Advances in Self-Consistent Accelerator modeling

John R. Cary
University of Colorado and Tech-X Corporation
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Advances in Self-Consistent Electromagnetic Modeling

- Complex cavity computations with particles have been improved through algorithms, including parallelization, making possible computations of wakefields in complex structures, intrabunch effects, injectors, …

- Summary of some of what has made this possible
  - Local charge and current deposition methods
  - Parallelization
  - Improved stability
  - Boundary representations

- Comparison with
  - Finite element approaches
  - Unitary separation approaches
The goals of modeling?

• Part of the design process
  – Create
  – Simulate
  – Build
  – Test

• Simulation for prediction of
  – Cavity losses
  – Instability

• In general for
  – Exploration
  – Confirmation
  – Elucidation
Modeling allows one to answer questions without construction cost

NLC

ILC (Tesla)
Basic problem in charge particles moving in EM fields

- Maxwell
  \[
  \frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E} \\
  \frac{\partial \mathbf{E}}{\partial t} = c^2 \left[ \nabla \times \mathbf{B} - \mu_0 \mathbf{j} \right]
  \]

- Particle sources
  \[
  \mathbf{j} = \sum q_i v_i \delta(x - x_i)
  \]

- Particle dynamics
  \[
  \frac{d(\gamma \mathbf{v})}{dt} = \frac{q_i}{m_i} \left[ \mathbf{E}(x_i, t) + \mathbf{v}_i \times \mathbf{B}(x_i, t) \right] \\
  \frac{d\mathbf{x}_i}{dt} = \mathbf{v}_i
  \]

Auxiliary equations

- \( \nabla \cdot \mathbf{B} = 0 \)
- \( \nabla \cdot \mathbf{E} = \rho / \varepsilon_0 \)
- \( \rho = \sum q_i \delta(x - x_i) \)
With much other physics added for a complete model

- Particle injection
- Dark currents
- Multipacting
- Photon (short wavelength) production
- Surface resistance
- Secondary emission
ELECTROMAGNETICS
Yee: 2nd order accurate spatial differentiation

\[ \frac{\partial B_x}{\partial t} = -\frac{\partial E_z}{\partial y} + \frac{\partial E_y}{\partial z} \]

- At the midpoint
  \[ \frac{\partial E_z}{\partial y} = \frac{E_{z,j+1} - E_{z,j}}{\Delta y} + O(\Delta y^2) \]

- Leads to special layout of values in a cell
- *Yee mesh* gives 2nd order accuracy of spatial derivatives
Second-order in time by leap frog

Time centered differences give second order accuracy in $\Delta t$

- Can get time-collocated values by half-stepping in $B$
- Similar for $E$ update, except $c^2$ factor

\[
\frac{\partial B_x}{\partial t} = -\frac{\partial E_z}{\partial y} + \frac{\partial E_y}{\partial z}
\]

\[
B_{x,i,j,k}^{n+1/2} - B_{x,i,j,k}^{n-1/2} = \Delta t \left( \frac{E_{z,i,j,k}^n - E_{z,i,j+1,k}^n}{\Delta y} + \frac{E_{y,i,j,k+1}^n - E_{y,i,j,k}^n}{\Delta z} \right)
\]
Matrix representation useful for stability

\[
\frac{dB_{x,i,j,k}}{dt} = \left( \frac{E_{z,i,j,k} - E_{z,i,j+1,k}}{\Delta y} + \frac{E_{y,i,j,k+1} - E_{y,i,j,k}}{\Delta z} \right)
\]

\[
\frac{db}{dt} = -C \cdot e \quad \frac{de}{dt} = c^2 C' \cdot b \quad \frac{d^2 b}{dt^2} = -c^2 C \cdot C' \cdot b = -D \cdot b
\]

