Exponential Recursion for Multi-Scale Problems in Electromagnetics

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Computational Aspects of Time Dependent Electromagnetic Wave Problems in Complex Materials
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Outline

1. Introduction and Motivation
2. Havriliak-Negami Model
3. Wave Solver
4. Conclusions
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1. Introduction and Motivation
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4. Conclusions
Exponential recursion is a simple concept, but a powerful tool. We focus on EM wave propagation in complex media.

(1) Anomalous dielectric relaxation (fractional relaxation models)
   1. Complex heterogeneous materials (soil, biological tissues)
   2. Empirical dispersion models involve $(i\omega)^\alpha$.
   3. Power-law decay, requires time history of fields.
   4. Useful for similar problems in acoustics, solid mechanics, etc.

(2) Plasmas
   1. Plasma phenomena occur at vastly disparate time scales.
   2. Geometry, fine spatial scales must be resolved.
   3. Experiments often have non-local effects.
   4. Pros and Cons of kinetic vs. fluid models of plasma.
In time, exponential recursion truncates time history. Consider

\[ \dot{\phi} + y\phi = f(t), \quad 0 < t < T \]

Multiply by integrating factor, and integrate over \([t - \delta, t]\)

\[
\int_{t - \delta}^{t} (e^{yt}\phi)' \, dt = \int_{t - \delta}^{t} e^{yt} f(t) \, dt \\
e^{yt}\phi(t) - e^{y(t-\delta)}\phi(t - \delta) = \int_{t - \delta}^{t} e^{y\tau} f(\tau) \, d\tau
\]

Rearranging, we find the exponential recursion

\[
\phi(t) = e^{-y\delta}\phi(t - \delta) + \int_{0}^{\delta} e^{-yu} f(t - u) \, du.
\]

Discretize using any exponential integrator.
In space, exponential recursion localizes the solution. Consider

\[ w - \frac{1}{\alpha^2} w'' = u \quad \implies \quad w_p(x) = \frac{\alpha}{2} \int_{a}^{b} e^{-\alpha|x-y|} u(y) \, dy \]

Split the integral at \( y = x \), and let \( w_p = w_L + w_R \). Then

\[ w_L(x) = \frac{\alpha}{2} \int_{a}^{x} e^{-\alpha(y-x)} u(y) \, dy, \quad w_R(x) = \frac{\alpha}{2} \int_{x}^{b} e^{-\alpha(x-y)} u(y) \, dy. \]

A few steps of algebra produce the exponential recursion

\[ w_L(x) = e^{-\alpha \delta_L} w_L(x - \delta_L) + \int_{0}^{\delta_L} e^{-\alpha z} u(x - z) \, dz \]

\[ w_R(x) = e^{-\alpha \delta_R} w_R(x + \delta_R) + \int_{0}^{\delta_R} e^{-\alpha z} u(x + z) \, dz. \]

Discretize using any collocation method.
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Consider EM propagation through a region $\Omega$

\[
\begin{align*}
\frac{\partial D}{\partial t} &= \nabla \times H - J, & \nabla \cdot D &= \rho \\
\frac{\partial B}{\partial t} &= -\nabla \times E, & \nabla \cdot B &= 0
\end{align*}
\]

- In the absence of external charges and currents, $\rho = 0$, $J = 0$.
- Assume the material is non-magnetic, so $B = \mu_0 H$.
- Anomalous dielectric relaxation, $\hat{D} = \epsilon_0 \hat{\epsilon} \hat{E}$, where

\[
\hat{\epsilon}(s) = \epsilon_\infty + \frac{\Delta \epsilon}{1 + (s\tau)^\alpha}^\beta
\]

with $\epsilon_\infty \geq 1$, $\Delta \epsilon > 0$, $0 < \alpha, \beta \leq 1$. 
Decompose $D = \epsilon_0 (\epsilon_\infty E + P)$, where

$$(I + \tau^\alpha \frac{c}{D} D_t^\alpha)^\beta P = \Delta \epsilon E \quad \text{fractional PDO!}$$

Solve for the polarization using Laplace transforms.

