A Fast Implicit Maxwell Solver

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Collaborators:
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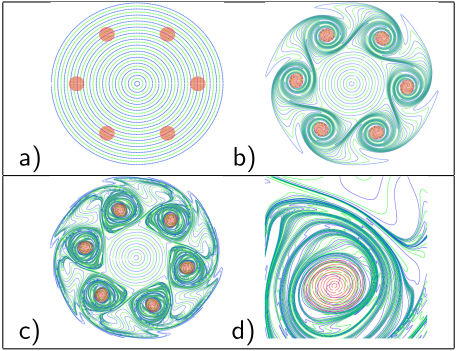
Goal

Penning Trap:



Goal: Address temporal scale separation in Plasmas.

Approach: Implicit methods – step over plasma oscillation time scale.

What do we need?

1. An implicit Maxwell solver (This talk - Progress on this front)
2. An implicit particle push (Just starting work on this)

Implicit Maxwell Solvers in Plasma Physics – IMEX Maxwell:

1. the direct method:
   1. A. Friedman, AB Langdon, and BI Cohen, Comments Plasma Physics Controlled Fusion (1981)
   2. DC Barnes, T. Kamimura, J.N. Leboeuf, and T. Tajima, Journal of Computational Physics 52 (1983), no. 3, 480502.
   3. A.B. Langdon, B.I. Cohen, and A. Friedman, Journal of Computational Physics 51 (1983), no. 1, 107138.
   4. A. Friedman, SE Parker, SL Ray, and CK Birdsall, Journal of Computational Physics 96 (1991), no. 1, 5470.
   5. GB Jacobs and JS Hesthaven, Computer Physics Communications 180 (2009), no. 10, 1760 1767.
2. the implicit moment method:
   1. J.U. Brackbill, D.B. Kothe, and H.M. Ruppel, Computer Physics Communications 48 (1988), no. 1, 2538
   2. R.J. Mason, Journal of Computational Physics 41 (1981), no. 2, 233244.
   3. P. Ricci, G. Lapenta, and JU Brackbill, Journal of Computational Physics 183 (2002), no. 1, 117141.
   4. G. Lapenta, JU Brackbill, and P. Ricci, Physics of Plasmas 13 (2006), 055904.
3. Darwin:
   1. A Kaufman, P Rostler, Physics of Fluids 14 (1971), no.2, 446–449
   2. D Hewett, C Nielson Journal of Computational Physics 29 (1978), no.2, 219–236
   3. D Hewett, Journal of Computational Physics 38 (1980), no.3, 378–395
   4. D Hewett . . .
   5. H Schmitz, R Grauer, Journal of Computational Physics 214 (2006), no.2, 738–756
   6. P Gibbon, R Speck, B Berberich, A Karmakar,L Arnold, M Mašek, NIC Symposium 2010: Proceedings, 24-25 February 2010, Jülich, Germany

4 ADI Implicit Maxwell

1 M. Lees, Journal of the Society for Industrial Applied Mathematics 10 (1962), no. 4, 610–616.
2 T. Namiki, IEEE Transactions on Microwave Theory and Techniques 47 (1999), no. 10, 20032007.
3 F Zheng, Z Chen, J Zhang, IEEE Microwave and Guided Wave Letters 9 (1999), no. 11, 441–443. ??
4 B Fornberg, J Zuev, J Lee, Journal of Computational and Applied Mathematics 200 (2007), no. 1, 178–192.
5 X Shao, Thesis–Electrical Engineering–University of Maryland (2004)
6 M Lyon, O Bruno, Journal of Computational Physics 229 (2010), no. , 2009–2033
7 M Lyon, O Bruno, Journal of Computational Physics 229 (2010), no. , 3358–3381

So whats NEW?????

In Addition to Implicit Maxwell based on ADI, we Leverage

1. Method of Lines Transpose (aka Rothe's method)
    1. U Hornung, Manuscripta Mathematica, 39 (1982), no.2, 155–172
    2. Kacur, Institute of Applied Matheamtics, Comenius University Mlynska doling, 842 15 Britishava, Czenchoslovakia 1986.
    3. U Ascher, R Mattheij, R Russell, Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA, 1995. Corrected reprint of the 1988 original
    4. A Mazzia, F Mazzia, Journal of Computational and Applied Mathematics, 82 (1997), no.1, 299–311
    5. R Chapko, R Kress. Rothes, Journal of Integral Equations and Applications, 9 (1997), 47–69
    6. J Jia, J Huang, Journal of Computational Physics 227 (2008), no.3, 1739–1753
    7. M Kropinski, B Quaife, Computer and Mathematics with Applications , 61 (2011), 2346–2446
2. Multi Derivative Methods
    1. G Dahlquist, Bit Numerical Mathematics 18 (1978), no. 2, 133–136.
    2. B Ehle, , Bit Numerical Mathematics 8 (1968), no. 4, 276278.
    3. E Hairer, G Wanner, Computing (Arch. Elektron. Rechnen) 11(3), 287303 (1973)
    4. S Stavroyiannis, TE Simos, Applied Numerical Mathematics 59 (2009), no. 10, 24672474.
    5. D Seal, Y Gl, A Christlieb, *arXiv, submitted* (2013).

Last Year:

We introduced an:

- A-Stable $O(\Delta t^2)$ wave propagation.
- Developed an ADI splitting for our wave solver.
- Dirichlet, Neumann and periodic boundary conditions.
- Developed outflow based on converting spatial integral to a temporal integral.
- Developed domain decomposition–Expect REALLY good scaling
- Developed an $O(N)$ fast convolution. $CFL > 2$ beat Yee method in time to solution.

Past Four Mounts:

- Non convex complex geometry
- Extension to particle methods
- $O(N)$ A-Stable to ALL Orders (removed splitting error)

Model Forumulation

In the Lorenz gauge, the scalar and vector potentials satisfy wave equations:

$$\frac{1}{c^2}\frac{\partial^2 \phi}{\partial t^2} - \nabla^2 \phi = \rho/\epsilon_0$$
$$\frac{1}{c^2}\frac{\partial^2 \vec{A}}{\partial t^2} - \nabla^2 \vec{A} = \mu_0 \vec{J}$$

which we couple to a Lagrangian description of phase space:

$$\frac{d\vec{x}_i}{dt} = \vec{v}_i$$
$$\frac{d\vec{v}_i}{dt} = \frac{q_i}{m_i}\left(-\nabla\phi - \frac{\partial \vec{A}}{\partial t} + \vec{v}_i \times \nabla \times \vec{A}\right)$$

Time discretization: Method of Lines Transpose (MOL^T)

$$\frac{1}{c^2}\phi_{tt} - \nabla^2\phi = \frac{\rho}{\epsilon_0}$$

M. Causley, A. Christlieb, B. Ong and L. Van Groningen, Method of Lines Transpose: An Implicit Solution to the One Dimensional Wave Equation, to appear, Math. Comp.

