Combining
Time and Mimetic Spatial Discretizations

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Connections in Geometric Numerical Integration and Structure-Preserving Discretization

Introduction

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Showing that energy is conserved requires the use of adjoint operators.

K.S. Yee, 1966 and A.A. Samarski, 1977

Non Mimetic Finite Differences

Let $f = f(x)$ be a smooth function, $\Delta x > 0$ and then define $f_i = f(x_i)$. The second-order accurate cental finite difference approximation of the first derivative is

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This is **NOT** mimetic. Multidimensional analogs cause problems like far field oscillations for finite differences and hourglass modes for finite elements.

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$\vec{\nabla}$, $\vec{\nabla}\times$, $\vec{\nabla}\cdot$ is and *exact sequence* of operators.

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$O^{**} = O$. Does this require that the dual of a dual grid be the grid?

Fix The First Derivative

Define the left and right differences:

$$L\,f_i = \frac{f_i - f_{i-1}}{\Delta x}\,, \quad R\,f_i = \frac{f_{i+1} - f_i}{\Delta x}\,.$$

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$$L\,R\,f_i = R\,L\,f_i = \frac{f_{i+1} - 2\,f_i + f_{i-1}}{\Delta x}$$

The adjoint $L^* = -R$ so $-L\,R$ and $-R\,L$ are positive operators.

Material Properties

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$$= - \int \mathbf{K} \vec{\nabla} T \, \vec{\nabla} T \, dV = - \langle \vec{\nabla} T \,, \vec{\nabla} T \rangle$$

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Accuracy? Groundwater modeling?

Harmonic Oscillator

Harmonic oscillator:

$$u'' + \omega^2 u = 0\,.$$

Here $u = u(t)$ is a smooth function of time t and $u' = du/dt$, $u'' = d^2u/dt^2$ and $\omega > 0$ is a real constant.

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This is conserved quantity because

$$E' = u''\,u' + \omega^2 u\,u' = \left(u'' + \omega^2 u\right)\,u' = 0\,.$$

First Order System

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Note that C is a constant multiple of the energy E.

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Given $u(0)$ and $u'(0)$ set $u^0 = u(0)$ and $u^1 = u(0) + \Delta t\,u'(0)$ and then

$$u^{n+1} = (2 - (\omega\Delta t)^2)u^n - u^{n-1}, n \geq 1\,.$$

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Stability for $\Delta t < 2/\omega$!! Accuracy for $\Delta t < \frac{2\pi}{5}/\omega$??

