Explicit Time Mimetic Discretizations *

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Abstract

This paper is part of a program to combine a staggered time and staggered spatial discretization of continuum mechanics problems so that any property of the continuum that is proved using vector calculus can be proven in an analogous way for the discretized system. We require that the discretizations be second order accurate and have a conserved quantity that approximates the energy for the system and guarantees stability for a reasonable constraint on the time step. We also require that the discretization is time explicit so as to avoid the solution of large system of possibly nonlinear algebraic equations. The well known Yee grid discretization of Maxwell’s equations is the same as our discretization and is an early example of using a staggered space and time grid.

To motivate our discussion we begin by studying the staggered time or leapfrog discretization of the harmonic oscillator and use this to introduce the modification of the energy that is conserved. Next we use systems of linear equations to motivate the definition of the modified energy for more complex systems of ordinary differential equations and then apply our ideas to the scalar wave equation in one spatial dimension. We finish by discretizing the three dimensional scalar wave and Maxwell’s equations. Because the spatial discretization is mimetic, we obtain that the divergence of the electric and magnetic fields are constant when there are no sources. Using the mimetic properties the proof of this trivial and is essentially the same as in the continuum.

Key Words: mimetic discretization, leapfrog, energy conservation
1 Introduction

For an introduction to the relationship of vector calculus to differential forms see the notes [2].

Mimetic discretizations have been used extensively to create simulation programs for problems in continuum mechanics, see [21] and the volume [19] in which this paper is published. In [30] it is shown that, in the spatial context, one can introduce a staggered grid discretization of the gradient, curl and divergence that satisfy most and perhaps all of the important properties of the continuum operators. For example the discrete divergence of the discrete curl operator is identically zero. Another is that the adjoint of the discrete gradient is the minus the discrete divergence.

However, for time dependent properties like the conservation of energy, many discretizations of time will not preserve the property although sometimes they will preserve an approximation of the property [14, 13, 9, 10, 29]. It appears that all of the energy preserving methods are implicit.

Because of the properties of mimetic discrete gradient, curl and divergence and the explicit leapfrog discretization time the derivation of the conservation of energy for several different systems can be modified to produce a conservation law that is a second order accurate approximation of the continuum energy. The new conserved quantity will be written as

\[ Q(t) = E(t) - \Delta t^2 R(t), \]

where \( E \) is a constant multiple of the classical energy, \( \Delta t \) is the discrete time step and \( R \) is positive. The minus sign introduces a constraint on the time step that is less restrictive than a modest accuracy constraint.

Our main result is that simulations show that the three dimensional scalar wave equation and Maxwell’s equations without sources, \( Q(t) \) is constant to less than one part in \( 10^{15} \). Additionally, for the scalar wave equation the curl of the velocity is constant to less than one part in \( 10^{13} \) and the divergence of the electric and magnetic fields are constant to less than one part in \( 10^{13} \), see ScalarWave.m and Maxwell.m. For an idea of the problems that discretizing Maxwell’s equations see [7].

The leapfrog discretization requires that the differential equations be written as a system of first order equations. The examples we study are wave equations in the sense that all solutions of the ordinary or partial differential equation will be oscillatory or constant in time. So the differential equations have time reversal symmetry.

In Section 2 the discussion begins with the harmonic oscillator for which it is well known that the implicit Crank-Nicolson discretization conserves energy; see Appendix A. For complex three dimensional nonlinear systems of partial differential equations, implicit methods can be expensive and it is possible that explicit time discretizations provide significant advantages. So to illustrate the ideas used here, the energy for harmonic oscillator is modified to make a conserved quantity in discrete time. Simulation show that this new quantity is conserved to one part in \( 10^{15} \), see StaggeredOscillator.m. Additionally, if the frequency of the oscillator is one then the time step must be less than 2 for stability. To obtain reasonably
accurate solutions the time step must be less than $1/10$ as shown in Figure 1. Consequently
the stability constraint does not play a significant role. Section A contains some additional
comments about the Crank-Nicolson discretization of the harmonic oscillator.

In Section 3, conserved quantities for possibly infinite systems of first order ordinary
differential equations that have form analogous to the 3D scalar wave equation and Maxwell’s
equations are derived. These conserved quantities provide significant insight in how to find
and understand conserved quantities for partial differential equations. Also the equations
studied are more general than linear Hamiltonian systems which is important for extending
the harmonic oscillator methods to partial differential equations. Simulations show that the
new quantity is conserved to about 2 parts in $10^{15}$, see SystemsODE.m.

In Section 4, the scalar wave equation in time and one space dimension is written as a
system of two first order equations and discretized using a grid staggered in space and time.
This is basically a tutorial in how to do staggered space time discretization like those used in
Yee methods [41]. The conserved quantities are extended to cover this 1D case. Simulation
show that the new quantities is conserved to one part in $10^{14}$, see OneDWave.m.

In Section 5 we introduce a double exact sequence of continuum differential operators
which will be important for understanding discretizations using staggered grids. This concept
from differential geometry is critical for understanding mimetic spatial discretizations. We
introduce spatial units (meters, feet, · · · ) of the dependent variables and use them to greatly
simplify the understanding how to create mimetic discretizations compared to the discussion
in 30.

In Section 6 we introduce primal and dual staggered grids (as in [41]) and show how to
discretize the gradient, curl and divergence on such grids as in 30. Because of the dual grids
we end up two versions of these difference operators that are best understood using a double
exacted sequence analogous to that used for the continuum operators. Recently the paper
22 used a dual grid differential form method to discretize the Navier-Stokes Equations.

In Section 7 we show how to create conserved quantities for the scalar wave equation
that are constant to one part in $10^{15}$, see ScalarWave.m. We also show that the curl of the
velocity field is constant to one part in $10^{13}$.

In Section 8 we show how to create a conserved quantity for Maxwell’s equations that is
constant to one in $10^{15}$, and also show that the divergence of the electric and magnetic fields
are constant to one part in $10^{13}$, see Maxwell.m.

One complexity of mimetic spatial discretizations is caused by having primary and dual
grids. In fact we can interchange the primary and dual grids and not change the discretiza-
tion. This is what leads to there being a primary gradient, curl, and divergence and dual
gradient, curl and divergence. We label the dual operators with a star *. This complexity
was already present in the paper by Yee [41] which has evolved into the FDTD discretization
method [40].

As we proceed, we will discover that there are several minor problems that need to
resolved. For example our second order equations are not exactly equivalent to first order
system that we change them to. Additionally, for the discrete equations there are problems
in converting the initial data for the second order equations to data for the first order
equations. Additionally, because our equations are linear if they conserve some quantity, they will conserve infinitely many quantities and in thus we have a choice in what the conserved quantity we study.

This paper was inspired by the paper [39] and [41]. We note that in [33] (see equation (45)) the same stability constraint was found as the one in this paper for conserving the classical energy but modifying the discretization of Maxwell’s equations. In [11] an implicit (ADI) method is developed that has a modified energy that is similar to ours but the added term has a plus sign. For a finite element approach that produce many of the same results that are in this paper see [36, 4].

There has been substantial effort made in creating discretizations for continuum mechanics problems that exactly preserve energy and other important properties. The paper [32] gives an overview of energy conserving methods for Navier-Stokes equations and develops some implicit Runge-Kutta methods for doing this. The thesis [5] address energy conservation for turbulent flows. For a differential forms approach to discretization see [27, 37] and additionally for multisymplectic time integration approach to Maxwell’s equations see [35]. For two dimensional problems see [6, 26, 25, 31, 8, 23]. The papers [38, 39] take a novel approach to finding discrete models. For the latest, see the minisimposium at a recent SIAM meeting [34].

1.1 Notes

For function depending on three spatial variables and time, the spatial variables will be discretized using mimetic finite differences as described in [30] while time variable will be discretized using the well known leapfrog finite differences.

The extension of ideas closely related to the work here to logically rectangular grids in 2-D is described in [16, 17].
2 The Harmonic Oscillator

To motivate the results for the three dimensions scalar wave equation and Maxwell’s equations, conserved quantities that depend on the time step are derived for finite difference discretizations of the simple harmonic oscillator. First the second-order harmonic oscillator equation is discretized and then a conserved quantity is derived. Next the oscillator equation is written as a first order system of ODEs and then discretize using a staggered time grid and two similar conserved quantities are derived. The first section in [3] has a complementary discussion of energy conservation for the harmonic oscillator.

Appendix A reviews the implicit Crank-Nicholson discretization of the oscillator which conserves a natural discretization of the continuum energy and that the methods used in [39] produce a discretization equivalent to the Crank-Nicholson method.

2.1 The Harmonic Oscillator and Conserved Quantities

The linear harmonic oscillator equation is given by

\[ u'' + \omega^2 u = 0, \]

where \( u = u(t) \) is a smooth function of time \( t \) and \( u' = du/dt, u'' = d^2u/dt^2 \) and \( \omega > 0 \) is a real constant. The total energy or Hamiltonian which is the sum of the kinetic and potential energies is

\[ E = \frac{(u')^2 + (\omega u)^2}{2}. \]

This is conserved quantity because

\[ E' = (u'' u' + \omega^2 u u') = (u'' + \omega^2 u) u' = 0. \]

To use a staggered time or leapfrog discretization, the oscillator equation is written as a first order system by introducing \( v = v(t) \) and requiring

\[ u' = \omega v, \quad v' = -\omega u. \quad (2.1) \]

The minus sign can be put in either equation. The energy is a constant multiple of the quantity \( C = C(t) \) where

\[ C = \frac{1}{2} (u^2 + v^2). \quad (2.2) \]

This quantity is conserved because

\[ C' = uu' + vv' = u\omega v - v\omega u = 0. \]

Note that \( C = E/\omega^2 \). The condition that \( \omega > 0 \) and not that \( \omega \geq 0 \) is important because for \( \omega = 0 \) the second order equation has the solutions \( u(t) = t \) for which the energy is unbounded. However, for \( \omega = 0 \) the system only has constant solutions which have bounded energy. Also because the system is linear with constant coefficients, the time derivatives of \( u \) and \( v \) also satisfy the system thus creating an infinity of conserved quantities.
2.2 Discretizing the Second Order Oscillator Equation

If $\Delta t > 0$ then a standard discretization of the second order oscillator equation using the discrete times $t^n = n \Delta t$, $-\infty < n < \infty$ is

$$
\frac{u^{n+1} - 2u^n + u^{n-1}}{\Delta t^2} + \omega^2 u^n = 0.
$$

Given the two initial conditions $u(0)$ and $u'(0)$ set $u^0 = u(0)$ and $u^1 = u(0) + \Delta t u'(0)$. The discrete solution is then

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

A natural proposal for a second-order accurate discrete conserved quantity is

$$
C^n = (u^n)^2 + \left(\frac{u^{n+1} - u^{n-1}}{2 \omega \Delta t}\right)^2.
$$

A little algebra shows that $C^n$ is not conserved. However this computation shows that

$$
C^n = \left(1 - \left(\frac{\omega \Delta t}{2}\right)^2\right)(u^n)^2 + \left(\frac{u^{n+1} - u^{n-1}}{2 \omega \Delta t}\right)^2
$$

is conserved. The program Oscillator2ndOrder.m produced Figure 1 confirming that the algorithm is stable for $0 < \Delta t/\omega < 2$ and that $C^n$ is constant to less than one part in $10^{10}$.

It is important that the constraint $\Delta t/\omega < 2$ is less restrictive than requiring an accurate solution and thus there seems to be no advantage to using a discretization that is stable for all $\Delta t$.

Figure 1: Phase plane plots for the second order harmonic oscillator model with $\omega = 1$ and $\Delta t = 3/2, 1, 1/2, 1/10$. 
2.3 Staggering the Time Discretization

A time staggered grid is used to discretize the first order system \( u^{n+1} - u^n = \omega v^{n+1/2} \) and \( v^{n+3/2} - v^{n-1/2} = -\omega u^n \), where \( \Delta t > 0 \) and \(-\infty < n < \infty\) is an integer. The staggered or leap-frog discretization of the harmonic oscillator is then given by

\[
\frac{u^{n+1} - u^n}{\Delta t} = \omega v^{n+1/2}, \quad \frac{v^{n+1/2} - v^{n-1/2}}{\Delta t} = -\omega u^n, \tag{2.3}
\]

The minus sign can be put in either equation, but it is important to have an \( \omega \) in both equations. As before, the initial conditions \( u(0) \) and \( u'(0) \) are given and then \( u^0 = u(0) \) and

\[
\omega v^{1/2} = \frac{u^1 - u^0}{\Delta t} \approx u'(0),
\]

that is, \( v^{1/2} = u'(0)/\omega \). The division by \( \omega \) will cause problems later. The update algorithm starts with \( u^0 \) and \( v^{1/2} \) and then for \( n \geq 0 \)

\[
u^{n+1} = u^n + \Delta t \omega v^{n+1/2}, \quad v^{n+3/2} = v^{n+1/2} - \Delta t \omega u^{n+1}.
\]

Note that the second equation depends on the update in the first equation, so the order of evaluation is critical.

This staggered grid discretization gives two standard single grid discretization of the second order oscillator equation:

\[
\frac{u^{n+2} - 2 u^{n+1} + u^n}{\Delta t^2} + \omega^2 u^{n+1} = 0; \quad \frac{v^{n+3/2} - 2 v^{n+1/2} + v^{n-1/2}}{\Delta t^2} + \omega^2 v^{n+1/2} = 0.
\]

So the solution of the fractional step methods will be identical to the solution of the second order equations.

Again a simple proposed conserved quantity for \( u \) is

\[
C^n = \frac{1}{2} \left( (u^n)^2 + \left( \frac{v^{n+1/2} + v^{n-1/2}}{2} \right)^2 \right), \tag{2.4}
\]

A little algebra gives

\[
C^{n+1} - C^n = \frac{\omega^2 \Delta t^2}{4} \left( (u^{n+1})^2 - (u^n)^2 \right).
\]

So \( C^n \) is not conserved. However, set

\[
\alpha = \frac{\omega \Delta t}{2},
\]

and then the following two quantities are conserved:

\[
C^n = \frac{1}{2} \left( (1 - \alpha^2) (u^n)^2 + \left( \frac{v^{n+1/2} + v^{n-1/2}}{2} \right)^2 \right); \tag{2.5}
\]

\[
\alpha = \frac{\omega \Delta t}{2},
\]
\[ C^{n+1/2} = \frac{1}{2} \left( \left( \frac{u^{n+1} + u^n}{2} \right)^2 + (1 - \alpha^2) \left( v^{n+1/2} \right)^2 \right). \] (2.6)

The important properties for the staggered scheme is that it is explicit, second order accurate and stable for \( \omega \Delta t/2 < 1 \). By modifying the discretization, a similar result was obtained in [33], Equation 45, for the Yee time discretization of Maxwell’s equations.

The code StaggeredOscillator.m confirms that the two energies are constant to one part in \( 10^{15} \). The phase plane plots for the staggered grid and the second order equation are identical. The code also estimates that for \( \omega = 1 \), \( \Delta t < 2 \) is required for stability, but for such a large \( \Delta t \) the numerical solution is very inaccurate, as made clear in Figure 1.