Time discretization: Method of Lines Transpose (MOL^T)

$$\frac{1}{c^2}\phi_{tt} - \nabla^2\phi = \frac{\rho}{\epsilon_0}$$

Discretize ϕ_{tt} in time

$$\phi_{tt}(x, t_n) \approx \frac{\phi^{n+1} - 2\phi^n + \phi^{n-1}}{\Delta t^2}.$$

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The Laplacian is treated semi-implicitly using

$$\nabla^2\phi(x, t_n) \approx \nabla^2\left(\phi^n + \frac{\phi^{n+1} - 2\phi^n + \phi^{n-1}}{\beta^2}\right), \quad 0 < \beta \leq 2$$

M. Causley, A. Christlieb, B. Ong and L. Van Groningen, Method of Lines Transpose: An Implicit Solution to the One Dimensional Wave Equation, to appear, Math. Comp.

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$$\frac{\phi^{n+1} - 2\phi^n + \phi^{n-1}}{(c\Delta t^2)} - \nabla^2\left(\phi^n + \frac{\phi^{n+1} - 2\phi^n + \phi^{n-1}}{\beta^2}\right) \approx \frac{\rho^n}{\epsilon_0}.$$

M. Causley, A. Christlieb, B. Ong and L. Van Groningen, Method of Lines Transpose: An Implicit Solution to the One Dimensional Wave Equation, to appear, Math. Comp.

Time discretization: Method of Lines Transpose (MOL^T)

The semi-discrete equation is

$$\mathcal{L}_\beta \left[\phi^n + \frac{\phi^{n+1} - 2\phi^n + \phi^{n-1}}{\beta^2}\right] = -\phi^n - \left(\frac{1}{\alpha^2}\right)\frac{\rho^n}{\epsilon_0}, \qquad (1)$$

where the modified Helmholtz operator is

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

Inversion of the Helmholtz operator

$$\mathcal{L}_\beta^{-1}[\rho](x) = \int_\Omega G(x,x')\rho(x')dx' + \int_{\partial\Omega}\left[G_n\phi - G\phi_n\right]dS$$

using free space **Green's function**

$$G(x,x') = \alpha^2 \frac{e^{-\alpha|x-x'|}}{4\pi|x-x'|}.$$

The full update equation is

$$\phi^{n+1} = (2-\beta^2)\phi^n - \phi^{n-1} + \frac{\beta^2}{2}\mathcal{L}_\beta^{-1}\left[\phi^n + \frac{\rho^n}{\alpha^2\epsilon_0}\right].$$

In one spatial dimension, we instead have

$$\mathcal{L}_\beta^{-1}[\phi](x) := \underbrace{\alpha\int_a^b \phi(y)e^{-\alpha|x-y|}dy}_{\text{Particular Solution}} + \underbrace{Ae^{-\alpha(x-a)} + Be^{-\alpha(b-x)}}_{\text{Homogeneous Solution}}.$$

For delta point sources, $\mathcal{L}_\beta^{-1}$ gives an exact expression!

Theorem: This scheme is A-stable for $\beta \in (0,2]$. The A-stable scheme with the smallest error constant corresponds to $\beta = 2$.

M. Causley, A. Christlieb, Y. Guclu and E. Wolf, Method of Lines Transpose: A Fast Implicit Wave Propagator, submitted, Mathematics of Computation.

Outflow Boundary conditions

Use free space solution to write

$$A = \alpha \int_{-\infty}^{a} \phi(y) e^{-\alpha(a-y)} dy, \quad B = \alpha \int_{b}^{\infty} \phi(y) e^{-\alpha(y-b)} dy, \quad x \in [a, b].$$

Outflow boundary conditions allow the free space solution to flow out of the computational domain, without spurious reflections

$$\phi_t - c\phi_x = 0, \quad x \leq a, \quad \phi_t + c\phi_x = 0, \quad x \geq b.$$

If the initial support of ϕ is $[a, b]$, then for $t > 0$,

$$A^n = \alpha \int_{a-ct_n}^{a} e^{-\alpha(a-y)} \phi^n(y) dy, \quad B^n = \alpha \int_{b}^{b+ct_n} e^{-\alpha(y-b)} \phi^n(y) dy.$$

Considering $x < a$, we only have a left traveling wave, so $\phi(x, t) = \phi(x + ct)$. By tracing backward along a characteristic ray we find

$$\phi(a - y, t) = \phi\left(a, t - \frac{y}{c}\right), \quad y > 0.$$

Outflow Boundary conditions (cont'd.)

$$
\begin{aligned}
A^n &= \alpha \int_{a-ct_n}^{a} e^{-\alpha(a-y)} \phi(y, t_n) dy \\
&= \alpha \int_0^{c\Delta t} e^{-\alpha y} \phi^n(a-y, t_n) dy + \alpha \int_{c\Delta t}^{cn\Delta t} e^{-\alpha y} \phi^n(a-y, t_n) dy \\
&= \alpha \int_0^{c\Delta t} e^{-\alpha y} \phi^n(a-y, t_n) dy + e^{-\alpha c \Delta t} \alpha \int_0^{c(n-1)\Delta t} e^{-\alpha y} \phi^n(a-y, t_n) dy \\
&= e^{-\alpha c \Delta t} A^{n-1} + \alpha \int_0^{c\Delta t} e^{-\alpha y} \phi^n(a-y) dy.
\end{aligned}
$$

The final integral is outside the domain, but since

$$
\phi(a-y, t_n) = \phi\left(a, t_n - \frac{y}{c}\right), \quad \text{for } 0 < y < c\Delta t,
$$

the coefficient can be updated using only $\phi(a, t)$, $t \in [t_{n-1}, t_n]$.

