A2. Mesh Refinement in Field Solvers

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Outline

- Why mesh refinement?
- Potential issues
- Electrostatic mesh refinement
  - spurious self-force example
  - spurious self-force mitigation
  - application to the modeling of HCX injector
- Electromagnetic mesh refinement
  - spurious reflection of waves
  - spurious reflection of waves mitigation
  - Application to the modeling beam-induced plasma wake
- Special mesh refinement for particle emission
- Summary

Why mesh refinement?

To resolve density spikes & gradients.

Injector

Emitter

Beam edge

Electron cloud

Plasma accelerator

Electron density spikes Small electron beams

Coupling of AMR to PIC: issues

Mesh refinement implies:

- jump of resolution at coarse-fine interface,
- some procedure for coupling the solutions at the interface.

Consequences:

- loss of symmetry: self-force,
- loss of conservation laws,
- EM: waves reflection.
Solution to Poisson is a boundary value problem.
We can define the following simple procedure:
1. solve on coarse grid,
2. interpolate on fine grid boundaries,
3. solve on fine grid.
Illustration potential problem: spurious self-force

Assume one charged macroparticle in a box with metallic BC.

Illustration potential problem: spurious self-force

The macroparticle is attracted by its image from the closest metallic wall.

Illustration potential problem: spurious self-force

We apply specular reflection at the boundary.

Illustration potential problem: spurious self-force

The particle moves up and down.
Illustration potential problem: spurious self-force

Now add a refinement patch.
- Particle is trapped in patch by "spurious self-force"

<table>
<thead>
<tr>
<th>Time</th>
<th>Position</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>100</td>
<td>10</td>
</tr>
<tr>
<td>200</td>
<td>20</td>
</tr>
<tr>
<td>300</td>
<td>30</td>
</tr>
<tr>
<td>400</td>
<td>40</td>
</tr>
<tr>
<td>500</td>
<td>50</td>
</tr>
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</table>

Spurious self-force: magnitude map

Map of spurious self-force as a function of particle position in refinement patch

$E = \sqrt{(E_x - E_{x,0})^2 + (E_y - E_{y,0})^2}$

Mesh refinement
Physical field

Spurious self-force decreases rapidly
In patch

Spurious self-force: mitigation

Add buffer region surrounding refined area

Example with 2 and 4 guard cells buffer region

No buffer: particle trapped in patch.

1 - solve on coarse grid,
2 - Interpolate on fine grid boundaries,
3 - solve on fine grid,
4 - disregard fine grid solution close to edge when gathering force onto particles.

Thickness of buffer region provides user control of relative magnitude of spurious force.
Spurious self-force: mitigation

Example with 2 and 4 guard cells buffer region

With buffer: no more trapping

Buffer region is very effective.

Electrostatic AMR PIC example: HCX

High Current Experiment
(High Brightness Beam Transport Campaign, 2005)

1 MeV, 0.18 A, t = 5 μs,
6x10^12 K+/pulse

Heavy Ion Fusion program, LBNL

WARP simulation of HCX
Electrostatic AMR PIC example: HCX

Very high resolution needed to model the source.

Source region is axisymmetric and is well captured with RZ simulations.

Modeling of source critical - determines initial shape of beam.

Axisymmetric (RZ) time-dependent simulations.

<table>
<thead>
<tr>
<th>Run</th>
<th>Grid size</th>
<th>Nb particles</th>
</tr>
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<tbody>
<tr>
<td>Low res.</td>
<td>50x540</td>
<td>~1M</td>
</tr>
<tr>
<td>Medium res.</td>
<td>112x1280</td>
<td>~4M</td>
</tr>
<tr>
<td>High res.</td>
<td>224x2560</td>
<td>~16M</td>
</tr>
<tr>
<td>Very High res.</td>
<td>448x5120</td>
<td>~64M</td>
</tr>
</tbody>
</table>

Normalized RMS emittance

A fairly high resolution is needed to reach convergence.

First MR attempt - 1 MR block surrounding emitter.

Refining around the emitter area is enough to recover emittance from converged high-resolution case.