Phase Plane

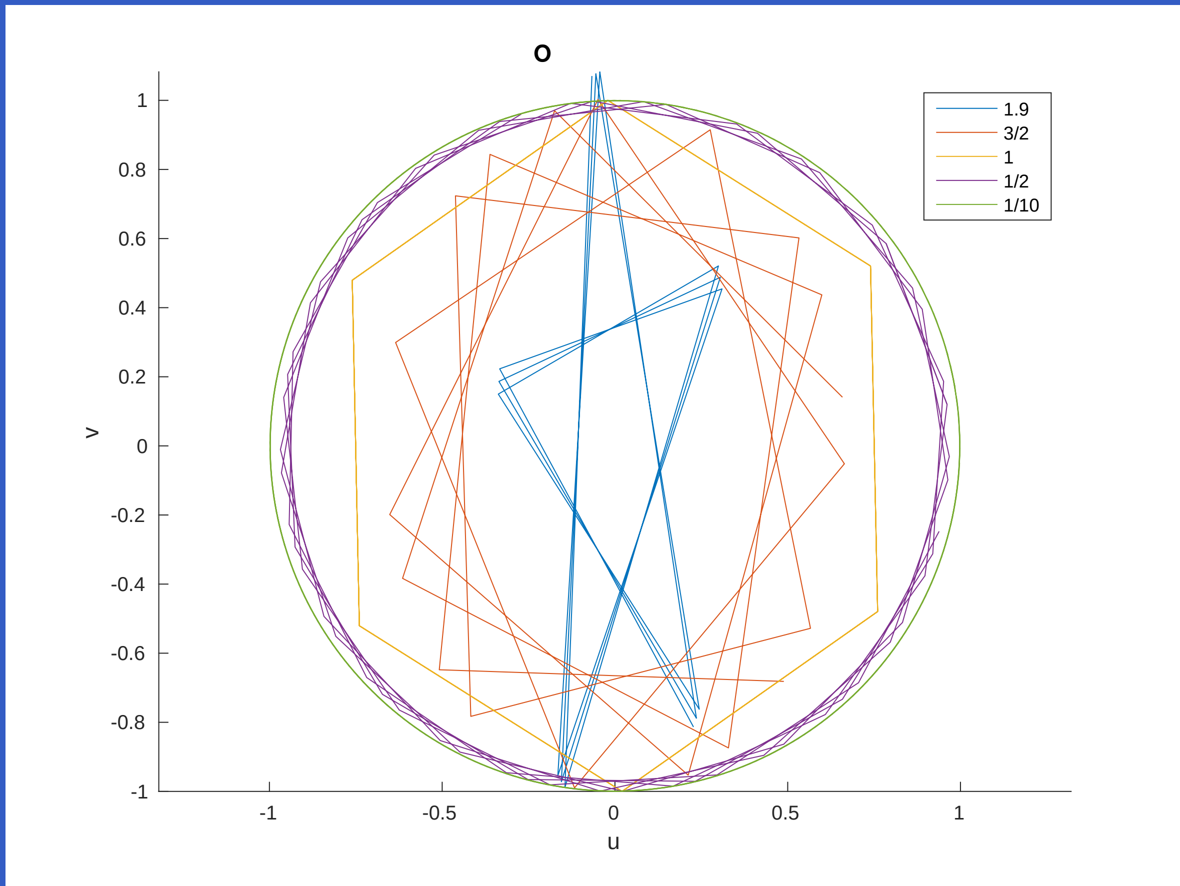

Figure 1: $\omega = 1$ and $\Delta t = 1.9,\ 3/2,\ 1,\ 1/2,\ 1/10$

Staggered Time

Primary grid: $t^n = n\,\Delta t\,.$ Dual grid: $t^{n+1/2} = (n + 1/2)\,\Delta t.$

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The leap-frog discretization:

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$$u^0 = u(0)\,, \quad v^{1/2} = u'(0)/\omega\,.$$

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Given u^0 and $v^{1/2}$ update using

$$\boxed{u^{n+1}} = u^n + \Delta t\,\omega\, v^{n+1/2}\,, \qquad v^{n+3/2} = v^{n+1/2} - \Delta t\,\omega\,\boxed{u^{n+1}}.$$

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Same as the discretization of the second order equation.

Conserved Quantities

$$C^n = \frac{1}{2}\left(\left(1-\alpha^2\right)\left(u^n\right)^2 + \left(\frac{v^{n+1/2} + v^{n-1/2)}}{2}\right)^2\right);$$

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- stable for $\alpha = \omega\,\Delta t/2 < 1$
- explicit
- second order accurate

Systems of ODEs

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where $f = f(t) \in X$ and $g = g(t) \in Y$.

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Here X and Y are linear spaces with inner product $\langle f, g \rangle$ and norm $||f||^2 = \langle f, f \rangle$. Also A is a linear map from X to Y and A^* is the adjoint of A: $X \stackrel{A}{\to} Y\,; \quad Y \stackrel{A^*}{\to} X\,.$

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$$C(t) = \frac{1}{2}\left(||f(t)||^2 + ||g(t)||^2\right)$$

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Conserved quantity:

$$C^n = ||f^n||^2 - \frac{\Delta t^2}{4}\, ||A^*\, f^n||^2 + \left|\left| \frac{g^{n+1/2} + g^{n-1/2}}{2} \right|\right|^2$$

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Stability:

$$||C^n|| \geq \left(1 - \frac{\Delta t^2}{4}\, ||A^*||^2\right) ||f^n||^2 + \left|\left| \frac{g^{n+1/2} + g^{n-1/2}}{2} \right|\right|^2$$

1D-Wave

The 1D wave equation is

$$u_{tt} = c^2 \, u_{xx} \; ,$$

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The initial conditions for this equation are $u(0, x)$ and $u_t(0, x)$.