A Novel approach: A fast algorithm in 1D

$$I[\phi](x) = \alpha \int_a^b e^{-\alpha|x-y|}\phi(y)dy$$
$$= \alpha \int_a^x e^{-\alpha(x-y)}\phi(y)dy + \alpha \int_x^b e^{-\alpha(y-x)}\phi(y)dy =: I^L + I^R$$

I^L and I^R are the "characteristics" of I, which satisfy first order IVPs

$$(I^L)'(y) + \alpha I^L(y) = \alpha u(y), \quad a < y < x, \quad I^L(a) = 0$$
$$(I^R)'(y) - \alpha I^R(y) = -\alpha u(y), \quad x < y < b, \quad I^R(b) = 0.$$

Spatial discretization of the particular solution

Define the partition of $[a, b]$ by the subintervals $[x_{j-1}, x_j]$, where $x_0 = a$, $x_N = b$. Then, using exponential recursion,

$$\begin{aligned} I^L(x_j) =& \alpha \int_a^{x_{j-1}} e^{-\alpha(x_j - y)} \phi(y) dy + \alpha \int_{x_{j-1}}^{x_j} e^{-\alpha(x_j - y)} \phi(y) dy \\ =& e^{-\alpha(x_j - x_{j-1})} I^L(x_{j-1}) + \alpha \int_{x_{j-1}}^{x_j} e^{-\alpha(x_j - y)} \phi(y) dy \end{aligned}$$

This expression is still exact, and only the remaining localized integral needs to be approximated. **The convolution is computed in $O(N)$ operations.**

$$I^L(x_j) = e^{-\alpha(x_j - x_{j-1})} I^L(x_{j-1}) + \alpha \int_{x_{j-1}}^{x_j} e^{-\alpha(x_j - y)} \phi(y) dy$$

Theorem: For consistency, approximate ϕ with splines of order ≥ 2.

Compact Simpson's rule

To be precise, $\phi(x_j + z\Delta x_j)$ is approximated by

$$p_j^{(2)}(z) = (1-z)\phi_j + z\phi_{j+1} + \left(\frac{z^2 - z}{2}\right)\Delta x_j^2 \phi''(\xi_j),$$

so that

$$\begin{aligned} I_j^L =& d_j I_{j-1}^L + a_j\phi_j + b_j\phi_{j-1} + c_j\Delta x_j^2\phi''(\xi_j) \\ I_j^R =& d_{j+1} I_{j+1}^R + a_{j+1}\phi_j + b_{j+1}\phi_{j+1} + c_{j+1}\Delta x_j^2\phi''(\xi_j), \end{aligned}$$

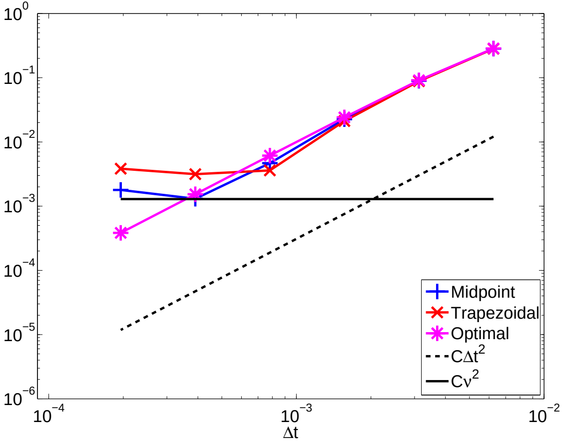
where

$$\begin{aligned} h_j =& x_j - x_{j-1}, \quad \nu_j = \alpha h_j, \quad d_j = e^{-\nu_j} \\ a_j =& 1 - \frac{1-d_j}{\nu_j} \quad b_j = -d_j + \frac{1-d_j}{\nu_j} \\ c_j =& \frac{1}{2\nu_j^2}(2(1-d_j) - \nu_j(1+d_j)). \end{aligned}$$

Remark: Same $p_j^{(2)}(z)$ for I_j^L and I_j^R for convergence as $\Delta t \to 0$.

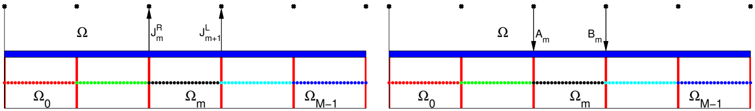
Convergence for compact Simpson's rule

Linear interpolation $p_j^{(1)}(z)$ not sufficient to ensure second order accuracy! Spatial and temporal error couple. $\nu = \frac{\Delta x}{c\Delta t}$



Domain Decomposition

The solution is computed simultaneously on a coarse and fine mesh. All communication is at coarse mesh points.



(a) Fine-Coarse Pass (b) Coarse-Fine Pass

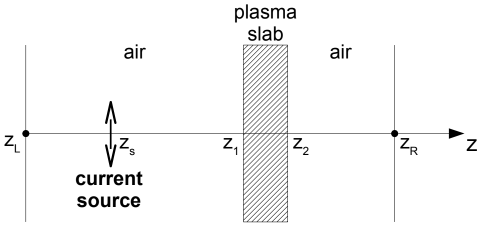
$$I^L(X_j) = e^{-\alpha(X_j - X_{j-1})} I^L(X_{j-1}) + J^L(X_j), \quad J^L(X_j) = \alpha \int_{X_{j-1}}^{X_j} e^{-\alpha(X_j - y)} \phi(y) dy$$

1. Each local particular solution on Ω_j is first computed separately.
2. The global particular solution is computed in $O(M)$ operations, using global recurrence relations.
3. Boundary conditions are imposed, translated across the coarse mesh, and communicated back to Ω_j.

