Explicit Time Mimetic Discretizations Of Wave Equations *

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Abstract

Updated versions of this paper will appear at arXiv. This version has been revised thru Section 4.

This paper is part of a program to combine a staggered time and staggered spatial discretization of continuum wave equations so that important properties of the continuum that are proved using vector calculus can be proven in an analogous way for the discretized system. The spatial discretizations are second order accurate and mimetic. The time discretizations are second order accurate explicit leapfrog schemes. The discretizations have a conserved quantity that guarantees stability for a reasonable constraint on the time step. The conserved quantities are closely related to the energy for the continuum equations. The well known Yee grid discretization of Maxwell's equations [62] is the same as discretization described here and is an early example of using a staggered space and time grids.

Motivation of the discussion begins by studying the discretization of the harmonic oscillator and then use this to introduce the modification of the usual discrete energy that is conserved. Next the discretization and creation of a conserved quantity for possibly infinite linear systems of constant coefficient wave equations is used to show how to create conserved quantities for partial differential equations.

As an introduction to discretizing higher dimensional wave equations the one dimensional wave equation with variable coefficients is used to motivate the rest of this paper. The discussion begins with the constant coefficient wave equation and is then extended to variable coefficients. The conserved quantity contains a term proportional to the square of the time step. Requiring that the conserved quantity is positive is the well known Courant-Friedrichs-Lewy (CFL) condition for stability. For constant material properties and some variable material properties the simulation codes are second order accurate but for other materials they are only close to second order accurate. The cause and importance of this is under study.

To study partial differential equations in higher dimensions the notion of exact sequences and diagram chasing from differential geometry are used to produce second order variable coefficient differential operators that are self adjoint and either positive or negative and thus can be used to define many of the known wave equations. These operators are then used to define second order wave equations and their equivalent first order systems.

Next mimetic spatial finite difference approximations and leap-frog time discretization are used to discretize the first order systems of wave equations in one, two and three dimensional spaces. The discretization also provide solutions of the second order wave equation that are equivalent to the first order system. The discretizations are at least second order accurate and have a conserved quantity that guarantees stability for a modest restriction on the time step. The conserved quantities imply the conservation of energy.

MatLab simulation codes are provided for all of equations studied.

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

The main goal is to show that second-order accurate mimetic finite difference spatial discretizations can be combined with an explicit second order accurate leapfrog finite difference time discretizations to discretize wave equations to produce stable second-order accurate simulations and then to create a general method for extending mimetic discretizations to model waves in inhomogeneous and anisotropic materials. Most importantly, discrete conserved quantities that have simple relationships to the energy are introduced. These discrete conserved quantities are positive quadratic forms for modest restrictions on the time step and consequently imply the discretizations are stable. It is important that the material properties do not depend on the solution of the differential equation so that the equation are linear and additionally that the material properties do not depend on time. The techniques depend on writing second order wave equations as systems of two first order equations. The spatial and temporal units of variables play an important role in the discussion. Simulation codes are provided for all the examples discussed. It is an open question if these ideas can be extended to higher order discretizations or to nonlinear differential equations. Simulation programs are provided for the differential equations. These codes confirm that the conserved quantities are constant to within a small multiple of machine epsilon $\varepsilon$. For constant and some variable material properties the codes confirm the second order accuracy. For other variable material properties the codes are only close to second order accurate. The cause of this is currently under investigation.

In Section 2 The Harmonic Oscillator and Conserved Quantities the standard second-order harmonic oscillator ordinary differential equation is written as a first order system which is discretized using the standard leapfrog or staggered in time method. For this discretization a conserved quantity is created that is closely related to the oscillator energy. This quantity depends on the time step and is positive for small time steps thus guaranteeing stability of the discretization. The constraint on the time step for reasonable accuracy is much smaller than the constraint for stability.

In Section 3 Systems of Ordinary Differential Equations the results for the harmonic oscillator are extended to possibly infinite systems of first order linear and constant coefficient ordinary differential equations that are wave equations. For the discrete system conserved quantities that are generalization of those for the harmonic oscillator are derived. Simple generalizations of these conserved quantities will provide conserved quantities for variable material properties wave equations.

In Section 4 Discretizing the One Dimensional Wave Equation the discussion of spatial discretizations of partial differential equations begins by discretizing wave equations with variable material properties in one spatial dimension. First the second order one dimensional wave equation is derived from the continuum conservation of energy to make clear the correct form of a wave equation with variable material properties. The second order equation is then written as a first order system and then this provides another second order wave equation. The critical point is that weighted inner products can be introduced so that the system has the same form as the equations in Section 3. This immediately gives a conserved quantity.
that implies the conservation of energy.

First the constant coefficient system is discretized followed by the variable coefficient case. These discretizations use the same grids that are staggered in space and time. In space, as in standard in mimetic discretizations, two grids are used where a point in one of the grids is at the midpoint of the cells in the other grid. The time discretization is the standard leapfrog scheme. This results in each first order equation being discretized on separate space and time grids. The discussion in Section 3 then easily provides a conserved quantities that contains a term that is proportional to minus the square of the time step times a positive quantity.

In the constant coefficient discretization the wave speed $c$ is introduced so that it will be easy to compare the mimetic discretization to the usual discretizations found in the literature. Importantly, requiring the conserved quantity to be positive produces the standard Courant-Friedrichs-Lewy (CFL) condition for stability. For the variable coefficient case an estimate of the maximum wave speed can be introduced that provides an analog of the CFL condition for stability.

Two codes `Wave1DCMP.m` and `Wave1DVMP.m` that implement the constant material properties CMP and variable material properties VMP discretizations are described. For the constant materials case both codes produce the same results. Both codes keep a their conserved quantity constant to within a small multiple of machine epsilon $\epsilon$. Simulations confirm that the CMP code is second order accurate. A significant puzzle is that in some cases the VMP code solution has oscillatory errors that start near the boundary and propagate to the interior of the spatial domain. The convergence rate is reduce but is still greater than 1. In a sense made clear in this section the VMP discrete solutions are close to second order accurate. On the other hand when the material properties are given by $1 + (2x(1-x))^2$ the VMP code is second order accurate and there are no small oscillatory errors.

The first 4 sections have been revised. Still working on the following sections. The plan is to first create the three dimensional theory and codes and then use this to implement the two dimensional codes because mimetic differential operators are easier to understand in three dimensions than in two dimensions. In particular the mimetic three dimensional method naturally produces the gradient, curl and divergence operators.

In Section 5 *Three Dimensional Variable Coefficient Differential Operators* the notions of exact sequences and diagram chasing used in differential geometry are used to create twelve second order differential operators with variable coefficients. These operators are built using the gradient, curl and divergence and have coefficients that are positive functions or real symmetric 3 by 3 positive matrices that are smooth functions of the spatial variables. These functions correspond to the star operators in differential geometry. An additional 4 operators that are a linear combination of two of the above operators are also be defined.

The second order operators are next written as a product of two first order operators with variable coefficients. Weighted inner products are introduced and used to compute the adjoint operators of the first order operators and the show that the second order operators are self adjoint and either positive or negative. Thus the negative operators and minus the positive operators can be used to define second order wave equations. It is not clear
if all of the 16 general equations are useful but they do provide flexibility in dealing with spatially dependent material properties. When the scalar coefficients are constant and the matrix coefficient are a constant multiple of the identity matrix the second order operators are reduced to 4 unique operators.

Revisions done to here.

In Section 6 *3D Wave Equations With Variable Material Properties* second order variable coefficient wave equations are defined. Diagram chasing is used to write the second order equations as first order systems. These systems have the same form as those in Section 3 which then easily provides conserved quantities for all of the equations. This section ends by showing the relationship of the diagram chasing wave equations to the standard wave equations in the literature.

In Section 7 *Mimetic 3D Discretizations* three dimensional staggered grids are introduced and used to define mimetic discretizations of the gradient, curl and divergence [46]. This type of discretization is motivated by the use of exact sequences from differential geometry, except here there are two grids so the exact sequence becomes a double exact sequence. This is combined with a leapfrog discretization. The spatial discretization uses two grids where the corners of cells in one grid are the same points as the centers of the cells in the other grid and the centers of the edges on one grid are the cell face centers in the other grid. An early example of this type of spatial and time discretization was given by Yee [62] for Maxwell’s equations. Mimetic spatial discretizations have been used extensively to create simulation programs for problems in continuum mechanics, see [34] and the volume [31] in which this work appeared. They have also been used to model inhomogeneous and anisotropic materials in two dimensions [26, 25]. For a comparison of mimetic finite difference, finite volume and finite element discretizations see [3].

The mimetic spatial discretization studied here are extensions of those described in [46] where it is shown that mimetic discretizations of the gradient, curl and divergence satisfy important properties of the continuum operators. For example the discrete divergence of the discrete curl operator is identically zero and the adjoint of the discrete gradient is the minus the discrete divergence. To extend this work to anisotropic materials it is critical that in three dimensions the anisotropic properties of many important materials are describe by a $3 \times 3$ symmetric positive definite matrix [38], see Chapter 4, Sections 1 and 4, for the permittivity. Additionally, [34, 5, 24, 29] discuss the incorporation of material properties into mimetic discretizations using symmetric positive definite matrices.

In Section 8 the results in Section 7 are used to discretize the scalar wave equation and Maxwell’s equations for general material proprieties. Three case will be considered: trivial material properties where the scalar material property is 1 and the matrix material property is the identity matrix; constant material proprieties where the scalar material properties is a positive constant and the matrix material properties is a multiple of the identity matrix and finally general material proprieties where the scalar material property is a positive smooth function and the matrix material proprieties are given by positive definite matrix and both material properties are smooth functions of the spatial variable.

The code Wave3DTMP.m shows that for the scalar wave equation with trivial material
proprieties the solution is forth order accurate and the conserved quantity is conserved quantity is constant to a small multiple of machine epsilon $\epsilon$. Note that the one spatial dimension scalar wave equation could also produce forth order accurate solutions in some simple cases.

Too be done are the scalar wave equation with general material properties and Maxwell’s equations with general material properties.

It would be interesting to use ghost points to implement general Robin boundary conditions as was done in [9].
2 The Harmonic Oscillator

The goal is to use the time discretization of the harmonic oscillator to motivate time discretizations of special systems of ordinary differential equation that are wave equations, and then this is used to discretize wave equations in 1, 2 and 3 dimensional spaces. The discretizations are second order accurate, explicit and conserve a quantity that is a second order approximation of a constant multiple of the energy. Requiring this quantity to be positive gives the standard constraint on the time step for stability and is far less restrictive that a reasonable accuracy constraint.

First the explicit second order discretization of the second order continuum oscillator equation is described and the novel conserved discrete quantity is introduced. This quantity contains a term that is minus the square of the time step times a positive quantity. The space and time units of the conserved quantity is that of energy. The simulation program $\text{Oscillator2ndOrder.m}$ confirms that the discretization is second order accurate and that the conserved quantity is constant within a small multiple of machine epsilon $\epsilon$.

Next the second order equation is written as a first order system and then this system is discretized using staggered grids which is typically called a leapfrog discretization. This discretization gives solutions that are equivalent to solutions of the discretized second order equation. Next a conserved quantity for the discrete system is described. As before the simulation code $\text{OscillatorSystem.m}$ confirms that the method is second order accurate and that conserved quantity gives a second order accurate approximation of a constant multiple continuum energy. This system was used to make the phase plane plot 2.1 for the harmonic oscillator that illustrates how well the new conserved quantity approximates the continuum conserved quantity.

The constraint on the time step to keep the quantity positive becomes the Courant-Friedrichs-Lewy (CFL) condition for spatially dependent wave equations. Appendix A reviews the implicit Crank-Nicholson discretization of the oscillator which conserves a natural second order accurate discretization of the continuum energy. The paper [58] uses a natural discretization of the classical energy to derive a discretization of the oscillator equation that is equivalent to the Crank-Nicholson discretization. This discretization is implicit.

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 $\omega$ is a positive constant. The total energy is a multiple of the average of the kinetic and potential energies which is

$$E = \frac{(u')^2 + (\omega u)^2}{2}.$$
This is conserved quantity because
\[ E' = u''u' + \omega^2 uu' = (u'' + \omega^2 u) u' = 0. \]

In general conserved quantities are labeled \( C \) but if the conserved quantity is a constant multiple of the energy it will usually be labeled with \( E \).

In this paper time and spatial units are used extensively to help construct appropriate models. For the energy note that \( u \) has units of distance, \( t \) has units of time, \( u' \) has units distance over time and \( \omega \) has units of reciprocal time:
\[
\begin{align*}
    u & \sim d; \\
    t & \sim t; \\
    u' & \sim d/t; \\
    \omega & \sim 1/t \\
    E & \sim d^2/t^2.
\end{align*}
\]

So both the differential equation and the conserved quantity are dimensionally consistent.