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</tr>
<tr>
<td>Medium res. + MR</td>
<td>112x1280</td>
<td>~64M</td>
</tr>
</tbody>
</table>

First MR attempt - 1 MR block surrounding emitter (2).

However, it is not enough for recovering details of distribution.

(pLOTS FROM DATA AT Z=0.4M)
Full adaptive mesh refinement implementation -- speedup from AMR: x10

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</tr>
</thead>
<tbody>
<tr>
<td>Low res</td>
<td>96 x 640</td>
<td>~1M</td>
</tr>
<tr>
<td>Medium res</td>
<td>112 x 1200</td>
<td>~4M</td>
</tr>
<tr>
<td>High res</td>
<td>224 x 2560</td>
<td>~90M</td>
</tr>
<tr>
<td>Low res + AMR</td>
<td>56 x 640</td>
<td>~1M</td>
</tr>
</tbody>
</table>

Example of AMR at edge of beam

- Test using script testxy_amr.py:
  - Run with case="lowres", then "highres" and "AMR".
  - Observe how using AMR enables accurate simulation at reduced CPU cost.

Summary of electrostatic AMR-PIC

- Simple method for electrostatic AMR-PIC was presented.
- Buffer region mitigates spurious self-force effect very effectively.
- Speedups of x10 demonstrated on simulation of injector.
- Alternate methods such as multipole expansions have other advantages/drawbacks.
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1-D FDTD EM wave equation

- We consider 1d wave equation (natural units)
  \[
  \frac{\partial E_j}{\partial t} = \frac{\partial B_j}{\partial x}, \quad \frac{\partial B_j}{\partial t} = \frac{\partial E_j}{\partial x}
  \]
- staggered on a regular space time grid using finite-difference time-domain (FDTD) centered scheme

\[
\begin{align*}
E_j^{n+1} - E_j^n &= B_{j+1/2}^{n+1/2} - B_{j-1/2}^{n+1/2} \\
B_{j+1/2}^{n+1} - B_{j-1/2}^{n+1} &= E_j^{n+1} - E_j^n
\end{align*}
\]

1-D MR-EM: space refinement

uncentered finite-difference

centered finite-difference

- finite-difference at positions $j$
- finite-volume (=uncentered FD) at $j$
- jump' inside fine grid at $j$
1-D MR-EM: coefficients of spurious reflection

Test to measure spurious reflection \( R \) at interface at \( j \) of signal injected on fine grid.

\[ \delta x_2 = n \delta x_1 \]

\( \phi: E, \phi B \)

Reflection

Total energy

\( \lambda \leq \lambda_{\text{min}} \) of coarse grid are reflected with amplification of total energy!

Warp's Electromagnetic MR uses PML and substitution to prevent reflections

Warp's electromagnetic MR solver

- Termination of patches with Perfectly Matched Layers (PML) to avoid spurious reflections
- Buffer zone used for mitigating spurious self-force

Inside patch at \( L_{n+1} \):

\[ F_{n+1}(a) = |F_{n+1}(a)| + F_{n+1}(f) \]

Main grid: \( F_n(a) \)

MR procedure is recursive, accommodating an arbitrary number of levels

Example with two levels of refinement

Inside patch at \( L_{n+2} \):

\[ F_{n+2}(a) = |F_{n+2}(a)| + F_{n+2}(f) \]

Main grid: \( F_n(a) \)

Example: simulation of beam-induced plasma wake

Plasma

Ion beam

High resolution is needed to capture details.
Example: simulation of beam-induced plasma wake

- Mesh refinement
  - 2 levels
  - Fields only

- Low resolution
  - MR
  - 2 levels
  - Fields only particles

3-D

Speedup x10 in 3D (using the same time steps for all refinement levels).

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3-D WARP simulation of HCX showed beam head scraping

- Head cleaner with shorter voltage rise-time.
- Questions:
  - What is the optimal rise-time?
  - Can we produce and model very-fast rise-time?