1D Example: Reflectance and absorbance in a plasma slab

We study the plasma response of small amplitude waves, i.e. near-equilibrium solutions. In this regime, we may safely consider a *linear* plasma response. We further assume an non-magnetic ($B = 0$) plasma, so that the response is isotropic. Now, it is safe to consider a transverse electromagnetic mode.

$$\hat{J} = \sigma \left(\frac{\nu}{\nu + i\omega} \right) \hat{E} \quad \Longrightarrow \quad \frac{\partial J}{\partial t} + \nu J = \omega_p^2 \epsilon_0 E$$



1D Example: Reflectance and absorbance in a plasma slab

$$\frac{\partial^2 E}{\partial z^2} - \frac{1}{c^2}\frac{\partial^2 E}{\partial t^2} = \mu_0 \frac{\partial J}{\partial t}, \quad \frac{\partial J}{\partial t} + \nu J = \omega_p^2 \epsilon_0 E$$

- Unconditional stability for the fully implicit scheme

$$\mathcal{L}_\beta \left[E^n + \frac{E^{n+1} - 2E^n + E^{n-1}}{\beta^2} \right] = -E^n + \mu_0 \frac{J^{n+1} - J^{n-1}}{2\Delta t},$$

$$J^{n+1} = e^{-\nu \Delta t} J^n + \left(1 - \frac{1 - e^{-\nu\Delta t}}{\nu \Delta t}\right) E^{n+1} + \left(\frac{1 - e^{-\nu\Delta t}}{\nu \Delta t} - e^{-\nu\Delta t}\right) E^n$$

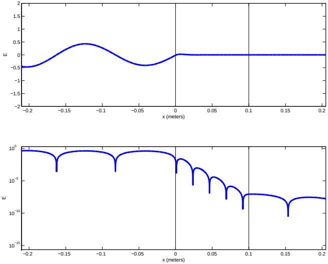
- For a semi-implicit scheme, the time step must obey $\Delta t < \frac{2\nu}{\omega_p^2}$

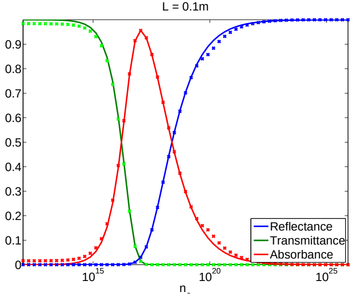
$$\mathcal{L}_\beta \left[E^n + \frac{E^{n+1} - 2E^n + E^{n-1}}{\beta^2} \right] = -E^n + \mu_0 \left(\omega_p^2 \epsilon_0 E^n - \nu J^n\right),$$

$$J^{n+1} = e^{-\nu \Delta t} J^n + \left(1 - \frac{1 - e^{-\nu\Delta t}}{\nu \Delta t}\right) E^{n+1} + \left(\frac{1 - e^{-\nu\Delta t}}{\nu \Delta t} - e^{-\nu\Delta t}\right) E^n$$

1D Example: Reflectance and absorbance in a plasma slab

Plasma reflection and transmission coefficients constructed as a function of excitation frequency ω, and plasma density n. Results agree well with those of [Verboncoeur, 2000].

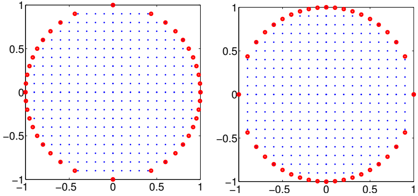




Higher Dimensions: ADI Splitting

$$\frac{1}{\alpha^2}\nabla^2 - I = \left(\frac{1}{\alpha^2}\frac{\partial^2}{\partial x^2} - I\right)\left(\frac{1}{\alpha^2}\frac{\partial^2}{\partial y^2} - I\right)\left(\frac{1}{\alpha^2}\frac{\partial^2}{\partial z^2} - I\right) + O\left(\frac{1}{\alpha^2}\right)$$

Now, each spatial differential operator is separated, and the update equation is found after sweeps along lines in each dimension. The fast 1D algorithm is used, and the **boundary conditions** are applied line-by-line.



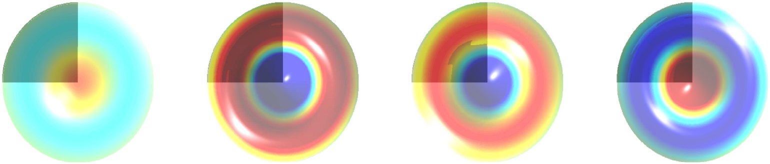
(a) x-sweep (b) y-sweep

Example 1: symmetry on a quarter circle

First, we solve the Dirichlet problem, with initial conditions

$$u(x, y, 0) = J_0\left(z_{20}\frac{r}{R}\right), \quad u_t(x, y, 0) = 0,$$

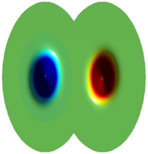
and exact solution $u = J_0\left(z_{20}\frac{r}{R}\right)\cos\left(z_{20}\frac{ct}{R}\right)$. We also use the symmetry of the mode to construct the solution restricted to the second quadrant.



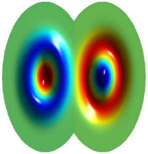
(a) $t = 0.25$ (b) $t = 0.50$ (c) $t = 0.75$ (d) $t = 1.00$

Example 2: Waves in a double-circle cavity.

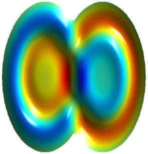
Two localized pulses are propagated through a wave guide with circular geometry. Second order convergence in space and time is observed. A highly refined reference solution is used as the "exact" solution.



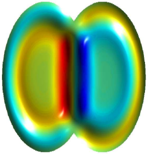
(a) $t = 0$



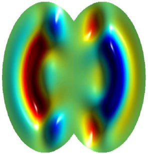
(b) $t = 0.1$



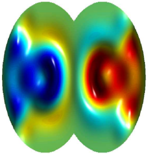
(c) $t = 0.2$



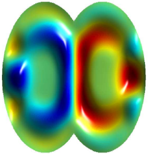
(d) $t = 0.25$



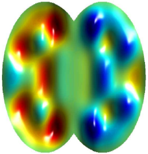
(e) $t = 0.45$



(f) $t = 0.7$



(g) $t = 0.8$



(h) $t = 1.0$

ADI with outflow

$$
\begin{aligned}
I(x,y) =& \alpha^2 \iint\limits_{\Omega_0} e^{-\alpha(|x-x'|+|y-y'|)} \phi^n(x',y') dx' dy' \\
&+ S_{\mathrm{L}}^n(y) e^{-\alpha|x-x_0|} + S_{\mathrm{R}}^n(y) e^{-\alpha|x-x_N|} \\
&+ S_{\mathrm{B}}^n(x) e^{-\alpha|y-y_0|} + S_{\mathrm{T}}^n(x) e^{-\alpha|y-y_M|}
\end{aligned}
$$