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Where $c > 0$ and $u = u(t, x)$ is a smooth real valued function of the real variables x and t such that $u(t, \pm\infty) = 0$. Also $u_t = \partial u / \partial t$, $u_x = \partial u / \partial x$, $u_{tt} = \partial^2 u / \partial t^2$, and $u_{xx} = \partial^2 u / \partial x^2$.
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First order system:

$$u_t = c \, v_x \, , \quad v_t = c \, u_x \, .$$

Energy 1D-Wave

The inner product and norm are

$$\langle f, g\rangle = \int_{-\infty}^{\infty} f(x)\, g(x)\, dx\,, \quad ||f||^2 = \langle f, f\rangle\,.$$

If $f(\pm\infty) = 0$ and $g(\pm\infty) = 0$ then integration by parts gives $\langle f', g\rangle = \langle f, -g'\rangle$, so

$$\frac{\partial}{\partial x}^* = -\frac{\partial}{\partial x}\,.$$

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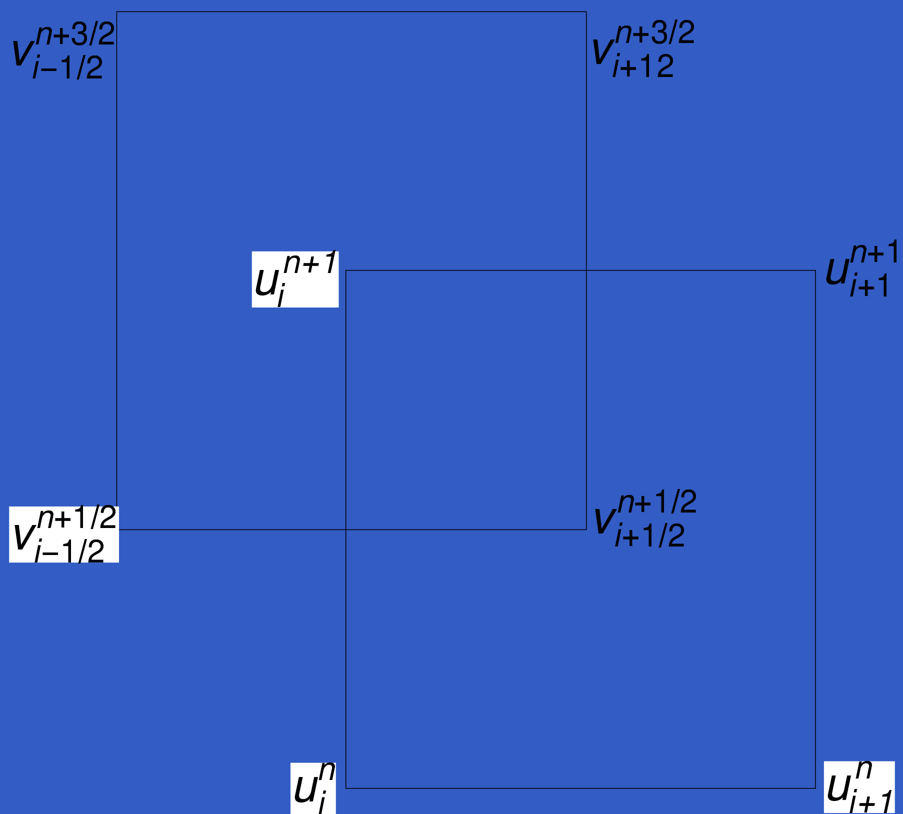
So the wave equation has the same form as the equations in the previous sections.

Energy and conserved quantity:

$$E = \frac{1}{2}\left(\langle u_t\,,\, u_t \rangle + c^2 \langle u_x\,,\, u_x \rangle\right)\,, \quad C = \frac{1}{2}\left(\langle u, u \rangle + \langle v, v \rangle\right)$$

Space-Time Staggered Grid



Discrete Wave Equation

Primary and dual grid points:

$$(t^n, x_i) = (n \triangle t, i \triangle x) \ ,$$

$$\left(t^{n+1/2}, x_{i+1/2}\right) = ((n+1/2) \triangle t, (i+1/2) \triangle x) \ ,$$

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\end{aligned}
$$

The discretized first order system

$$
\begin{aligned}
\frac{u_i^{n+1} - u_i^n}{\triangle t} &= c \, \frac{v_{i+1/2}^{n+1/2} - v_{i-1/2}^{n+1/2}}{\triangle x} \\
\frac{v_{i+1/2}^{n+1/2} - v_{i+1/2}^{n-1/2}}{\triangle t} &= c \, \frac{u_{i+1}^n - u_i^n}{\triangle x}
\end{aligned}
$$