### 2.4 Summary

If conserved quantities for the harmonic oscillator are allows to depend on \( \Delta t \) then it is possible to derive conserved quantities that converges quadratically to the energy of the continuum differential equation. The restriction on \( \Delta t \) to keep the conserved quantity positive is less stringent than the restriction for reasonably accurate solutions. All discretizations considered are second order accurate.
3 Systems of Ordinary Differential Equations

The next task is to consider a special class of systems of linear ordinary differential equations that are wave equations. Here the conservation laws are easy to find by following the harmonic oscillator example. xxx but there are some issues with unbounded solutions and initial conditions.

3.1 Continuous Time

Let $X$ and $Y$ be linear spaces (finite or infinite dimensional). It is important that we are not assuming that $X$ and $Y$ have the same dimension. If $f$ and $g$ are in $X$ then their inner product is $\langle f, g \rangle$ and the norm of $f$ is given by $||f||^2 = \langle f, f \rangle$, with the same notation for $Y$. Let $A$ be a linear operator mapping $X$ to $Y$ with adjoint $A^*$. This is summarized by

$$X \xrightarrow{A} Y, \quad Y \xrightarrow{A^*} X,$$

and if $f \in X$ and $g \in Y$ then

$$\langle Af, g \rangle = \langle f, A^* g \rangle.$$

Next, if $f = f(t) \in X$ and $g = g(t) \in Y$ then a generalization of the harmonic oscillator is given by

$$f' = A g, \quad g' = -A^* f,$$

or in matrix form

$$\begin{bmatrix} f' \\ g' \end{bmatrix} = \begin{bmatrix} 0 & A \\ -A^* & 0 \end{bmatrix} \begin{bmatrix} f \\ g \end{bmatrix}.$$  \hfill (3.1)

Because the matrix

$$\begin{bmatrix} 0 & A \\ -A^* & 0 \end{bmatrix}$$

is skew adjoint, it must have purely imaginary spectra and the solutions of this system must be made up of oscillatory waves and possibly constant solutions. In particular all solutions are bounded in $t$. Both $f$ and $g$ are solutions of a second order linear differential equation:

$$f'' + A^* Af = 0; \quad g'' + AA^* g = 0.$$

The main difference between the system of equations (3.1) and the system (2.1) for the harmonic oscillator is that is was assumed that $\omega \neq 0$ while here $A$ is not assumed to be invertible. The analogous operators for the scalar wave equation and Maxwell’s equations are also not invertible.

If $f \in X$ and $g \in Y$ then

$$\langle A^* Af, f \rangle = \langle Af, Af \rangle = \langle f, A^* Af \rangle$$

$$\langle A A^* g, g \rangle = \langle A^* g, A^* g \rangle = \langle g, A A^* g \rangle.$$
Consequently both $AA^*$ and $A^*A$ are self-adjoint positive operators, but they may not be positive definite. Also if $h \neq 0$ and $Ah = 0$ then $g(t) = th$ is an unbounded solution solution of the second equation while if $A^*h = 0$ then $f(t) = th$ is an unbounded solution of the first equation. For this $f(t)$ the system becomes $h = Ag(t), \quad g'(t) = 0$. So $g(t) = k$ a constant and then $\langle h, h \rangle = \langle h, Ak \rangle = \langle A^*h, k \rangle = 0$, that is $h = 0$ and then $f(t) = 0$ and $g(t) = k$ and $Ak = 0$. So the unbounded solution of the second order equation is not a solution of the system, an advantage of using the system. If $f$ and $g$ are vectors of the same length and $A$ is invertible then the system and second order equations are consistent.

There is also a problem with the initial conditions for the system and the second order equations. If $A$ is an $n$ by $m$ matrix, then $A^*$ is $m$ by $n$ matrix and consequently $AA^*$ is an $n$ by $n$ matrix and $A^*A$ is an $m$ by $m$ matrix. So the first of the second order equation needs $2n$ initial conditions, and the second of the second-order equations needs $2m$ initial conditions. The system needs $n + m$ initial conditions. If $n = m$ then the number of initial conditions are the same for all three variants of the ordinary differential equations. If $n \neq m$, then the three formulations of the ODE are not equivalent! The $n \neq m$ is far more analogous to the situation for the scalar wave and Maxwell’s equations than the $n = m$ case.

### 3.2 Continuous Time Conserved Quantities

In the previous section it was assumed that that $\omega$ was nonzero equations could be multiplied and divided by $\omega$. Here it is not assumed that $A$ or $A^*$ are invertible, so the choice of a conserved quantity need to be a bit more careful:

\[
C(t) = \frac{1}{2} (||f(t)||^2 + ||g(t)||^2),
\]

which is analogous to (2.2). Then the time derivative is

\[
C'(t) = \langle f'(t), f(t) \rangle + \langle g'(t), g(t) \rangle = \langle Ag(t), f(t) \rangle + \langle -A^*f(t), g(t) \rangle = 0,
\]

so this quantity is conserved.

For the second order equations, an analog of the total energy that is the sum of the kinetic plus the potential energy is given by

\[
E(t) = \frac{1}{2} \left( ||f'(t)||^2 + ||A^*f(t)||^2 \right)
= \frac{1}{2} \left( ||Ag(t)||^2 + ||g'(t)||^2 \right)
= \frac{1}{2} \left( ||f'(t)||^2 + ||g'(t)||^2 \right), \quad (3.2)
\]

is conserved because if $f, g$ are a solutions of the system then so are $f'$ and $g'$. Note that the linearly growing solution has constant energy but $C(t)$ is unbounded.

The $C(t)$ type conserved quantities will used from now on.
3.3 Staggered Time Discretization

A leapfrog discretization for the first order system is
\[
\frac{f_{n+1} - f^n}{\Delta t} = A g_{n+1/2}, \quad \frac{g_{n+1/2} - g_{n-1/2}}{\Delta t} = -A^* f^n.
\]

Assuming that \(f^0\) and \(g^{1/2}\) are given then for \(n \geq 0\) the leapfrog time stepping scheme is
\[
f_{n+1} = f^n + \Delta t A g_{n+1/2}, \quad g_{n+3/2} = g_{n+1/2} - \Delta t A^* f^{n+1}.
\]

Again note that the order of evaluation is important.

If \(f(0)\) and \(f'(0)\) are given, then
\[
A g^{1/2} = f'(0) - \frac{\Delta}{2} A A^* f(0),
\]

need to be solved for \(g^{1/2}\). If \(A\) is not invertible then it may not be possible to solve this equation and then system is not consistent with the second order equation. However, if \(f(0)\) and \(g(0)\) are given then
\[
\frac{g_{1/2} - g^0}{\Delta t/2} \approx -A^* f^0,
\]

and then
\[
g^{1/2} = g^0 - \frac{\Delta t}{2} A^* f^0.
\]

Both \(f\) and \(g\) satisfy a second order difference equation. Also a second order average is important for computing conserved quantities. For \(f\)
\[
\frac{f_{n+1} - 2f^n + f^{n-1}}{\Delta t^2} = -A A^* f^n,
\]
and for \(g\)
\[
\frac{g_{n+3/2} - 2g_{n+1/2} + g_{n-1/2}}{\Delta t^2} = -A^* A g_{n+1/2}.
\]
\[
\frac{g_{n+3/2} + 2g_{n+1/2} + g_{n-1/2}}{4} = g_{n+1/2} - \frac{\Delta t^2}{4} A^* A g_{n+1/2}.
\]

For the equation for \(f\) it is usual to specify \(f(0)\) and \(f'(0)\) and the set \(f^0 = f(0)\) and \(f^1 \approx f(0) + \Delta t f'(0)\) with a similar specification for \(g\).

When comparing this discretization to the simple oscillator discretization it is important that \(\omega > 0\), while here one or both or the operators \(A\) and \(A^*\) may not be invertible.
3.4 Discrete Time Conserved Quantities

To show that $A$ not being invertible is not serious problem a detailed derivation of the conservation laws that are analogs of (2.6) and (2.5) are given. Let

$$C_1^{n+1/2} = \left| \frac{f^{n+1} + f^n}{2} \right|^2,$$

$$C_2^{n+1/2} = \left| g^{n+1/2} \right|^2,$$

$$C_3^{n+1/2} = \Delta t^2 \left| A g^{n+1/2} \right|^2.$$

As before compute:

$$C_1^{n+1/2} - C_1^{n-1/2} = \langle f^{n+1} + 2 f^n + f^{n-1}, f^{n+1} - f^{n-1} \rangle$$

$$= \langle f^n - \frac{\Delta t^2}{4} A A^* f^n, f^{n+1} - f^{n-1} \rangle;$$

$$C_2^{n+1/2} - C_1^{n-1/2} = \langle g^{n+1/2} + g^{n-1/2}, g^{n+1/2} - g^{n-1/2} \rangle$$

$$= \langle g^{n+1/2} + g^{n-1/2}, -\Delta t A^* f^n \rangle$$

$$= -\Delta t \langle A g^{n+1/2} + A g^{n-1/2}, f^n \rangle$$

$$= -\Delta t \langle f^{n+1} - f^{n-1}, f^n \rangle$$

$$= \langle -f^n, f^{n+1} - f^{n-1} \rangle;$$

$$C_3^{n+1/2} - C_1^{n-1/2} = \Delta t^2 \langle A g^{n+1/2} - A g^{n-1/2}, A g^{n+1/2} + A g^{n-1/2} \rangle$$

$$= \Delta t^2 \langle A \left( g^{n+1/2} - g^{n-1/2} \right), \frac{f^{n+1} - f^{n-1}}{\Delta t} \rangle$$

$$= \Delta t^2 \langle -\Delta t A^* f^n, \frac{f^{n+1} - f^{n-1}}{\Delta t} \rangle$$

$$= -\Delta t^2 \langle A A^* f^n, f^{n+1} - f^{n-1} \rangle.$$

Consequently $C = C_1 + C_2 - C_3/4$ is a conserved quantity:

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

This implies that

$$C^{n+1/2} \geq \left| \frac{f^{n+1} + f^n}{2} \right|^2 + \left( 1 - \frac{\Delta t^2}{4} \left| A \right|^2 \right) \left| g^{n+1/2} \right|^2.$$
Consequently $C^{n+1/2} \geq 0$ for $\Delta t$ sufficiently small provided $||A||$ is finite.

Next let

$$C_1^n = \left\| \frac{g^{n+1/2} + g^{n-1/2}}{2} \right\|^2,$$

$$C_2^n = ||f^n||^2,$$

$$C_3^n = \Delta t^2 ||A^* f^n||^2.$$

$$C_1^{n+1} - C_1^n = \left\langle \frac{g^{n+3/2} + 2g^{n1/2} + g^{n-1/2}}{4}, g^{n+3/2} - g^{n-1/2} \right\rangle$$

$$= \left\langle g^{n+1/2} - \frac{\Delta t^2}{4} A^* A g^{n+1/2}, g^{n+3/2} - g^{n-1/2} \right\rangle.$$

$$C_2^{n+1} - C_2^n = \langle f^{n+1} - f^n, f^{n+1} + f^n \rangle$$

$$= \langle \Delta t A g^{n+1/2}, f^{n+1} + f^n \rangle$$

$$= \Delta t \langle g^{n+1/2}, A^* f^{n+1} + A^* f^n \rangle$$

$$= \Delta t \langle g^{n+1/2}, g^{n+3/2} - g^{n-1/2} \frac{\Delta t}{\Delta t} \rangle$$

$$= \langle -g^{n+1/2}, g^{n+3/2} - g^{n-1/2} \rangle.$$

$$C_3^{n+1} - C_3^n = \Delta t^2 \langle A^* f^{n+1} - A^* f^n, A^* f^{n+1} + A^* f^n \rangle$$

$$= \Delta t^2 \langle A^* f^{n+1} - A^* f^n, \frac{g^{n+3/2} - g^{n-1/2}}{\Delta t} \rangle$$

$$= \Delta t^2 \langle \Delta t A^* A g^{n+1/2}, g^{n+3/2} - g^{n-1/2} \frac{\Delta t}{\Delta t} \rangle$$

$$= \Delta t^2 \langle A^* A g^{n+1/2}, g^{n+3/2} - g^{n-1/2} \rangle.$$

Consequently $C^n = C_1^n + C_2^n - C_3^n/4$ is a conserved quantity:

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

This implies that

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

so $||C^n||$ is positive for sufficiently small $\Delta t$.

Program SystemsODEs.m tests these conservation laws for $A$ a $2 \times 3$ random matrix showing that the energies are constant with an error less than one part in $10^{14}$.
4 The Wave Equation in 1D

Let $u = u(t, x)$ be a smooth real valued function of the real variables $x$ and $t$ such that $u(t, \pm \infty) = 0$. Then let $u_t = \partial u/\partial t$, $u_x = \partial u/\partial x$, $u_{tt} = \partial^2 u/\partial t^2$, and $u_{xx} = \partial^2 u/\partial x^2$. The 1D wave equation is then

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

where $c > 0$. The initial conditions for this equation are $u(0, x)$ and $u_t(0, x)$. This equation can also be written as a system

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

(4.1)

where again $v$ is smooth and $v(t, \pm \infty) = 0$. The initial conditions are $u(0, x)$ and $v(0, x)$. As before $v$ also satisfies a second order wave equation

$$v_{tt} = c^2 v_{xx}.$$

The inner product of two functions $f = f(x)$ and $g = g(x)$ is

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

If $f(\pm \infty) = 0$ and $g(\pm \infty) = 0$ then integration by parts gives $\langle f', g \rangle = \langle f, -g' \rangle$, so if $A = \partial/\partial x$ then $-A^* = A$. So the wave equation has the same form as the equations in the previous sections.

The usual energy $E = E(t)$ for the wave equation is the kinetic plus the potential energies:

$$E = \frac{1}{2} \int_{\infty}^{-\infty} \left( u_t^2 + c^2 u_x^2 \right) \, dx.$$

Use integration by parts to see that

$$E' = \int_{\infty}^{-\infty} \left( u_t u_{tt} + c^2 u_x u_{tx} \right) \, dx.$$

$$= \int_{\infty}^{-\infty} \left( u_t u_{tt} - c^2 u_{xx} u_t \right) \, dx = 0,$$

that is, the energy $E(t)$ is conserved. A preferred conserved quantity is $C = C(t)$ where

$$C = \frac{1}{2} \int_{\infty}^{-\infty} \left( u^2 + v^2 \right) \, dx,$$

(4.2)
Figure 2: Space-Time Staggered Grid
because

\[ C' = \int_{-\infty}^{\infty} (u u_t + v v_t) \, dx , \]
\[ = \int_{-\infty}^{\infty} (u c v_x + v c u_x) \, dx , \]
\[ = \int_{-\infty}^{\infty} c (u v_x + v u_x) \, dx , \]
\[ = \int_{-\infty}^{\infty} c (u v)_x \, dx , \]
\[ = 0 . \]

Again note that if \( u, v \) are solutions of the system (4.1) then so are \( u_t, v_t \) and then (4.2) implies that a conserved quantity is given by the energy

\[ \frac{1}{2} \int_{-\infty}^{\infty} (u_t^2 + v_t^2) \, dx = \frac{1}{2} \int_{-\infty}^{\infty} (u_i^2 + c^2 u_x^2) \, dx = E . \]

So if \( C \) is conserved then so is \( E \).