$$P(x, t) = \int_0^t \chi(u) E(x, t - u) \, du, \quad \hat{\chi}(s) = \frac{\Delta \epsilon}{(1 + (s\tau)^\alpha)^\beta}$$

$$\chi(t) \sim \begin{cases} t^{\alpha\beta-1} & t \ll 1 \\ t^{-\alpha-1} & t \gg 1 \end{cases}$$
We first re-cast the susceptibility as an integral over $\mathbb{R}$

$$\chi(t) = \frac{\Delta \epsilon}{2\pi i} \int_{\zeta - i\infty}^{\zeta + i\infty} \frac{e^{st}}{(1 + (s\tau)^\alpha)^\beta} ds$$

$$= \int_0^\infty f(y)e^{-yt/\tau} \, dy$$

$$= \int_{-\infty}^\infty f(e^z)e^{z - e^z t/\tau} \, dz,$$

where

$$f(y) = \frac{\Delta \epsilon}{\pi \tau} \sin \left( \beta \cos^{-1} \left\{ \frac{y^\alpha \cos(\pi \alpha) + 1}{\sqrt{y^{2\alpha} + 2 \cos(\pi \alpha) y^\alpha + 1}} \right\} \right).$$
In general, consider

$$K(t) = \int_{0}^{\infty} f(y)e^{-yt} \, dy$$

for non-negative $f \in L^1(\mathbb{R}^+)$. We set $y = e^z$. Then, for $h > 0$ the Poisson summation formula yields

$$h \sum_{n=-\infty}^{\infty} f(e^{nh})e^{nh}e^{-nh}t = \sum_{k=-\infty}^{\infty} \hat{f} \left( \frac{2\pi k}{h} \right)$$

where

$$\hat{f}(k) = \int_{-\infty}^{\infty} [f(z)e^{z}e^{-z}t] e^{ikz} \, dz, \quad \hat{f}(0) = K(t)$$

Under mild assumptions, the integrand is analytic for $Im\{z\} \leq \theta$.

$$|\hat{f}(k)| \leq C_k e^{-|k|\theta}.$$
\begin{align*}
K(t) &= h \sum_{n=-\infty}^{\infty} f(e^{nh})e^{nh-e^{nh}t} - \sum_{k \neq 0} \hat{f} \left( \frac{2\pi k}{h} \right) \\
&\approx h \sum_{nh<z_r} f(e^{nh})e^{nh-e^{nh}t} + \mathcal{O} \left( e^{-\pi^2/h} \right)
\end{align*}
Given $\epsilon > 0$, for $t \in [\Delta t, T]$

1. **Discretization**: Choose $h$ so that $e^{-\pi^2/h} \approx \epsilon$.

2. **Truncation**: Choose $z_r$ so that $hf(e^{z_r})e^{z_r-\Delta te^{z_r}} \approx \epsilon$.

3. **Compression**: Choose $z_\ell$ so that a minimal number $J$ (typically 2 or 3) compressed nodes satisfies

$$h \sum_{z \leq z_\ell} f(e^{nh})e^{nh-e^{nh}T} = \sum_{j=1}^{J} w_j e^{-y_j T} + O(\epsilon)$$

Next, merge the weights and nodes. Then, we have a uniform relative error bound

$$\max_{\Delta t < t < T} \left| K(t) - \sum_{m=1}^{M} w_m e^{-y_mt} \right| \leq K(t)\epsilon$$
Introduction and Motivation

Havriliak-Negami Model

Wave Solver

Conclusions

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Exponential Recursion

Relative error, $K(t) = t^{-\alpha}$

$t$

Relative error, $K(t) = \chi(t), \ (\alpha, \beta) = (0.5, 0.5)$

$t$
For \( t \in [0, T] \),

\[
P(x, t) = \int_0^{\Delta t} \chi(u)E(x, t - u) \, du + \sum_{m=1}^M w_m \phi_m(t) + \mathcal{E}(t)
\]

where we have the diagonized linear system

\[
\dot{\phi}_m + y_m \phi_m = E.
\]