- Magnetic and electric spaces are different
- \( C, C' \) are adjoints, so \( D \) is self-adjoint (symmetric)
- Diagonalize into separate harmonic oscillators
- Leap frog for harmonic oscillator, stability limit at

\[
\omega_{\text{max}} \Delta t_{\text{CFL}} = 2 \quad \Delta t_{\text{CFL}} = \frac{1}{c \sqrt{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2}}}
\]
Gershgorin Circle Theorem gives stability bound

- Frequencies are eigenmodes of \( D = c^2 \ C’C \)
- Eigenvalues in range

\[
0 < \omega^2 < \max \left( \sum_j |D_{ij}| \right) \text{ over } i
\]

- Gives precise range for infinite grid
- Points to relation between coefficients and frequencies for other cases
Many other methods available

- Finite element - later
- Hamiltonian splitting (de Raedt): into exactly solvable parts
  \[
  \frac{d(b, e)}{dt} = A \cdot (b, e) = M \cdot N \cdot (b, e)
  \]
- known:
  \[
  \frac{dU_M}{dt} = M \cdot U_M \quad \frac{dU_N}{dt} = N \cdot U_N
  \]
- stable approximate solution (since unitary):
  \[
  U(\Delta t) = U_N(\Delta t/2) \cdot U_M(\Delta t) \cdot U_N(\Delta t/2)
  \]
- Similar to drift-kick of symplectic integration
- Smith, Cary, Carlsson now have implicit, charge-conserving algorithm
PARTICLES
Computing particle-particle interactions is prohibitive

- Coulomb interaction leads to $N_p^2$ force computations

$$\frac{d\gamma_i v_i}{dt} = \frac{q_i}{\varepsilon_0 m_i} \sum_j q_j \frac{x_i - x_j}{|x_i - x_j|^3}$$

- Lenard-Weichert (retarded potentials) - worse due to need to keep history

$$\frac{d\gamma_i v_i}{dt} = \frac{q_i}{\varepsilon_0 m_i} \sum_j q_j F_{ij}(x_i, x_j(t - \tau))$$
Particle In Cell (PIC) reduces to $N_p$ scaling

- Particle contributions to charges and currents are added to each cell: $O(N_p)$ operations
- Forces on a particle are found from interpolation of the cell values: $O(N_p)$ operations
Finding the force: interpolation (gather)

- Linear weighting for each dimension
  - 1D: linear
  - 2D: bilinear = area weighting
  - 3D: trilinear = volume weighting

- Force obtained through 1st order, error is 2nd order

- For simplicity, no loss of accuracy, weight first to nodal points
Efficiency

Avoiding Poisson
Only certain EM algorithms ensure Poisson satisfied

\[ \nabla \cdot \mathbf{E} = \rho / \varepsilon_0 \]

satisfied always if

\[ \frac{\Delta E_x}{\Delta x} + \frac{\Delta E_y}{\Delta y} + \frac{\Delta E_z}{\Delta z} = \rho / \varepsilon_0 \]

finite difference version

\[ \frac{\partial \mathbf{E}}{\partial t} = c^2 [\nabla \times \mathbf{B} - \mu_0 \mathbf{j}] \]

and

\[ \mathbf{E} \times \mathbf{B} = \rho / \varepsilon_0 \]

initially

\[ \frac{\Delta E_x}{\Delta x} + \frac{\Delta E_y}{\Delta y} + \frac{\Delta E_z}{\Delta z} = \rho / \varepsilon_0 \]

and

\[ \frac{\partial \rho}{\partial t} = -\nabla \cdot \mathbf{j} \]

\[ \frac{\Delta \rho}{\Delta t} = -\frac{\Delta j_x}{\Delta x} + \frac{\Delta j_y}{\Delta y} + \frac{\Delta j_z}{\Delta z} \]
A special scatter ensures finite difference charge conservation