4.1 A Staggered Discretization of the Wave Equation

Let \( \Delta t > 0 \) and \( \Delta x > 0 \) be given and then the primary and dual grids points are given by

\[ (t^n, x_i) = (n \Delta t, i \Delta x) , \]
\[ (t^{n+1/2}, x_{i+1/2}) = ((n + 1/2) \Delta t, (i + 1/2) \Delta x) , \]

where \(-\infty < n < \infty \) and \(-\infty < i < \infty \). Then \( u \) discretized on the primary grid and \( v \) on the dual grid as \( u_i^n \) and \( v_{i+1/2}^{n+1/2} \). Then the system (4.1) is discretized as

\[ \frac{u_i^{n+1} - u_i^n}{\Delta t} = c \frac{v_{i+1/2}^{n+1/2} - v_{i-1/2}^{n+1/2}}{\Delta x} , \]
\[ \frac{v_{i+1/2}^{n+1/2} - v_{i-1/2}^{n-1/2}}{\Delta t} = c \frac{u_{i+1}^n - u_i^n}{\Delta x} . \]

Assume that \( u^0 \) and \( v^{1/2} \) are given then the leapfrog time stepping scheme is

\[ u_i^{n+1} = u_i^n + c \frac{\Delta t}{\Delta x} (v_{i+1/2}^{n+1/2} - v_{i-1/2}^{n+1/2}) , \]
\[ v_{i+1/2}^{n+3/2} = v_{i+1/2}^{n+1/2} + c \frac{\Delta t}{\Delta x} (u_{i+1}^{n+1} - u_i^{n+1}) . \]
This implies that both $u$ and $v$ satisfy a discretization of the second order wave equation:

$$
\frac{u_{i+1}^{n+1} - 2u_i^n + u_{i-1}^{n-1}}{\Delta t^2} = \frac{1}{\Delta t} \left( \frac{u_{i+1}^{n+1} - u_i^n}{\Delta t} - \frac{u_i^n - u_{i-1}^{n-1}}{\Delta t} \right)
$$

$$
= \frac{c}{\Delta t} \left( \frac{v_{i+1/2}^{n+1/2} - v_{i-1/2}^{n+1/2}}{\Delta x} - \frac{v_{i+1/2}^{n-1/2} - v_{i-1/2}^{n-1/2}}{\Delta x} \right)
$$

$$
= \frac{c}{\Delta x} \left( \frac{v_{i+1/2}^{n+1/2} - v_{i-1/2}^{n-1/2}}{\Delta t} - \frac{v_{i+1/2}^{n-1/2} - v_{i-1/2}^{n-1/2}}{\Delta t} \right)
$$

$$
= \frac{c^2}{\Delta x} \left( \frac{u_{i+1}^n - u_i^n}{\Delta x} - \frac{u_i^n - u_{i-1}^n}{\Delta x} \right)
$$

$$
= c^2 \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\Delta x^2}.
$$

A similar calculation shows that

$$
\frac{v_{i-1/2}^{n+1/2} - 2v_{i-1/2}^{n-1/2} + v_{i-3/2}^{n-3/2}}{\Delta t^2} = \frac{c^2}{\Delta x^2} \left( v_{i+1/2}^{n-1/2} - 2v_{i-1/2}^{n-1/2} + v_{i-3/2}^{n-3/2} \right).
$$

The inner product of two grid functions $a = (\cdots, a_{-1}, a_0, a_1, \cdots)$ and $b = (\cdots, b_{-1}, b_0, b_1, \cdots)$ is given by

$$
\langle a, b \rangle = \sum_{i=-\infty}^{\infty} a_i b_i , \quad ||a||^2 = \langle a, a \rangle.
$$

Similarly, if $c = (\cdots, c_{-1/2}, c_{1/2}, c_{3/2}, \cdots)$ and $d = (\cdots, d_{-1/2}, d_{1/2}, d_{3/2}, \cdots)$ then

$$
\langle c, d \rangle = \sum_{i=-\infty}^{\infty} c_{i+1/2} d_{i+1/2} , \quad ||c||^2 = \langle c, c \rangle.
$$

Also, the discrete analogs of the integration by parts formula will be needed so let

$$
\delta(a)_{i+1/2} = a_{i+1} - a_i , \quad \delta(c)_i = c_{i+1/2} - c_{i-1/2}.
$$

Then the summation by parts formula is given by

$$
\langle \delta(a), c \rangle = \sum_{i=-\infty}^{\infty} (a_{i+1} - a_i) c_{i+1/2}
$$

$$
= \sum_{i=-\infty}^{\infty} a_{i+1} c_{i+1/2} - \sum_{i=-\infty}^{\infty} a_i c_{i+1/2}
$$

$$
= \sum_{i=-\infty}^{\infty} a_i c_{i-1/2} - \sum_{i=-\infty}^{\infty} a_i c_{i+1/2}
$$

$$
= -\sum_{i=-\infty}^{\infty} a_i (c_{i+1/2} - c_{i-1/2})
$$

$$
= -\langle a, \delta(c) \rangle.
$$
The difference equations (4.3) can now be written
\[
\begin{align*}
\frac{u_{i}^{n+1} - u_{i}^{n}}{\Delta t} &= c \frac{\delta(v_{i}^{n+1/2})}{\Delta x}, \\
\frac{v_{i+1/2}^{n+1/2} - v_{i+1/2}^{n-1/2}}{\Delta t} &= c \frac{\delta(u_{i}^{n})}{\Delta x}.
\end{align*}
\] (4.4)

To find a conserved quantity define:
\[
\begin{align*}
C_1(n) &= ||u^n||^2; \\
C_2(n) &= \left|\left|\frac{v^{n+1/2} + v^{n-1/2}}{2}\right|\right|^2; \\
C_3(n) &= ||\delta(u^n)||^2.
\end{align*}
\]

Now
\[
C_1(n + 1) - C_1(n) = \langle u^{n+1} - u^n, u^{n+1} + u^n \rangle
\]
\[
= c \frac{\Delta t}{\Delta x} \langle \delta(v^{n+1/2}), u^{n+1} + u^n \rangle \quad \text{see (4.4)}
\]
\[
= c \frac{\Delta t}{\Delta x} \langle v^{n+1/2}, -\delta(u^{n+1} + u^n) \rangle
\]
\[
= -c \frac{\Delta t}{\Delta x} \langle v^{n+1/2}, \delta(u^{n+1}) + \delta(u^n) \rangle
\]
\[
= -\langle v^{n+1/2}, v^{n+3/2} - v^{n-1/2} \rangle \quad \text{see (4.4)}.
\]

\[
C_2(n + 1) - C_2(n) = \frac{1}{4} \langle v^{n+3/2} + v^{n+1/2} + v^{n+1/2} + v^{n-1/2}, v^{n+3/2} + v^{n+1/2} - v^{n+1/2} - v^{n-1/2} \rangle
\]
\[
= \frac{1}{4} \langle v^{n+3/2} + 2v^{n+1/2} + v^{n-1/2}, v^{n+3/2} - v^{n-1/2} \rangle
\]
\[
= \langle v^{n+1/2}, v^{n+3/2} - v^{n-1/2} \rangle + \frac{1}{4} \langle v^{n+3/2} - 2v^{n+1/2} + v^{n-1/2}, v^{n+3/2} - v^{n-1/2} \rangle
\]
\[
xxx = \langle v^{n+1/2}, v^{n+3/2} - v^{n-1/2} \rangle + \frac{\Delta t}{4 \Delta x} \langle \delta(u^{n+1}) - \delta(u^n), v^{n+3/2} - v^{n-1/2} \rangle
\]
\[
= \langle v^{n+1/2}, v^{n+3/2} - v^{n-1/2} \rangle + \left(\frac{c \frac{\Delta t}{2 \Delta x}}{2} \right)^2 \langle \delta(v^{n+1/2}), v^{n+3/2} - v^{n-1/2} \rangle
\]

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\[ C3(n+1) - C3(n) = \langle \delta (u^{n+1}) - \delta (u^n), \delta (u^{n+1}) + \delta (u^n) \rangle \\
= \langle \delta (u^{n+1} - u^n), \delta (u^{n+1}) + \delta (u^n) \rangle \\
= c \frac{\Delta x}{\Delta t} \langle \delta (u^{n+1}) - \delta (u^n), v^{n+3/2} - v^{n-1/2} \rangle \\
= \langle \delta (\delta (v^{n+1/2})), v^{n+3/2} - v^{n-1/2} \rangle \\
\]

Consequently we have the conserved quantity

\[ C(n) = ||u^n||^2 - \left( \frac{c \Delta t}{2 \Delta x} \right)^2 ||\delta u^n||^2 + \left| \left| \frac{v^{n+1/2} + v^{n-1/2}}{2} \right| \right| \]

A similar argument shows that

\[ C(n + 1/2) = ||v^{n+1/2}||^2 - \left( \frac{c \Delta t}{2 \Delta x} \right)^2 ||\delta v^{n+1/2}||^2 + \left| \left| \frac{u^{n+1} + u^n}{2} \right| \right| \]

is a conserved quantity. The program \texttt{OneDWave.m} shows that the energies are constant to within an error of less than 10e-14.

The conserved quantity will be positive provided that

\[ \frac{c \Delta t}{2 \Delta x} \frac{||\delta u^n||}{||u^n||} < 1. \]

But

\[ \frac{||\delta u^n||}{||u^n||} \leq ||\delta||, \]

so the conserved quantity will be positive if

\[ \frac{c \Delta t}{\Delta x} < \frac{2}{||\delta||}. \]

Because ||\delta|| = 2 (see \texttt{Normdelta.m}) this is the Courant-Friedrichs-Lewy (CFL) condition for stability.
5 The Continuum Scalar and Vector Wave Equations

The differential equations studied here are linear and written in terms of a time derivative and the three spatial differential operators: the gradient $\vec{\nabla}$, the curl or rotation $\vec{\nabla} \times$, and the divergence $\vec{\nabla}$·. An important step is to introduce two positive functions $a = a(x, y, z)$ and $b = b(x, y, z)$ and two $3 \times 3$ symmetric positive definite matrices $A = A(x, y, z)$ and $B = B(x, y, z)$ that will be used to describe properties of non-homogeneous and anisotropic materials and additionally to increase the order of the spatial finite differences. A critical assumption is that $a > 0$ and $b > 0$ and that the matrices $A$ and $B$ are symmetric positive definite. Additionally as a function of $(x, y, z)$ these functions and matrices are bounded from above and below by positive constants. Consequently $a^{-1}$, $b^{-1}$, $A^{-1}$ and $B^{-1}$ are bounded as function of $(x, y, z)$.

5.1 Mimetic Properties

Next let $H_P$ and $H_V$ be linear spaces of smooth scalar functions depending on $(x, y, z)$ and $H_C$ and $H_S$ be linear spaces of smooth vector functions that depend on $(x, y, z)$ then the differential operators $\vec{\nabla}$, $\vec{\nabla} \times$, and $\vec{\nabla}$· and the functions $a$, $b$, $A$ and $B$ create mappings:

\[
\begin{align*}
\text{if } f & \in H_P \text{ then } \vec{\nabla} f \in H_C; \\
\text{if } \vec{v} & \in H_C \text{ then } \vec{\nabla} \times \vec{v} \in H_S; \\
\text{if } \vec{w} & \in H_S \text{ then } \vec{\nabla} \cdot \vec{w} \in H_V; \\
\text{if } f & \in H_P \text{ then } a f \in H_V; \\
\text{if } v & \in H_C \text{ then } A v \in H_S; \\
\text{if } w & \in H_C \text{ then } B w \in H_S; \\
\text{if } g & \in H_P \text{ then } b g \in H_V.
\end{align*}
\]

5.1 Mimetic Properties

It is also assumed that the functions in $H_P$, $H_C$, $H_S$ and $H_V$ go to zero as point $(x, y, z)$ goes to infinity. The multiplicative operators have an inverse because they are bounded below. In the function space names the subscripts stand for point, curve, surface and volume. Reasons for the notation will be given later.

Mimetic methods [30] will be used to discretize the spatial differential operators so here
is a summary of the properties of the continuum differential operators that will be mimicked:

\begin{align}
\text{if } f \in H_P \text{ is constant function then } \vec{\nabla} f &= 0 ; \\
\text{if } f \in H_P \text{ then } \vec{\nabla} \times \vec{\nabla} f &= 0 ; \\
\text{if } \vec{v} \in H_C \text{ then } \vec{\nabla} \cdot \vec{\nabla} \times \vec{v} &= 0 ; \\
\text{if } f \in H_P \text{ and } \vec{\nabla} f = 0 \text{ then } f \text{ is constant } ; \\
\text{if } \vec{v} \in H_C \text{ and } \vec{\nabla} \times \vec{v} = 0 \text{ then there exists } f \in H_P \text{ so that } \vec{v} = \vec{\nabla} f ; \\
\text{if } \vec{v} \in H_S \text{ and } \vec{\nabla} \cdot \vec{v} = 0 \text{ then there exists } \vec{w} \in H_C \text{ so that } \vec{v} = \vec{\nabla} \times \vec{w} .
\end{align}

(5.2)

If \((x, y, z)\) are restricted to a subregion of three dimensional space the existence of \(f\) and \(\vec{w}\) may not hold for the full region.

As is done in differential geometry, it is helpful to use an exact sequence of differential operators to record the properties to be mimicked. To include the multiplicative operators a double exact sequence as shown in Figure 3 is used. An additional advantage of the double sequence is that the spatial discretization of the differential operators will use two interlaced grids called primal and dual grids. In this case, in Figure 3 the upper row of spaces will be functions on the primal grid and the lower row of spaces will be functions on the dual grid.

An important example of a finite difference operator that is not mimetic is the central difference approximation of the first derivative. If \(f = f(x), \Delta x > 0, f_i = f(i \Delta x)\) and

\[ \delta(f)_i = \frac{f_{i+1} - f_i}{\Delta x}, \]

then \(\delta\) is not a mimetic approximation of the first derivative because \(\delta f = 0\) where \(f_i = (-1)^i\) and \(f\) is not constant. The use of mimetic discretizations using primal and dual grids restores the ability to make simple second order accurate approximations of the first derivative.

\subsection*{5.2 Using Spatial Units}

The discussion of mimetic methods in [30] was driven by the goal of proving that the mimetic properties of the discretized operators is correct. For application such detail not needed.
What is critical is the spatial unit $d$ (e.g., meter, foot) and less so the temporal unit $\tau$ (e.g., second, year) of the functions and operators used in the differential equations. The spatial variables (e.g., $x, y, z$) all have spatial dimension $d$ and the differential operators $\vec{\nabla}$, $\vec{\nabla} \times$, and $\vec{\nabla} \cdot$ all have dimension $1/d$. If we choose the function in $H_P$ to not have a spatial dimension and then because the differential operators have spatial dimension $1/d$ it must be that:

- the function in $H_P$ have spatial dimension 1;
- the function in $H_C$ have spatial dimension $1/d$;
- the function in $H_S$ have spatial dimension $1/d^2$;
- the function in $H_V$ have spatial dimension $1/d^3$.

The subscripts $P, C, S$ and $V$ corresponds to points having dimension 0, curves having dimension 1, surfaces having dimension 2 and volumes having dimension 3. This in turn implies that $a$ and $b$ must have dimension $1/d^k$ while the matrices $A$ and $B$ must have dimension $1/d$. For the exact-sequences in Figure 3 an integer $k$ above or below the $H$ indicates that the functions in that space have dimension $1/d^k$. The mappings given by $a, b, A$ and $B$ correspond to the star operators for differential forms.