A natural way to write the oscillator equation as a first order system is 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 consequence is that now \( v \) must have units \( d \) and thus is not a velocity. This could be fixed by setting \( v = u' \) but then this is inconsistent for what must be done when the material properties are variable and the density and tension are used to describe the physical properties of the material the waves are traveling in as is done in Section 4. In any case this simple example will be helpful for understanding more complex problems.

For the system, set
\[ C = \frac{1}{2} (u^2 + v^2). \quad (2.2) \]
This quantity is conserved because
\[ C' = uu' + vv' = u\omega v - v\omega u = 0, \]
Use (2.1) to remove \( v \) to get
\[ C = \frac{E}{\omega^2}. \quad (2.3) \]
For partial differential equations the relationship between energy and the conservation laws is similar but not so simple. Note that the phase plane plots using \((u(t), v(t))\) are circles where the radius \( r \) is given by \( r^2 = 2C \).

Because the second order equation is linear with constant coefficients the time derivative \( u' \) satisfies the same equation a \( u \). Similarly the time derivatives \( u' \) and \( v' \) also satisfy the system thus creating an infinity of conserved quantities.

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The condition that $\omega > 0$ and not that $\omega \geq 0$ is important because for $\omega = 0$ the second order equation with $u(0) = 0$ and $u'(0) = 1$ has the solution $u(t) = t$ for which the energy is unbounded. However, for $\omega = 0$ the system only has only constant solutions which have a bounded conserved quantity. So the second order equation and the system are not consistent for $\omega = 0$.

2.2 Discretizing the Second Order Oscillator Equation

If $\Delta t > 0$ then a standard explicit discretization of the second order oscillator equation using the discrete times $t_n = n \Delta t$, $0 \leq n < \infty$ is where $n$ is and integer and

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

Given the two initial conditions $u(0)$ and $u'(0)$ set

$$u^0 = u(0)$$
$$u^1 = u(\Delta t) = u(0) + \Delta t u'(0) - \frac{1}{2} \Delta t^2 \omega^2 u(0).$$

The discrete equation 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. Consequently for $0 < \Delta t/\omega < 2$ the discretization is stable. It is important that this constraint is less restrictive than requiring an accurate solution.

The initial condition given above is only first order accurate but a Taylor series expansion can be used to make the order of accuracy higher:

$$u^1 = u(0) + \Delta t u'(0) + \frac{1}{2} \Delta t^2 u''(0) + \frac{1}{6} \Delta t^3 u'''(0) + \cdots$$
$$= u(0) + \Delta t u'(0) - \frac{1}{2} \Delta t^2 \omega^2 u(0) - \frac{1}{6} \Delta t^3 \omega^2 u'(0) + \cdots$$

(2.4)

The program Oscillator2ndOrder.m confirms that the algorithm is stable for $0 < \Delta t/\omega < 2$ and is second order accurate. The discrete conserved quantity is second order accurate and constant to within a small multiple of machine epsilon $\epsilon$. As an exact solutions is known for the system the simulations codes uses the value $u(\Delta t)$ as the initial condition.
2.3 Staggering the Time Discretization

A time staggered grid is used to discretize the first order system (2.1) which is given by a primal grid \( t^n = n \Delta t \) and a dual grid \( t^{n+1/2} = (n + 1/2) \Delta t \), where \( \Delta t > 0 \) and \( 0 \leq n < \infty \) is an integer. The staggered or leapfrog discretization of the harmonic oscillator is then given by

\[
\frac{u^{n+1} - u^n}{\Delta t} = -\omega v^{n+1/2}, \quad n \geq 0, \quad \frac{v^{n+1/2} - v^{n-1/2}}{\Delta t} = \omega u^n, \quad n \geq 1. \tag{2.5}
\]

The minus sign can be put in either equation, but it is important for consistent time units 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

\[
v^{1/2} = v \left( \frac{\Delta t}{2} \right)
= v(0) + \frac{\Delta t}{2} v'(0) + \frac{1}{2} \left( \frac{\Delta t}{2} \right)^2 v''(0) + \cdots
= v(0) + \frac{\Delta t}{2} \omega u(0) - \frac{1}{2} \left( \frac{\Delta t}{2} \right)^2 \omega^2 v(0) + \cdots \tag{2.6}
\]

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 \( u \) of the fractional step methods is identical to the solution of the second order equations.

Again a simple proposed conserved quantity for (2.5) is

\[
C^n = \frac{1}{2} \left( (u^n)^2 + \left( \frac{v^{n+1/2} + v^{n-1/2}}{2} \right)^2 \right). \tag{2.7}
\]

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

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

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and then the following two quantities are conserved:

\[
C^n = \frac{1}{2} \left( (1 - \alpha^2) (u^n)^2 + \left( \frac{u^{n+1/2} + u^{n-1/2}}{2} \right)^2 \right); \quad (2.8)
\]

\[
C^{n+1/2} = \frac{1}{2} \left( \left( \frac{u^{n+1} + u^n}{2} \right)^2 + (1 - \alpha^2) \left( v^{n+1/2} \right)^2 \right). \quad (2.9)
\]

The important properties for the staggered scheme are that it is explicit, second order accurate and stable for \( \alpha = \omega \Delta t / 2 < 1 \). By modifying the discretization, a similar result was obtained in [50], Equation 45, for the Yee time discretization of Maxwell’s equations.

The simulation program OscillatorSystems.m confirms that the numerical solutions are second order accurate and that the two conserved quantities are constant to within a small multiple of \( \text{eps} \).
2.4 Summary

For the second order harmonic oscillator and the first order harmonic oscillator conserved quantities are introduce that are second order accurate approximations of a multiple of the continuum energy but contain a term that is minus the square of the time step times a positive quantity. Requiring this conserved quantity to be positive gives the standard stability condition on the time step for the discrete oscillator. The restriction on $\Delta t$ to keep the conserved quantity positive is far less stringent than the restriction for reasonably accurate solutions. Simulations confirm that the discrete conserved quantities are constant up to a small multiple of machine epsilon $\epsilon$ and are second order accurate. For the simulations code it is a bit awkward to check but the systems code is stable for $\Delta t/\omega = 1.99$ and unstable for $\Delta t/\omega = 2.30$ supporting the stability condition $0 < \Delta t/\omega < 2$. A modified version of the systems code produced the phase plane plot in figure 2.1 using rather large time steps which confirms that the conserved quantity converges to the continuum conserved quantity rapidly.
3 Systems of Ordinary Differential Equations

The next task is to study a special class of systems of linear ordinary differential equations that are wave equations. Discrete conservation laws are easy to find by following the harmonic oscillator example. Most importantly, the discussion here will show how to find conservation laws for discretized spatially dependent wave equations. Consequently the notation here is set up to conveniently apply the results to these equations. To see how this is done note that the standard wave equation in 3D is given by the second time derivative of a scalar function equals the divergence of the gradient of the function. Critical points are that the adjoint operator of the divergence is minus the gradient and vice versa and the divergence of the gradient is a symmetric negative operator.

3.1 Continuous Time

Let \( X \) and \( Y \) be linear spaces (finite or infinite dimensional). It is important not to assume that \( X \) and \( Y \) have the same dimension. If \( f_1 \) and \( f_2 \) are in \( X \) then their inner product is \( \langle f_1, f_2 \rangle_X \) and the norm of \( f_1 \) is given by \( \| f_1 \|_X^2 = \langle f_1, f_1 \rangle_X \) with a similar notation for \( Y \).

Let \( A \) be a linear operator mapping \( X \) to \( Y \) with adjoint \( A^* \) that maps \( Y \) to \( X \):

\[
X \xrightarrow{A} Y; \quad Y \xrightarrow{A^*} X.
\]

Consequently, if \( f \in X \) and \( g \in Y \) then

\[
\langle Af, g \rangle_Y = \langle f, A^* g \rangle_X.
\]

Next, if \( f = f(t) \in X \) and \( g = g(t) \in Y \) then the generalization of the harmonic oscillator system that was studied in the previous section is given by

\[
f' = -A^* g, \quad g' = Af.
\] (3.1)

Consequently

\[
f'' = -A^* Af, \quad g'' = -AA^* g.
\]

Note that \( A^* A \) and \( AA^* \) are symmetric positive operators. If they are positive definite then the solutions will be oscillatory. When studying spatially dependent wave equations \( A \) will correspond to the gradient and \( -A^* \) will correspond to the divergence so that \( -AA^* \) corresponds to the divergence of the gradient that is the Laplacian in the scalar wave equation. Also \( -A^* A \) corresponds to the gradient of the divergence that occurs in the second order vector wave equation.

The matrix form of the system is

\[
\begin{bmatrix}
  f' \\
  g'
\end{bmatrix} = \begin{bmatrix}
  0 & -A^* \\
  A & 0
\end{bmatrix} \begin{bmatrix}
  f \\
  g
\end{bmatrix}.
\]

The coefficient matrix is skew adjoint, so it must have purely imaginary spectra so the solutions of this system must be made up of waves and constant functions. Additionally,
the adjoint of the product of two operators $A$ and $B$ is $(AB)^* = B^*A^*$ so both $AA^*$ and $A^*A$ are self-adjoint and positive. If $A^*A$ is positive then the second order equations have solution that are made up of waves. However if $A^*A$ has a zero eigenvalue then the second order equation can have solutions that grow linearly in time.

There are three natural initial conditions: for the system specify $f(0)$ and $g(0)$; for the second order equation in $f$ specify, $f(0)$ and $f'(0)$; and for the second order equation in $g$ specify, $g(0)$ and $g'(0)$. Note that if $f(0)$ and $f'(0)$ are given then to use the first order system, Equation (3.1) must be solved for $g(0)$ which may not be possible. So the system and the second order equations may not be equivalent.

If the dimensions of $X$ and $Y$ are the same so that it make sense to assume that $A$ is inevitable then the system (3.1) will have properties similar to the harmonic oscillator system (2.1) when $\omega > 0$. The most interesting case is when the dimensions of the spaces are different which provides insight in to the discretization of the scalar and vector wave equation and also the Maxwell equations. Also the case when $A$ is self-adjoint, $A^* = A$, provides insight into the discretization of Maxwell’s equations.

### 3.2 Continuous Time Conserved Quantities

An interesting point here is that there is a conserved quantity that is not the energy but implies that an analog of the energy is conserved. This fundamental conserved quantity is

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

which is analogous to (2.2). Because

$$ C'(t) = \langle f'(t), f(t) \rangle_X + \langle g'(t), g(t) \rangle_Y \\
= \langle -A^*g(t), f(t) \rangle_Y + \langle Af(t), g(t) \rangle_Y \\
= -\langle g(t), Af(t) \rangle_X + \langle Af(t), g(t) \rangle_Y \\
= 0 , $$

this quantity is conserved.

Additionally because the system of equations is linear and constant coefficient, if $f$ and $g$ are solutions then so are $f'$ and $g'$. Consequently

$$ E(t) = \frac{1}{2} \left( ||f'(t)||_X^2 + ||g'(t)||_Y^2 \right) , $$

$$ = \frac{1}{2} \left( ||A^*f(t)||_X^2 + ||A^*f(t)||_Y^2 \right) , $$

$$ = \frac{1}{2} \left( ||Af(t)||_X^2 + ||g'(t)||_Y^2 \right) $$

(3.2)
is constant. For the wave equations to be studied later this is essentially the total energy that is the sum of the kinetic and potential energies. The \( C(t) \) type conserved quantities will used from now on.

### 3.3 Staggered Time Discretization

A second order centered leapfrog discretization for the first order system is

\[
\frac{f^{n+1} - f^n}{\Delta t} = -A^* g^{n+1/2}, \quad \frac{g^{n+1/2} - g^{n-1/2}}{\Delta t} = A f^n. \tag{3.3}
\]

Assuming that \( f^0 \) and \( g^{1/2} \) are given then for \( n \geq 0 \) the leapfrog time stepping scheme is

\[
f^{n+1} = f^n - \Delta t A^* g^{n+1/2}, \quad g^{n+3/2} = g^{n+1/2} + \Delta t A f^{n+1}.
\]

The order of evaluation is important.

The initial conditions for the discretized system require \( f^0 = f(0) \) and \( g^{1/2} = g(\Delta t/2) \). If \( f(0) \) and \( g(0) \) are given then

\[
g^{1/2} \approx g(0) + \frac{\Delta t}{2} g'(0) + \frac{\Delta t^2}{2} g''(0) = g(0) + \frac{\Delta t}{2} A f(0) - \frac{\Delta t^2}{2} A A^* g(0).
\]

The remaining cases require the solution of a system of equations, that is one of the operators \( A A^* \) or \( A^* A \) needs to inverted. These operators are symmetric and positive but under our assumptions cannot be guaranteed to be definite. In the other cases, if \( g(0) \) and \( g'(0) \) are given then solve

\[
A^* g'(0) = A^* A f(0)
\]

for \( f(0) \) and if \( f(0) \) and \( f'(0) \) are given solve

\[
A f'(0) = -A A^* g(0)
\]

for \( g(0) \).