Discretize using any exponential integrator. For \( E \in L^2([0, T]) \),

\[
\|\mathcal{E}(t)\|_{L^2} \leq \left\| \chi(t) - \sum_{m=1}^M w_m e^{-y_m t} \right\|_{L^1} \left\| E(x, t) \right\|_{L^2}
\]

\[
\leq T \left\| \chi(t) - \sum_{m=1}^M w_m e^{-y_m t} \right\|_{L^\infty} \left\| E(x, t) \right\|_{L^2}
\]

\[
\leq \varepsilon T \left\| E(x, t) \right\|_{L^2}
\]
Replace the electric field with a polynomial interpolant, and perform product integration to arrive at

\[ P(t) = \sum_{\ell=0}^{L} A_{\ell} E(x, t - \ell \Delta t) + \sum_{m=1}^{M} w_{m} \phi_{m}(t) \]

\[ \phi_{m}(x, t) = e^{-y_{m} \Delta t} \phi_{m}(x, t - \Delta t) + \sum_{\ell=0}^{L} B_{\ell, m} E(x, t - \ell \Delta t). \]

The polarization law can now be evaluated with \( L \) levels of time history, and \( M = \mathcal{O}(\log N_{t}) \) terms in memory.

The operation count is \( \mathcal{O}(LM) \). Here, \( N_{t} = \lceil \frac{T}{\Delta t} \rceil \).

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\(^{1}\) JCP 2013, with S. Jiang and P. Petropoulos
**Theorem.** The numerical scheme, based on the second order accurate FDTD method, and is stable under the standard CFL stability condition.

We solve a signaling problem (1d TEM wave) using the finite difference time domain (FDTD) technique, with square pulse

\[ E(0, t) = \frac{1}{t_d} (H(t) - H(t - t_d)). \]
Similar asymptotics for Cole-Cole, Cole-Davidson models.  

2IEEE Trans. Ant. 2011 with P. Petropoulos
Consider the Vlasov-Maxwell system for a plasma

\[
\epsilon_0 \mu_0 \frac{\partial E}{\partial t} = \nabla \times B - \mu_0 J, \quad \nabla \cdot E = \frac{\rho}{\epsilon_0}
\]

\[
\frac{\partial B}{\partial t} = -\nabla \times E, \quad \nabla \cdot B = 0
\]

\[
\rho = q \int_v f(x, v, t) \, dv, \quad J = q \int_v v f(x, v, t) \, dv
\]

\[
\frac{\partial f}{\partial t} + v \cdot \nabla_x f + \frac{F}{m} \cdot \nabla_v f = 0
\]

\[
F = q (E + v \times B)
\]
Define EM fields using scalar potential $\phi$ and vector potential $A$ by

$$E = -\frac{\partial A}{\partial t} - \nabla \phi, \quad B = \nabla \times A.$$ 

Impose the Lorenz gauge $\frac{1}{c^2} \frac{\partial \phi}{\partial t} + \nabla \cdot A = 0$, so that

$$\frac{1}{c^2} \frac{\partial^2 A}{\partial t^2} - \nabla^2 A = \mu_0 J \quad \frac{1}{c^2} \frac{\partial^2 \phi}{\partial t^2} - \nabla^2 \phi = \frac{1}{\epsilon_0 } \rho$$
1. **Apply the method of lines transpose (MOL\(^T\))**
   - Discretize in time first.
   - Re-formulate as a semi-discrete boundary integral.
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2. **Build a (1d) spatial solver**
   - Spatial discretization over a (perhaps nonuniform) mesh.
   - Fast \(O(N)\) matrix-free convolution, via exponential recursion.
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3. **Multi-dimensional solver**
   - Spatial solver works in a "line-by-line" fashion.
   - Embedded boundaries.
   - Local interpolation for normal derivatives.
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4. **Raise order of accuracy in time**
   - Taylor expansion reformulated with convolution operators.
   - Coefficients determined with resolvent expansion.
   - Stability guaranteed by introducing a free parameter \(\beta > 0\).
\[ \frac{1}{c^2} u_{tt} - \nabla^2 u = S \]
\[
\frac{1}{c^2} u_{tt} - \nabla^2 u = S
\]

Discretize \(u_{tt}\) in time

\[
u_{tt}(x, t_n) \approx \frac{u^{n+1} - 2u^n + u^{n-1}}{\Delta t^2}.
\]

\(^2\text{Math Comp. 2014 with A. Christlieb, B. Ong, and L. Van Groningen}\)
\[
\frac{1}{c^2} u_{tt} - \nabla^2 u = S
\]

Discretize \( u_{tt} \) in time

\[
u_{tt}(x, t_n) \approx \frac{u^{n+1} - 2u^n + u^{n-1}}{\Delta t^2}.
\]