Conserved Quantity

A conserved quantity is:

$$C(n) = ||u^n||^2 - \left(\frac{c\,\triangle t}{2\,\triangle x}\right)^2 ||\delta u^n||^2 + \left|\left|\frac{v^{n+1/2} + v^{n-1/2}}{2}\right|\right|^2 .$$

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The difference operators:

$$\delta(u)_{i+1/2} = u_{i+1} - u_i\,, \quad \delta(v)_i = v_{i+1/2} - v_{i-1/2}\,.$$

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Because $||\delta|| = 2$ the conserved quantity will be positive if

$$c\,\frac{\triangle t}{\triangle x} < 1\,,$$

which is the Courant-Friedrics-Lewy condition for stability.

3 Dimensions

Continuum exact sequence:

$$
\begin{array}{ccccccc}
\overset{0}{H_P} & \xrightarrow{\vec{\nabla}} & \overset{1}{H_C} & \xrightarrow{\vec{\nabla}\times} & \overset{2}{H_S} & \xrightarrow{\vec{\nabla}\cdot} & \overset{3}{H_V} \\
a \Big\downarrow & & \mathbf{A} \Big\downarrow & & \Big\uparrow \mathbf{B} & & \Big\uparrow b \\
\underset{3}{H_V} & \xleftarrow{\vec{\nabla}\cdot} & \underset{2}{H_S} & \xleftarrow{\vec{\nabla}\times} & \underset{1}{H_C} & \xleftarrow{\vec{\nabla}} & \underset{0}{H_P}
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\end{array}
$$

Laplacian: $\Delta = \dfrac{1}{a}\,\vec{\nabla}\cdot\,\mathbf{A}\,\vec{\nabla} f$

curl curl: $\mathbf{A}^{-1}\,\vec{\nabla}\times\,\mathbf{B}^{-1}\,\vec{\nabla}\times\,\vec{v}$

useful: $\mathbf{B}\,\vec{\nabla}\,b^{-1}\,\vec{\nabla}\cdot\,\vec{w}$

Units for Maxwell's Equations

quantity	units	name
$\vec{B}$	$1/d^2$	magnetic flux
$\vec{H}$	$1/d$	magnetic field
μ	$1/d$	permittivity
$\vec{D}$	$1/d^2$	electric displacement
$\vec{E}$	$1/d$	electric field
ϵ	$1/d$	permeability tensor
$\vec{J}$	$1/d^2$	current
$\vec{\nabla}\times$	$1/d$	curl operator
$\partial/\partial t$	$1/t$	time derivative

Maxwell's Equations

$$\frac{\partial \vec{B}}{\partial t} + \vec{\nabla} \times \vec{E} = 0 \,, \qquad \frac{\partial \vec{D}}{\partial t} - \vec{\nabla} \times \vec{H} = \vec{J} \,.$$

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$$\vec{B} = \mu\,\vec{H}\,, \qquad \vec{D} = \epsilon\,\vec{E}\,.$$

Maxwell's Equations

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$$\langle\vec{v}_1,\vec{v}_2\rangle_\epsilon = \int_{\mathbb{R}^3} \epsilon\,\vec{v}_1\cdot\vec{v}_2 dx\,dy\,dz\,, \quad \langle\vec{v}_1,\vec{v}_2\rangle_\mu = \int_{\mathbb{R}^3} \mu\,\vec{v}_1\cdot\vec{v}_2\,dx\,dy\,dz\,.$$