Both \( f \) and \( g \) satisfy a second order difference equation:

\[
\begin{align*}
\frac{f^{n+1} - 2 f^n + f^{n-1}}{\Delta t^2} &= -A^* A f^n; \\
\frac{g^{n+3/2} - 2 g^{n+1/2} + g^{n-1/2}}{\Delta t^2} &= -A A^* g^{n+1/2}.
\end{align*}
\tag{3.4}
\]

Additionally a second order average is needed for computing conserved quantities. So multiply the above equations by \( \Delta t^2/4 \) and then add \( f^n \) to the first equation and \( g^{n+1/2} \) to the second equation to get:

\[
\begin{align*}
\frac{f^{n+1} + 2 f^n + f^{n-1}}{4} &= f^n - \frac{\Delta t^2}{4} A^* A f^n; \\
\frac{g^{n+3/2} + 2 g^{n+1/2} + g^{n-1/2}}{4} &= g^{n+1/2} - \frac{\Delta t^2}{4} A A^* g^{n+1/2}.
\end{align*}
\tag{3.5}
\]
When comparing this discretization to the simple oscillator discretization it is important that \( \omega > 0 \), while here the operators \( A \) and \( A^* \) may not be invertible which is typically the case when studying spatially dependent partial differential wave equations.

### 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 (2.8) and (2.9) are given. So let

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

\[
C_2^n = \|f^n\|_X^2,
\]

\[
C_3^n = \|Af^n\|_Y^2.
\]

As above compute the changes in \( C_1, C_2 \) and \( C_3 \) over a time step:

\[
C_1^{n+1} - C_1^n = \left\langle \frac{g^{n+3/2} + 2g^{n+1/2} + g^{n-1/2}}{4}, g^{n+3/2} - g^{n-1/2} \right\rangle_Y;
\]

\[
= \left\langle g^{n+1/2} - \frac{\Delta t^2}{4} AA^* g^{n+1/2}, g^{n+3/2} - g^{n-1/2} \right\rangle_Y;
\]

\[
= \langle g^{n+1/2}, g^{n+3/2} - g^{n-1/2} \rangle_Y - \frac{\Delta t^2}{4} \langle AA^* g^{n+1/2}, g^{n+3/2} - g^{n-1/2} \rangle_Y.
\]

\[
C_2^{n+1} - C_2^n = \left\langle f^{n+1} - f^n, f^{n+1} + f^n \right\rangle_X;
\]

\[
= \left\langle \Delta t A^* g^{n+1/2}, f^{n+1} + f^n \right\rangle_X;
\]

\[
= \Delta t \left\langle g^{n+1/2}, Af^{n+1} + Af^n \right\rangle_Y;
\]

\[
= \Delta t \left\langle g^{n+1/2}, -\frac{g^{n+3/2} - g^{n-1/2}}{\Delta t} \right\rangle_Y;
\]

\[
= -\langle g^{n+1/2}, g^{n+3/2} - g^{n-1/2} \rangle_Y.
\]

\[
C_3^{n+1} - C_3^n = \left\langle Af^{n+1} - Af^n, Af^{n+1} + Af^n \right\rangle_Y;
\]

\[
= \left\langle Af^{n+1} - Af^n, -\frac{g^{n+3/2} - g^{n-1/2}}{\Delta t} \right\rangle_Y;
\]

\[
= -\left\langle \Delta t A A^* g^{n+1/2}, g^{n+3/2} - g^{n-1/2} \right\rangle_Y;
\]

\[
= -\langle AA^* g^{n+1/2}, g^{n+3/2} - g^{n-1/2} \rangle_Y.
\]

Consequently

\[
C^n = C_1^n + C_2^n - \left( \frac{\Delta t}{2} \right) C_3^n.
\]
is a conserved quantity. Moreover, if $||A||$ is the operator norm of $A$ then
\[
||C^n|| \geq \left( 1 - \frac{\Delta t^2}{4} ||A||^2 \right) ||f^n||^2 + \left( \frac{g^{n+1/2} + g^{n-1/2}}{2} \right)^2,
\]
so $C^n$ is positive for $\Delta t \leq 2/||A||$.

Next let
\[
C_1^{n+1/2} = \left\| \frac{f^{n+1} + f^n}{2} \right\|^2_X, \\
C_2^{n+1/2} = \left\| g^{n+1/2} \right\|^2_Y, \\
C_3^{n+1/2} = \left\| A^* g^{n+1/2} \right\|^2_X.
\]

Now compute the changes in $C_1$, $C_2$ and $C_3$ over a time step:
\[
C_1^{n+1/2} - C_1^{n-1/2} = \langle \left( \frac{f^{n+1} + f^n}{2}, \frac{f^{n+1} + f^n}{2} \right), \frac{f^n + f^{n-1}}{2} \rangle_X = \langle \left( \frac{f^{n+1} + 2f^n + f^{n-1}}{4}, f^{n+1} - f^{n-1} \right), \frac{f^n + f^{n-1}}{2} \rangle_X = \langle \left( f^n + \frac{\Delta t^2}{4} A^* A f^n, f^{n+1} - f^{n-1} \right), \frac{f^n + f^{n-1}}{2} \rangle_X = \langle \left( f^n, f^{n+1} - f^{n-1} \right), \Delta t \Delta t \left( A^* A f^n, f^{n+1} - f^{n-1} \right) \rangle_X.
\]
\[
C_2^{n+1/2} - C_2^{n-1/2} = \langle \left( g^{n+1/2}, g^{n+1/2} \right), \frac{g^n + g^{n-1}}{2} \rangle_Y = \langle \left( g^{n+1/2}, g^{n+1/2} \right), \frac{g^n + g^{n-1}}{2} \rangle_Y = \langle \left( g^{n+1/2} + g^{n-1/2}, g^{n+1/2} - g^{n-1/2} \right), \frac{g^n + g^{n-1}}{2} \rangle_Y = \langle \left( g^{n+1/2} + g^{n-1/2}, \Delta t A f^n \right), \frac{g^n + g^{n-1}}{2} \rangle_Y = \Delta t \langle \left( -A^* g^{n+1/2} - A^* g^{n-1/2}, f^n \right), \frac{g^n + g^{n-1}}{2} \rangle_X = \Delta t \langle \left( f^{n+1} - f^{n-1}, f^n \right), \frac{g^n + g^{n-1}}{2} \rangle_X = -\langle \left( f^n, f^{n+1} - f^{n-1} \right), \frac{g^n + g^{n-1}}{2} \rangle_X.
\]
\[
C_3^{n+1/2} - C_3^{n-1/2} = \langle A^* g^{n+1/2} - A^* g^{n-1/2}, A^* g^{n+1/2} + A^* g^{n-1/2} \rangle_X = \langle A^* \left( g^{n+1/2} - g^{n-1/2} \right), \frac{f^{n+1} - f^n}{\Delta t} \rangle_X = \langle \Delta t A^* A f^n, \frac{f^{n+1} - f^n}{\Delta t} \rangle_X = \langle A^* A f^n, f^{n+1} - f^{n-1} \rangle_X.
\]
Consequently
\[ C^{n+1/2} = C_1^{n+1/2} + C_2^{n+1/2} - \left( \frac{\Delta t}{2} \right)^2 C_3^{n+1/2} \]  
(3.8)
is a conserved quantity. Moreover, if \( \|A^*\| \) is the operator norm of \( A^* \) then
\[ C^{n+1/2} \geq \left\| \frac{f_{n+1} + f_n}{2} \right\|^2_X + \left( 1 - \frac{\Delta t^2}{4} \|A^*\|^2 \right) \|g^{n+1/2}\|^2_Y, \]
so \( C^{n+1/2} \) is positive for \( \Delta t \leq 2/\|A^*\| \).

The program SystemODEs.m confirms that the solutions of the system are second order accurate and that the conserved quantities are second order accurate and are constant to a small multiple of eps.

3.5 Notes

Both \( AA^* \) and \( A^* A \) are self-adjoint positive operators, but may not be positive definite. So if \( h \neq 0 \) and \( Ah = 0 \) then \( g(t) = th \) is an unbounded solution of the second second order equation while if \( A^* h = 0 \) then \( f(t) = th \) is an unbounded solution of the first second order equation. For this \( f(t) \) the system becomes \( h = Ag(t), g'(t) = 0 \). 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. So the second order equations and the system are not exactly consistent.

There is also a problem with the initial conditions for the system and the second order equations. If \( A \) is an \( n \times m \) matrix, then \( A^* \) is \( m \times n \) matrix and consequently \( AA^* \) is an \( n \times n \) matrix and \( A^* A \) is an \( m \times m \) 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. However, for example, if one knows \( f(t) \) then \( g(t) \) can be found using simple integration and the initial condition for \( g(t) \) and conversely for knowing \( g(t) \).

If \( n = m \) then the number of initial conditions are the same for all three variants of the ordinary differential equations. If \( A \) is inevitable then the system and second order equations are consistent. Unfortunately, the \( n \neq m \) is far more analogous to the situation for equations modeling waves in spaces of dimension 1 or larger.
4 Discretizing the One Dimensional Wave Equation

| quantity | units | name               |
|----------|-------|-------------------|
| $x$      | $d$   | spatial position  |
| $dx$     | $d$   | spatial increment |
| $L$      | $d$   | end of spatial interval |
| $t$      | $t$   | time              |
| $u$      | $d$   | displacement      |
| $v$      | $d/t$ | velocity          |
| $u_t$    | $d/t$ | velocity          |
| $u_x$    | 1     | slope             |
| $\rho$   | $1/d$ | 1D density        |
| $\tau$   | $d/t^2$ | 1D Young’s Modulus |
| $E$      | $d^2/t^2$ | energy           |

Table 4.1: Quantities and their one dimensional space-time units.

The physical model used to motivate this discussion is piece of string or wire pinned at both ends that is under tension and whose mass and strength varies along the string or wire. To better understand the correct form of the one dimensional wave equation in such materials, three forms of this equation will be derived from the conservation of energy. The three forms are two second order equations and most importantly a first order system of two equations. An important tool for obtaining correct equations is to use the one dimensional units for distance $d$ and time $t$ units of the variables in the equations that are given in Table 4.1 so that the equations are dimensionally consistent.

The discussion of the continuum problem begins by introducing the energy of the string using this to derive the second order wave equation the describes the motion of the string. The energy then suggests how to write the second order equation as a system of two first order equations and also how to introduce two weighted inner products so the system has the same form as the system of ODEs studied in Section 3. The results in Section 3 then motivate the discretization of the system so that the discrete system has conserved quantities.

For spatially dependent differential equations two case will be studied: CMP standing for constant material properties and VMP standing for variable material properties. The simulation codes are created first for the CMP case and then extended to the VMP case. For the VMP case two functions are introduced to represent the material properties, one is the one dimensional density $\rho(x)$ while the other is the one dimensional Young’s modulus $\tau(x)$ that depends on the strength of the material and the force applied to the string. Two inner products weighted by $\rho$ and $\tau$ and their related norms are also introduced and used to show that this system of equations again has the same form as the system studied in Section 3. This is then used to introduce conserved quantities that are defined in terms of the weighted norms. The conserved quantities have a simple relationship to the energy that was used to
derive the differential equations and thus imply the conservation of energy. For the CMP case it is assumed that $\rho$ and $\tau$ are constant and then the wave speed $c^2 = \tau/\rho$ is introduced.

The discussion of the discretizations begins with constant material properties CMP followed by variable material properties VMP. Two reasons: the CMP case is what is commonly studied in the literature and is relatively simple; the VMP case requires the introduction of weighted inner products and is more complicated. More importantly, the CMP as done in the literature doesn’t provide a good motivation for VMP case. In both cases a variable $v$ is introduced to define the first order system, however the units of $v$ in the two cases are different. In the CMP case the wave speed is introduced which is commonly used in text books. In this case $v$ has units distance $v \sim d$. In the VMP case the material is characterized by the one dimensions density $\rho$ and the one dimensional Young’s modulus $\tau$. In this case a natural first order system is obtained by introducing a velocity $v$ with units $v \sim d/t$.

The discretization of the system begins by introducing a grid staggered in both space and time and the using central differences in both space and time so that the discretizations are second order accurate. The time discretization is the same as leapfrog discretization used in Section 3 while the spatial discretization is the 3D mimetic discretization [46] specialized to one dimension. In this case the spatial discretization is also a simple staggered discretization. The discretization of the system also gives a standard discretization of the two second order wave equations. The resulting discrete system can be put in the form used to study system of ODEs studied in the section 3 and consequently the results in that section provide two discrete conserved quantities.