The Laplacian is treated semi-implicitly, so that

\[
u^{n+1} - 2u^n + u^{n-1}
\]

\[
\frac{1}{c \Delta t^2} - \nabla^2 \left( u^n + \frac{u^{n+1} - 2u^n + u^{n-1}}{\beta^2} \right) \approx S^n,
\]

with \( 0 < \beta \leq 2 \).

\[^2\text{Math Comp. 2014 with A. Christlieb, B. Ong, and L. Van Groningen}\]
\[ \mathcal{L} \left[ u^n + \frac{u^{n+1} - 2u^n + u^{n-1}}{\beta^2} \right] = u^n + \frac{S^n}{\alpha^2}, \]

where the modified Helmholtz operator is

\[ \mathcal{L}[u](x) := \left( 1 - \frac{1}{\alpha^2} \nabla^2 \right) u(x), \quad \alpha = \frac{\beta}{c\Delta t}. \]

Update equation

\[ u^{n+1} = 2u^n - u^{n-1} - \beta^2 D[u^n](x) + \beta^2 \mathcal{L}^{-1} \left[ \frac{S^n}{\alpha^2} \right] (x), \]

where

\[ D[u](x) := u(x) - \mathcal{L}^{-1}[u](x) \approx -\frac{1}{\alpha^2} \nabla^2 u. \]
Rather than invert the 3d Helmholtz operator, we utilize dimensional splitting

\[ \mathcal{L} \approx \mathcal{L}_x \mathcal{L}_y \mathcal{L}_z \]

In one spatial dimension,

\[ u^{n+1} = 2u^n - u^{n-1} - \beta^2 D[u^n](x) + \beta^2 \mathcal{L}^{-1} \left[ \frac{S^n}{\alpha^2} \right](x), \]

where

\[ \mathcal{L}^{-1}[u](x) := \frac{\alpha}{2} \int_a^b u(y)e^{-\alpha|x-y|} dy + Ae^{-\alpha(x-a)} + Be^{-\alpha(b-x)}. \]

**Theorem:** This semi-discrete scheme is second order accurate in time, and A-stable for \( \beta \in (0, 2] \).
\[ w_p(x) = I[u](x) = \frac{\alpha}{2} \int_a^b e^{-\alpha|x-y|} u(y) dy. \]

Split the particular solution at \( y = x \),

\[
I[u](x) = \frac{\alpha}{2} \int_a^x e^{-\alpha(x-y)} u(y) dy + \frac{\alpha}{2} \int_x^b e^{-\alpha(y-x)} u(y) dy.
\]

Each "characteristic" is updated using exponential recursion

\[
I^L(x + \delta) = e^{-\alpha \delta} I^L(x) + \frac{\alpha}{2} \int_x^{x+\delta} e^{-\alpha(x_j-y)} u(y) dy
\]

\[
I^R(x - \delta) = e^{-\alpha \delta} I^R(x) + \frac{\alpha}{2} \int_x^{x-\delta} e^{-\alpha(y-x_j)} u(y) dy.
\]
Partition \([a, b]\) into \(N\) subintervals \([x_{j-1}, x_j]\), \(h_j = x_j - x_{j-1}\).

Replace \(u\) with a local Lagrange interpolant, of order \(2M\). Then

\[
I^L(x_j) = e^{-\alpha h_j} I^L(x_{j-1}) + \sum_{k=-M}^{M} w^L_k u(x_{j+k}), \quad j = 1, \ldots N,
\]

\[
I^R(x_j) = e^{-\alpha h_{j+1}} I^R(x_{j+1}) + \sum_{k=-M}^{M} w^R_k u(x_{j+k}), \quad j = N - 1, \ldots 0.
\]

Convolution computed in \(O(MN)\) operations.
Transmission conditions can be formulated, for domain decomposition and (1d) outflow BCs.

\[ \mathcal{L}^{-1}[u](x) := \frac{\alpha}{2} \int_a^b u(y)e^{-\alpha|x-y|} \, dy + Ae^{-\alpha(x-a)} + Be^{-\alpha(b-x)}. \]

**Particular Solution**

**Homogeneous Solution**

Compare with the free space solution. Then, for \( x \in [a, b] \), we see

\[ A(t) = \alpha \int_0^\infty u(a - y, t)e^{-\alpha y} \, dy. \]