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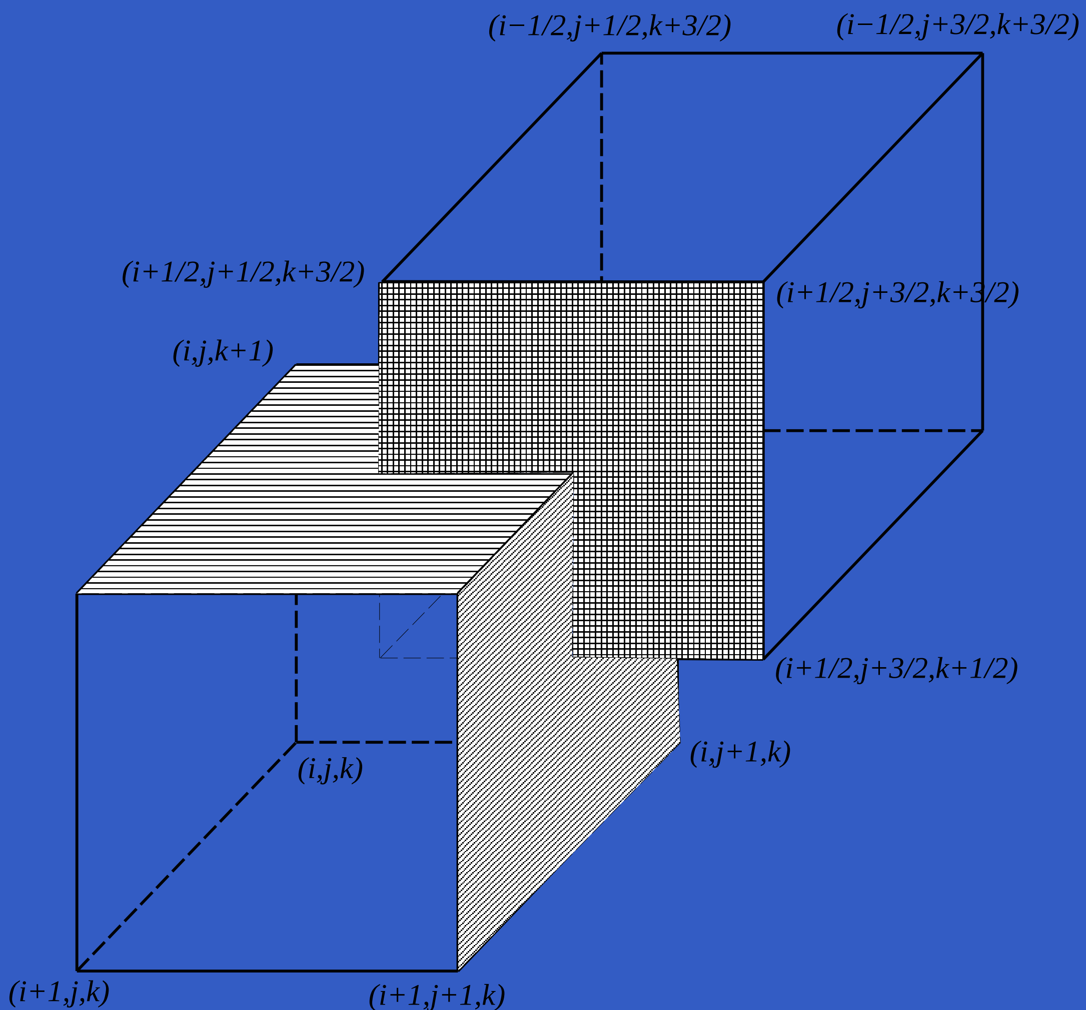
Conserved quantity: $C = \dfrac{\langle \vec{E}, \vec{E} \rangle_\epsilon + \langle \vec{H}, \vec{H} \rangle_\mu}{2}$

3d Staggered Grid



3D Discrete Functions

units	primal	dual	units
1	$s_{i,j,k}$	$d^\star_{i,j,k}$	$1/d^3$
$1/d$	$t_{i+\frac{1}{2},j,k}$ $t_{i,j+\frac{1}{2},k}$ $t_{i,j,k+\frac{1}{2}}$	$n^\star_{i+\frac{1}{2},j,k}$ $n^\star_{i,j+\frac{1}{2},k}$ $n^\star_{i,j,k+\frac{1}{2}}$	$1/d^2$
$1/d^2$	$n_{i,j+\frac{1}{2},k+\frac{1}{2}}$ $n_{i+\frac{1}{2},j,k+\frac{1}{2}}$ $n_{i+\frac{1}{2},j+\frac{1}{2},k}$	$t^\star_{i,j+\frac{1}{2},k+\frac{1}{2}}$ $t^\star_{i+\frac{1}{2},j,k+\frac{1}{2}}$ $t^\star_{i+\frac{1}{2},j+\frac{1}{2},k}$	$1/d$
$1/d^3$	$d_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}$	$s^\star_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}$	1
units	primal	dual	units