The simulation codes Wave1DCMP.m and Wave1DVMP.m test the developed theory for the constant and variable material properties cases. For both cases the simulation programs show that the discrete solution converges at least order 2 to the continuum solution and that conserved quantities are second order accurate and constant to within small multiple of machine epsilon $\epsilon$ that increases slowly with decreasing time and space step sizes. Surprisingly, for the CMP code if the final time is a multiple of half of the period of the solution then the convergence rate is order 4. For the CMP code it is important that the condition that guarantees the conserved quantities are positive is the same as the Courant-Friedrichs-Lewy (CFL) condition for stability. This condition guarantees that the conserved quantity is positive and consequently the discretization is stable.

Next the VMP equations are discretized in the same manner as the CMP equations and again the results of Section 3 can be applied. As in the continuum, weighted inner products and norms of discrete functions are introduced and used to define discrete weighted conservation laws. Again, these conserved quantities are positive for constraints on the time step that are a generalization of the CFL condition. The discretization is stable when the conserved quantities are positive.

For constant material properties the simulation program Wave1DVMP.m will produce the same results as the constant properties code Wave1DCMP.m if $\rho = 1/c$ and $\tau = c$. Both codes show that two conserved quantities are constant and second order accurate. For the CMP case it is easy to find exact solutions for wave equation and thus estimate the error in the solution and the convergence rate. For the general variable coefficient case it is not
possible to find exact solutions of the wave equation so an alternative method of estimating the convergence rate is used.

For the VMP case the convergence rates is computed by comparing the discrete solution on a given grid to the solution on a grid where each cell is cut in half and the time step is also cut in half. The accuracy of the solution on the original grid is estimated by the difference of the two solutions on the course grid. The convergence rate is easily estimated but is a bit noisy. It is far more informative divide the error estimate by the square of the size of the cells in the course grid and plot the results. If the plots overlap with decreasing step size then this shows that the solutions converge at least order 2. Most example are order 2 but for some examples the plots increase indicating that the convergence rate order is less than 2. In all cases the convergence rate order is at least 1. There are a several examples given in Wave1DVM. The "method of manufactured solutions" could be used to compute the order of convergence of trivially modified equations but that was not done here.

4.1 Derivation of the VMP 1D Wave Equation

Consider a piece of string that is pinned at both ends and whose displacement from equilibrium is given by \( u(x,t) \) for \( 0 \leq x \leq 1 \) and \( t \geq 0 \). The boundary conditions are then \( u(0,t) = u(1,t) = 0 \). The derivatives of functions will be given by subscripts: \( u_t = \partial u/\partial t; \) \( u_x = \partial u/\partial x; \) \( u_{tt} = \partial^2 u/\partial t^2; \) \( u_{xx} = \partial^2 u/\partial x^2 \). The derivation of the variable material properties wave equation will start with the conservation of the energy of a vibrating string which is the average of the kinetic and potential energies,

\[
E = \frac{1}{2} \int_0^1 \rho u_t^2 \, dx + \frac{1}{2} \int_0^1 \tau u_x^2 \, dx.
\]

Here \( \rho = \rho(x) \) is the one dimensional density and \( \tau = \tau(x) \) is the one dimensional Young’s modulus. It is assumed \( \rho \) and \( \tau \) are bounded above and below by positive constants. Table 4.1 shows that the energy \( E \) has space and time units \( d^2/t^2 \).

The wave equation is derived by assuming the energy \( E \) is conserved and the using integration by parts. First

\[
\frac{dE}{dt} = \int_0^1 (\rho u_t u_{tt} + \tau u_x u_{xt}) \, dx. \tag{4.1}
\]

However

\[
\int_0^1 (\tau u_x u_t) \, dx = \int_0^1 (\tau u_x) u_t \, dx + \int_0^1 \tau u_x u_{xt} \, dx \\
= \tau (1) u_x(1,t) u_t(1,t) - \tau (0) u_x(0,t) u_t(0,t).
\]

Consequently

\[
\frac{dE}{dt} = \int_0^1 u_t (\rho u_{tt} - (\tau u_x)_x) \, dx + \tau (1) u_x(1,t) u_t(1,t) - \tau (0) u_x(0,t) u_t(0,t).
\]
But $u(0, t) = u(1, t) = 0$ for $t \geq 0$ so $u_t(0, t) = u_t(1, t) = 0$ and thus the energy will be conserved provided that
\[ \rho u_{tt} = (\tau u_x)_x, \]
which is the 1D wave equation with variable material properties.

It is also common to derive the wave equation from Newton’s law, which gives the mass times acceleration is equal to the force which is the form of this equation. The form of the equation used here is
\[ u_{tt} = \frac{1}{\rho} (\tau u_x)_x. \tag{4.2} \]
In [13] the same form is given for the wave equation but there $\tau$ is a function both $x$ and $t$.

This second order wave equation can be written as a system by introducing a velocity $v = v(x, t)$ with units $d/t$ where
\[ u_t = \frac{1}{\rho} v_x, \quad v_t = \tau u_x. \tag{4.3} \]
Also $v$ satisfies a second order differential equation
\[ v_{tt} = \tau \left( \frac{1}{\rho} v_x \right)_x. \]
The second order equation can be expanded to
\[ u_{tt} = \frac{\tau}{\rho} u_{xx} + \frac{\tau_x}{\rho} u_x, \quad v_{tt} = \frac{\tau}{\rho} v_{xx} - \frac{\tau \rho_x}{\rho^2} v_x. \tag{4.4} \]
This brings up a concern that if either $\rho_x/\rho$ or $\tau_x/\tau$ are large then the first order terms involving $u_x$ or $v_x$ will dominate the second order terms and then the solution second order equations and consequently the first order equations could have non wave like behavior?

To apply the ideas in Section 3 to the 1D wave equation two inner products of functions defined on $[0, 1]$ are needed. First, if $u1 = u1(x)$ and $u2 = u2(x)$ have dimensions $d$ then let
\[ \langle u1, u2 \rangle_{\rho} = \int_0^1 u1(x) u2(x) \rho(x) \, dx, \tag{4.5} \]
Note that $\rho \, dx$ has units 1 so the inner product has units $d^2$. Next, if $v1 = v1(x)$ and $v2 = v2(x)$ have units $d/t$ then let
\[ \langle v1, v2 \rangle_{\tau} = \int_0^1 v1(x) v2(x) \tau^{-1}(x) \, dx. \tag{4.6} \]
Again, note that $\tau^{-1}(x) \, dx$ has units $t^2$ and then because $v1$ and $v2$ have units $d/t$ the inner product has units $d^2$.

To apply the ideas in Section 3 define the operator $A$ as
\[ Au = \tau u_x. \]
If \( u(0) = u(1) = 0 \) then integration by parts gives
\[
\langle Au, v \rangle_{\tau} = \langle \tau u_x v \rangle_{\tau} \\
= \int_0^1 \tau u_x v \tau^{-1} \, dx, \\
= \int_0^1 u_x v \, dx, \\
= -\int_0^1 uv_x \, dx, \\
= -\int_0^1 \frac{1}{\rho} v_x \rho \, dx, \\
= \langle u A^* v \rangle_{\rho}.
\]
(4.7)

Consequently the adjoint of \( A \) is given by
\[
A^* v = -\frac{1}{\rho} v_x.
\]

Now the system (4.3) can be written in the form given in (3.1):
\[
u_t = -A^* v; \quad v_t = Au.
\]
(4.8)

Additionally \( u \) and \( v \) will satisfy the second order equations
\[
u_{tt} = -A^* Au; \quad v_{tt} = -AA^* v.
\]
(4.9)

Next
\[
\langle AA^* v_1, v_2 \rangle_{\tau} = \langle A^* v_1, A^* v_2 \rangle_{\rho} = \langle v_1, AA^* v_2 \rangle_{\tau},
\]
and
\[
\langle A^* Au_1, u_2 \rangle_{\rho} = \langle Au_1, Au_2 \rangle_{\tau} = \langle u_1, A^* Au_2 \rangle_{\rho}.
\]
Consequently both \( AA^* \) and \( A^* A \) are self adjoint and positive so that (4.9) are wave equations.

As in Section 3 a conserved quantity is given by
\[
C(t) = \frac{1}{2} ||u||^2_{\rho} + \frac{1}{2} ||v||^2_{\tau}
\]
because if \( u(0) = u(1) = 0 \) then
\[
C_t = \langle u, u_t \rangle_{\rho} + \langle v, v_t \rangle_{\tau}
\]
\[
= \int_0^1 u(x) \frac{1}{\rho(x)} v_x(x) \rho(x) \, dx + \int_0^1 v(x) \tau(x) u_x(x) \frac{1}{\tau(x)} \, dx
\]
\[
= \int_0^1 u(x) v_x(x) + v(x) u_x(x) \, dx
\]
\[
= \int_0^1 (u(x) v(x))_x \, dx
\]
\[
= 0.
\]
Now note that \( u_t \) and \( v_t \) are also a solution of the system (4.3) implying that
\[
E = \frac{1}{2} \left| |u_t|\right|^2_\rho + \frac{1}{2} \left| |v_t|\right|^2_\tau
\]
is constant. Also the units of \( E \) are \( d^2/t^2 \). A little algebra shows that \( E \) is the energy of the second order 1D wave equation.

### 4.2 The Constant Material Properties Wave Equation

The following standard formulation of the constant material properties (CMP) 1D wave equation provides insight into the variable material properties case. The wave equation in constant materials is different from just assuming that \( \rho \) and \( \tau \) are constant in the above discussion because of the introduction of the wave speed \( c \).

If \( \rho \) and \( \tau \) are constant then (4.2) becomes
\[
 u_{tt} = \frac{\tau}{\rho} u_{xx}.
\] (4.10)

Note that \( \tau/\rho \) has dimension \( d^2/t^2 \). For constant material properties the 1D wave equation is typically given as
\[
 u_{tt} = c^2 u_{xx},
\]
where \( c > 0 \) is the constant wave speed with units \( d/t \). So
\[
 c^2 = \frac{\tau}{\rho}.
\]

This equation can also be written as a system
\[
 u_t = c v_x, \quad v_t = c u_x,
\] (4.11)
but now \( v \) must have units \( d \) not \( d/t \) as will be the case for variable material properties, so \( v \) is not a velocity. So this system is not the same as the first order system for variable material properties that will be described below. Note that interchanging \( u \) and \( v \) doesn’t change the system. As before \( v \) also satisfies a second order wave equation
\[
 v_{tt} = c^2 v_{xx}.
\]

It is easy to check that for \( u(0,t) = u(1,t) = 0 \)
\[
 C = \frac{1}{2} \int_0^1 (u^2 + v^2) \, dx,
\] (4.12)
is a conserved quantity. Again note that if \( u, v \) are solutions of the system then so are \( u_t, v_t \) and then a conserved quantity is given by
\[
 E = \frac{1}{2} \int_0^1 (u_t^2 + v_t^2) \rho dx = \frac{1}{2} \int_0^1 (c^2 u_x^2 + u_t^2) \rho dx.
\]
The constant $\rho$ is included so that $E$ has dimensions $d^2/t^2$ which is correct for energy. So if $C$ is conserved then so is $E$.

The constant material properties simulation code Wave1DCMP.m will be tested for $t \geq 0$ and the interval $0 \leq x \leq 1$ using the solution

$$u(x,t) = \cos(m \pi ct) \sin(m \pi x),$$
$$v(x,t) = \sin(m \pi ct) \cos(m \pi x).$$

where $m$ is a positive integers and $c$ is a positive constant. Note that the arguments of the $\sin$ and $\cos$ should be dimensionless but they are not. This can be fixed by multiplying the arguments by the density $\rho$ of the string and then assuming $\rho = 1$. Note that $u(0,t) = u(1,t) = 0$ so this solution satisfies homogeneous Dirichlet boundary conditions while $v$ satisfies homogeneous Neumann boundary conditions. Also, interchanging $u$ and $v$ gives a solution of the second order equation that satisfies Neumann boundary conditions. For the test solution the quantity (4.12) is $C(t) = 1/2$. An important topic not included is general boundary conditions for the wave equation.