Using **exponential recursion**, storing time history at the boundary

\[ A^n = \alpha \int_{a-ct_n}^a e^{-\alpha(a-y)} u(y, t_n) \, dy \]

\[ = e^{-\beta} A^{n-1} + \alpha \int_0^{c\Delta t} e^{-\alpha y} u \left( a, t_n - \frac{y}{c} \right) \, dy. \]
The exponential recursion can also be employed hierarchically.\(^3\)

\[ I^L(X_j) = e^{-\alpha(X_j-X_{j-1})} I^L(X_{j-1}) + J^L(X_j), \]
\[ J^L(X_j) = \alpha \int_{X_{j-1}}^{X_j} e^{-\alpha(X_j-y)} u(y)dy \]

1. Compute each local particular solution on \(\Omega_j\).
2. Find particular solution using global exponential recursion.
3. Pass transmission conditions, boundary conditions to each \(\Omega_j\).

\(^3\)Arxiv, with A. Christlieb, **Y. Guclu** and E. Wolf
### CPU vs GPU Run Time Data

<table>
<thead>
<tr>
<th>dx</th>
<th>CFL</th>
<th># Grid Points</th>
<th>CPU Run Time (Sec)</th>
<th>GPU 1 Domain Run Time (Sec)</th>
<th>GPU 4 domain Run Time (Sec)</th>
<th>GPU 8 domain Run Time (Sec)</th>
<th>GPU 16 domain Run Time (Sec)</th>
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<td>6.76 (unstable)</td>
<td>6.38 (unstable)</td>
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#### 2D CPU vs GPU runtime comparison

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<th>Grid Width</th>
<th>CPU Run Time (Sec)</th>
<th>GPU Run Time (Sec)</th>
<th>GPU Speed Up %</th>
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<td>3100</td>
</tr>
</tbody>
</table>

Undergraduate thesis with C. Seipp
In order to approximate higher order powers of the Laplacian operator using dimensional splitting\(^4\), we first define

\[
\mathcal{L}_\gamma := 1 - \frac{\partial^2}{\alpha^2}, \quad \mathcal{D}_\gamma := 1 - \mathcal{L}_\gamma^{-1}, \quad \gamma = x, y, z,
\]

and

\[
\mathcal{C}_{xyz} := \mathcal{L}_y^{-1} \mathcal{L}_z^{-1} \mathcal{D}_x + \mathcal{L}_z^{-1} \mathcal{L}_x^{-1} \mathcal{D}_y + \mathcal{L}_x^{-1} \mathcal{L}_y^{-1} \mathcal{D}_z.
\]

so that

\[
\left(-\nabla^2/\alpha^2\right)^m = \mathcal{C}_{xyz}^m \sum_{p=m}^{\infty} \binom{p-1}{m-1} \mathcal{D}_{xyz}^{p-m}.
\]

\(^4\)SINUM 2013, with A. Christlieb
\[ u^{n+1} - 2u^n + u^{n-1} = \sum_{m=1}^{\infty} \frac{2\beta^{2m}}{(2m)!} \left( \frac{\nabla^2}{\alpha^2} \right)^m u^n \]

\[ = \sum_{m=1}^{\infty} (-1)^m \frac{2\beta^{2m}}{(2m)!} C^m \sum_{p=m}^{\infty} \binom{p-1}{m-1} D^{p-m}[u^n] \]

\[ = \sum_{p=1}^{\infty} \sum_{m=1}^{p} (-1)^m \frac{2\beta^{2m}}{(2m)!} \binom{p-1}{m-1} C^m D^{p-m}[u^n] \]

\[ = \sum_{p=1}^{P} \sum_{m=1}^{p} A_{p,m}(\beta) C^m D^{p-m}[u^n] + O(\Delta t^{2P+2}). \]
<table>
<thead>
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<th>$P = 1$</th>
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<th></th>
<th>$P = 2$</th>
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<th>$P = 3$</th>
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<td>Error</td>
<td>Rate</td>
<td>Time (s)</td>
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<td>Rate</td>
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<td>186.2</td>
</tr>
</tbody>
</table>

Table: Refinement and computational efficiency for a 2d rectangular mode $u(x, y, 0) = \sin(\pi x) \sin(\pi y)$. The mesh is held fixed at $\Delta x = \Delta y = 0.003125$.