### 5.3 Second Order Differential Operators

Second order operators have domain and range in the same space and are created using diagram chasing.

To create scalar operators For example starting in the upper left corner of each square in Figure 3 gives

\[
\begin{align*}
    f &\in H_P, \\
    \vec{\nabla} f &\in H_C, \\
    A \vec{\nabla} f &\in H_S, \\
    \vec{\nabla} \cdot A \vec{\nabla} f &\in H_V \\
\end{align*}
\]

\[
\begin{align*}
    \vec{\nabla} \times \vec{v} &\in H_S, \\
    B^{-1} \vec{\nabla} \times \vec{v} &\in H_C, \\
    \vec{\nabla} b^{-1} \vec{\nabla} \cdot \vec{w} &\in H_P \\
\end{align*}
\]

\[
\begin{align*}
    \vec{\nabla} \times \vec{\nabla} \times \vec{v} &\in H_S, \\
    B^{-1} \vec{\nabla} \times \vec{\nabla} \times \vec{v} &\in H_C, \\
    B \vec{\nabla} b^{-1} \vec{\nabla} \cdot \vec{w} &\in H_S \\
\end{align*}
\]

If $a = b = 1$ and $A = B = I$ the identity matrix then the second order operators become:

\[
\Delta f = \vec{\nabla} \cdot \vec{\nabla} f, \quad \vec{\nabla} \times \vec{\nabla} \times \vec{v}, \quad \vec{\nabla} \vec{\nabla} \cdot \vec{w}.
\]

So it is reasonable to call the operator generated in the first column of (5.3) the generalized Laplacian or just the Laplacian

\[
\Delta f = a^{-1} \vec{\nabla} \cdot A \vec{\nabla} f. \quad (5.4)
\]
Several other operators can be created but starting with the right corners of the squares in Figure 3 will create the same operators but with \( a \) and \( b \) interchanged and \( A \) and \( B \) interchanged. An example of a scalar operator is to start with \( g = g(x, y, z, t) \in H_V \) to get

\[
\vec{\nabla} \cdot \mathbf{A} \vec{\nabla} (a^{-1} g) . \tag{5.5}
\]

There is a one additional operator that is used quite frequently. First start with \( \vec{v} \in H_C \) and diagram chase the first square to get \( \vec{\nabla} a^{-1} \vec{\nabla} \cdot \mathbf{A} \vec{v} \) which under the above simplifying assumptions becomes \( \vec{\nabla} \vec{\nabla} \cdot \vec{v} \). This operator has the same domain and range as that the operator in the second column of (5.3) so these operators can be linearly combined to define the vector Laplacian by

\[
\Delta \vec{v} = \vec{\nabla} a^{-1} \vec{\nabla} \cdot \mathbf{A} \vec{v} - \mathbf{A}^{-1} \vec{\nabla} \times \mathbf{B}^{-1} \vec{\nabla} \times \vec{v} .
\]

Under the simplifying assumptions this becomes

\[
\Delta \vec{v} = \vec{\nabla} \vec{\nabla} \cdot \vec{v} - \vec{\nabla} \times \vec{\nabla} \times \vec{v} ,
\]

which in Cartesian coordinates this gives (see CurlCurl.nb)

\[
\Delta (v_1, v_2, v_3) = (\Delta v_1, \Delta v_2, \Delta v_3) .
\]

### 5.4 Scalar Wave Equations

If \( u = u(x, y, z, t) \) then in dimensionless variables and homogeneous and isotropic materials the scalar wave is

\[
\frac{\partial^2 u}{\partial t^2} = \Delta u = \vec{\nabla} \cdot \vec{\nabla} u , \tag{5.6}
\]

while in dimensioned variables the wave equations is

\[
\frac{\partial^2 u}{\partial t^2} = v^2 \Delta u = v^2 \vec{\nabla} \cdot \vec{\nabla} u , \tag{5.7}
\]

where \( v \) is a scalar velocity (speed of sound or light) with dimension \( d/\tau \), \( t \) has dimension \( \tau \) and \( \vec{\nabla} \) and \( \vec{\nabla} \cdot \) have dimension \( 1/d \).

For general material properties diagram chasing gives the scalar wave equation as

\[
\frac{\partial^2 u}{\partial t^2} = \Delta u = \frac{1}{a} \vec{\nabla} \cdot \left( \mathbf{A} \vec{\nabla} u \right) . \tag{5.8}
\]

This equation has consistent spatial dimension and time dimensions.

The operator in (5.5) can also be used to define a wave equation

\[
\frac{\partial^2 g}{\partial t^2} = \vec{\nabla} \cdot \mathbf{A} \vec{\nabla} (a^{-1} g) , \tag{5.9}
\]
but letting $u = a^{-1} g$ converts this equation to (5.8) thus gives nothing new.

Under the assumption that $a = 1$ and $A = I$ (5.8) reduces to (5.6) and if $A = I$ and $a = 1/v^2$ then this equation reduces to (5.7). However, diagram chasing requires that $a$ have spatial dimension $1/d^3$ and $A$ should have spatial dimension $1/d$.

Taking a hint from the acoustic wave equation literature [18] let $\rho = \rho(x, y, z)$ be the density of the material with dimension $1/d^3$ and $v = v(x, y, z)$ be a velocity with dimension $d/\tau$ and then as in Figure 4 set

$$a = b = \rho, \quad A = B = \rho v^2 I,$$

where $I$ is the identity matrix and $\rho v^2$ has units $1/d \tau^2$ is the bulk modulus [18] (Chapter 2, equation 2.14). Because of this assumption starting with the lower righ corners of the squares in 4 gives the same results as starting with the upper left corners. Now $a, b, A$ and $B$ have the correct spatial dimension and the general wave equation becomes

$$\frac{\partial^2 u}{\partial t^2} = \frac{1}{\rho} \nabla \cdot \left( \rho v^2 \nabla u \right). \quad (5.10)$$

Of course the $v^2$ can be replaced by any matrix (tensor) with the same units.

Equation (5.10) is close to but exactly the acoustic wave equation given in the literature. For example [18], (Chapter 2, equation 2.14), [1] (equation 2.3 page 23), [12] (equation 2 page 2) and [20] (equation 2.2 page 589) give the acoustic wave equation for the pressure $p = p(x, y, x, t)$ as

$$\frac{\partial^2 p}{\partial t^2} = \rho v^2 \nabla \cdot \left( \frac{1}{\rho} \nabla p \right).$$

Diagram chasing cannot produce this equation.

**5.5 Vector Wave Equations**

For general materials the vector wave equation is given by diagram chasing $\vec{w} \in H_S$ in the right square in Figure 3

$$\frac{\partial^2 \vec{w}}{\partial t^2} = B \nabla \frac{1}{b} \nabla \cdot \vec{w}. \quad (5.11)$$

The equations in (5.14) can be combined to produce this equation with $a = b$ and $A = B$. 27
To obtain the acoustic version of this equation (ILS, page 67, equation 2.16) choose \( b = 1/(\rho v^2) \) and \( B = 1/\rho I \) to get
\[
\frac{\partial^2 \vec{w}}{\partial t^2} = \frac{1}{\rho} \vec{\nabla} \left( \rho v^2 \vec{\nabla} \cdot \vec{w} \right).
\] (5.12)

5.6 Inner Products

Applying the ideas developed in the previous sections requires the adjoints of the operators involved in the wave equation written as a system and this requires inner products on the spaces \( H_P, H_C, H_S \) and \( H_V \). The standard inner products on scalar functions \( f(x, y, z) \) and \( g(x, y, z) \) and vector function \( \vec{v}(x, y, z) \) and \( \vec{w}(x, y, z) \) are
\[
\langle f, g \rangle = \int_{\mathbb{R}^3} f(x, y, z) g(x, y, z) \, dx \, dy \, dz, \quad \langle \vec{v}, \vec{w} \rangle_C = \int_{\mathbb{R}^3} \vec{v}(x, y, z) \cdot \vec{w}(x, y, z) \, dx \, dy \, dz.
\]

An important requirement for the inner product is that they do not have a spatial dimension. Consequently, the inner product on our function spaces must use a weight function when we use dimensioned variables. Consequently, the weighted inner products can be used to define conserved quantities. Because \( dx, dy \) and \( dz \) all have spatial dimension \( d \) the integrand in the definition of the inner products must have spatial dimension \( 1/d^3 \).

For \( u_1 \in H_P \) and \( u_2 \in H_P \) set
\[
\langle u_1, u_2 \rangle_P = \int_{\mathbb{R}^3} a(x, y, z) u_1(x, y, z) u_2(x, y, z) \, dx \, dy \, dz.
\]
The integrand has dimension \( 1/d^3 \) because \( a \) has dimension \( 1/d^3 \) and \( u_1 \) and \( u_2 \) are dimensionless.

For \( \vec{v}_1 \in H_C \) and \( \vec{v}_2 \in H_C \) set
\[
\langle \vec{v}_1, \vec{v}_2 \rangle_C = \int_{\mathbb{R}^3} A(x, y, z) \vec{v}_1(x, y, z) \cdot \vec{v}_2(x, y, z) \, dx \, dy \, dz.
\]
The dimension of \( A \) is \( 1/d^3 \) and the dimensions of \( \vec{v}_1 \) and \( \vec{v}_2 \) are \( 1/d \) so the integrand has dimension \( 1/d^3 \).

For \( \vec{w}_1 \in H_S \) and \( \vec{w}_2 \in H_S \) set
\[
\langle \vec{w}_1, \vec{w}_2 \rangle_S = \int_{\mathbb{R}^3} A^{-1}(x, y, z) \vec{w}_1(x, y, z) \cdot \vec{w}_2(x, y, z) \, dx \, dy \, dz.
\]
The dimension of \( A^{-1} \) is \( d \) while the dimensions of \( \vec{w}_1 \) and \( \vec{w}_2 \) are \( 1/d^2 \) so the integrand has dimension \( 1/d^3 \).

For \( g_1 \in H_V \) and \( g_2 \in H_V \) set
\[
\langle g_1, g_2 \rangle_V = \int_{\mathbb{R}^3} a^{-1}(x, y, z) g_1(x, y, z) g_2(x, y, z) \, dx \, dy \, dz.
\]
The integrand has dimension \( 1/d^3 \) because \( a^{-1} \) has dimension \( d^3 \) and \( u_1 \) and \( u_2 \) have dimensions \( 1/d^3 \).

Similar inner product can be made by replacing \( a \) by \( b \) and \( A \) by \( B \).
5.7 Adjoint Operators

Adjoint operators are commonly defined for operators mapping a space into itself but most of the operators used here are mapping between two different spaces, so the adjoint is defined as in Section 3.1. The notation in that section shows that

\[ X \xrightarrow{A} Y \xrightarrow{B} Z, \quad Z \xrightarrow{B^*} Y \xrightarrow{A^*} X, \]

and thus

\[ (BA)^* = A^* B^*. \]

Because the diagram chasing gives operators as compositions of other operators, this will be used many times. Also, \((A^*)^* = A\).

For the operator \(\vec{\nabla}\) let \(u \in H_P\) and \(\vec{v} \in H_C\) so that

\[
\langle \vec{\nabla} u, \vec{v} \rangle_C = \langle A \vec{\nabla} u, \vec{v} \rangle \\
= \langle \vec{\nabla} u, A \vec{v} \rangle \\
= -\langle u, \vec{\nabla} \cdot A \vec{v} \rangle \\
= -\langle a u, a^{-1} \vec{\nabla} \cdot A \vec{v} \rangle \\
= -\langle u, a^{-1} \vec{\nabla} \cdot A \vec{v} \rangle_P
\]

For the operator \(A\) let \(\vec{v} \in H_C\) and \(\vec{w} \in H_S\) so that

\[
\langle A \vec{v}, \vec{w} \rangle_S = \langle A^{-1} A \vec{v}, \vec{w} \rangle \\
= \langle A \vec{v}, A^{-1} \vec{w} \rangle \\
= \langle \vec{v}, A^{-1} \vec{w} \rangle_C
\]

For the operator \(\vec{\nabla} \cdot\) let \(\vec{w} \in H_S\) and \(g \in H_V\) so that

\[
\langle \vec{\nabla} \cdot \vec{w}, g \rangle_V = \langle a^{-1} \vec{\nabla} \cdot \vec{w}, g \rangle \\
= \langle \vec{\nabla} \cdot \vec{w}, a^{-1} g \rangle \\
= -\langle \vec{w}, \vec{\nabla} (a^{-1} g) \rangle \\
= -\langle A A^{-1} \vec{w}, \vec{\nabla} (a^{-1} g) \rangle \\
= -\langle A^{-1} \vec{w}, A \vec{\nabla} (a^{-1} g) \rangle \\
= -\langle \vec{w}, A \vec{\nabla} (a^{-1} g) \rangle_S
\]

For the operator \(a^{-1}\) let \(g \in H_V\) and \(f \in H_P\) so that

\[
\langle a^{-1} g, f \rangle_P = \langle a a^{-1} g, f \rangle \\
= \langle a^{-1} g, a f \rangle \\
= \langle g, af \rangle_V
\]
In summary

\[ \tilde{\nabla}^* = -a^{-1} \tilde{\nabla} \cdot A, \]
\[ \tilde{\nabla} \cdot ^* = -A \tilde{\nabla} a^{-1}, \]
\[ A^* = A^{-1}, \]
\[ a^* = a^{-1}. \]  

(5.13)

This then implies that the Laplacian is self adjoint because

\[ \Delta^* = \left( a^{-1} \tilde{\nabla} \cdot A \tilde{\nabla} \right)^* \]
\[ = \tilde{\nabla}^* A^* \tilde{\nabla}^* a^{-1*} \]
\[ = a^{-1} \tilde{\nabla} \cdot A A^{-1} A \tilde{\nabla} a^{-1} a \]
\[ = a^{-1} \tilde{\nabla} \cdot A \tilde{\nabla} \]
\[ = \Delta. \]

5.8 Conserved Quantity

The second order wave equation (5.8) can be written as a system of two equations by introducing \( \tilde{v} = \tilde{v}(x, y, z, t) \in H_S \) that has dimension \( 1/d^2 \) so that

\[ \frac{\partial u}{\partial t} = \frac{1}{a} \tilde{\nabla} \cdot \tilde{v}, \quad \frac{\partial \tilde{v}}{\partial t} = A \tilde{\nabla} u. \]  

(5.14)

Next note that

\[ \left( \frac{1}{a} \tilde{\nabla} \cdot \right)^* = -A \tilde{\nabla} a^{-1} a = -A \tilde{\nabla} \]

so the system has the same form as the systems of equation in the previous sections. This suggests that a conserved quantity is given by

\[ C(t) = \frac{\langle u, u \rangle_P + \langle \tilde{v}, \tilde{v} \rangle_S}{2}. \]