### 4.3 Staggered Discretizations of the 1D Wave Equations

As illustrated in Figure 4.1 two grids that are staggered in space and time grids will be used to discretize the first order constant materials properties (CMP) system (4.11) and the
variable material properties (VMP) system (4.3). The simulation region is $a \leq x \leq b$ and $0 \leq t \leq T$ where $L = b - a > 0$ and $T > 0$. One grid is the primal grid and the other is the dual grid. For the primal grid $N_x$ is the number of discretization points in the spatial region. Consequently the number of cells in the spatial grid is $N_x - 1$ so set $\Delta x = L / (N_x - 1)$. If $N_t$ is the number of time steps then $\Delta t = T / N_t$. Then the primal grids points are given by

$$\left( t^n, x_i \right) = (n \Delta t, a + i \Delta x), \quad 0 \leq n \leq N_t, \ 0 \leq i \leq N_x - 1,$$

(4.13)

The dual grid points are at the centers of the cell in the primal grid,

$$\left( t_{n+1/2}^{n+1/2}, x_{i+1/2}^{n+1/2} \right) = ((n + 1/2) \Delta t, a + (i + 1/2) \Delta x), \quad 0 \leq n \leq N_t, \ 0 \leq i \leq N_x - 2.$$

(4.14)

The discretization of $u(x,t)$ on the primal grid the discretization of $v(x,t)$ on the dual grid are:

$$u^n_i = u(x_i, t^n); \quad v^{n+1/2}_{i+1/2} = v(x_{i+1/2}, t^{n+1/2}).$$

(4.15)

### 4.4 Constant Material Proprieties (CMP)

For CMP the inner products and norms of the discrete functions are given by:

$$\langle u_1, u_2 \rangle = \sum_{i=0}^{N_x-1} u_1_i u_2_i \Delta x: \quad \langle v_1, v_2 \rangle = \sum_{i=0}^{N_x-2} v_{1,i+1/2} v_{2,i+1/2} \Delta x :$$

$$||u||^2 = \langle u, u \rangle: \quad ||v||^2 = \langle v, v \rangle.$$

To have the units of the norms be $d^2$, because $u$ and $v$ have units $d$, the norms can be multiplied by the constant density $\rho$ so that $\rho \Delta x$ is dimensionless, and then assume that $\rho = 1$. The CMP system (4.11) is discretized as

$$\frac{u^{n+1}_{i} - u^n_{i}}{\Delta t} = c \frac{v^{n+1/2}_{i+1/2} - v^{n+1/2}_{i-1/2}}{\Delta x},$$

$$\frac{v^{n+1/2}_{i+1/2} - v^{n-1/2}_{i+1/2}}{\Delta t} = c \frac{u^n_{i+1} - u^n_{i}}{\Delta x}.$$  

(4.16)

The initial conditions are $u^n_0$ and $v^{1/2}_{n+1/2}$. Introduce the finite difference operators

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

so that the system can be written

$$\frac{u^{n+1}_{i} - u^n_{i}}{\Delta t} = c \frac{\delta(v^{n+1/2})_i}{\Delta x}, \quad \frac{v^{n+1/2}_{i+1/2} - v^{n-1/2}_{i+1/2}}{\Delta t} = c \frac{\delta(u^n)_{i+1/2}}{\Delta x}.$$  

(4.17)
To use the discussion in Section 3 this system must be put into the form (3.3):

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

(4.18)

So

\[
A = c \frac{\delta}{\Delta x}, \quad A^* = -c \frac{\delta}{\Delta x}.
\]

It is easy to check that \(A^*\) is the adjoint operator of \(A\).

Now (3.6) and (3.8) give the conserved quantities

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

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

(4.19)

and

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

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

(4.20)

The conserved quantities will be positive provided

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

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

\[
c \frac{\Delta t}{\Delta x} < 1.
\]

This is the Courant-Friedrichs-Lewy (CFL) condition for stability of the second order discrete equations that are derived below from the first order discrete system.

### 4.5 Variable Material Properties

For variable material properties \(\rho\) is discretized on the primal grid while \(\tau\) is discretized on the dual grid:

\[
\rho_i = \rho(x_i); \quad \tau_{i+1/2} = \tau(x_{i+1/2}).
\]

Then the system (4.3) is discretized as

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

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

(4.21)
As before assume that $u^0$ and $v^0$ are given then the leapfrog time stepping scheme for $n \geq 0$ is

$$u_i^{n+1} = u_i^n + \frac{1}{\rho_i} \frac{\Delta t}{\Delta x} \left( v_i^{n+1/2} - v_i^{n+3/2} \right), \quad v_i^{n+3/2} = v_i^{n+1/2} + \tau_{i+1/2} \frac{\Delta t}{\Delta x} (u_i^{n+1} - u_i^n).$$

To use the discussion in Section 3 to study the discretized wave equation, the system (4.21) must be put into the form (3.3):

$$\frac{u^{n+1} - u^n}{\Delta t} = -A^* v^{n+1/2}, \quad \frac{v^{n+1/2} - v^{n-1/2}}{\Delta t} = A u^n. \quad (4.22)$$

The difference equations (4.21) can be written as

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \frac{1}{\rho_i} \delta(v^{n+1/2})_i, \quad \frac{v_i^{n+1/2} - v_i^{n-1/2}}{\Delta t} = \tau_i^{1/2} \frac{\delta(u^n)_{i+1/2}}{\Delta x}. \quad (4.23)$$

Consequently

$$A^* = -\frac{\delta}{\rho \Delta x}, \quad A = \frac{\tau \delta}{\Delta x}.$$

Below it will be shown that $A^*$ is the adjoint of $A$.

The second order variable material properties wave equation for $u$ is:

$$\frac{u_i^{n+1} - 2u_i^n + u_i^{n-1}}{\Delta t} = -A^* v_i^{n+1/2} - (-A^*) v_i^{n-1/2}; \quad \frac{u_i^{n+1} - u_i^n}{\Delta t} = \frac{1}{\rho_i} \delta(v^{n+1/2})_i - \frac{1}{\rho_i} \delta(v^{n-1/2})_i; \quad \frac{u_i^{n+1} - u_i^n}{\Delta t} = \frac{1}{\rho_i} \frac{v_i^{n+1/2} - v_i^{n+3/2}}{\Delta x} - \frac{1}{\rho_i} \frac{v_i^{n-1/2} - v_i^{n-3/2}}{\Delta x}; \quad \frac{u_i^{n+1} - 2u_i^n + u_i^{n-1}}{\Delta t} = \frac{1}{\Delta x \rho_i} \left( u_i^{n+1/2} - u_i^{n-1/2} - \left( \tau_{i+1/2} u_i^{n+1/2} + \tau_{i-1/2} u_i^{n-1/2} \right) \right); \quad \frac{u_i^{n+1} - 2u_i^n + u_i^{n-1}}{\Delta t^2} = \frac{1}{\Delta x \rho_i} \left( \tau_{i+1/2} \frac{u_i^{n+1} - u_i^n}{\Delta x} - \tau_{i-1/2} \frac{u_i^{n} - u_i^{n-1}}{\Delta x} \right); \quad \frac{u_i^{n+1} - 2u_i^n + u_i^{n-1}}{\Delta t^2} = \frac{1}{\Delta x \rho_i} \left( \tau_{i+1/2} u_i^{n+1} - (\tau_{i+1/2} + \tau_{i-1/2}) u_i^n + \tau_{i-1/2} u_i^{n-1} \right).$$

A similar argument gives the second order equation for $v$ as

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

(4.24)
To study the conservation properties of the discretized system (4.21) weighted inner products and norms analogous to (4.5) and (4.6) will be needed. So if \( u_i = u_1(x_i) \) and \( u_2 = u_2(x_i) \) and \( \rho_i = \rho(x_i) \) then let

\[
\langle u_1, u_2 \rangle_\rho = \sum_{i=1}^{N_x} u_1 u_2 \rho_i \Delta x. \tag{4.25}
\]

Next, if \( v_{1/2} = v_1(x_{1/2}) \) and \( v_{1/2} = v_2(x_{1/2}) \) then let

\[
\langle v_1, v_2 \rangle_\tau = \sum_{i=0}^{N_x-1} v_{1/2} v_{1/2} \tau_{i+1/2}^{-1} \Delta x. \tag{4.26}
\]

As above, let the inner products and norms with no subscript be the standard mean square norm and the norm with the subscript \( \infty \) be the maximum of the absolute value.

First, these inner products can be used to show that the adjoint of \( A \) is \( A^* \) that was defined above because

\[
\langle Au, v \rangle_\tau = \left\langle \frac{\tau \delta u}{\Delta x}, v \right\rangle_\tau,
\]

\[
= \sum_{i=0}^{N_x-1} \frac{\tau_{i+1}}{2} \frac{\delta u_{i+1}}{\Delta x} \frac{\tau_i}{2} \Delta x,
\]

\[
= -\sum u_i \delta v_i,
\]

\[
= -\sum u_i \frac{\delta v_i}{\rho_i \Delta x} \rho_i \Delta x,
\]

\[
= \langle u, -\frac{\delta v}{\rho} \rangle_\rho,
\]

\[
= \langle u, A^* v \rangle_\rho.
\]

The discrete wave equation has conserved quantities that can be derived from those defined in (3.6) and which are (3.8)

\[
C^n = \|u^n\|_\rho^2 + \left\| \frac{v^{n+1/2} + v^{n-1/2}}{2} \right\|_\tau^2 - \left( \frac{\Delta t}{2} \right)^2 \|A u^n\|_\tau^2,
\]

\[
= \|u^n\|_\rho^2 + \left\| \frac{v^{n+1/2} + v^{n-1/2}}{2} \right\|_\tau^2 - \left( \frac{\Delta t}{2} \right)^2 \left\| \tau \frac{\delta u^n}{\Delta x} \right\|_\tau^2.
\]
\[ C^{n+1/2} = \| v^{n+1/2} \|_\tau^2 + \left\| \frac{u^{n+1} + u^n}{2} - \left( \frac{\Delta t}{2} \right)^2 A^* v^{n+1/2} \right\|_\rho^2, \]
\[ = \| v^{n+1/2} \|_\tau^2 + \left\| \frac{u^{n+1} + u^n}{2} - \left( \frac{\Delta t}{2} \right)^2 \frac{\delta v^{n+1}}{\rho \Delta x} \right\|_\rho^2 . \]

To estimate when the conserved quantity is positive compute
\[
\left\| \frac{\tau \delta u^n}{\Delta x} \right\|_\tau^2 = \left\langle \frac{\tau \delta u^n}{\Delta x}, \frac{\tau \delta u^n}{\Delta x} \right\rangle_	au
\leq \max(\tau) \frac{\Delta x^2}{\Delta x^2} \left\langle \delta u^n, \delta u^n \right\rangle
\leq \max(\tau) \frac{\Delta x^2}{\Delta x^2} \left\| \delta u^n \right\|^2
\leq \max(\tau) \left( \frac{2}{\Delta x} \right)^2 \| u^n \|^2
\leq \max(\tau) \left( \frac{2}{\Delta x} \right)^2 \left\langle u^n, u^n \right\rangle_ho
\leq \max(\tau) \left( \frac{2}{\Delta x} \right)^2 \frac{1}{\min(\rho)} \left\langle u^n, u^n \right\rangle_ho
\leq \max(\tau) \left( \frac{2}{\Delta x} \right)^2 \left\| u^n \right\|_\rho^2 .
\]

As noted above when \( \rho \) and \( \tau \) are constant the wave speed \( c \) is given by \( c^2 = \tau/\rho \). So in the variable materials case
\[
s = \sqrt{\frac{\max(\tau)}{\min(\rho)}} \quad (4.27)
\]
gives an estimate for the maximum wave speed. Consequently
\[
C^n \geq \left( 1 - \left( s \frac{\Delta t}{\Delta x} \right)^2 \right) \| u^n \|_\rho^2 + \left\| \frac{u^{n+1/2} + u^{n-1/2}}{2} \right\|_\rho^2 .
\]

Similarly
\[
C^{n+1/2} \geq \left\| \frac{u^{n+1} + u^n}{2} \right\|_\tau + \left( 1 - \left( s \frac{\Delta t}{\Delta x} \right)^2 \right) \left\| v^{n+1/2} \right\|_\tau^2 .
\]
To assure that both conserved quantities are positive requires that \( s\Delta t/\Delta x \leq 1 \) which corresponds to the standard CFL stability condition when \( \rho \) and \( \tau \) are constant. So for this constraint the discretization is stable. Note that if \( \rho \) goes to zero or \( \tau \) becomes large then \( \Delta t \) must go to zero to maintain stability. So it is important for density to be bounded below and the Young’s modulus to be bounded above.