Require symmetric implementation to access both intermediate variables

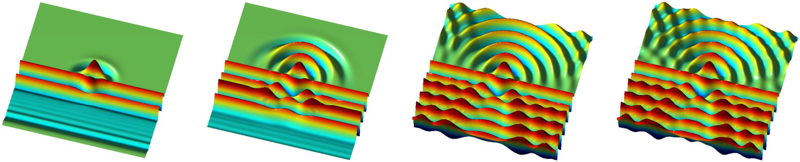
$$
w(x,y) = \alpha \int e^{-\alpha|x-x'|} \phi^n(x',y) dx', \quad v(x,y) = \alpha \int e^{-\alpha|y-y'|} \phi^n(x,y') dy'
$$

$$
S_{\mathrm{L}}^n = \int_0^{t_n} e^{-\alpha cs} w_Y(x_0, y, t_n - s) ds, \quad S_{\mathrm{R}}^n = \int_0^{t_n} e^{-\alpha cs} w_Y(x_N, y, t_n - s) ds,
$$

$$
S_{\mathrm{B}}^n = \int_0^{t_n} e^{-\alpha cs} w_X(x, y_0, t_n - s) ds, \quad S_{\mathrm{T}}^n = \int_0^{t_n} e^{-\alpha cs} w_X(x, y_M, t_n - s) ds
$$

Example 3: Periodic Slit Diffraction Grating

A preliminary test of outflow boundary conditions in higher dimensions.

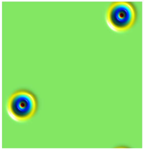


(a) $t = 0.31$ (b) $t = 0.51$ (c) $t = 1.01$ (d) $t = 2.01$

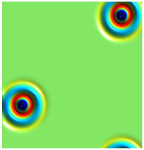
The outflow boundary conditions allow the waves to propagate outside the domain, with no visible reflections at the artificial boundaries.

Example 4: Point Sources and various BCs

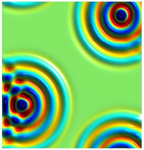
Two point-sources, located at non-mesh points, generate time-varying signals. Homogeneous Dirichlet boundary conditions are employed at $x = 0$; outflow at $x = 1$; and periodic BCs are given in the y direction. The spatial grid has 200×200 points, and $\Delta t = 0.01$.



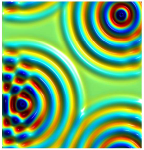
(a) $t = 0.05$

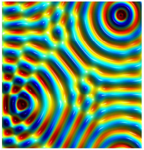


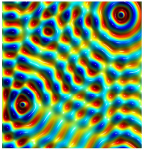
(b) $t = 0.08$



(c) $t = 0.16$

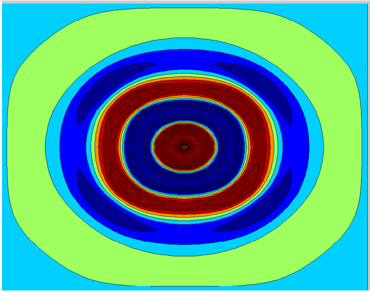






ADI Splitting ERROR

Point sources are part of plasma particle simulations.
HOWEVER: CFL of 2 with point sources in center of 80×80 mesh.



(a) 2nd order

High order solution?

Breaking the “Dahlquist barrier”

Theorem (Dahlquist's order barrier)

The order, p, of an A-stable linear muttistep method cannot exceed 2. The smallest error constant, is obtained for the trapezoidal rule, $k = 1$.

Multiderivative and *A*-stable

- **[Obreschkoff, 1940], [Turan, 1950]**, **[Stancu & Stroud, 1963], ...**
- **[Ehle, 1965]** "High order *A*-stable methods for the numerical solution of systems of D.E.'s."
- **[Hairer & Wanner, 1973]** "Multistep-multistage-multiderivative methods for ordinary differential equations."
- **[Jeltsch, 1974]** "Necessary and sufficient conditions for *A*-stability".

Our basic second order scheme is

$$u^{n+1} - (2-\beta^2)u^n + u^{n-1} = \beta^2 \mathcal{L}^{-1}\left[u^n\right] \quad 0 < \beta \leq 2$$

with

$$\mathcal{L}^{-1}[u] := \frac{\alpha}{2} \int e^{-\alpha|x-y|} u(y) dy, \quad \alpha = \frac{\beta}{c\Delta t}.$$

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Or,

$$u^{n+1} - 2u^n + u^{n-1} = -\beta^2 \mathcal{D}\left[u^n\right]$$

with

$$\mathcal{D}[u] := u - \mathcal{L}^{-1}[u].$$

Thus

$$-\beta^2 \mathcal{D}[u] \approx (c\Delta t)^2 u_{xx} + O(\Delta t^4)!$$

Let $\hat{D} = \mathcal{F}[\mathcal{D}]$. Then

$$\hat{D} = 1 - \frac{1}{1 + (k/\alpha)^2} = \frac{(k/\alpha)^2}{1 + (k/\alpha)^2} \quad \implies \left(\frac{k}{\alpha}\right)^2 = \frac{\hat{D}}{1 - \hat{D}}.$$

Using binomial series,

$$\left(\frac{k}{\alpha}\right)^{2m} = \left(\frac{\hat{D}}{1 - \hat{D}}\right)^m = \sum_{p=m}^{\infty} \binom{p-1}{m-1} \hat{D}^p$$

$$\implies \quad \left(\frac{\partial_{xx}}{\alpha^2}\right)^m = (-1)^m \sum_{p=m}^{\infty} \binom{p-1}{m-1} \mathcal{D}^p.$$

Why is this useful?

Let's expand the left hand side of the equation

$$u^{n+1} - 2u^n + u^{n-1} = 2\sum_{m=1}^{\infty} \frac{\Delta t^{2m}}{(2m)!} \left(\partial_{tt}\right)^m u^n$$

Let's expand the left hand side of the equation

$$u^{n+1} - 2u^n + u^{n-1} = 2\sum_{m=1}^{\infty} \frac{\Delta t^{2m}}{(2m)!} (\partial_{tt})^m u^n$$

But from the wave equation, $(\partial_{tt})^m = \left(c^2\partial_{xx}\right)^m$, so

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But from the wave equation, $(\partial_{tt})^m = \left(c^2\partial_{xx}\right)^m$, so

$$\begin{aligned} u^{n+1} - 2u^n + u^{n-1} &= 2\sum_{m=1}^{\infty} \frac{(c\Delta t)^{2m}}{(2m)!} (\partial_{xx})^m u^n \\ &= 2\sum_{m=1}^{\infty} \frac{\beta^{2m}}{(2m)!} \left(\frac{\partial_{xx}}{\alpha^2}\right)^m u^n \quad \left(\alpha = \frac{\beta}{c\Delta t}\right) \\ &= 2\sum_{m=1}^{\infty} \frac{\beta^{2m}}{(2m)!}(-1)^m \sum_{p=m}^{\infty} \binom{p-1}{m-1} \mathcal{D}^p[u^n]. \end{aligned}$$

This expression is exact! And, it uses recursive applications of $\mathcal{D}$ to reconstruct spatial derivatives!

$$u^{n+1} - 2u^n + u^{n-1} = 2\sum_{p=1}^{P} A_p(\beta)\mathcal{D}^p[u^n] + O\left(\Delta t^{2P+2}\right)$$

with

$$A_p(\beta) = 2\sum_{m=1}^{p}(-1)^m \binom{p-1}{m-1}\frac{\beta^{2m}}{(2m)!}.$$

This family of schemes are stable for any Δt, and some range of β.

