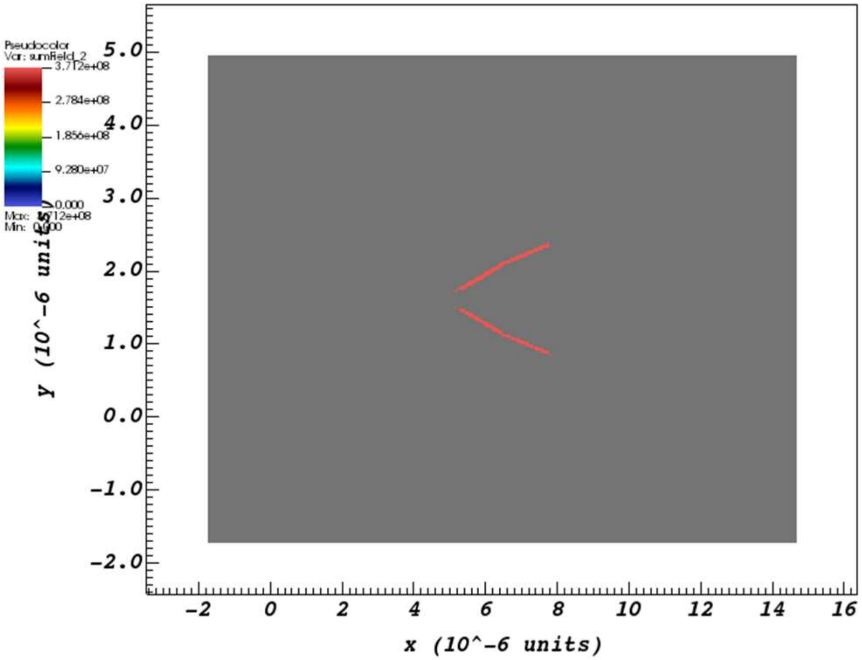
$$\mathrm{T} = \int dy \left| \frac{\partial^2 D_z}{\partial x \partial y} \right|^2 \qquad \frac{\partial T}{\partial D_z} = \frac{\partial^4 D_z}{\partial x^2 \partial y^2}$$

$$\frac{\partial T}{\partial p_k} = \omega^2 \int dV \mathbf{D}_A \cdot \frac{\partial \varepsilon^{-1}}{\partial p_k} \cdot \mathbf{D}$$

Mode matching shows location of inner product; better solution obtained



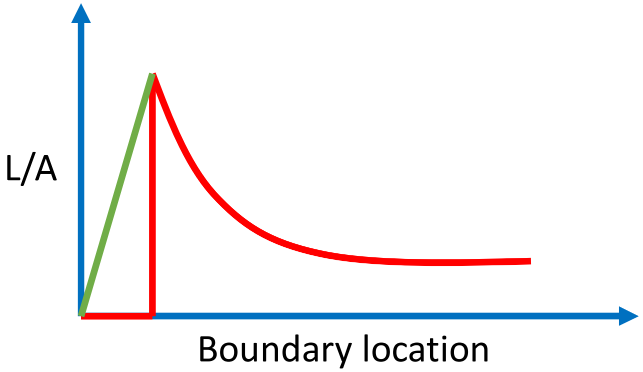




Research needed, as the PEC cut-cell operator is not differentiable

$$\frac{\partial T}{\partial p_k} = \omega^2 \int dV \mathbf{D}_A \cdot \frac{\partial \varepsilon^{-1}}{\partial p_k} \cdot \mathbf{D} \quad \longrightarrow \quad \frac{\partial T}{\partial p_k} = \omega^2 \int dV \mathbf{E}_A \cdot \mathbf{C}^T \frac{\partial\left(\mathbf{A}^{-1}\mathbf{CL}\right)}{\partial p_k} \cdot \mathbf{E}$$

- Averaged permittivity is piece-wise continuous function of boundary location
- But length over inverse area increases until dropped
- Possible solutions
  - Write in terms of surface fields
  - Create a piecewise differentiable operator