In fact

\[ C' = \langle u', u \rangle_P + \langle \tilde{v}', \tilde{v} \rangle_S \]
\[ = \langle \frac{1}{a} \tilde{\nabla} \cdot \tilde{v}, u \rangle_P + \langle A \tilde{\nabla} u, \tilde{v} \rangle_S \]
\[ = \langle \frac{1}{a} \tilde{\nabla} \cdot \tilde{v}, u \rangle_P - \langle u, \frac{1}{a} \tilde{\nabla} \cdot \tilde{v} \rangle_P \]
\[ = 0, \]

so \( C \) is a conserved quantity.
5.9 Maxwell’s Equation

Maxwell’s Equations

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

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

provide an applied example that was studied by Yee [41] with essentially the same ideas that are used in this paper. Here $\vec{B}, \vec{E}, \vec{D}$ and $\vec{H}$ are vector functions of $(x, y, z, t)$ while $\mu$ and $\epsilon$ are symmetric positive definite matrices that depend only on the spatial variables. The meaning of variables and their distance units are:

| quantity | units | name               | spaces        |
|----------|-------|--------------------|---------------|
| $\vec{E}$ | 1/d   | electric field     | $H_{CU}$      |
| $\epsilon$ | 1/d   | permeability tensor| $H_{CU} \rightarrow H_{SD}$ |
| $\vec{D}$ | 1/d^2 | electric displacement | $H_{SD}$      |
| $\vec{H}$ | 1/d   | magnetic field     | $H_{CD}$      |
| $\mu$    | 1/d   | permittivity tensor| $H_{CD} \rightarrow H_{SU}$ |
| $\vec{B}$ | 1/d^2 | magnetic flux      | $H_{SU}$      |
| $\nabla \times$ | 1/d   | curl operator      | $H_{CU} \rightarrow H_{SU}$ |
| $\nabla \times$ | 1/d   | curl operator      | $H_{CD} \rightarrow H_{SD}$ |
| $\partial / \partial t$ | 1/\tau | time derivative    |               |
| $\vec{J}$ | 1/d^2 | current            | $\vec{J} \in H_{SD}$ |

Table 1: Quantities and their units in Maxwell’s equations. For details see https://www.spec2000.net/06-electromag.htm

Representing Maxwell’s equations using diagram chasing uses the center square in Figure 8 which is reproduced in Figure 5 using notation appropriate to Maxwell’s equations, that is, by setting $\bf{A} = \epsilon$ and $\bf{B} = \mu$. The situation here is a bit different from the scalar wave equation because in Figure 5 the upper left space and the lower right space are the same as well as the upper right space is the same as the lower left space. To clarify which space is being used they are relabeled as $H_{CU}, H_{CD}, H_{SU}$ and $H_{SD}$. To obtain Maxwell’s equation
the choice of \( A \) and \( B \) requires that \( \vec{E} \in H_{CU}, \vec{H} \in H_{CD}, \vec{B} \in H_{SU} \) and \( \vec{D} \in H_{SD} \). In this discussion it is assumed that \( \vec{J} = 0 \), but if this is not the case then \( \vec{J} \in H_{SD} \). Now it is easy to check Maxwell’s equation are dimensionally consistent. Next eliminate \( \vec{B} \) and \( \vec{D} \) from the equation to get

\[
\vec{E}' = \epsilon^{-1} \vec{\nabla} \times H, \quad \vec{H}' = -\mu^{-1} \vec{\nabla} \times E. \tag{5.15}
\]

### 5.10 Adjoint Operators

To find the adjoint operators each of the spaces will require an inner product:

\[
\langle \vec{v}_1, \vec{v}_2 \rangle_{CU} = \int_{\mathbb{R}^3} \epsilon \vec{v}_1 \cdot \vec{v}_2 \, dx \, dy \, dz ,
\]

\[
\langle \vec{v}_1, \vec{v}_2 \rangle_{CD} = \int_{\mathbb{R}^3} \mu \vec{v}_1 \cdot \vec{v}_2 \, dx \, dy \, dz ,
\]

\[
\langle \vec{w}_1, \vec{w}_2 \rangle_{SU} = \int_{\mathbb{R}^3} \mu^{-1} \vec{w}_1 \cdot \vec{w}_2 \, dx \, dy \, dz ,
\]

\[
\langle \vec{w}_1, \vec{w}_2 \rangle_{SD} = \int_{\mathbb{R}^3} \epsilon^{-1} \vec{w}_1 \cdot \vec{w}_2 \, dx \, dy \, dz .
\]

For the curl operator in the upper part of Maxwell Exact Sequences Figure 5 let \( \vec{v} \in H_{CU} \) and \( \vec{w} \in H_{SU} \) and then compute

\[
\langle \vec{\nabla} \times \vec{v}, \vec{w} \rangle_{SU} = \langle \mu^{-1} \vec{\nabla} \times \vec{v}, \vec{w} \rangle \\
= \langle \vec{v}, \vec{\nabla} \times \mu^{-1} \vec{w} \rangle \\
= \langle \epsilon \vec{v}, \epsilon^{-1} \vec{\nabla} \times \mu^{-1} \vec{w} \rangle \\
= \langle \vec{v}, \epsilon^{-1} \vec{\nabla} \times \mu^{-1} \vec{w} \rangle_{CU}.
\]

For the curl operator in the upper part of Maxwell Exact Sequences Figure 5 let \( \vec{v} \in H_{CL} \) and \( \vec{w} \in H_{SL} \) and then compute

\[
\langle \vec{\nabla} \times \vec{v}, \vec{w} \rangle_{SD} = \langle \epsilon^{-1} \vec{\nabla} \times \vec{v}, \vec{w} \rangle \\
= \langle \vec{v}, \vec{\nabla} \times \epsilon^{-1} \vec{w} \rangle \\
= \langle \mu \vec{v}, \mu^{-1} \vec{\nabla} \times \epsilon^{-1} \vec{w} \rangle \\
= \langle \vec{v}, \mu^{-1} \vec{\nabla} \times \epsilon^{-1} \vec{w} \rangle_{CD}.
\]
In summary

\begin{align*}
\tilde{\nabla} \times^* &= \epsilon^{-1} \tilde{\nabla} \times \mu^{-1} \quad \text{upper row,} \\
\tilde{\nabla} \times^* &= \mu^{-1} \tilde{\nabla} \times \mu^{-1} \quad \text{lower row,} \\
\epsilon^* &= \epsilon^{-1} \\
\mu^* &= \mu^{-1}
\end{align*}

Now this implies that

\[
(\mu^{-1} \tilde{\nabla} \times)^* = \epsilon^{-1} \tilde{\nabla} \times \mu^{-1} \mu = \epsilon^{-1} \tilde{\nabla} \times,
\]

so the Maxwell system (5.13) has the same form as the systems of equations in the previous sections.

Additionally (5.13) can be written as two different second order in time equations:

\[
\tilde{E}'' = -\epsilon^{-1} \tilde{\nabla} \times \mu^{-1} \tilde{\nabla} \times E, \quad \tilde{H}'' = -\mu^{-1} \tilde{\nabla} \times \epsilon^{-1} \tilde{\nabla} \times H. \tag{5.16}
\]

But

\[
(\epsilon^{-1} \tilde{\nabla} \times \mu^{-1} \tilde{\nabla} \times)^* = \epsilon^{-1} \tilde{\nabla} \times \mu^{-1} \mu \mu^{-1} \tilde{\nabla} \times \epsilon^{-1} \epsilon = \epsilon^{-1} \tilde{\nabla} \times \mu^{-1} \tilde{\nabla} \times.
\]

and

\[
(\mu^{-1} \tilde{\nabla} \times \epsilon^{-1} \tilde{\nabla} \times)^* = \mu^{-1} \tilde{\nabla} \times \epsilon^{-1} \epsilon \mu \mu^{-1} \mu = \mu^{-1} \tilde{\nabla} \times \epsilon^{-1} \tilde{\nabla} \times.
\]

so both of the operators in (5.16) are self-adjoint.

### 5.11 Maxwell Conservation Law

Consider the quantity

\[
C = \frac{(\tilde{E}, \tilde{E})_{CV} + (\tilde{H}, \tilde{H})_{CD}}{2} = \frac{1}{2} \int_{\mathbb{R}^3} \epsilon \tilde{E} \cdot \tilde{E} + \mu \tilde{H} \cdot \tilde{H} \, dx \, dy \, dz,
\]

where the integrand is the standard energy density. A vector identity is needed to see that the energy is constant:

\[
\tilde{\nabla} \cdot (\tilde{E} \times \tilde{H}) = (\tilde{\nabla} \times \tilde{E}) \cdot \tilde{H} - \tilde{E} \cdot (\tilde{\nabla} \times \tilde{H}).
\]
The time derivative of the energy is

\[
Q' = \int_{\mathbb{R}^3} \left( \epsilon \vec{E}' \cdot \vec{E} + \mu \vec{H}' \cdot \vec{H} \right) dx \, dy \, dz,
\]

\[
= \int_{\mathbb{R}^3} \left( \nabla \times \vec{H} \cdot \vec{E} - \nabla \times \vec{E} \cdot \vec{H} \right) dx \, dy \, dz,
\]

\[
= - \int_{\mathbb{R}^3} \nabla \cdot (\vec{H} \times \vec{E}) \, dx \, dy \, dz,
\]

\[
= \int_{\mathbb{R}^3} \nabla \cdot (\vec{E} \times \vec{H}) \, dx \, dy \, dz,
\]

\[
= \int_{\mathbb{R}^3} \nabla \cdot \vec{S} 
\]

\[
= 0.
\]

where \( \vec{S} = \vec{E} \times \vec{H} \) is called the Poynting vector which has spatial units \(1/d^2\). The last integral is zero because we assume that \( \vec{E} \) and \( \vec{H} \) are zero far from the origin.
6 Mimetic Discretizations

Again, our discussion and notation will follow that in [30]. However, that work was set up to rigorously prove that the discrete operators in mimetic discretizations have the same properties as the continuum operators used in vector calculus. Here we will focus on applying mimetic methods to physical problems by adding a time variable and its discretization and focus on how to use physical spatial units to correctly discretize physical problems.

6.1 Primal and Dual Grids

Mimetic discretizations use primal and dual spatial grids as shown in Figure 6. The points in the grids are given in Table 2. The grids are made up of cells, faces of cells, edges of the faces and nodes that are the corners of the cells as indicated in Table 2.

Figure 6: The Primal and Dual Grids Taken From [30]
Table 2: Notation for the primal and dual, scalar and vector fields where \(-\infty < i < \infty, -\infty < j < \infty \) and \(-\infty < k < \infty\).

### 6.2 Primal and Dual Scalar and Vector Fields

As summarized in Table 2 there two types of scalar fields and also two type of vector fields on both the primal and dual grids. On the primary grid there are scalar fields \(s\) that do not have a spatial dimensions, vector fields \(\vec{t}\) (for tangent) that have dimension \(1/d\), vector fields \(\vec{n}\) (for normal) that have units \(1/d^2\), and scalar fields with dimension \(1/d^3\) (as in densities) while the dual grid has the same types of fields labeled with a superscript star as in \(s^*\).

It is important that at each point in the grid there is a value from both the primal and dual fields, but why don’t we just take them to be the same? Because their spatial dimensions are not the same. Historically, this appeared in the Yee grid for Maxwell equations [41] which we will discuss in Section 8.

### 6.3 Difference Operators

The discrete gradient \(\mathcal{G}\), curl or rotation \(\mathcal{R}\) and divergence \(\mathcal{D}\) are difference operators on a scalar or vector fields. The formulas for the dual grid are obtained by making the changes \(i \rightarrow i + 1/2, j \rightarrow j + 1/2\) and \(k \rightarrow k + 1/2\).

**The Gradient:** If \(s \in S_N\) is a discrete scalar field, then its gradient \(\mathcal{G}s \in V_e\) is an edge vector field. In terms of components

\[
(\mathcal{G}s)_{i+\frac{1}{2},j,k} = \frac{s_{i+1,j,k} - s_{i,j,k}}{\Delta x};
(\mathcal{G}s)_{i,j+\frac{1}{2},k} = \frac{s_{i+1,j,k} - s_{i,j,k}}{\Delta y};
(\mathcal{G}s)_{i,j,k+\frac{1}{2}} = \frac{s_{i,j,k+1} - s_{i,j,k}}{\Delta z}.
\]
The Curl: If \( \vec{t} \in V_E \) is a discrete edge vector field, then its curl \( \mathcal{R} \vec{t} \in V_F \) is a discrete face vector field. In terms of components

\[
(\mathcal{R} \vec{t})_{i,j+\frac{1}{2},k+\frac{1}{2}} = \frac{t_{i,j+1,k+\frac{1}{2}} - t_{i,j,k+\frac{1}{2}} - t_{i,j+\frac{1}{2},k+1} + t_{i,j+\frac{1}{2},k}}{\Delta y} ;
\]
\[
(\mathcal{R} \vec{t})_{i+\frac{1}{2},j,k+\frac{1}{2}} = \frac{t_{i+1,j,k+\frac{1}{2}} - t_{i,j+\frac{1}{2},k+1} - t_{i+\frac{1}{2},j,k} + t_{i,j,k}}{\Delta x} ;
\]
\[
(\mathcal{R} \vec{t})_{i+\frac{1}{2},j+\frac{1}{2},k} = \frac{t_{i+1,j+1,k} - t_{i,j+1,k} - t_{i+\frac{1}{2},j,k} + t_{i,j,k}}{\Delta z} .
\]

The Divergence: If \( \vec{n} \in V_F \) is a discrete face vector field, then its divergence \( \mathcal{D} \vec{n} \in S_C \) is a cell scalar field. In terms of components

\[
(\mathcal{D} \vec{n})_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} = \frac{n_{i+1,j+\frac{1}{2},k+\frac{1}{2}} - n_{i,j+\frac{1}{2},k+\frac{1}{2}} - n_{i+\frac{1}{2},j,k+\frac{1}{2}} + n_{i,j,k+\frac{1}{2}}}{\Delta x} + \frac{n_{i+\frac{1}{2},j+1,k+\frac{1}{2}} - n_{i+\frac{1}{2},j,k+\frac{1}{2}} - n_{i+\frac{1}{2},j+\frac{1}{2},k} + n_{i+\frac{1}{2},j,k}}{\Delta y} + \frac{n_{i+\frac{1}{2},j+\frac{1}{2},k+1} - n_{i+\frac{1}{2},j+\frac{1}{2},k}}{\Delta z} .
\]

The Star Gradient: If \( s^* \in S_{N^*} \) is a discrete star scalar field then its star gradient \( G^* s^* \in V_{E^*} \) is a star edge vector field. In terms of components

\[
(G^* s^*)_{i,j+\frac{1}{2},k+\frac{1}{2}} = \frac{s^*_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} - s^*_{i-\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}}{\Delta x} ;
\]
\[
(G^* s^*)_{i+\frac{1}{2},j,k+\frac{1}{2}} = \frac{s^*_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} - s^*_{i+\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2}}}{\Delta y} ;
\]
\[
(G^* s^*)_{i+\frac{1}{2},j+\frac{1}{2},k} = \frac{s^*_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} - s^*_{i+\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}}}{\Delta z} .
\]