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

P	1	2	3	4	5
Order	2	4	6	8	10
β_{max}	2	1.4840	1.2345	1.0795	0.9715

Table : The scheme is stable for $\beta \le \beta_{max}$, satisfying $S(\beta_{max}, 1) = 4$.

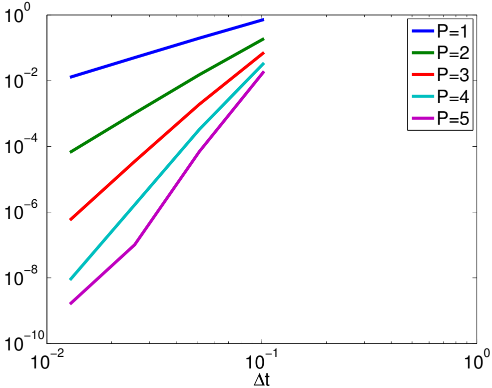


Figure : Convergence in the L^2-norm of a 1d standing wave, with Dirichlet boundary conditions. The spatial resolution is held fixed at $\Delta x = 0.0001$.

In 2D

$$u^{n+1} - 2u^n + u^{n-1} = \sum_{p=1}^{\infty} \sum_{m=1}^{p} (-1)^m \frac{2\beta^{2m}}{(2m)!} \binom{p-1}{m-1} \bar{D}_{xy}^m \mathcal{D}_{xy}^{p-m} [u^n].$$

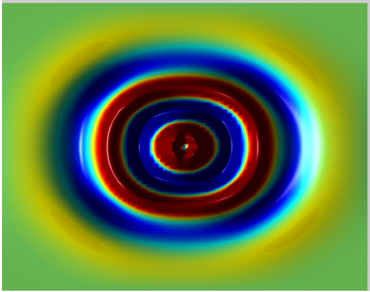
with

$$\mathcal{D}_{xy} := 1 - \mathcal{L}_x^{-1} \mathcal{L}_y^{-1}, \quad \bar{D}_{xy} := \mathcal{D}_{xy} - (1 - \mathcal{L}_x^{-1})(1 - \mathcal{L}_y^{-1})$$

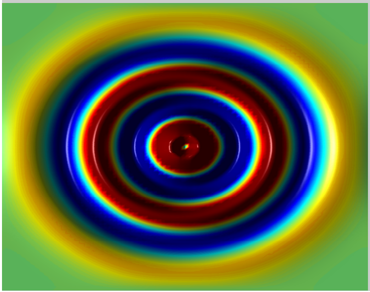
and

$$\mathcal{L}_x^{-1}[u] = \frac{\alpha}{2} \int e^{-\alpha|x-x'|} u(x', y) dx',$$
$$\mathcal{L}_y^{-1}[u] = \frac{\alpha}{2} \int e^{-\alpha|y-y'|} u(x, y') dy'.$$

Higher order removes anisotropy due to ADI splitting

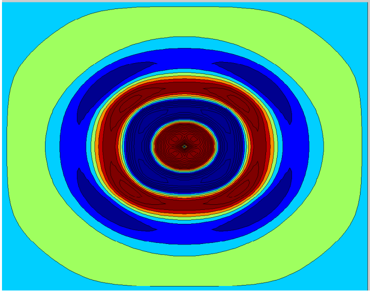


(a) 2nd order

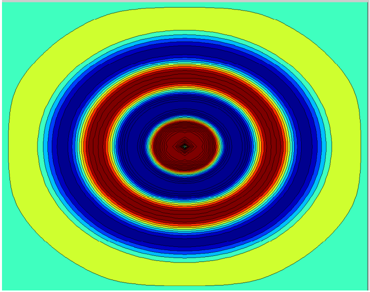


(b) 4th order

Higher order removes anisotropy due to ADI splitting

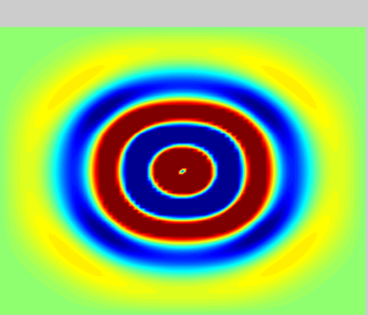


(a) 2nd order

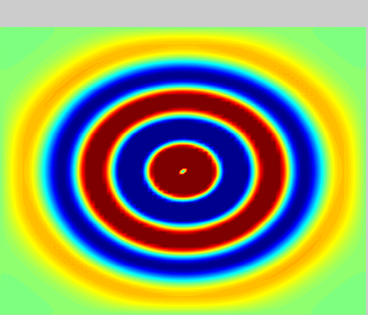


(b) 4th order

Higher order removes anisotropy due to ADI splitting



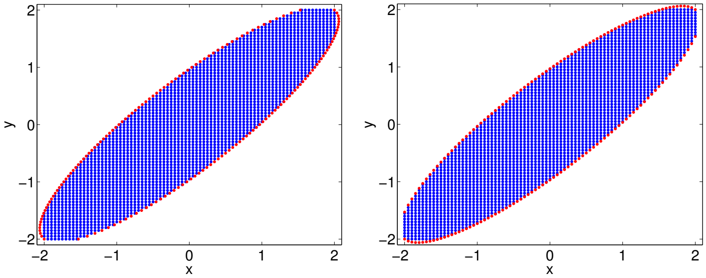
(a) 2nd order



(b) 4th order

A Gaussian initial condition is placed inside the ellipse, whose boundary is given by

$$C = \left\{ (x, y) : \left(\frac{x+y}{4} \right)^2 + (x-y)^2 = 1 \right\}.$$



(a) x-sweep

(b) y-sweep

Figure : Discretization of the ellipse, showing the regular Cartesian points (blue), and the additional boundary points (red) for the x and y sweeps.