4.6 Implementing the Discrete Systems

Two codes will be created, \texttt{Wave1DCMP.m} for constant material properties and a more complex \texttt{Wave1DVMP.m} for variable material properties. The notation for the spatial derivatives is based on the notation in three dimensions where \( u \) will be a scalar while \( v \) is a vector. So then in the system (4.18) \( A \) must be the gradient while \( -A^* \) must be the divergence. So the simulation codes will use the notation

\[
\text{CMP} \quad A = c \text{Grad1} \quad A^* = -c \text{Div1}, \\
\text{VMP} \quad A = \tau \text{Grad1} \quad A^* = -\frac{1}{\rho} \text{Div1}.
\]

The spatial primal grid is obtained by replacing \( i \) by \( i - 1 \) in 4.13 to get

\[
xp(i) = a + (i - 1) \Delta x \quad 1 \leq i \leq Nx.
\]

The dual spatial grid is obtained by replacing \( i \) by \( i - 1 \) in 4.14 to get

\[
xd(i) = a + (i - 1/2) \Delta x, \quad 1 \leq i \leq Nx - 1.
\]

Because \( \Delta x = (b - a)/(Nx - 1) \), \( xp(1) = a \) and \( xp(Nx) = b \). Also note that

\[
xd(1) = a + \Delta x/2 \\
xd(Nx - 1) = a + (i - 1 - 1/2)\Delta x \\
= a + (i - 1)\Delta x - \Delta x/2 \\
= a - (b - a)\Delta x/2. \\
= b - \Delta x/2.
\]

The time grids are not stored in arrays so there in no need for a special notation.

In 4.15 the function \( u(x, t) \) is discretized on the primal grid while the function \( v(x, t) \) discretized on the dual grid. So in the simulation programs

\[
u^n_i \approx u(xp(i), n \Delta t), \quad v^n_i \approx v(xd(i), (n + 1/2)\Delta t), \quad 0 \leq n \leq Nt.
\]

Note that for \( n = Nt \), \( t^{n+1/2} = (Nt + 1/2) \Delta t = T + \Delta t/2 \) and that this value of \( v \) will be used to estimate \( v \) at the final time \( T \) using

\[
v^{Nt}_{i+1/2} = \frac{v^{Nt+1/2}_{i+1/2} + v^{Nt-1/2}_{i+1/2}}{2}.
\]
Both simulation codes will start with the initial data \( u^0 = u(x, 0) \) and \( v^0 = v(x, \Delta x/2) \). Then the update equations for the simulation code are obtained from 4.18. For \( u \) replace \( n + 1/2 \) by \( n \) in the first equation while for \( v \) replace \( n \) by \( n + 1 \) in the second equation and then replace \( n + 3/2 \) by \( n + 1 \) and \( n + 1/2 \) by \( n \) to obtain

\[
 u_i^{n+1} = u_i^n + \Delta t c (\text{Div}v^n)_i, \quad v_i^{n+1} = v_i^n + \Delta t c (\text{Grad}u^{n+1})_i, \quad 0 \leq i \leq Nt - 1. \tag{4.28}
\]

Not that the second equation depends on the results of the first equation so the order of evaluation is critical.

The implementation of the code \texttt{Wave1DVMP.m} is essentially the same as that of \texttt{Wave1DCMP.m}. Also see the simulation codes for the implementation of the conserved quantities. Consequently a preliminary test for variable materials simulation code is given by assuming the material properties \( \rho \) and \( \tau \) are constant and then use the analytic solution

\[
 u(x, t) = \cos(m \pi \frac{1}{\rho} t) \sin(m \pi x), \\
 v(x, t) = \sin(m \pi \tau t) \cos(m \pi x).
\]

where \( m \) is a positive integer. Note that if \( c = 1/\rho = \tau \) then this is the same as the solution for the constant material code. In fact both codes give the same result in this case.

### 4.7 Simulation Results

Simulations show that for \texttt{Wave1DCMP.m} and \texttt{Wave1DVMP.m} the conserved quantities are constant within a small multiple of \( \text{eps} \) and that the constant increases slowly with increasing grid size. The constant material code \texttt{Wave1DCMP.m} produces at least second order accurate solutions but computes the solution to forth order accuracy when the final time is a multiple of the half period of the solution. The situation for \texttt{Wave1DVMP.m} is more complex as it does not alway achieve second order accuracy but is at least first order accurate. A large number of simulations are presented in an attempt to understand this. The results are noisy especially when the errors are small.

Because the simulation codes use centered differences it is to be expected that the simulations should have order of convergence 2, that is, for decreasing \( \Delta x \) and \( \Delta t \) the error in the solution should behave like

\[
 Er = C_1 \Delta x^2 + C_2 \Delta t^2
\]

where \( C_1 \) and \( C_2 \) are constants. This was tested by setting \( \Delta t = C_3 \Delta x \) for some constant \( C_3 \) and then for a sequence of decreasing spatial step sizes \( \Delta x \) the errors should behave like \( Er = C \Delta x^2 \) for some constant \( C \). To estimate the order of convergence, use two simulations with different values of \( \Delta x \) and assume that \( Er_1 = C \Delta x_1^p \) and \( Er_2 = C \Delta x_2^p \) and then \( p \) can be estimated by

\[
 p = \frac{\ln(Er_1) - \ln(Er_2)}{\ln(\Delta x_1) - \ln(\Delta x_2)}.
\]
Because it is easy to find analytic solutions for the constant coefficient wave equation
the code Wave1DCMP.m is tested by computing the errors using an analytic solution. For
variable material properties, typically there are no analytic solutions. So in Wave1DVMP.m
the errors are estimated by choosing the number of spatial grids point $N_x = 2^k + 1$ for some
$k > 0$. Increasing $k$ to $k + 1$ will cause the refined grid points to be at the edges and centers
of the course grid cells. The difference between the course grid solution and the fine grid
solution at the course grid points gives an estimate for the error in $u$ on the course grid
points. In the error analysis it more informative to choose a decreasing sequence of
$\Delta x_k$ and then estimate the error in the solution $E_{r_k}(x_i)$ and then plot $E_{r_k}(x_i)/\Delta x_k^2$ as a function of
$x_i$. It is important that this illuminates where in space the errors are occurring.

For the time discretizations it is important for stability to keep the ratio of $dx/dt$ constant.
First if $N_x = 2^k + 1$ then $\Delta x = L/2^k$. Next for some integer $f$ choose $N_t = 2^{k+f}$ so that
$\Delta t = T/2^{k+f}$ and then $\Delta x/\Delta t = 2^{-f} L/T$ is constant for all $k$. The value of $f$ is chosen so
that the simulations are stable for all $k$.

Figure 4.2 displays the results of seven simulations run by Wave1DCMP.m. The number
of spatial grid points for each simulation is given in figure 4.2 part D. The initial data were
$u(x, 0) = \sin(\pi x)$ and $v(x, 0) = 0$. Parts A and B of figure 4.2 show the numerical and exact
solutions $u$ and $v$ at the final time for for the run using the most grid points. These solution
are identical up to graphics resolution. Part C of figure 4.2 shows the value of the solution
at the midpoint of the interval for the run using the largest number of grid points. So the
time interval used was slightly smaller than the period of the solution. Part D of figure 4.2
plots the error in the solution divided by $\Delta x^2$ for each of the seven simulations. Again all of
these plots are identical up to graphics resolution confirming the second order convergence
of the solution.

The situation for Wave1DVMP.m is a bit more complex. The first test was to define the
material properties functions in terms of the wave speed, that is, $\rho(x) = 1/c$ and $\tau(x) = c$
and then show that Wave1DVMP.m gave the same results as Wave1DCMP.m. The results from
the two codes are the same. In the case that at least one of $\rho$ and $\tau$ are not constant the
solutions can have small oscillatory errors that cause the convergence rate to be less that
2 but still larger than 1. To illustrate this, the errors $E_r(x)$ divided by $\Delta x^2$ are plotted
for several examples in figures 4.3, 4.4, 4.5, 4.7 and 4.8. If the numerical solutions are
converging at order 2 then the plots of $E_r(x)/\Delta x^2$ will be essentially independent of $\Delta x$.
When the order of convergence is less than 2 these plot will show increasing $E_r(x)/\Delta x^2$.
The legend gives the number of points in the grids and then $\Delta x = 1/(N_x - 1)$.

A simple case to start with is to choose one of $\rho$ and $\tau$ to be a linear function. As shown
in Figure 4.3 there are some surprises. First the legends give the number of spatial points $N_x$
so for $N_x = 1025$ the errors are order $10^{-6}$. As the length of the interval is 1, $\Delta x^2 \approx 10^{-6}$ so
the errors are small. Note that constant $\rho$ simulations are second order accurate so it is the
variable $\tau$ that causes the small oscillatory error. Next Figure 4.4 shows that for one choice
of $\rho$ and $\tau$ the larger errors start at the boundary and move to the interior. The final times
double from frame to frame so roughly the oscillatory errors move away from the boundary
linearly and grow linearly.
Figure 4.2: Simulations using Wave1DCMP.m.
Figure 4.3: Simulations using `Wave1DVMP.m` with linear material properties.
Figure 4.4: Errors Near The Boundary for Wave1DVM.m.
Figure 4.5: Boundary Errors For The Bump in Wave1DVMP.m.
Figure 4.6: Piecewise Linear Material Property

In Figure 4.5

\[ \rho(x) = 1 + (2x(1-x))^p, \quad \tau(x) = 1 + (2x(1-x))^q. \]

The panels contain plots of the solution errors for several values of \( p \) and \( q \). The number of grid points are given in the legend. The final time \( t = 2 \) is close to a "period" of the solution. Note that for \( p > 1 \) and \( q > 1 \) the derivatives of \( \rho \) and \( \tau \) are zero at the boundary while if \( p = 1 \) and \( q = 1 \) the derivatives are not zero. For \( q = 2 \) and \( p = 1 \) or \( p = 2 \) there are no oscillatory errors while if \( q = 1 \) and \( p = 1 \) or \( p = 2 \) there are oscillatory errors. It seems that the derivative of \( \tau \) not being zero at boundary causes the oscillatory errors.

To test the hypothesis that nonzero derivatives at the boundary cause the oscillatory errors in the next examples either \( \rho \) or \( \tau \) is a piecewise linear function as shown in Figure 4.6. If \( H \) is the Heaviside function, that is, \( H(x) = 1 \) if \( x \geq 0 \) and \( H(x) = 0 \) for \( x < 0 \) then \( \rho \) or \( \tau \) are given by

\[ c(1 - H(x - a)) + dH(x - b) + \frac{(a d - b c) + (c - d)x}{a - b}(H(x - a) - H(x - b)). \] (4.29)

In Figure 4.6 and in the simulations \( a = 1/4, b = 3/4, c = 1, d = 2 \).
Figure 4.7 shows that the solutions errors. Note that \( y'(0) = y'(1) = 0 \). So the conjecture above that the derivative at the boundary being zero eliminates the oscillations is not correct. Additionally the discontinuities in the derivative \( d\tau/dx \) do cause similar oscillatory errors. Again the errors are a small multiple of \( \Delta x^2 \) that grows slowly with decreasing \( \Delta x \).

The final test is to see what discontinuities in \( \rho \) and \( \tau \) do to the errors, that is one of \( \rho \) or \( \tau \) jumps up or down:

\[
\rho(x) = 1 \pm H(x)/2; \quad \tau(x) = 1 \pm H(x)/2.
\]

Figure 4.8 show that the jump causes oscillations similar to those seen in the previous figures near the boundary of the \( x \) interval.
Figure 4.8: $\rho$ or $\tau$ have a jump at $x = 1/2$ in Wave1DVMP.m.
5 Three Dimensional Variable Coefficient Differential Operators

This section introduces terminology based on that used in differential geometry of exact sequences and diagram chasing that are used to create second order variable coefficient differential operators that are be used to create second order wave equations. However, using the ideas from differential geometry in the mimetic finite difference [46] setting poses a new problem as there are two interlaced discretization grids. Consequently two exact sequences as shown in Figure 5.1 are need to study the discretizations. In the continuum the two exact sequences are not needed but are useful when the continuum is discretized. The use of diagram chasing is critical to obtain differential operators that can be discretized using the mimetic finite difference methods as described in [46].

After the operators are defined, inner products are introduced and the adjoints of all of the operators obtained from the double exact sequence are computed. This is then used to show that the second order operators are self-adjoint and either positive or negative and thus suitable for defining wave equations. In this continuum setting there are two equivalent derivations of each operator. In the discrete setting these operators will be different.

5.1 Exact Sequences

In the double exact sequence diagram 5.1 the bottom row is the same as the top row written in opposite order. For reasons which will become clear when the operators are discretized, $P$ stands for points, $C$ stands for curves, $S$ stands for surfaces, $V$ stands for volumes. In this diagram $H_P$ and $H_V$ are linear spaces of smooth scalar functions depending on the spatial variables $(x, y, z)$ and $H_C$ and $H_S$ are linear spaces of smooth vector valued functions that also depend on $(x, y, z)$. In this discussion all of the functions converge rapidly to zero as $x^2 + y^2 + z^2$ becomes large.