The Star Curl: If \( \vec{t}^* \in S_{C^*} \) is a discrete star edge vector field then its curl \( \mathcal{R}^* \vec{t}^* \in V_{F^*} \) is a discrete star face vector field. In terms of components

\[
(R^* \vec{t}^*)_{i+\frac{1}{2},j,k} = \frac{t^*_{i+\frac{1}{2},j+\frac{1}{2},k} - t^*_{i+\frac{1}{2},j-\frac{1}{2},k} - t^*_{i+\frac{1}{2},j,k+\frac{1}{2}} + t^*_{i+\frac{1}{2},j,k-\frac{1}{2}}}{\Delta y} ;
\]
\[
(R^* \vec{t}^*)_{i,j+\frac{1}{2},k} = \frac{t^*_{i,j+\frac{1}{2},k+\frac{1}{2}} - t^*_{i,j+\frac{1}{2},k-\frac{1}{2}} - t^*_{i+\frac{1}{2},j,k+\frac{1}{2}} + t^*_{i+\frac{1}{2},j,k-\frac{1}{2}}}{\Delta z} ;
\]
\[
(R^* \vec{t}^*)_{i,j,k+\frac{1}{2}} = \frac{t^*_{i,j+\frac{1}{2},k+\frac{1}{2}} - t^*_{i,j+\frac{1}{2},k-\frac{1}{2}} - t^*_{i+\frac{1}{2},j,k+\frac{1}{2}} + t^*_{i+\frac{1}{2},j,k-\frac{1}{2}}}{\Delta x} .
\]

The Star Divergence: If \( \vec{n}^* \in V_{F^*} \) is a discrete star face vector field then it divergence
\( D^* \vec{n}^* \in S_C \) is a discrete star cell field. In terms of components

\[
(D^* \vec{n}^*)_{i,j,k} = \frac{n^*_{i+\frac{1}{2},j,k} - n^*_{i-\frac{1}{2},j,k}}{\Delta x} + \frac{n^*_{i,j+\frac{1}{2},k} - n^*_{i,j-\frac{1}{2},k}}{\Delta y} + \frac{n^*_{i,j,k+\frac{1}{2}} - n^*_{i,j,k-\frac{1}{2}}}{\Delta z}.
\]

### 6.4 Multiplication Operators

The simplest form of the multiplication by the scalar functions \( a = a(x, y, z) \) and \( b = b(x, y, z) \) and the matrix functions \( A \) and \( B \) is given by assuming that \( A \) is scalar function \( A = A(x, y, z) \) times the identity matrix and \( B \) is is scalar function \( B = B(x, y, z) \) times the identity matrix and the multiplication is point wise. For \( A \) define \( A \) on the edges in the primal grid to be

\[
A_{(i+\frac{1}{2}, j, k)} = A((i + \frac{1}{2}) \Delta x, j \Delta y, k \Delta z),
\]

\[
A_{(i, j+\frac{1}{2}, k)} = A(i \Delta x, (j + \frac{1}{2}) \Delta y, k \Delta z),
\]

\[
A_{(i, j, k+\frac{1}{2})} = A(i \Delta x, j \Delta y, (k + \frac{1}{2}) \Delta z),
\]

so that \( \vec{n}^* = A \vec{t} \) is given by

\[
n^*_{(i+\frac{1}{2}, j, k)} = A_{(i+\frac{1}{2}, j, k)} t_{(i+\frac{1}{2}, j, k)},
\]

\[
n^*_{(i, j+\frac{1}{2}, k)} = A_{(i, j+\frac{1}{2}, k)} t_{(i, j+\frac{1}{2}, k)},
\]

\[
n^*_{(i, j, k+\frac{1}{2})} = A_{(i, j, k+\frac{1}{2})} t_{(i, j, k+\frac{1}{2})}.
\]

The formulas for multiplication by \( a, b \) and \( A \) are similar to the above as are the formulas for multiplication by \( 1/a, A^{-1} B^{-1} \) and \( 1/b \). If we take \( a, b, A \) and \( B \) to be the constant 1, then this says that the quantities in Table 2 that are at the same point in the grid are equal. Unfortunately, this is not dimensionally consistent! So we need the functions \( a \) and \( b \) to have spatial dimensions \( 1/d^3 \) and \( A \) and \( B \) to have spatial dimensions \( 1/d \).

### 6.5 Dual Exact Sequences

The actions of the difference and multiplication operators are summarized in the double exact sequence shown in Figure 7. A critical point here is that this diagram has a big difference from the continuum diagram given in Figure 3: the primal and dual spaces such as \( S_N \) and \( S_{N^*} \) are not the same as was the case in the continuum. The upper row are discrete scalar
and vector fields on the primary grid while the lower row are vector and scalar fields on the dual grid. What is important is that each of the difference operators increases the spatial dimension of the grid quantities by one and the spatial dimensions of the grid quantities are correctly handled by the multiplication operators.

If \( c \) is a constant scalar field then a direct computation \[30\] shows that:

\[
Gc \equiv 0, \quad R\!\!G \equiv 0, \quad D\!\!R \equiv 0, \quad G^\ast c \equiv 0, \quad R\!\!G^\ast \equiv 0, \quad D\!\!R^\ast \equiv 0.
\] (6.7)

These realtionships we checked in MimeticTest.m. These properties are summarized by saying that the discretization is \textit{exact} or that the sequences in Figure 7 are \textit{exact}, see \[30\] for a precise definition of \textit{exact} and a proof that the diagram is \textit{exact}.

### 6.6 Inner Products and Adjoint Operators

To study conserved quantities we need an inner product for each of the eight linear spaces in the dual exact sequences Figure 7. An important property of the inner products is that they need to be dimensionless.

If \( s1, s2 \in S_N \) then

\[
\langle s1, s2 \rangle_N = \sum_{i,j,k} a_{i,j,k} s1_{i,j,k} s2_{i,j,k} \Delta x \Delta y \Delta z.
\]

If \( s1^\ast, s2^\ast \in S_N^\ast \) then

\[
\langle s1^\ast, s2^\ast \rangle_{N^\ast} = \sum_{i,j,k} b_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} s1^\ast_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} s2^\ast_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} \Delta x \Delta y \Delta z.
\]

If \( \vec{t}1, \vec{t}2 \in V_E \) then

\[
\langle \vec{t}1, \vec{t}2 \rangle_E = \sum_{i,j,k} (A_{i+\frac{1}{2},j+\frac{1}{2},k} t1_{i+\frac{1}{2},j+\frac{1}{2},k} t2_{i+\frac{1}{2},j+\frac{1}{2},k} +
A_{i,j+\frac{1}{2},k} t1_{i,j+\frac{1}{2},k} t2_{i,j+\frac{1}{2},k} +
A_{i,j+\frac{1}{2},k} t1_{i,j+\frac{1}{2},k} t2_{i,j+\frac{1}{2},k} \Delta x \Delta y \Delta z.
\]
If \( t^1^*, t^2^* \in V_\mathcal{C} \), then
\[
\langle t^1^*, t^2^* \rangle_{\mathcal{E}} = \sum_{i,j,k} (B_{i,j,k} + \frac{1}{2}) t^1_{i,j,k} + \frac{1}{2} t^2_{i,j,k} +
\]
\[
B_{i,j,k} + \frac{1}{2} t^1_{i,j,k} + \frac{1}{2} t^2_{i,j,k} +
\]
\[
B_{i,j,k} + \frac{1}{2} t^1_{i,j,k} + \frac{1}{2} t^2_{i,j,k} \triangle x \triangle y \triangle z
\]

If \( n^1, n^2 \in V_\mathcal{F} \) then
\[
\langle n^1, n^2 \rangle_{\mathcal{F}} = \sum_{i,j,k} (B_{i,j,k} + \frac{1}{2}) n^1_{i,j,k} + \frac{1}{2} n^2_{i,j,k} +
\]
\[
B_{i,j,k} + \frac{1}{2} n^1_{i,j,k} + \frac{1}{2} n^2_{i,j,k} +
\]
\[
B_{i,j,k} + \frac{1}{2} n^1_{i,j,k} + \frac{1}{2} n^2_{i,j,k} \triangle x \triangle y \triangle z
\]

If \( n^1^*, n^2^* \in V_\mathcal{F} \), then
\[
\langle n^1^*, n^2^* \rangle_{\mathcal{F}} = \sum_{i,j,k} (A_{i,j,k}^{-1} n^1^*_{i,j,k} + \frac{1}{2} n^2^*_{i,j,k} +
\]
\[
A_{i,j,k}^{-1} n^1^*_{i,j,k} + \frac{1}{2} n^2^*_{i,j,k} +
\]
\[
A_{i,j,k}^{-1} n^1^*_{i,j,k} + \frac{1}{2} n^2^*_{i,j,k} \triangle x \triangle y \triangle z
\]

If \( d_1, d_2 \in S_\mathcal{C} \) then
\[
\langle d_1, d_2 \rangle_{\mathcal{N}} = \sum_{i,j,k} b_{i,j,k} d_1_{i,j,k} + \frac{1}{2} d_2_{i,j,k} + \frac{1}{2} \triangle x \triangle y \triangle z.
\]

If \( d_1^*, d_2^* \in S_\mathcal{C}^* \), then
\[
\langle d_1^*, d_2^* \rangle_{\mathcal{C}} = \sum_{i,j,k} a_{i,j,k}^{-1} d_1^*_{i,j,k} + d_2^*_{i,j,k} \triangle x \triangle y \triangle z.
\]

### 6.7 Adjoint Operators

We now note that the discrete difference operators satisfy adjoint relationships analogous to the continuum differential operators \( \nabla, \nabla \times \) and \( \nabla \cdot \). The best way to see why these formulas are correct is to trace the actions of the operators around the squares in Figure 7. The top row of operators give us three formulas, the bottom row of operators give the same formulas. If \( s \in S_\mathcal{N} \) and \( \mathcal{n}^* \in V_\mathcal{F} \), then
\[
\langle A G s, \mathcal{n}^* \rangle_{\mathcal{F}} = -\langle s, \frac{1}{a} D^* \mathcal{n}^* \rangle_{\mathcal{N}}
\]  \quad (6.8)
If \( \vec{t} \in V \) and \( \vec{t}^* \in V^* \), then

\[
\langle B^{-1} \mathcal{R} \vec{t}, \vec{t}^* \rangle_{E^*} = -\langle \vec{t}, A^{-1} \mathcal{R}^* \vec{t}^* \rangle_{E}
\]  

(6.9)

If \( \vec{n} \in V \) and \( \vec{t}^* \in S_{N^*} \), then

\[
\langle b^{-1} \mathcal{D} \vec{n}, \vec{s}^* \rangle_{N^*} = -\langle \vec{n}, B \mathcal{G} \vec{s}^* \rangle_{F}
\]  

(6.10)

The proofs of the adjoint formulas rely on summation by parts which we will illustrate by computing

\[
\sum_{i,j,k} \left( s_{i+1,j,k} - s_{i,j,k} \right) n^*_{i+\frac{1}{2},j,k} - \sum_{i,j,k} s_{i,j,k} n^*_{i+\frac{1}{2},j,k} = \sum_{i,j,k} s_{i,j,k} n^*_{i-\frac{1}{2},j,k} - \sum_{i,j,k} s_{i,j,k} n^*_{i+\frac{1}{2},j,k}
\]

For an example, we will consider (6.8):

\[
\langle A \mathcal{G} s, \vec{n}^* \rangle_{F^*} = \sum_{i,j,k} \left( \frac{s_{i+1,j,k} - s_{i,j,k}}{\Delta x} n^*_{i+\frac{1}{2},j,k} + \frac{s_{i,j,k+1} - s_{i,j,k}}{\Delta y} n^*_{i,j,k+\frac{1}{2}} + \frac{s_{i,j,k+1} - s_{i,j,k}}{\Delta z} n^*_{i,j,k+\frac{1}{2}} \right) \Delta x \Delta y \Delta z
\]

\[
\langle s, \frac{1}{a} \mathcal{D}^* \vec{n}^* \rangle_{N^*} = \sum_{i,j,k} \left( \frac{n^*_{i+\frac{1}{2},j,k} - n^*_{i-\frac{1}{2},j,k}}{\Delta x} + \frac{n^*_{i,j,k+\frac{1}{2}} - n^*_{i,j,k-\frac{1}{2}}}{\Delta y} + \frac{n^*_{i,j,k+\frac{1}{2}} - n^*_{i,j,k-\frac{1}{2}}}{\Delta z} \right) \Delta x \Delta y \Delta z.
\]

Three integration by parts will prove (6.8). The remaining formulas (6.9) and (6.10) can be proved in the same way.

### 6.8 An Important Identity

An important operator identity for quantum mechanics is

\[
\vec{\nabla} \times \vec{\nabla} \times \vec{v} = \vec{\nabla} (\vec{\nabla} \cdot \vec{v}) - \Delta \vec{v}.
\]

xxx explain this xxx
Discretizing the Scalar Wave Equation in 3D

This system can be written in matrix form:

\[
\begin{bmatrix}
    u' \\
    v'
\end{bmatrix} = \begin{bmatrix}
    0 & \frac{1}{a} \nabla \\
    \nabla & 0
\end{bmatrix} \begin{bmatrix}
    u \\
    v
\end{bmatrix}.
\]

(7.1)

We will discretize the scalar wave equation written as a first order system as in (7.1) using the discrete operators described in Section 6. Actually we will changing the notation in Section 3.3 to accomplish this by changing \( f^n \) to \( u^n \), \( g^{n+\frac{1}{2}} \) to \( v^{n+\frac{1}{2}} \), \( A \) to \( a^{-1} D^{*} \) and \( A^{*} \) to \( -AG \). So let \( u \in S_{N} \) and \( v \in V_{F} \), then define the time discretization by

\[
\frac{u^{n+1} - u^n}{\Delta t} = a^{-1} D^{*} v^{n+\frac{1}{2}}, \quad \frac{v^{n+\frac{1}{2}} - v^{n-\frac{1}{2}}}{\Delta t} = AG u^n.
\]

We assume that we are given \( u^0 \) and \( v^{\frac{1}{2}} \) and then the leapfrog scheme for \( n \geq 0 \) is

\[
u^{n+1} = u^n + \Delta t a^{-1} D^{*} v^{n+\frac{1}{2}}, \quad v^{n+\frac{3}{2}} = v^{n+\frac{1}{2}} + \Delta t AG u^{n+1}.
\]

As before we will need the second order discrete equation and a second order average:

\[
\frac{u^{n+1} - 2 u^n + u^{n-1}}{\Delta t^2} = a^{-1} D^{*} v^{n+\frac{1}{2}} - D^{*} v^{n-\frac{1}{2}}
\]

\[
= a^{-1} D^{*} v^{n+\frac{1}{2}} - v^{n-\frac{1}{2}}
\]

\[
= a^{-1} D^{*} AG u^n
\]

\[
\frac{u^{n+1} + 2 u^n + u^{n-1}}{4} = u^n + \frac{u^{n+1} - 2 u^n + u^{n-1}}{4}
\]

\[
= u^n + \frac{\Delta t^2 u^{n+1} - 2 u^n + u^{n-1}}{\Delta t^2}
\]

\[
= u^n + \frac{\Delta t^2}{4} a^{-1} D^{*} AG u^n
\]

To find a conserved quantity let

\[
C_{1_{n+1/2}} = \left\| \frac{u^{n+1} + u^n}{2} \right\|_{N}^2,
\]

\[
C_{2_{n+1/2}} = \left\| v^{n+1/2} \right\|_{F_{*}}^2,
\]

\[
C_{3_{n+1/2}} = \Delta t^2 \left\| a^{-1} D^{*} v^{n+1/2} \right\|_{N}^2.
\]