Gradient and Star Gradient

$$(\mathcal{G}s)_{i+\frac{1}{2},j,k} \equiv \frac{s_{i+1,j,k} - s_{i,j,k}}{\triangle x} \;;$$

$$(\mathcal{G}s)_{i,j+\frac{1}{2},k} \equiv \frac{s_{i,j+1,k} - s_{i,j,k}}{\triangle y} \;;$$

$$(\mathcal{G}s)_{i,j,k+\frac{1}{2}} \equiv \frac{s_{i,j,k+1} - s_{i,j,k}}{\triangle z} \;.$$

$$(\mathcal{G}^\star s^\star)_{i,j+\frac{1}{2},k+\frac{1}{2}} \equiv \frac{s^\star_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} - s^\star_{i-\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}}{\Delta x};$$

$$(\mathcal{G}^\star s^\star)_{i+\frac{1}{2},j,k+\frac{1}{2}} \equiv \frac{s^\star_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} - s^\star_{i+\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2}}}{\Delta x};$$

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Exact Sequence 3D

$$
\begin{array}{ccccccc}
S_{\mathcal{N}} & \xrightarrow{\mathcal{G}} & V_{\mathcal{E}} & \xrightarrow{\mathcal{R}} & V_{\mathcal{F}} & \xrightarrow{\mathcal{D}} & S_{\mathcal{C}} \\
a \downarrow & & \mathbf{A} \downarrow & & \mathbf{B} \uparrow & & b \uparrow \\
S_{\mathcal{C}^\star} & \xleftarrow{\mathcal{D}^\star} & V_{\mathcal{F}^\star} & \xleftarrow{\mathcal{R}^\star} & V_{\mathcal{E}^\star} & \xleftarrow{\mathcal{G}^\star} & S_{\mathcal{N}^\star}
\end{array}
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\end{array}$$

$$\mathcal{G}c \equiv 0\,, \quad \mathcal{R}\mathcal{G} \equiv 0\,, \quad \mathcal{D}\mathcal{R} \equiv 0\,, \quad \mathcal{G}^\star c \equiv 0\,, \quad \mathcal{R}^\star\mathcal{G}^\star \equiv 0\,, \quad \mathcal{D}^\star\mathcal{R}^\star \equiv 0\,.$$

Adjoint Operators

$$\langle s1, s2 \rangle_{\mathcal{N}} = \sum_{i,j,k} a_{i,j,k}\, s1_{i,j,k}\, s2_{i,j,k} \triangle x \triangle y \triangle z \,.$$

$$\langle s1^\star, s2^\star \rangle_{\mathcal{N}^\star} = \sum_{i,j,k} b_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}\, s1^\star_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}\, s2^\star_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} \triangle x \triangle y \triangle z \,.$$

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$$\langle \mathbf{A}\, \mathcal{G}\, s, \vec{n}^{\star} \rangle_{\mathcal{F}^{\star}} = -\langle s, \frac{1}{a}\, \mathcal{D}^{\star}\, \vec{n}^{\star} \rangle_{\mathcal{N}}$$

$$\langle \mathbf{B}^{-1}\, \mathcal{R}\vec{t}, \vec{t}^{\star} \rangle_{\mathcal{E}^{\star}} = +\langle \vec{t}, \mathbf{A}^{-1} \mathcal{R}^{\star} \vec{t}^{\star} \rangle_{\mathcal{E}}$$

$$\langle b^{-1}\, \mathcal{D}\vec{n}, s^{\star} \rangle_{\mathcal{N}^{\star}} = -\langle \vec{n}\,, \mathbf{B}\mathcal{G}^{\star}\, \vec{s}^{\star} \rangle_{\mathcal{F}}$$

Discrete Maxwell's Equations

This is the Yee discretization (1966) that has has become the FDTD method!!

$$\frac{\vec{E}^{n+1} - \vec{E}^{n}}{\triangle t} = \epsilon^{-1}\,\mathcal{R}^{\star}\vec{H}^{n+\frac{1}{2}}\,, \qquad \frac{\vec{H}^{n+\frac{1}{2}} - \vec{H}^{n-\frac{1}{2}}}{\triangle t} = -\mu^{-1}\,\mathcal{R}\vec{E}^{n}\,.$$

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Conserved quantity:

$$C_{n+1/2} = \left\|\frac{\vec{E}^{n+1} + \vec{E}^{n}}{2}\right\|_{\mathcal{E}}^{2} + \left\|\vec{H}^{n+1/2}\right\|_{\mathcal{E}^{\star}}^{2} - \frac{\Delta t^{2}}{4}\left\|\epsilon^{-1}\,\mathcal{R}^{\star}\,\vec{H}^{n+1/2}\right\|_{\mathcal{E}}^{2}\,.$$

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Big success!!!