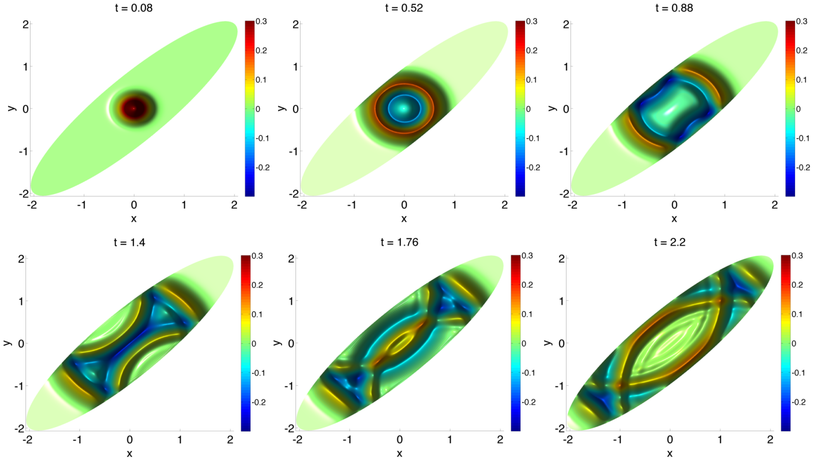


Figure : Time evolution of a Gaussian field through an elliptical cavity.

Conclusions

- Developed a novel implicit Maxwell solver (IMS), which is second order and A-stable.
- Combines ADI splitting and a fast $O(N)$ 1D algorithm for speed.
- Accurately addresses complex geometries.
- Implementation of periodic, outflow, Dirichlet and Neumann BC's
- Exact spatial treatment of point sources
- Incorporated domain decomposition, and uneven mesh spacing.
- Higher order methods in space and time

Future Directions

- Parallel Implementation of Domain Decomposition in higher dimensions
- Couple the IMS to a Vlasov solver
- Fast implementation of particle sums (P3M) using modified kernel
- Higher order outflow

Thank you!

References

[1] Causley, M., Christlieb, A., Ong, B., and Van Groningen, L., "*Method of Lines Transpose: An Implicit Solution to the One Dimensional Wave Equation*", *to appear*, Mathematics of Computation, 2013.

[2] Causley, M., Güçlü, Y., Christlieb, A. and Wolf, E., "*Method of Lines Transpose: A Fast Implicit Wave Propagator*", *submitted*, Mathematics of Computation, 2013.

[3] Causley, M., and Christlieb, A., "*Higher Order A-stable Schemes for the Wave Equation Using a Recursive Convolution Approach*", *submitted*, SIAM Numerical Analysis, 2013.

1D PIC – Quasi-electrostatic Model

For simplicity, we drop $\vec{A}$ and consider a quasi-electrostatic model, valid when $v/c << 1$:

$$\frac{1}{c^2}\frac{\partial^2 \phi}{\partial t^2} - \nabla^2 \phi = \rho/\epsilon_0$$

$$\frac{d\vec{x}_i}{dt} = \vec{v}_i, \quad \frac{d\vec{v}_i}{dt} = -\frac{q_i}{m_i}\nabla\phi, \quad \rho = \sum_{i=1}^{N_p} q_i S(\vec{x} - \vec{x}_i)$$

$S(\vec{x})$: particle shape function

1D Particle-in-Cell (PIC) Method

Based on this model,

Wave Equation Solver $+$ **Particle Mover** $\rightarrow$ **PIC Method**

The success of the method relies on

- the use of diffusive version of the wave solver, and
- the exact integration of particle shapes.

Exact Integration of Particle Shapes

For typical particle shapes $S(x)$, the integrals

$$I[S](x) = \alpha \int e^{-\alpha|x-y|} S(y) dy$$

can be computed exactly. This replaces the charge accumulation step of typical electrostatic PIC codes.

Exponential recursion allows for the exact computation of $I[\rho](x) = \alpha \int e^{-\alpha|x-y|} \rho(y) dy$ in $O(N)$ operations.

On a uniform grid with linear particle shapes, one evaluation of an exponential function is required per particle per time step.

Numerical Results

We consider several standard electrostatic test problems, posed with periodic boundary conditions in a domain of length L. Time quantities are scaled by the plasma frequency ω_p, and spatial quantities by the Debye length λ_D. We use N_p electrons with a fixed uniform neutralizing background charge distribution.

In all problems, we use 100 cells in the domain, and take $\Delta t = 0.1$, and set $c = 1000$. The initial electron distribution $f(x, v, t = 0)$ is specified in each problem. Start up values for the wave solver are provided through finite difference Poisson solves.

Numerical Results - Cold Plasma Oscillation

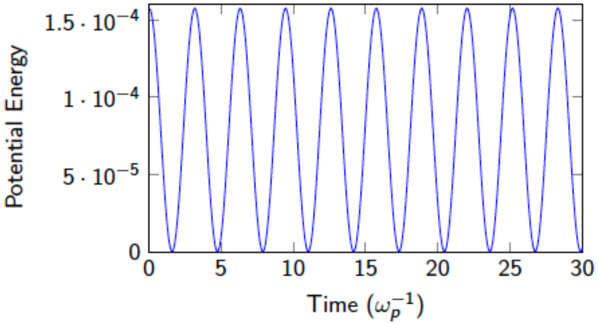


Figure : IC: $f(x, v, t = 0) = \delta(v)(1 + 0.01\sin(2\pi x/L))$ Parameters: $L = 2\pi$, $N_p = 10000$

Numerical Results - Landau Damping

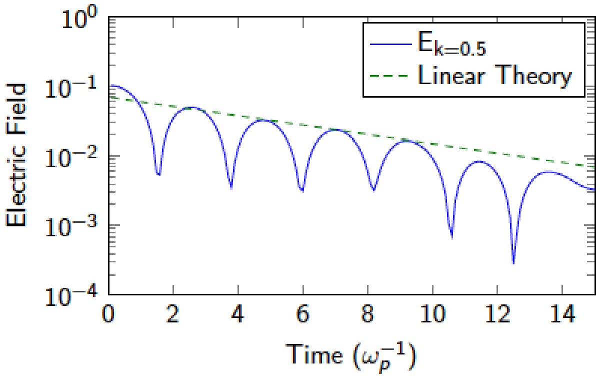


Figure : IC: $f(x, v, t = 0) = \tilde{f}(v)(1 + 0.1\sin(2\pi x/L))$. $\tilde{f}(v)$ is a Maxwellian.
Parameters: $L = 4\pi$, $N_p = 300000$