• Principle: apportion via some weighting
• Computing the charge density
  – Compute the current density and find the charge density from finite difference
  – Directly weight particles to the grid
• If these two methods do not agree, then one can have false charge buildup from the Ampere-Maxwell equation. Requires Poisson solve to remove.
• Villasenor/Buneman explicitly conserves charge, but is noisier
EM algorithm must take *numerically divergenceless* to *numerically divergenceless*

\[
\frac{\Delta E_x^n}{\Delta x} + \frac{\Delta E_y^n}{\Delta y} + \frac{\Delta E_z^n}{\Delta z} = 0
\]

and

\[E^{n+1} = M \cdot E^n\]

implies

\[
\frac{\Delta E_{x}^{n+1}}{\Delta x} + \frac{\Delta E_{y}^{n+1}}{\Delta y} + \frac{\Delta E_{z}^{n+1}}{\Delta z} = 0
\]
Charge conservation in electromagnetic PIC codes; spectral comparison of Boris/DADI and Langdon-Marder methods

P.J. Mardahl ¹, J.P. Verboncoeur

Cory Hall Box 173, Department of Electrical Engineering and Computer Science, University of California, Berkeley, CA 94720-1770, USA

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Parallelism: domain decomposition
Parallelism rules of thumb

- Communication is expensive
- Global solves are really expensive
Overlap of communication and computation needed for speed

- Non overlap algorithms:
  - Compute domain
  - Send skin (outer edge)
  - Receive guard
  - Repeat

- Overlap algorithms
  - Compute skin
  - Send skin
  - Compute interior
  - Receive guard
  - Repeat
Similar overlap possible for particles

- Move particles and weight currents to grid
- Send currents needed by neighboring processors
- Send particles to neighboring processors
- Update B for half step
- Receive currents and add in
- Update E, B
- Receive particles

Without charge conserving current deposition, further costly global solve
VORPAL implements basic algorithms in a highly scalable manner.

Object-oriented and flexible
(Arbitrary dimensional)
• Self-consistent EM modeling
  – Full EM or electrostatic + cavity mode
  – Particle in cell with relativistic or nonrelativistic dynamics
• But has other capabilities
  – Impact and field ionization
  – Fluid methods for plasma or neutral gases
  – Implicit EM
  – Secondary emission
• And is modern
  – Serial or Parallel (general domain decomposition)
  – Cross-platform (Linux, AIX, OS X, Windows)
  – Cross-platform binary data (HDF5)
Simplest algorithm allows complex computations

- Example: formation of beams in laser-plasma interaction
Elucidation: long pulses shorten to resonance, capture, loading, acceleration
Simulations have found the hosing problem
Complications: boundaries
Modes computed with combination of FFT and fitting

- Spherical cavity
- Resonant current driver
- FFT measurement of frequency, for accuracy by fitting
Early work on structured meshes had **stair-step** boundary conditions

- \( N \left( \frac{L}{\Delta x} \right) \) cells in each direction
- Error of \((\Delta x / L)^3\) at each surface cell
- \( O(N^2) \) cells on surface
- Error = \( N^2(\Delta x / L)^3 = O(1/N) \)

\[ 120 \times 24 \times 24 = 71,424 \text{ cells} \]
\[ = 215,000 \text{ degrees of freedom} \]
Convergence studies confirm result, indicate modeling problem

- Stair-step error is $10^{-3}$ at 5000 cells per dimension, error linear with cell size
- $10^{11}$ cells for 3D problem

This approach will not give answer even on large, parallel hardware
Finite elements give one approach to improved boundary modeling

- Tau3P, HFSS, ...