Positive Solutions

Solutions of the transport and diffusion equations should be positive because they are things like density $\rho(x,t) \geq 0$.

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Conservation does not use a quadratic form but is given by the total amount of material so

$$\int_{-\infty}^{\infty} \rho(x,t)\,dx = \text{constant.}$$

Transport

Assume $v = v(x)$ is a given velocity and then

$$\frac{\partial \rho}{\partial t} + \frac{\partial \, v \, \rho}{\partial x} = 0 \, ,$$

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Units dictate that we use a cell centered discretization as is done in finite volumes:

$$\frac{\rho_{i+\frac{1}{2}}^{n+3/2} - \rho_{i+\frac{1}{2}}^{n+\frac{1}{2}}}{\Delta t} + \frac{v_{i+1}\,\rho_{i+\frac{1}{2}}^{n+\frac{1}{2}} - v_i\,\rho_{i-\frac{1}{2}}^{n+\frac{1}{2}}}{\Delta x} = 0\,.$$

Upwind

$$\text{if } v_i \geq 0 \text{ then} \quad \rho_{i-\frac{1}{2}}^{n+3/2} = \rho_{i-\frac{1}{2}}^{n+3/2} - v_i \frac{\Delta t}{\Delta x} \rho_{i-\frac{1}{2}}^{n+\frac{1}{2}} \;;$$

$$\rho_{i+\frac{1}{2}}^{n+3/2} = \rho_{i+\frac{1}{2}}^{n+3/2} + v_i \frac{\Delta t}{\Delta x} \rho_{i-\frac{1}{2}}^{n+\frac{1}{2}} \;;$$

$$\text{if } v_i \leq 0 \text{ then} \quad \rho_{i-\frac{1}{2}}^{n+3/2} = \rho_{i-\frac{1}{2}}^{n+3/2} - v_i \frac{\Delta t}{\Delta x} \rho_{i+\frac{1}{2}}^{n+\frac{1}{2}} \;;$$

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If $V = \max(|v_i|)$ then to keep $\rho \geq 0$ it must be that $V \frac{\Delta t}{\Delta x} \leq 1$.

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So all is OK!! This solution is very diffusive:(

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Forward time centered space finite difference discretization:

$$\frac{\rho_{i+\frac{1}{2}}^{n+\frac{1}{2}} - \rho_{i+\frac{1}{2}}^{n-\frac{1}{2}}}{\Delta t} = \frac{1}{\Delta x}\left(D_{i+1} \frac{\rho_{i+\frac{3}{2}}^{n-\frac{1}{2}} - \rho_{i+\frac{1}{2}}^{n-\frac{1}{2}}}{\Delta x} - D_i \frac{\rho_{i+\frac{1}{2}}^{n-\frac{1}{2}} - \rho_{i-\frac{1}{2}}^{n-\frac{1}{2}}}{\Delta x} \right)$$

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This algorithm will preserve positive solutions for

$$\left(D_{i+1} + D_i \right) \frac{\Delta t}{\Delta x^2} \leq 1 \,,$$

which is the standard stability constraint for this discretization.

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Search for “arXiv Stanly Steinberg” (arXiv:1605.08762v2 [math.NA].)

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Discretizations are second order accurate, stable and explicit.

Conserved quantities converge to the continuum energy.

For Maxwell's, divergence of $\vec{B}$ and $\vec{D}$ are constant is trivial.

I studied rectangualr grids. Will work for logically rectangular grids!

Higher order is not difficult.

There are papers on mimetic methods for general grids.

Finite elements using differential geometery are strong competitors.

Search for "arXiv Stanly Steinberg" (arXiv:1605.08762v2 [math.NA].)

Email me for codes for rectangular grids.