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As before we compute:
\[
C_{1,n+1/2} - C_{1,n-1/2} = \frac{\Delta t^2}{4} a^{-1} \mathcal{D}^* A\mathcal{G} u^n, u^{n+1} - u^{n-1} \rangle_N
\]
\[
= \langle u^n + \frac{\Delta t^2}{4} a^{-1} \mathcal{D}^* A\mathcal{G} u^n, u^{n+1} - u^{n-1} \rangle_N;
\]
\[
= \langle u^n, u^{n+1} - u^{n-1} \rangle_N + \frac{\Delta t^2}{4} \langle a^{-1} \mathcal{D}^* A\mathcal{G} u^n, u^{n+1} - u^{n-1} \rangle_N;
\]
Using the adjoint equation (6.8) gives
\[
C_{2,n+1/2} - C_{1,n-1/2} = (v^{n+1/2} + v^{n-1/2}, v^{n+1/2} - v^{n-1/2})_{\mathcal{F}^*},
\]
\[
= \langle v^{n+1/2} + v^{n-1/2}, \Delta t A\mathcal{G} u^n \rangle_{\mathcal{F}^*},
\]
\[
= -\Delta t \langle a^{-1} \mathcal{D}^* v^{n+1/2} + a^{-1} \mathcal{D}^* v^{n-1/2}, u^n \rangle_N
\]
\[
= -\Delta t \langle \frac{u^{n+1} - u^{n-1}}{\Delta t}, u^n \rangle_N
\]
\[
= -\langle u^n, u^{n+1} - u^{n-1} \rangle_N;
\]
Also
\[
C_{3,n+1/2} - C_{1,n-1/2} = \Delta t^2 \langle a^{-1} \mathcal{D}^* v^{n+1/2} - a^{-1} \mathcal{D}^* v^{n-1/2}, a^{-1} \mathcal{D}^* v^{n+1/2} + a^{-1} \mathcal{D}^* v^{n-1/2} \rangle_N
\]
\[
= \Delta t^2 \langle a^{-1} \mathcal{D}^* \left( v^{n+1/2} - v^{n-1/2} \right), \frac{u^{n+1} - u^{n-1}}{\Delta t} \rangle_N
\]
\[
= \Delta t^2 \langle -\Delta t a^{-1} \mathcal{D}^* - A\mathcal{G} u^n, \frac{u^{n+1} - u^{n-1}}{\Delta t} \rangle_N
\]
\[
= \Delta t^2 \langle a^{-1} \mathcal{D}^* A\mathcal{G} u^n, u^{n+1} - u^{n-1} \rangle_N.
\]
Consequently \( C = C_1 + C_2 - C_3/4 \) is a conserved quantity:
\[
C_{n+1/2} = \left\| \frac{u^{n+1} + u^n}{2} \right\|^2 + \left\| v^{n+1/2} \right\|^2 - \frac{\Delta t^2}{4} \left\| a^{-1} \mathcal{D}^* v^{n+1/2} \right\|^2.
\]
This implies that
\[
C_{n+1/2} \geq \left\| \frac{u^{n+1} + u^n}{2} \right\|^2 + \left( 1 - \frac{\Delta t^2}{4} \left\| a^{-1} \mathcal{D}^* \right\|^2 \right) \left\| v^{n+1/2} \right\|^2.
\]
So \( C_{n+1/2} \geq 0 \) for \( \Delta t \) sufficiently small provided \( \left\| a^{-1} \mathcal{D}^* \right\| \) is finite.

Next we look for an analog \( C_n \) of the scaler conserved quantity
\[
C_{1,n} = \left\| \frac{v^{n+1/2} + v^{n-1/2}}{2} \right\|^2_{\mathcal{F}^*},
\]
\[
C_{2,n} = \left\| u^n \right\|^2_N ,
\]
\[
C_{3,n} = \Delta t^2 \left\| A\mathcal{G} u^n \right\|^2_{\mathcal{F}^*}.
\]
First we compute
\[ C_{1n+1} - C_{1n} = \left( \frac{v^{n+3/2} + 2v^{n1/2} + v^{n-1/2}}{4}, v^{n+3/2} - v^{n-1/2} \right) \mathcal{F}^* \]
\[ = \left( \frac{\Delta t^2}{4} \right) (\mathcal{A} \mathcal{G} a^{-1} \mathcal{D}^* v^{n+1/2}, v^{n+3/2} - v^{n-1/2}) \mathcal{F}^*. \]

Using the adjoint equation (6.8) gives
\[ C_{2n+1} - C_{2n} = \langle u^{n+1} - u^n, u^{n+1} + u^n \rangle_N \]
\[ = \langle \Delta t a^{-1} \mathcal{D}^* v^{n+1/2}, u^{n+1} + u^n \rangle_N \]
\[ = \Delta t \langle v^{n+1/2}, -\mathcal{A} \mathcal{G} u^n + \mathcal{A} \mathcal{G} u^{n+1} \rangle \]
\[ = \Delta t \langle v^{n+1/2}, -\frac{v^{n+3/2} - v^{n-1/2}}{\Delta t} \rangle \]
\[ = -\langle v^{n+1/2}, v^{n+3/2} - v^{n-1/2} \rangle. \]

Also
\[ C_{3n+1} - C_{3n} = \Delta t^2 \langle \mathcal{A} \mathcal{G} u^n, \mathcal{A} \mathcal{G} u^{n+1} \rangle \mathcal{F}^* \]
\[ = \Delta t^2 \langle \mathcal{A} \mathcal{G} u^n, \frac{v^{n+3/2} - v^{n-1/2}}{\Delta t} \rangle \mathcal{F}^* \]
\[ = \Delta t^2 \langle \Delta t \mathcal{A} \mathcal{G} a^{-1} \mathcal{D}^* v^{n+1/2}, v^{n+3/2} - v^{n-1/2} \rangle \]
\[ = \Delta t^2 \langle \mathcal{A} \mathcal{G} a^{-1} \mathcal{D}^* v^{n+1/2}, v^{n+3/2} - v^{n-1/2} \rangle. \]

Consequently \( C_n = C_{1n} + C_{2n} - C_{3n}/4 \) is a conserved quantity:
\[ C_n = ||u^n||^2 - \frac{\Delta t^2}{4} ||\mathcal{A} \mathcal{G} u^n||^2 + \left| \left| \frac{v^{n+1/2} + v^{n-1/2}}{2} \right| \right|^2. \]

This implies that
\[ ||C_n|| \geq \left( 1 - \frac{\Delta t^2}{4} ||\mathcal{A} \mathcal{G}||^2 \right) ||u^n||^2 + \left| \left| \frac{v^{n+1/2} + v^{n-1/2}}{2} \right| \right|^2, \]
so \( ||C_n|| \) is positive for sufficiently small \( \Delta t \) if \( ||\mathcal{A} \mathcal{G} u^n|| \) is finite.

We used the programs ScalarWave.m and ScalarWaveStar.m to show that the energies \( C_n \) and \( C_{n+1}/4 \) are constant to less than 1 part in \( 10^{15} \) for the discretization described above and the one that changes \( \mathcal{G} \) to \( \mathcal{G}^* \) and \( \mathcal{D} \) to \( \mathcal{D}^* \).
8 Maxwell’s Equations

We assume that $\vec{E} \in V_\epsilon$ and $\vec{H} \in V_\epsilon^*$, then using the notation in the previous sections we will discretized the Maxwell system 5.15 as

$$\frac{\vec{E}^{n+1} - \vec{E}^n}{\Delta t} = \epsilon^{-1} R^* \vec{H}^{n+\frac{1}{2}}, \quad \frac{\vec{H}^{n+\frac{1}{2}} - \vec{H}^{n-\frac{1}{2}}}{\Delta t} = -\mu^{-1} R \vec{E}^n.$$  

where in Exact Sequence diagram (7) we choose $A = \epsilon$ and $B = \mu$. Here $\epsilon$ and $\mu$ can be symmetric positive definite matrices. If we write $\vec{E} = (Ex, Ey, Ez)$ and $\vec{H} = (Hx, Hy, Hz)$ then from Table 2 we see that $Ex$ and $Hx$ are indexed as $Ex^n_{i,j,k+\frac{1}{2}}$, $Hx^n_{i,j+\frac{1}{2},k+\frac{1}{2}}$ just as in Yee’s paper [41]. If we are given $\vec{E}^0$ and $\vec{H}^\frac{1}{2}$ and then the leapfrog scheme for $n \geq 0$ is

$$\vec{E}^{n+1} = \vec{E}^n + \Delta t \epsilon^{-1} R^* \vec{H}^{n+\frac{1}{2}}, \quad \vec{H}^{n+3/2} = \vec{H}^{n+\frac{1}{2}} - \Delta t \mu^{-1} R \vec{E}^{n+1}.$$  

To study conserved quantities for Maxwell’s equations we will need the second order discrete difference and average:

$$\bar{\vec{E}}^{n+1} - 2 \bar{\vec{E}}^n + \bar{\vec{E}}^{n-1} = -\epsilon^{-1} R^* \mu^{-1} R \bar{\vec{E}}^n$$

$$\bar{\vec{E}}^{n+1} + 2 \bar{\vec{E}}^n + \bar{\vec{E}}^{n-1} = \bar{\vec{E}}^n - \frac{\Delta t^2}{4} \epsilon^{-1} R^* \mu^{-1} R \bar{\vec{E}}^n$$

To find a conserved quantity $C_{n+1/2}$ let

$C_{1/2} = \left| \frac{\bar{\vec{E}}^{n+1} + \bar{\vec{E}}^n}{2} \right|^2_{\mathscr{E}}$,

$C_{2/2} = \left| \bar{\vec{H}}^{n+1/2} \right|^2_{\mathscr{E}^*}$,

$C_{3/2} = \Delta t^2 \left| \epsilon^{-1} R^* \bar{\vec{H}}^{n+1/2} \right|^2_{\mathscr{E}}$.

As before we compute:

$$C_{1/2}^{n+1} - C_{1/2}^{n-1} = \left( \frac{\bar{\vec{E}}^{n+1} + 2 \bar{\vec{E}}^n + \bar{\vec{E}}^{n-1}}{4}, \bar{\vec{E}}^{n+1} - \bar{\vec{E}}^{n-1} \right)_{\mathscr{E}}$$

$$= \left( \bar{\vec{E}}^n - \frac{\Delta t^2}{4} \epsilon^{-1} R^* \mu^{-1} R \bar{\vec{E}}^n, \bar{\vec{E}}^{n+1} - \bar{\vec{E}}^{n-1} \right)_{\mathscr{E}};$$

$$= \left( \bar{\vec{E}}^n, \bar{\vec{E}}^{n+1} - \bar{\vec{E}}^{n-1} \right)_{\mathscr{E}} - \frac{\Delta t^2}{4} \left( \epsilon^{-1} R^* \mu^{-1} R \bar{\vec{E}}^n, \bar{\vec{E}}^{n+1} - \bar{\vec{E}}^{n-1} \right)_{\mathscr{E}};$$

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Using the adjoint equation (6.8) gives

\[ C_{2n+1/2} - C_{1n-1/2} = \langle \bar{H}^{n+1/2} + \bar{H}^{n-1/2}, \bar{H}^{n+1/2} - \bar{H}^{n-1/2} \rangle_{\mathcal{F}^*} \]
\[ = \langle \bar{H}^{n+1/2} + \bar{H}^{n-1/2}, -\Delta t \mu^{-1} \mathcal{R} \bar{E}^n \rangle_{\mathcal{F}^*} \]
\[ = -\Delta t \langle \epsilon^{-1} \mathcal{R}^* \bar{H}^{n+1/2} + \epsilon^{-1} \mathcal{R}^* \bar{H}^{n-1/2}, \bar{E}^n \rangle \]
\[ = -\Delta t \left( \frac{\bar{E}^{n+1} - \bar{E}^{n-1}}{\Delta t} \right) \bar{E}^n \]
\[ = -\langle \bar{E}^n, \bar{E}^{n+1} - \bar{E}^{n-1} \rangle \epsilon ; \]

Also

\[ C_{3n+1/2} - C_{1n-1/2} = \Delta t^2 \langle \epsilon^{-1} \mathcal{R}^* \bar{H}^{n+1/2} - \epsilon^{-1} \mathcal{R}^* \bar{H}^{n-1/2}, \epsilon^{-1} \mathcal{R}^* \bar{H}^{n+1/2} + \epsilon^{-1} \mathcal{R}^* \bar{H}^{n-1/2} \rangle \epsilon \]
\[ = \Delta t^2 \langle \epsilon^{-1} \mathcal{R}^* \left( \bar{H}^{n+1/2} - \bar{H}^{n+1/2} \right), \frac{\bar{E}^{n+1} - \bar{E}^{n-1}}{\Delta t} \rangle \epsilon \]
\[ = \Delta t^2 \langle -\Delta t \epsilon^{-1} \mathcal{R}^* \mu^{-1} \mathcal{R} \bar{E}^n, \frac{\bar{E}^{n+1} - \bar{E}^{n-1}}{\Delta t} \rangle \epsilon \]
\[ = -\Delta t^2 \langle \epsilon^{-1} \mathcal{R}^* \mu^{-1} \mathcal{R} \bar{E}^n, \bar{E}^{n+1} - \bar{E}^{n-1} \rangle \epsilon . \]

Consequently \( C = C_1 + C_2 - C_3/4 \) is a conserved quantity:

\[ C_{n+1/2} = \left\| \frac{\bar{E}^{n+1} + \bar{E}^n}{2} \right\|_\epsilon^2 + \left\| \bar{H}^{n+1/2} \right\|_{\mathcal{F}^*}^2 - \frac{\Delta t^2}{4} \left\| \epsilon^{-1} \mathcal{R}^* \bar{H}^{n+1/2} \right\|_{\mathcal{F}^*}^2 . \]

This implies that

\[ C_{n+1/2} \geq \left\| \frac{\bar{E}^{n+1} + \bar{E}^n}{2} \right\|_\epsilon^2 + \left( 1 - \frac{\Delta t^2}{4} \left\| \epsilon^{-1} \mathcal{R}^* \right\|_\epsilon^2 \right) \left\| \bar{H}^{n+1/2} \right\|_{\mathcal{F}^*}^2 . \]

So \( C_{n+1/2} \geq 0 \) for \( \Delta t \) sufficiently small provided \( \left\| \epsilon^{-1} \mathcal{R}^* \right\|_\epsilon \) is finite.