The algorithm scales linearly with the number of spatial points.
The characteristic polynomial satisfied by the amplification factor is

$$
\rho^2 - 2\rho + 1 = \rho \left( \sum_{p=1}^{P} A_p(\beta) \hat{D}^p \right), \quad \beta > 0, \quad 0 \leq \hat{D} \leq 1.
$$

**Def.** The scheme will be A-stable provided that $|\rho| \leq 1$.

**Theorem.** For each finite $P$, there exists $\beta_{\text{max}}$ such that the semi-discrete scheme will be A-stable for $0 < \beta \leq \beta_{\text{max}}$, and where

$$
\sum_{p=1}^{P} A_p(\beta_{\text{max}}) = 4.
$$

<table>
<thead>
<tr>
<th>$P$</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
</tr>
</thead>
<tbody>
<tr>
<td>Order</td>
<td>2</td>
<td>4</td>
<td>6</td>
<td>8</td>
<td>10</td>
</tr>
<tr>
<td>$\beta_{\text{max}}$</td>
<td>2</td>
<td>1.4840</td>
<td>1.2345</td>
<td>1.0795</td>
<td>0.9715</td>
</tr>
</tbody>
</table>
(a) 2nd order  
(b) 4th order

**Figure:** Propagation due to a point source in 2d, on a $80 \times 80$ mesh, with CFL number 2.
1. Add a **ghost point**, exterior to the domain.\(^5\)

2. Interpolate \(u_I\) and \(u_{II}\) from **local** interior grid points (bilinear).

3. Interpolant through \(u_I\) and \(u_{II}\), such that \(\frac{\partial u}{\partial n}(\xi_B) = 0\).

4. Extrapolate to find \(u_G\), and update **only** local grid points. Iterate to convergence.

---

\(^5\) J. Sci. Comp. 2017, with A. Christlieb and **E. Wolf**
\[ C = \left\{ (x, y) : \left( \frac{x + y}{4} \right)^2 + (x - y)^2 = 1 \right\} . \]

**Figure:** The boundary points (red) close each line of the $x$ and $y$ sweeps.
Solution is 6th order in time and space. No stability restriction.
(a) $t = 0$

(b) $t = 0.1$

(c) $t = 0.2$

(d) $t = 0.25$

(e) $t = 0.45$

(f) $t = 0.7$

(g) $t = 0.8$

(h) $t = 1.0$
Implicit PIC, quasi-electrostatics.  

**Initial Prediction**

1. **Charge:** \( \{\xi_i^n\} \rightarrow \rho^n . \)
2. **Potential (MOL\(^T\)):** \( \phi^{n-1}, \phi^n, \rho^n \rightarrow \phi^* . \)
3. **Positions:** \( \xi_i^* = \xi_i^n + \Delta t v_i^n . \)
4. **Fields:** \( \phi^* \rightarrow \vec{E}^* \rightarrow \vec{E}_i^* = \vec{E}^*(\xi_i^*) . \)

**Correction Iteration**

5. **Velocities:** \( v_i^* = v_i^n + \Delta t (\alpha \vec{E}_i^* + (1 - \alpha) \vec{E}_i^n). \)
6. **Positions:** \( \xi_i^* = \xi_i^n + \Delta t (\alpha v_i^* + (1 - \alpha) v_i^n). \)
7. **Charge:** \( \{\xi_i^*\} \rightarrow \rho^* . \)
8. **Potential/Fields:** \( \phi^{n-1}, \phi^n, \bar{\rho} \rightarrow \phi^* \rightarrow \vec{E}_i^* . \)
9. **Repeat steps 5-8 to convergence.**
50 periods of an electron-ion oscillatory system. The CFL is 10, with 100 cells in the domain. Standard spatial smoothing operators are applied to grid quantities. The relaxation parameter is varied, no grid heating is observed when $\alpha = 0.5$. 
Total energy is conserved, as the underlying field solver is non-dissipative.
Ph.D. thesis of M. Thavappiragasam
Ph.D. thesis of M. Thavappiragasam
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Future Work:

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2. Domain decomposition in multiple dimensions
3. Consistent treatment of particles
4. Fully parallel 3d Maxwell solver
Thank you!

References

The Christlieb Group