Numerical Results - Two Stream Instability

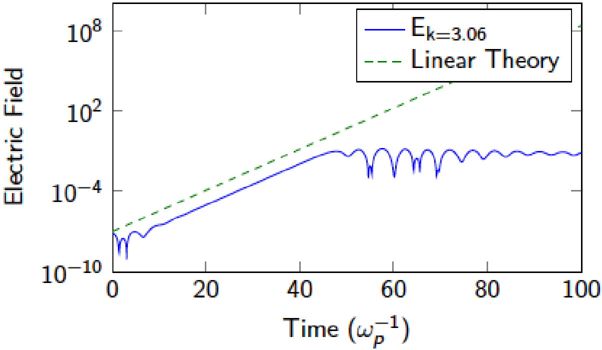


Figure : IC: $f(x, v, t = 0) = (\delta(v - 0.2) + \delta(v + 0.2))(1 + 0.001 \sin(2\pi x/L))$. Parameters: $L = 2\pi/3.06$, $N_p = 30000$. Linear theory: $k = 3.06$ mode of largest instability growth

Future work: fast particle sums

$$S(x,y) = \sum_i w_i e^{-\alpha|x-\xi_i|-\alpha|y-\eta_i|}$$

We will have many more source points (ξ_i, η_i) than grid points (x_j, y_k), so the particle sum must be done efficiently. For fixed k,

$$\sum_i w_i e^{-\alpha|x_j-\xi_i|-\alpha|y_k-\eta_i|} = S_{jk}^{BL} + S_{jk}^{BR} + S_{jk}^{TL} + S_{jk}^{TR}$$

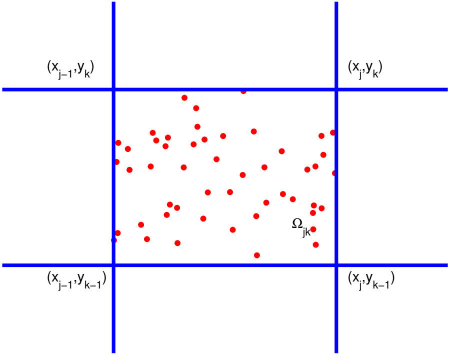
For instance, S_{jk}^{BL} is the sum of all particles to the bottom-left of the point (x_j, y_k). This quantity can be updated recursively by

$$\begin{aligned} S_{jk}^{BL} = {} & G_{jk}(x_{j-1}, y_k) S_{j-1,k}^{BL} + G_{jk}(x_j, y_{k-1}) S_{j,k-1}^{BL} \\ & - G_{jk}(x_{j-1}, y_{k-1}) S_{j-1,k-1}^{BL} + \sum_{\Omega_{jk}} w_i G_{jk}(\xi_i, \eta_i) \end{aligned}$$

where $G_{jk}(x,y) = e^{-\alpha(x_j - x + y_k - y)}$.

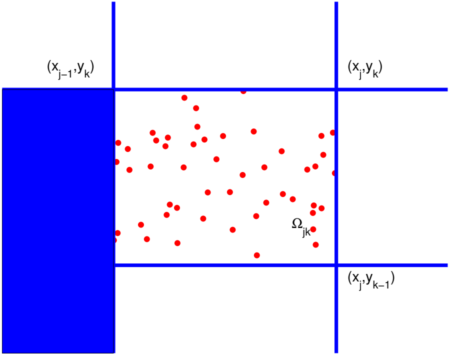
$$S_{jk}^{BL} =$$

The update for S_{jk}^{BL} proceeds from bottom to top, then from left to right.



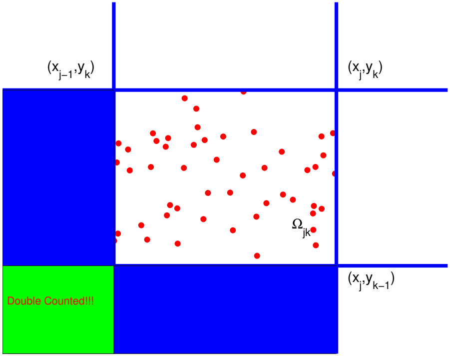
$$S_{jk}^{BL} = G_{jk}(x_{j-1}, y_k) S_{j-1,k}^{BL}$$

The update for S_{jk}^{BL} proceeds from bottom to top, then from left to right.



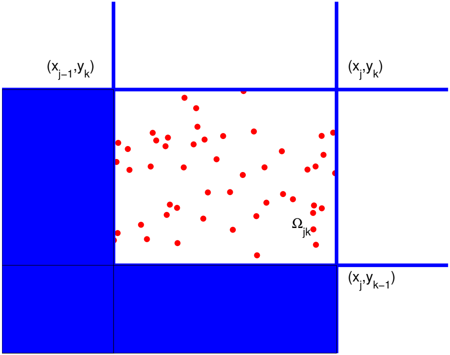
$$S_{jk}^{BL} = G_{jk}(x_{j-1}, y_k) S_{j-1,k}^{BL} + G_{jk}(x_j, y_{k-1}) S_{j,k-1}^{BL}$$

The update for S_{jk}^{BL} proceeds from bottom to top, then from left to right.



$$S_{jk}^{BL} = G_{jk}(x_{j-1}, y_k)S_{j-1,k}^{BL} + G_{jk}(x_j, y_{k-1})S_{j,k-1}^{BL} - G_{jk}(x_{j-1}, y_{k-1})S_{j-1,k-1}^{BL}$$

The update for S_{jk}^{BL} proceeds from bottom to top, then from left to right.



$$S_{jk}^{BL} = G_{jk}(x_{j-1}, y_k) S_{j-1,k}^{BL} + G_{jk}(x_j, y_{k-1}) S_{j,k-1}^{BL} - G_{jk}(x_{j-1}, y_{k-1}) S_{j-1,k-1}^{BL} + \sum_{\Omega_{jk}} w_i G_{jk}(\xi_i, \eta_i)$$

The update for S_{jk}^{BL} proceeds from bottom to top, then from left to right.