\[
\mathbf{B} = \sum b_k(t)\mathbf{u}_k^B(x) \quad \mathbf{E} = \sum e_\ell(t)\mathbf{u}_\ell^E(x)
\]

\[
\frac{\partial \mathbf{B}}{\partial t} = \sum \frac{db_k}{dt}(t)\mathbf{u}_k^B(x) \quad \nabla \times \mathbf{E} = \sum e_\ell(t)\nabla \times \mathbf{u}_\ell^E(x)
\]

\[
\sum \frac{db_k}{dt}(t)\mathbf{u}_k^B(x) = -\sum e_\ell(t)\nabla \times \mathbf{u}_\ell^E(x)
\]

\[
\int d^3x \sum \frac{db_k}{dt}(t)\mathbf{u}_k^B(x)\mathbf{u}_k^B(x) = -\int d^3x \sum e_\ell(t)\mathbf{u}_k^B(x) \cdot \nabla \times \mathbf{u}_\ell^E(x)
\]

\[
\mathbf{M}_b \cdot \frac{\mathbf{db}}{dt} = -\mathbf{C} \cdot \mathbf{e}
\]

\[
\mathbf{M}_e \cdot \frac{\mathbf{de}}{dt} = c^2 \mathbf{C}' \cdot \mathbf{b}
\]
Finite elements require global solves, more intense particle calculations

- Global mass matrix inversion required at each step
  \[ M_b \cdot \frac{db}{dt} = -C \cdot e \]
- Self consistency difficult and charge conservation not guaranteed
  \[ M_e \cdot \frac{de}{dt} = c^2 (C' \cdot b - \mu_0 j) \]
  \[ j \ell = \sum_{ptcls i} q_i v_i u_{\ell}^E (x_i ((n + 1/2) \Delta t)) \]
- Difficult to follow particles
  - List of regions
  - List of FE’s with support in that region
  - Complex FE element evaluation at each time step for each particle
Resurgence of regular grids: cut cells give same accuracy as finite elements

- For cells fully interior, use regular update
- For boundary cells:
  - Store areas and lengths
  - Update fluxes via
    \[ \dot{\Phi}_{xy} = -E_x \ell_x - E_y \ell_y \]
  - Update fields via
    \[ B_z = \Phi_{xy} / A_{xy} \]
Cut-cell boundary conditions accurately represent geometry

- Tesla 2000 cavities
- 312x56x56 ($10^6$) cells
Dey-Mittra (1997) cut-cells allow $10^{-4}$ accuracy

- Fewer than $10^7$ cells for cavity modeling at one part in $10^5$
- Implementation exists now in VORPAL
- No significant additional computational cost
Beam problems provide motivation for further work

- SRF accelerating cavities
- SRF guns
- Crab cavities
Regular, structured grids allow for self-consistent integration of particles

Wakefield for Tesla cavities computed by VORPAL in 3D
Self-consistent EM gun simulations in complex cavities

- Emitted beam
- Wakes from constrictions
Now simulating dipole modes in symmetric cavities
Crab cavity generation, visualization, computation of splitting

- CAD representations
- Python coding of shapes
Dey-Mittra problem: small triangles give high frequencies, small time steps

- B update matrix coefs $\sim$ length/area
- Length/area becomes infinite as area vanishes
- Get localized, high-frequency modes
- Must throw out small cell fragments
Improvement on cut-cell recently discovered

- New method gives error lower than Dey-Mittra
- Does not have reduction of stable $\Delta t$
- Favorable properties re particle introduction
- Now being implemented
Each new study inspires capability, brings requests

- Laser-plasma: self-consistency, parallelism
  - Higher-order particle shapes
- Accelerating cavities: shape modeling
  - Higher-order field to particle near walls
  - Resistive walls for complex shapes
  - Implicit EM solvers
- Electron guns
  - Better emission models
- Crab cavities
  - Notch filters, LOM couplers
Summary

- Self-consistent EM modeling has progressed
  - High-performance, self-consistent computations
  - Accurate treatment of boundaries
  - Secondary emission
  - Absolutely stable charge-conserving algorithm
- Remain algorithm needs
  - Conformal resistive walls
- Remain implementation needs
  - Surface resistance
  - Dark currents
  - Photonic emission
  - Absolutely stable charge-conserving algorithm
- Remains work in simulation setup
  - Defines cavity shapes
  - Define particle beams