The first order differential operators in the exact sequence 5.1 are the gradient $\vec{\nabla}$, curl or rotation $\vec{\nabla} \times$, and divergence $\vec{\nabla} \cdot$. The diagram is called exact because the curl of the gradient is zero $\vec{\nabla} \times \vec{\nabla} = 0$ and the divergence of the curl is zero $\vec{\nabla} \cdot \vec{\nabla} \times = 0$. The scalar functions $a$ and $b$ and also the matrix valued functions $A$ and $B$ are used to describe material properties and act by multiplication as described in Table 5.1. The functions $a$ and $b$ are bounded above and below by positive constants. The matrix functions are symmetric positive definite and the eigenvalues of the matrices are bounded above and below by positive constants. To
begin, these functions will be assumed smooth but later this will not be assumed so that
they can be used to describe discontinuous material properties.

So in Figure 5.1 the horizontal arrows represent the action of the differential operators
while the vertical arrows represent multiplication by scalar functions $a$ and $b$ and by $3 \times 3$
matrices $A$ and $B$ that are known as star operators in differential geometry. The differential
operators and material property functions give mappings between the spaces in the double
exact sequence as described in Table 5.1. Note that the differential operators are not invertible, but that the conditions on $a$, $b$, $A$ and $B$ imply that they are invertible. This will play
a critical role in diagram chasing.

The integers in the double exact sequence give the spatial dimension of the function in
the spaces, that is if $f \in H_P$ the $f$ has no spatial dimension while if $g \in H_V$ then $g$ has
spatial dimension $1/d^3$. Also if $\vec{v} \in H_C$ then $\vec{v}$ has spatial dimension $1/d$ and if $\vec{w} \in H_S$ then $\vec{w}$ has spatial dimension $1/d^2$. The differential operators all have dimension $1/d$. Moreover $a$ and $b$ have spatial dimensions $1/d^3$ while $A$ and $B$ have dimensions $1/d$. The directions
of the vertical arrows were chosen so that $a$, $b$, $A$ and $B$ have dimensions $1/d^k$ for $k > 0$. Importantly, the operators and spaces in Table 5.1 are dimensionally consistent! In some
applications $a$ and $b$ are densities.

### 5.2 Diagram Chasing and Second Order Operators

Table 5.2 gives all of the possible second order operators given by diagram chasing. As an
elementary of diagram chasing, consider $f \in H_P$ so that $\vec{\nabla} f \in H_C$ and then $A \vec{\nabla} f \in H_S$ so that
$\vec{\nabla} \cdot A \vec{\nabla} f \in H_V$ and finally $a^{-1} \vec{\nabla} \cdot A \vec{\nabla} f \in H_S$. Consequently $a^{-1} \vec{\nabla} \cdot A \vec{\nabla}$ maps $H_S$ into $H_S$.

For diagram chasing it is important that the mappings $a$, $b$, $A$ and $B$ are invertible
while $\vec{\nabla}$, $\vec{\nabla} \times$ and $\vec{\nabla} \cdot$ are not invertible. Consequently to create a second order operator,
only going clockwise around a square in Figure 5.1 is allowed. However it is possible to
start and any corner, so this gives twelve operators, four corners times three squares. In
the continuum some of these operators are essentially the same, for example $a^{-1} \vec{\nabla} \cdot A \vec{\nabla}$ and
$b^{-1} \vec{\nabla} \cdot B \vec{\nabla}$. What is important is that when these operators are discretized they will not be
the same. The assumptions that $B = A$ and $b = a$ reduces the number of operators to six.

When the material properties are constant it is useful to introduce that wave speed and then
then use the simplifying assumptions

$$a = 1/c^3, b = 1/c^3, A = I/c, B = I/c,$$  \hspace{1cm} (5.1)
Table 5.2: Fundamental second order differential operators. The left two columns start with spaces in the top row in Figure 5.1 while the right two columns start with spaces in the bottom row.

| Upper Row | Bottom Row |
|-----------|------------|
| $f \in H_P$ | $\vec{v} \in H_C$ | $\vec{w} \in H_S$ | $g \in H_V$ |
| $\nabla f \in H_C$ | $\mathbf{A}\vec{v} \in H_S$ | $\nabla \cdot \vec{w} \in H_V$ | $a^{-1}g \in H_P$ |
| $\mathbf{A}\nabla f \in H_S$ | $\nabla \cdot \mathbf{A}\vec{v} \in H_V$ | $a^{-1}\nabla \cdot \vec{w} \in H_P$ | $\nabla a^{-1}g \in H_C$ |
| $\nabla \cdot \mathbf{A}\nabla f \in H_V$ | $a^{-1}\nabla \cdot \mathbf{A}\vec{v} \in H_P$ | $\nabla a^{-1}\nabla \cdot \vec{w} \in H_C$ | $\mathbf{A}\nabla a^{-1}g \in H_S$ |
| $a^{-1}\nabla \cdot \mathbf{A}\nabla f \in H_P$ | $\nabla a^{-1}\nabla \cdot \mathbf{A}\vec{v} \in H_C$ | $\mathbf{A}\nabla a^{-1}\nabla \cdot \vec{w} \in H_S$ | $\nabla \cdot \mathbf{A}\nabla a^{-1}g \in H_V$ |

where $\mathbf{I}$ is the identity matrix then the operators simplify to those in Table 5.3. So under the simplifying assumptions there are only three distinct second order operators:

$$\Delta f = \nabla \cdot \nabla f; \quad \nabla \times \nabla \times \vec{v}; \quad \nabla \nabla \cdot \vec{w}.$$ 

where $\Delta$ is the scalar Laplacian.

### 5.3 Additional Second Order Operators

Note that in Table 5.2 there are two operators defined on $H_P$, four operators defined on $H_C$, four operators defined on $H_S$ and two operators defined on $H_V$. If linear operators are defined on the same space then linear combinations of these operators are again linear operators. The two operators defined on $H_P$ and the two defined on $H_V$ are essentially the same so linear combinations are not interesting. For any operator in the Top Row boxes, there is a similar operator in the Bottom Row that can be obtained by interchanging $a$ with
Table 5.3: The general operators can be simplified using the assumptions in 5.1.

\[
\begin{array}{|c|c|c|c|c|}
\hline
& f \in H_P & \vec{v} \in H_C & \vec{w} \in H_S & g \in H_V \\
\hline
\text{First Box} & c^2 \vec{\nabla} \cdot \vec{\nabla} f \in H_P & c^2 \vec{\nabla} \cdot \vec{\nabla} \cdot \vec{v} \in H_C & c^2 \vec{\nabla} \cdot \vec{\nabla} \cdot \vec{w} \in H_S & c^2 \vec{\nabla} \cdot \vec{\nabla} g \in H_V \\
\hline
\text{Second Box} & c^2 \vec{\nabla} \times \vec{\nabla} \times \vec{v} \in H_C & c^2 \vec{\nabla} \times \vec{\nabla} \times \vec{w} \in H_S & c^2 \vec{\nabla} \times \vec{\nabla} \times \vec{w} \in H_S & c^2 \vec{\nabla} \times \vec{\nabla} \times \vec{w} \in H_S \\
\hline
\text{Third Box} & c^2 \vec{\nabla} \cdot \vec{\nabla} \cdot \vec{w} \in H_S & c^2 \vec{\nabla} \cdot \vec{\nabla} g \in H_V & c^2 \vec{\nabla} \cdot \vec{\nabla} f \in H_P & c^2 \vec{\nabla} \cdot \vec{\nabla} \cdot \vec{v} \in H_C \\
\hline
\end{array}
\]

For \( \vec{v} \in H_C \) and for \( \vec{w} \in H_S \) define

\[
\begin{align*}
\text{VL}_1(\vec{v}) &= \vec{\nabla} a^{-1} \vec{\nabla} \cdot \vec{A} \vec{v} - \vec{A}^{-1} \vec{\nabla} \times \vec{B}^{-1} \vec{\nabla} \times \vec{v} \\
\text{VL}_2(\vec{w}) &= \vec{B} \vec{\nabla} b^{-1} \vec{\nabla} \cdot \vec{w} - \vec{\nabla} \times \vec{A}^{-1} \vec{\nabla} \times \vec{B}^{-1} \vec{w} \\
\text{VL}_3(\vec{v}) &= \vec{\nabla} b^{-1} \vec{\nabla} \cdot \vec{B} \vec{v} - \vec{B}^{-1} \vec{\nabla} \times \vec{A}^{-1} \vec{\nabla} \times \vec{v} \\
\text{VL}_4(\vec{w}) &= \vec{A} \vec{\nabla} a^{-1} \vec{\nabla} \cdot \vec{w} - \vec{\nabla} \times \vec{B}^{-1} \vec{\nabla} \times \vec{A}^{-1} \vec{w}
\end{align*}
\] (5.2)

Under the simplifying assumptions 5.1 and with \( a = b = 1 \) and \( \vec{A} = \vec{B} = 1 \) these operators become

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

where \( \Delta \) is the vector Laplacian

\[
\Delta \vec{v} = (\Delta v_1, \Delta v_2, \Delta v_3), \quad \Delta \vec{w} = (\Delta w_1, \Delta w_2, \Delta w_3).
\]

Operators like these appear in the elastic wave equation which will be studied in Section 6.12.

### 5.4 Inner Products

Applying the mimetic ideas to physical problems requires the use of inner products on the spaces \( H_P, H_C, H_S \) and \( H_V \). It is important that the inner products do not have a spatial dimension. Two bilinear forms will help simplify the notation. Let \( f = f(x, y, z) \in H_P \), \( g = g(x, y, z) \in H_V \), \( \vec{v} = v(x, y, z) \in H_C \) and \( \vec{w} = w(x, y, z) \in H_S \) and then define

\[
\langle \langle f, g \rangle \rangle = \int_{\mathbb{R}^3} f(x, y, z) g(x, y, z) \, dx \, dy \, dz,
\]

\[
\langle \langle \vec{v}, \vec{w} \rangle \rangle = \int_{\mathbb{R}^3} \vec{v}(x, y, z) \cdot \vec{w}(x, y, z) \, dx \, dy \, dz.
\] (5.3)
These bilinear forms are dimensionless because $dx$, $dy$ and $dy$ have dimension $d$ while $f$ has dimension 0, $g$ has dimension $1/d^3$, $\vec{v}$ has dimension $1/d$ and $\vec{w}$ has $1/d^2$.

The inner product on the function spaces must use a weight function to be dimensionless:

- for $f_1, f_2 \in H_P$ set $\langle f_1, f_2 \rangle_P = \langle \langle a f_1, f_2 \rangle \rangle$
- for $\vec{v}_1, \vec{v}_2 \in H_C$ set $\langle \vec{v}_1, \vec{v}_2 \rangle_C = \langle \langle A \vec{v}_1, \vec{v}_2 \rangle \rangle$
- for $\vec{w}_1, \vec{w}_2 \in H_S$ set $\langle \vec{w}_1, \vec{w}_2 \rangle_S = \langle \langle A^{-1} \vec{w}_1, \vec{w}_2 \rangle \rangle$
- for $g_1, g_2 \in H_V$ set $\langle g_1, g_2 \rangle_V = \langle \langle a^{-1} g_1, g_2 \rangle \rangle$

As usual $||f||_P^2 = \langle f, f \rangle_P$, $||\vec{v}||_C^2 = \langle \vec{v}, \vec{v} \rangle_C$, $||\vec{w}||_S^2 = \langle \vec{w}, \vec{w} \rangle_S$, $||g||_V^2 = \langle g, g \rangle_V$. Additional inner products can be made by replacing $a$ by $b$ and $A$ by $B$. To be inner products it is important that $a$ and $b$ are positive and that $A$ and $B$ are symmetric and positive definite matrices.

5.5 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 discussion in that section shows that if $X$, $Y$, and $Z$ are linear spaces and $O_1$ and $O_2$ are linear operators such that

$$X \xrightarrow{O_1} Y \xrightarrow{O_2} Z$$

then

$$Z \xrightarrow{O_2^*} Y \xrightarrow{O_1^*} X$$

and

$$(O_1 O_2)^* = O_2^* O_1^*. \quad (5.4)$$

Because diagram chasing gives operators as compositions of other operators, this will be used many times.