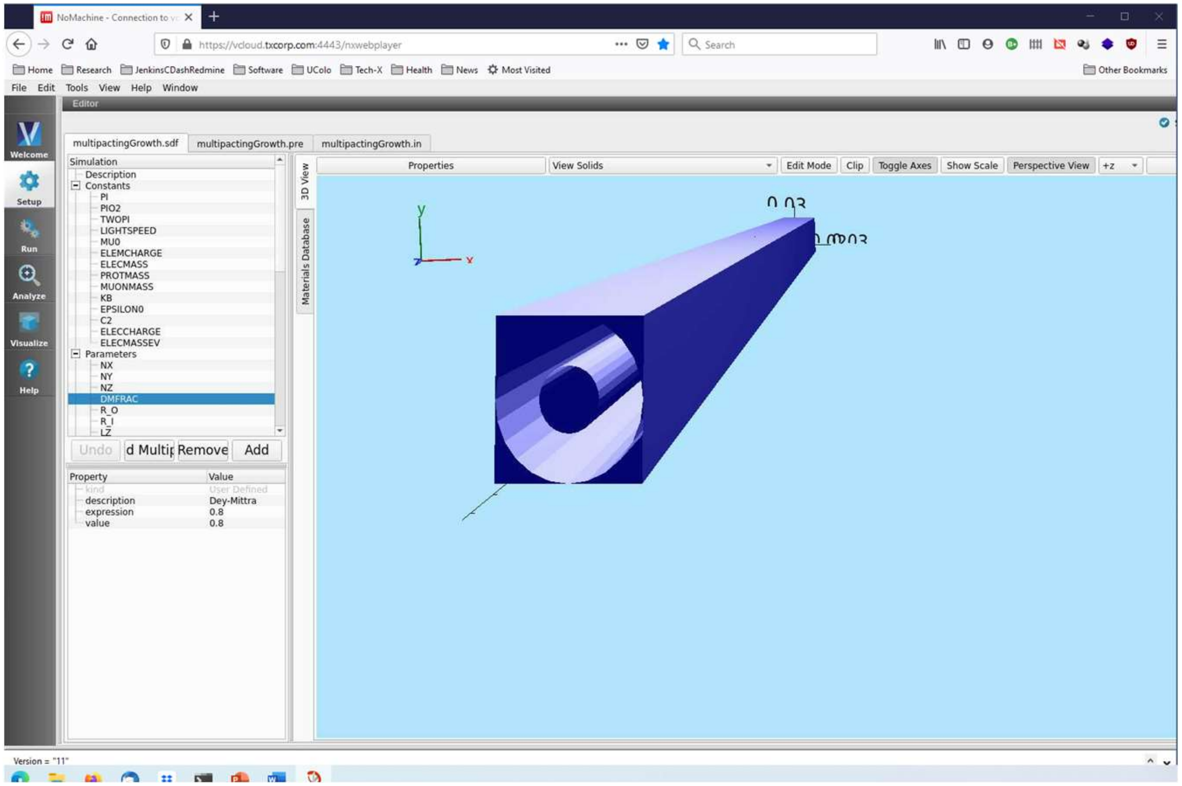
Adjoint optimization could give a direct approach to determining the effects of wake fields

- Compute the field at the bunch(es) of interest directly
- Optimize shape to minimize the wakefield kick

Define standard benchmarking problems for vetting codes

- Cavity basics
  - Surface fields
  - Higher order?
- Wake fields
  - Many-mode solver
  - Moving window
- Multipacting
  - “Multipactor and breakdown susceptibility and mitigation in space-based RF systems”, (MSU, UMich, UWisc, UNM, Texas Tech)
  - Something with HEP orientation?

All of this cheaper by using the cloud



Property	Value
kind	User Defined
description	Dey-Mittra
expression	0.8
value	0.8

- Get rid of capital expense of computers
- No need for installation
- No need to buy hardware
- Pay for what you use
- Green by natural incentive
  - Use what you need, not what you can

What about the rest?

- Any new computational applications should be able to export and import data and fields to the other applications
  - ANSYS mechanical
  - ANSYS thermal

Summary of directions

- RF modeling dominated by commercial sector, but innovations are no longer coming out of “established commercial codes”
  - Not developing algorithms, support has deteriorated.
  - Accelerators, charged particles not a large enough market, “the customer service is not anymore so much serving the accelerating community once code-XYZ became a successful suite of codes usable outside our community,”
  - Public-private model?
- There are many new directions in RF modeling ready to be brought into a product
  - PIC with Accurate surface fields
  - Multimode solvers
  - Adjoint optimization
- Commercial funding by itself insufficient. HEP Funding to create these capabilities insufficient. Public-private partnership?