Next we look for a conserved quantity \( C_n \):

\[ C_{1n} = \left\| \frac{\bar{H}^{n+1/2} + \bar{H}^{n-1/2}}{2} \right\|_{\mathcal{F}^*}^2 , \]
\[ C_{2n} = \left\| \bar{E}^n \right\|_{\mathcal{F}^*}^2 , \]
\[ C_{3n} = \Delta t^2 \left\| \mu^{-1} \mathcal{R} \bar{E}^n \right\|_{\mathcal{F}^*}^2 . \]

First we compute

\[ C_{n+1} - C_{1n} = \langle \bar{H}^{n+3/2} + 2 \bar{H}^{n+1/2} + \bar{H}^{n-1/2}, \bar{H}^{n+3/2} - \bar{H}^{n-1/2} \rangle_{\mathcal{F}^*} \]
\[ = \langle \bar{H}^{n+1/2}, \bar{H}^{n+3/2} - \bar{H}^{n-1/2} \rangle_{\mathcal{F}^*} + \frac{\Delta t^2}{4} \langle \mu^{-1} \mathcal{R} \epsilon^{-1} \mathcal{R} \bar{H}^{n+1/2}, \bar{H}^{n+3/2} - \bar{H}^{n-1/2} \rangle_{\mathcal{F}^*} . \]
Using the adjoint equation (6.8) gives

\[ C_{2n+1} - C_{2n} = \langle \vec{E}_{n+1}^2 - \vec{E}_n^2, \vec{E}_{n+1} + \vec{E}_n \rangle_e \]
\[ = \langle \Delta t \epsilon^{-1} \mathcal{R}^* \vec{H}_{n+1/2}^2, \vec{E}_{n+1} + \vec{E}_n \rangle_e \]
\[ = \Delta t \langle \vec{H}_{n+1/2}^2, -\mu^{-1} \mathcal{R} \vec{E}_{n+1} - \mu^{-1} \mathcal{R} \vec{E}_n \rangle_{\mathcal{F}_n^*} \quad \text{(adjoint)} \]
\[ = \Delta t \langle \vec{H}_{n+1/2}^2, -\frac{\vec{H}_{n+3/2} - \vec{H}_{n-1/2}}{\Delta t} \rangle_{\mathcal{F}_n^*} \]
\[ = -\langle \vec{H}_{n+1/2}^2, \vec{H}_{n+3/2} - \vec{H}_{n-1/2} \rangle_{\mathcal{F}_n^*}. \]

Also

\[ C_{3n+1} - C_{3n} = \Delta t^2 \langle \mu^{-1} \mathcal{R} \vec{E}_{n+1}^2 - \mu^{-1} \mathcal{R} \vec{E}_n^2, \mu^{-1} \mathcal{R} \vec{E}_{n+1} + \mu^{-1} \mathcal{R} \vec{E}_n \rangle_{\mathcal{F}_n^*} \]
\[ = \Delta t^2 \langle \mu^{-1} \mathcal{R} \vec{E}_{n+1}^2 - \mu^{-1} \mathcal{R} \vec{E}_n^2, \frac{\vec{H}_{n+3/2} - \vec{H}_{n-1/2}}{\Delta t} \rangle_{\mathcal{F}_n^*} \]
\[ = \Delta t^2 \langle \Delta t \mu^{-1} \mathcal{R} \epsilon^{-1} \mathcal{R}^* \vec{H}_{n+1/2}^2, \frac{\vec{H}_{n+3/2} - \vec{H}_{n-1/2}}{\Delta t} \rangle_{\mathcal{F}_n^*} \]
\[ = \Delta t^2 \langle \mu^{-1} \mathcal{R} \epsilon^{-1} \mathcal{R}^* \vec{H}_{n+1/2}^2, \vec{H}_{n+3/2} - \vec{H}_{n-1/2} \rangle_{\mathcal{F}_n^*}. \]

Consequently \( C_n = C_{1n} + C_{2n} - C_{3n}/4 \) is a conserved quantity:

\[ C_n = \left\| \vec{E}_n \right\|_e^2 - \frac{\Delta t^2}{4} \left\| \mu^{-1} \mathcal{R} \vec{E}_n \right\|_{\mathcal{F}_n^*}^2 + \left\| \frac{\vec{H}_{n+1/2} + \vec{H}_{n-1/2}}{2} \right\|_{\mathcal{F}_n^*}^2. \]

This implies that

\[ ||C_n|| \geq \left( 1 - \frac{\Delta t^2}{4} \left\| \mu^{-1} \mathcal{R} \right\|_e^2 \right) \left\| \vec{E}_n \right\|_e^2 + \left\| \frac{\vec{H}_{n+1/2} + \vec{H}_{n-1/2}}{2} \right\|_{\mathcal{F}_n^*}^2, \]

so \( ||C_n|| \) is positive for sufficiently small \( \Delta t \) if \( \left\| \mu^{-1} \mathcal{R} \vec{E}_n \right\|_e \) is finite.

The codes 'Maxwell.m' and 'MaxwellStar.m' confirm that our algorithms conserve \( C_{n+1/2} \) and \( C_n \) to two parts in \( 10^{16} \). Additionally, the divergence of the curl of the electric and magnetic fields are constant to one part in \( 10^{14} \) when there are no sources.
9 Conservation Laws and Positive Solutions

Conservation laws that say the total amount of some positive substance is conserved play an important role in modeling using partial differential equations, for example the Navier-Stokes equations [28](equations 1.5, 1.6 and 1.7) can be put into this form. To provided some insight into discretizing such conservation laws, we consider two important but simple cases. For a similar discussion see Chapter 11 in [24].

9.1 Transport

The transport equation in one dimension is given by

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

where $\rho = \rho(x,t)$ is a density and $v = v(x)$ is the velocity of transport. An important assumption is that $\rho \geq 0$ as it typically represents the density of some substance. The general solution of this equation is

$$\rho(x,t) = w(x - vt),$$

where $w(x) = \rho(x,0)$ is the initial data. This solution is a right translation of $w(x)$. This equation also has an important conservation law:

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

The conserved quantity is the total amount of material being transported. Also note that if $w(x) \geq 0$ then $\rho(x,t) \geq 0$ for all $t$. These two properties are central to this discussion. Our interest is in finite difference discretizations of equations that have a similar conservation law and maintain the positivity of the solution.

We assume that $\Delta x > 0$ and use two grids: a primary grid $x_i = i \Delta x$ that has cells $[x_i, x_{i+1}]$ and a grid of cell centers $x_{i+\frac{1}{2}} = (i + \frac{1}{2}) \Delta x$ where $-\infty < i < \infty$. Note that if $\rho$ is a density then it has spatial dimension $1/d_k$ in a space of dimension $k$ suggesting that $\rho$ should be in a cells. If we choose a primary grid then we get the discretization of $\rho$ is

$$\rho_{i+\frac{1}{2}}^{n+\frac{1}{2}}.$$

We will use the conservation of material

$$\Delta x \rho_{i+\frac{1}{2}}^{n+\frac{1}{2}}$$

in a cell to discretize this equation as

$$\Delta x \rho_{i+\frac{1}{2}}^{n+\frac{3}{2}} = \Delta x \rho_{i+\frac{1}{2}}^{n+\frac{1}{2}} + \Delta t v_i \rho_{i-\frac{1}{2}}^{n+\frac{1}{2}} - \Delta t v_{i+1} \rho_{i+\frac{1}{2}}^{n+\frac{1}{2}}.$$
Figure 8: A: Left transport of a square wave \( v \Delta t/\Delta x = -1 \). B: Right transport of a square wave with \( v = 0.4167 \). (See Transport.m)

Rewrite this as

\[
\frac{\rho_{i+1}^{n+1/2} - \rho_i^{n+1/2}}{\Delta t} + \frac{v_{i+1} \rho_{i+1}^{n+1/2} - v_i \rho_i^{n+1/2}}{\Delta x} = 0,
\]

to see that the discretization is a first order approximation of the differential equation. As an update of the density the equation becomes

\[
\rho_{i+1}^{n+3/2} = \rho_{i+1}^{n+1/2} + \frac{\Delta t}{\Delta x} v_i \rho_i^{n+1/2} - \frac{\Delta t}{\Delta x} v_{i+1} \rho_{i+1}^{n+1/2}.
\]

Now if

\[
\frac{\Delta t}{\Delta x} v_i \geq 0, \quad 1 - \frac{\Delta t}{\Delta x} v_{i+1} \geq 0,
\]

that is if

\[
v_i \geq 0, \quad \frac{\Delta t}{\Delta x} v_{i+1} \leq 1,
\]

then the discretization preserves the positivity of the discrete solution and is the well known upwind scheme. This scheme is not useful if the velocity \( v = v(x) \) has both negative and positive values. To fix this we will change our point of view from \( \rho \) to \( v \).

So consider the edges of the cells and compute the amount of material being transferred between the neighboring cells, that is for each time step \( n \), for all \( i \) compute the discrete
solution as follows:

\[
\begin{align*}
  \text{if } v_i \geq 0 \text{ then } & \quad \rho_{i-1/2}^{n+3/2} = \rho_{i-1/2}^{n+3/2} - v_i \frac{\Delta t}{\Delta x} \rho_{i-1/2}^{n+1/2}; \\
  \rho_{i+1/2}^{n+3/2} = \rho_{i+1/2}^{n+3/2} + v_i \frac{\Delta t}{\Delta x} \rho_{i+1/2}^{n+1/2}; \\
  \text{if } v_i \leq 0 \text{ then } & \quad \rho_{i-1/2}^{n+3/2} = \rho_{i-1/2}^{n+3/2} - v_i \frac{\Delta t}{\Delta x} \rho_{i-1/2}^{n+1/2}; \\
  \rho_{i+1/2}^{n+3/2} = \rho_{i+1/2}^{n+3/2} + v_i \frac{\Delta t}{\Delta x} \rho_{i+1/2}^{n+1/2}.
\end{align*}
\]

If \( v_i \) is positive then this removes some material from cell \( i - \frac{1}{2} \) and put it into cell \( i + \frac{1}{2} \) and conversely if \( v_i \) is negative. If \( V = \max(|v_i|) \) then the most material that can be removed from cell \( i - \frac{1}{2} \) is

\[
V \frac{\Delta t}{\Delta x} \rho_{i-1/2}^{n+1/2},
\]

so to keep \( \rho \geq 0 \) it must be that

\[
V \frac{\Delta t}{\Delta x} \leq 1.
\]

An interesting feature of this algorithm is that for \( v_i \Delta t / \Delta x = \pm 1 \) it gives an exact solution of solution as shown in Figure 8. This is an upwind scheme for velocities that change direction that keeps that preserves \( \rho \geq 0 \) and conserves the amount material being transported. As done in Transport.m this scheme can be implemented without the conditional in the update loop.

Not all discretizations preserve positive solutions, for example the Lax-Wendroff, Richtmyer, and MacCormac schemes do not for linear equations (see Lax-Wendroff-Positive.nb). This can also be seen by by choosing initial data \( f_i \) that are all zero except for one \( i \) where
\( f_i = 1. \) For linear equations the Richtmyer and MacCormac schemes produce the same solution as the Lax-Wendroff scheme.

### 9.2 Diffusion

The diffusion equation in one dimension is given by

\[
\frac{\partial \rho}{\partial t} = \frac{\partial}{\partial x} D \frac{\partial \rho}{\partial x},
\]

where \( \rho = \rho(x, t) \) is the heat density \( D = D(x) \geq 0 \) is the diffusion coefficient. For this discussion \( t \geq 0 \) and \( \rho \) is smooth and zero for large values of \( |x| \). Then integrating the differential equation gives

\[
\int_{-\infty}^{\infty} \rho(x, t) \, dx = 0.
\]

If \( \rho(x, 0) \geq 0 \) then the solution of the equation is given by convolution with a Gaussian so then \( \rho(x, t) \geq 0 \) for \( t \geq 0 \).

The standard forward time center space finite difference discretization of this equation is given by

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

or in computational form

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

This algorithm will preserve positive solutions for

\[
(D_{i+1} + D_i) \frac{\Delta t}{\Delta x^2} \leq 1,
\]

which is the standard stability constraint for this discretization.
10 Summary and Prospects

We have shown that a simple modification of the energy for several systems results in a conserved quantity that is constant essentially to machine precision. Moreover several other important properties of the continuum model are preserved. However, there are many remaining important problems. It seems clear that it will be easy to implement boundary condition in a way that the symmetry of the discrete first order system is preserved. Also the extension to logically rectangular grids seems straightforward. For more complex grids the dual of the dual grid being the original grid is lost which introduces a novel complexity in deriving conserved quantities. It is certainly unclear if the ideas presented here can be extended to higher-order time discretizations although there have been successes for related methods [15].
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A Energy Preserving Discretizations of the Harmonic Oscillator

Here we show the well-know fact that the Crank-Nicholson discretization conserves the discrete analog of the energy for the harmonic oscillator. We also show that the methods introduced in [39] produce a discretization that is equivalent to the Crank-Nicholson discretization.

A.1 Conserving the Simple Energy

The Crank-Nicholson discretization does preserve the simple energy (2.4):

$$\frac{u_{n+1} - u_n}{\Delta t} = -\omega \frac{v_{n+1} + v_n}{2}, \quad \frac{v_{n+1} - v_n}{\Delta t} = \omega \frac{u_{n+1} + u_n}{2}. $$

This gives a discretization of the second order differential equation:

$$\frac{u_{n+2} - 2 u_{n+1} + u_n}{\Delta t^2} + \frac{\omega^2}{4} \frac{u_{n+2} + 2 u_{n+1} + u_n}{4} = 0. \quad (A.1)$$

Then

$$C^2_{n+1} - C^2_n = \frac{1}{2} (v_{n+1} + v_n) (v_{n+1} - v_n) + \frac{1}{2} (u_{n+1} + u_n) (u_{n+1} - u_n)$$

$$= \frac{\Delta t \omega}{4} (v_{n+1} + v_n) (u_{n+1} + u_n) - \frac{\Delta t \omega}{4} (u_{n+1} + u_n) (v_{n+1} + v_n) \equiv 0,$$

so $C_n$ is conserved. If we write the system as

$$u_{n+1} + \frac{\Delta t \omega}{2} v_{n+1} = u_n - \frac{\Delta t \omega}{2} v_n$$

$$v_{n+1} + \frac{\Delta t \omega}{2} u_{n+1} = v_n + \frac{\Delta t \omega}{2} u_n,$$

then we see that the scheme is implicit, that is it involves the inversion of a $2 \times 2$ matrix. The coefficient matrix is always invertible, so there is no restriction on the size of $\Delta t$, that is, the scheme is unconditionally stable.

A.2 The Conservation Law First

We can show that the only reasonable discretization that conserves the simple conservation law (2.4) is equivalent to the Crank-Nicholson discretization following the discussion in [39]. First compute using (2.4) that

$$C^2_{n+1} - C^2_n = (u_{n+1} - u_n) (u_n + u_{n+1}) + \left(v_{n+\frac{1}{2}} - v_{n-\frac{1}{2}}\right) \frac{v_{n-\frac{1}{2}} + 2v_{n+\frac{1}{2}} + v_{n+\frac{3}{2}}}{4}. $$
Choosing

\[
\frac{u_{n+1} - u_n}{\Delta t} = -\omega \frac{v_{n-\frac{1}{2}} + 2v_{n+\frac{1}{2}} + v_{n+\frac{3}{2}}}{4}
\]

and

\[
\frac{v_{n+\frac{3}{2}} - v_{n-\frac{1}{2}}}{2 \Delta t} = \omega \frac{u_n + u_{n+1}}{2}
\]

will make the \( C_n \) constant. If \( \alpha = \Delta t \omega / 2 \) then these equations can be written

\[
\begin{align*}
  u_{n+1} + \frac{\alpha}{2} v_{n+3/2} &= u_n - \alpha v_{n+1/2} - \frac{\alpha}{2} v_{n-1/2} , \\
  -2 \alpha u_{n+1} + v_{n+3/2} &= 2 \alpha u_n + v_{n-1/2} ,
\end{align*}
\]

So the difference equations are implicit.

It is easy to check that \( u_n \) satisfies the second order difference equation \([A.1]\). Unfortunately, this discretization produces the same \( u_n \) values as the Crank-Nicholson scheme but with a greater computational cost. Setting

\[
v_n = \frac{v_{n+1/2} + v_{n-1/2}}{2} ,
\]

converts this scheme along with it’s conserved quantity to the Crank-Nicholson scheme along with it’s conserved quantity.