Test: 1-D time-dependent modeling of ion diode

- Analytic solution from Lampel-Tiefenback

- Child-Langmuir
**Test: 1D time-dependent modeling of ion diode (algo 1)**

Injection algorithm

- Emitter \( d \)
- Collector
- Virtual surface

Child-Langmuir solution + voltage drop between emitter and virtual surface determines current to inject.

\[ I = \chi \left( \frac{V - V_i}{d^2} \right)^{3/2}; \chi = \frac{4}{9} e_n \sqrt{\frac{2q}{m}} \]

\[ \Rightarrow \Delta Q = Nq = I \Delta t \]

Result:

- Lampel-Tiefenback waveform
- Analytic Simulation

Simulation result exhibits large unphysical oscillation.

N = 160
\( \Delta t = 1ns \)
d = 0.4m

*1:D = \( j_d \) (\( j_e \), \( s = 1 \))

**Unphysical oscillation related to Nb particles injected/time step (N)_i**

- Nb injected particles
- Time steps

Ideally,

\[ \frac{N}{\Delta t} = \frac{1}{2} \frac{1 - \left( \frac{V}{V_i} \right)^{3/2}}{\chi} \]

but the driving voltage is a continuous function derived analytically.

\[ \Rightarrow \text{Inconsistency due to infinitesimal solution applied in discrete world.} \]

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**Cure: derive voltage history numerically**

Injection algorithm

- Emitter \( d \)
- Collector
- Virtual surface

We apply Lampel-Tiefenback method at the discrete level.

\[ \Delta Q = Nq = I \Delta t \Rightarrow V - V_i = \left( \frac{Id^2}{\chi} \right) \]

solve for \( V \) using linearity of Poisson

\[ (V-V_i) = (V-V_i)_{v=0} + (V-V_i)_{d=0} \]

Result:

- Numerical waveform
- Lampel-Tiefenback waveform

Large unphysical oscillation has been suppressed but there is still a spike. Is it due to initial step \( V_0 \) in waveform?

N = 160
\( \Delta t = 1ns \)
d = 0.4m

**Cure #2: apply irregular gridded patch around emitter.**

Injection algorithm

- Emitter \( d \)
- Collector
- Virtual surface

- Apply irregular gridded patch covering \( d \)
- Mesh size such that number of particles per cell is a constant in patch assuming Child-Langmuir solution for \( p(x) \)
- Apply same injection algorithm as before in patch

Result:

- Numerical waveform

Spike still here

N = 160
\( \Delta t = 1ns \)
d = 0.4m
\( N_e = 200 \)
Cure #3: apply regularly gridded patch following front.

An Adaptive-Mesh-Refinement patch follows the front.

Result

- Applied Waveform
- Lampel-Tiefenback waveform

\[ V(\text{Vols}) \]
\[ N = 160 \]
\[ \Delta t = 1\text{ns} \]
\[ d = 0.4\text{mm} \]
\[ N_z = 200 \]
\[ \text{AMR ratio} = 16 \]

At this point, we declared victory!

Extension to three dimensions

- Specialized 1-D patch implemented in 3-D injection routine, as a 2-D array of 1-D patches.
- Extended Lampel-Tiefenback technique to 3-D, and implemented in WARP.
- Predicts a voltage waveform which extracts a nearly flat current at emitter.

\[ \text{Ion source diode} \]
\[ \text{MR patch} \]

- Without MR, WARP predicts overshoot.
- Run with MR predicts very sharp risetime (not square due to erosion)

Test of MR patch on modeling of STS500 Experiment.

Pierce diode: exercise

1. Open Pierce_diode.py. Run with w3d_injn - 0, 10, 20 and 100.
2. Observe convergence of voltage at t=0 toward 0. Notice very small dz required!

\[ \text{Current History (2:0.62m)} \]
\[ \text{Current History (2:0.62m)} \]

MR OFF

MR ON
AMR-PIC summary

- Mesh refinement (static or adaptive) can reduce simulation time by several.
- Care is needed to avoid spurious effects (spurious charge & reflections).
- Warp implementation has validated methods, but maintenance is lacking sufficient manpower:
  ➔ To be used with great care by experience users.
  ➔ Novel implementation with external AMR package (BoxLib) is planned.

References