The adjoints of the operators in Table 5.1 are

$$\nabla^* = -a^{-1} \nabla \cdot A, \quad \vec{\nabla}^* = -b^{-1} \vec{\nabla} \cdot B,$$

$$\nabla \times^* = A^{-1} \nabla \times B^{-1}, \quad \vec{\nabla} \times^* = B^{-1} \vec{\nabla} \times A^{-1},$$

$$\nabla \cdot^* = -B \nabla b^{-1}, \quad \vec{\nabla} \cdot^* = -A \vec{\nabla} a^{-1},$$

$$A^* = A^{-1}, \quad B^* = B^{-1},$$

$$a^* = a^{-1}, \quad b^* = b^{-1}, \quad (5.5)$$

where the column on the left contains differential operators from the top row in Figure 5.1 and the column on the right contains differential operators from the bottom row in Figure 5.1.
The proofs of the formulas in 5.5 are straight forward. For the gradient let $f \in H_P$ and $\vec{v} \in H_C$ so that

$$\langle \vec{\nabla} f, \vec{v} \rangle_C = \langle \langle A \vec{\nabla} f, \vec{v} \rangle \rangle$$

$$= \langle \langle \vec{\nabla} f, A \vec{v} \rangle \rangle$$

$$= -\langle \langle f, \vec{\nabla} \cdot A \vec{v} \rangle \rangle$$

$$= -\langle \langle a f, a^{-1} \vec{\nabla} \cdot A \vec{v} \rangle \rangle$$

$$= \langle \langle f, -a^{-1} \vec{\nabla} \cdot A \vec{v} \rangle \rangle_P$$

For the curl let $\vec{v} \in H_C$ and $\vec{w} \in H_S$ so that

$$\langle \vec{\nabla} \times \vec{v}, \vec{w} \rangle_S = \langle \langle A^{-1} \vec{\nabla} \times \vec{v}, \vec{w} \rangle \rangle$$

$$= \langle \langle \vec{\nabla} \times \vec{v}, A^{-1} \vec{w} \rangle \rangle$$

$$= \langle \langle \vec{v}, \vec{\nabla} \times A^{-1} \vec{w} \rangle \rangle$$

$$= \langle \langle B \vec{v}, B^{-1} \vec{\nabla} \times A^{-1} \vec{v} \rangle \rangle$$

$$= \langle \langle \vec{v}, B^{-1} \vec{\nabla} \times A^{-1} \vec{w} \rangle \rangle_C$$

For the divergence let $\vec{w} \in H_S$ and $g \in H_V$ so that

$$\langle \vec{\nabla} \cdot \vec{w}, g \rangle_V = \langle \langle a^{-1} \vec{\nabla} \cdot \vec{w}, g \rangle \rangle$$

$$= \langle \langle \vec{\nabla} \cdot \vec{w}, a^{-1} g \rangle \rangle$$

$$= -\langle \langle \vec{w}, \vec{\nabla} (a^{-1} g) \rangle \rangle$$

$$= -\langle \langle A^{-1} \vec{w}, A \vec{\nabla} (a^{-1} g) \rangle \rangle$$

$$= \langle \langle \vec{w}, -A \vec{\nabla} (a^{-1} g) \rangle \rangle_S$$

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

$$\langle A \vec{v}, \vec{w} \rangle_S = \langle \langle A^{-1} A \vec{v}, \vec{w} \rangle \rangle$$

$$= \langle \langle A \vec{v}, A^{-1} \vec{w} \rangle \rangle$$

$$= \langle \langle \vec{v}, A^{-1} \vec{w} \rangle \rangle_C$$

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For the operator $a$ let $f \in H_P$ and $g \in H_V$ so that
\[
\langle a f, g \rangle_V = \langle a^{-1} a f, g \rangle_V \\
= \langle a f, a^{-1} g \rangle_V \\
= \langle f, a^{-1} g \rangle_P
\]

Similar arguments give the adjoint operators for operators containing $b$ and $B$. To keep the notation easy to read it has not been specified whether to use $a$ or $b$ and whether to use $A$ or $B$ in the inner products when computing adjoints. This is clear from the context.

It is now straightforward to compute the adjoints of the second order operators in Table 5.2:

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

\[
\left(A^{-1} \vec{\nabla} \times B^{-1} \vec{\nabla} \times \right)^* = \vec{\nabla} \times^* B^{-1}^* \vec{\nabla} \times^* A^{-1}^* \\
= A^{-1} \vec{\nabla} \times B^{-1} B B^{-1} \vec{\nabla} \times A^{-1} A \\
= A^{-1} \vec{\nabla} \times B^{-1} \vec{\nabla} \times
\]

\[
\left(B \vec{\nabla} b^{-1} \vec{\nabla} \cdot \right)^* = \vec{\nabla} \cdot b^{-1}^* \vec{\nabla} \cdot B^* \\
= B \vec{\nabla} b^{-1} b b^{-1} \vec{\nabla} \cdot B B^{-1} \\
= B \vec{\nabla} b^{-1} \vec{\nabla}
\]

So these three operators are self-adjoint and similar arguments show that all operators in Table 5.2 are self-adjoint.

### 5.6 Positive and Negative Second Order Operators

Arguments like those in the previous sections can be used to show that the second order operators in Table 5.2 are either positive or negative, those that contain two curl operators are positive while those that contain a gradient and divergence are negative.

Let $f \in H_P$ and then consider
\[
\langle a^{-1} \vec{\nabla} \cdot A \vec{\nabla} f, f \rangle_P = \langle \vec{\nabla} \cdot A \vec{\nabla} f, a f \rangle_V \\
= -\langle A \vec{\nabla} f, A \vec{\nabla} a^{-1} a f \rangle_S \\
= -\langle A \vec{\nabla} f, A \vec{\nabla} f \rangle_S \\
\leq 0
\]
Let $\vec{v} \in H_C$ and then consider
\[
\langle A^{-1} \vec{\nabla} \times B^{-1} \vec{\nabla} \times \vec{v}, \vec{v} \rangle_C = \langle \vec{\nabla} \times B^{-1} \vec{\nabla} \times \vec{v}, A \vec{v} \rangle_S = \langle B^{-1} \vec{\nabla} \times \vec{v}, B^{-1} \vec{\nabla} \times A^{-1} A \vec{v} \rangle_C = \langle B^{-1} \vec{\nabla} \times \vec{v}, B^{-1} \vec{\nabla} \times \vec{v} \rangle_C \geq 0
\]

Let $\vec{w} \in H_S$ and then consider
\[
\langle B \vec{\nabla} b^{-1} \vec{\nabla} \cdot \vec{w}, \vec{w} \rangle_S = \langle \vec{\nabla} b^{-1} \vec{\nabla} \cdot \vec{w}, B^{-1} \vec{w} \rangle_S = \langle b^{-1} \vec{\nabla} \cdot \vec{w}, \vec{\nabla}^* B^{-1} \vec{w} \rangle_P = -\langle b^{-1} \vec{\nabla} \cdot \vec{w}, b^{-1} \vec{\nabla} \cdot B B^{-1} \vec{w} \rangle_P = -\langle b^{-1} \vec{\nabla} \cdot \vec{w}, b^{-1} \vec{\nabla} \cdot \vec{w} \rangle_P \leq 0
\]

These results capture the important features of the second order differential operators.
6 3D Wave Equations With Variable Material Properties

Wave equation can be derived from Newton’s law and thus have the form

$$\rho \frac{d^2W}{dt^2} = \mathcal{A} W,$$

(6.1)

where \(W = W(t,x,y,z)\) is a scalar or vector function, \(\rho\) is the density of the material that
the wave is traveling in and \(\mathcal{A}\) is a second order spatial differential operator. Here such
equations will written in the form

$$\frac{d^2W}{dt^2} = \mathcal{B} W, \quad \mathcal{B} = \frac{1}{\rho} \mathcal{A}.$$

(6.2)

where \(\mathcal{B}\) is one of the second order operators in Table 5.2. The general case provides 12
possible wave equations. Another four equations are obtained using the operators in (5.2).
Note that many of these equations are equivalent but will not be equivalent in the discrete
setting because of the use of two grids in the discretization. A critical point for wave equations
is that the operator \(\mathcal{B}\) must be negative definite so that all eigenvalues of this operator are
real and strictly less than zero. This will guarantee that the solutions are oscillatory. As
will be seen below, if the material properties are constant and trivial and \(c\) is the wave speed
then \(\mathcal{B}\) will be a \(c^2\) times one of \(\nabla \cdot \nabla\), \(\nabla \nabla \cdot\) or \(\nabla \times \nabla \times\).

Next the second order equations are written as first order systems that are created using
operators generated by going half way around the squares in the double exact sequence dia-
gram 5.1. Note that the dependent variables in the first order systems are not dimensionless
because they come from spaces containing function with different spatial units. As before,
the first order systems are used to create conservation laws.

Finally, the connection between the notation in the literature and the notation in this
paper for wave, Maxwell and elastic wave equation is discussed. The methods used here
cannot produce the general elastic wave equation.

6.1 Second order Wave Equations

The well known scalar wave equation is given by choosing \(W = f \in H_P\) and then choosing
\(\mathcal{B}\) to be the operator in the upper left cell of Table 5.2 to get

$$\frac{d^2f}{dt^2} = a^{-1} \nabla \cdot A \nabla f.$$

(6.3)

To understand how this equation relates to the standard wave equation assume that \(a\) is a
constant and that \(A\) is a constant \(A\) times the identity matrix. In this case \(A/a \sim d^2/t^2\) that
is \(A/a = c^2\) where \(c\) is the wave speed. So under these simplifying assumptions the above
equation becomes the standard scalar wave equation

$$\frac{d^2f}{dt^2} = c^2 \nabla \cdot \nabla f.$$

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The initial conditions for the second order equation are \( f(0) \) and \( f'(0) \).

A vector wave equation can be generated by choosing \( W = \vec{w} \in H_S \) and then choosing \( \mathcal{B} \) to be the operator in the lower left cell of Table 5.2 to get

\[
\frac{d^2 \vec{w}}{dt^2} = \mathcal{B} \vec{\nabla} b^{-1} \vec{\nabla} \cdot \vec{w}.
\]  

(6.4)

To understand how this equation relates to a standard wave equation assume that \( b \) is a constant and that \( \mathcal{B} \) is a constant \( B \) times the identity matrix. In this case \( B/b \sim d^2/t^2 \) that is \( B/b = c^2 \) where \( c \) is the wave speed. So under these simplifying assumptions the above equation becomes the standard vector wave equation

\[
\frac{d^2 \vec{w}}{dt^2} = c^2 \vec{\nabla} \vec{\nabla} \cdot \vec{w}.
\]

For this equation the initial conditions are \( \vec{w}(0) \) and \( \vec{w}'(0) \).

Maxwell’s second order equation can be generated by choosing \( W = \vec{v} \in H_C \) and \( \mathcal{B} \) the operator in the center left cell of Table 5.2 to get

\[
\frac{d^2 \vec{v}}{dt^2} = -\mathcal{A}^{-1} \vec{\nabla} \times \mathcal{B}^{-1} \vec{\nabla} \times \vec{v}.
\]  

(6.5)

Under the simplifying assumptions this becomes

\[
\frac{d^2 \vec{v}}{dt^2} = -c^2 \vec{\nabla} \times \vec{\nabla} \times \vec{v},
\]

which is Maxwell’s second order equation in uniform materials. In total twelve equations can be created all of which under the simplifying assumptions reduce to one of the three wave equations just discussed. However, in the discretization the twelve general equations offer flexibility in modeling physical problems with variable material properties.

Additional second order wave equations can be made from the two term second order operators \( \mathbf{VL}_1, \mathbf{VL}_2, \mathbf{VL}_3, \) and \( \mathbf{VL}_4 \) in (5.2). For example

\[
\frac{d^2 \vec{v}}{dt^2} = \vec{\nabla} a^{-1} \vec{\nabla} \cdot \mathcal{A} \vec{v} - \mathcal{A}^{-1} \vec{\nabla} \times \mathcal{B}^{-1} \vec{\nabla} \times \vec{v}.
\]

(6.6)

Under the simplifying assumptions this equation becomes

\[
\frac{d^2 \vec{v}}{dt^2} = c^2 \vec{\nabla} \vec{\nabla} \cdot \vec{v} - c^2 \vec{\nabla} \times \vec{\nabla} \times \vec{v},
\]

which is a special case of the elastic wave equation (6.14). All four equations created this way reduce to the elastic wave equation under the simplifying assumptions. Note that the space time units of the dependent variable do not play a role in the second order equations. The study of first order system will clarify what the units of \( a, b, \mathcal{A} \) and \( \mathcal{B} \) must be.
6.2 First Order Systems and Conserved Quantities

There is a natural way to use diagram chasing to write the second order wave equations as a system of first order equations and then use this to define conserved quantities. Note that the first order equations contain functions from different spaces with different spatial units. The main idea is to choose two function in diagonally opposite corners of one of the squares in Figure 5.1 and do a diagram chase. Consequently there are lots of first order systems!

For example for equation (6.3), because \( f \in H_P \), choose \( \vec{w} \in H_S \) and then set

\[
\frac{d \vec{w}}{dt} = A \vec{\nabla} f, \quad \frac{df}{dt} = a^{-1} \vec{\nabla} \cdot \vec{w}
\]

The initial conditions for this system are \( f(0) \) and \( \vec{w}(0) \) This also gives the vector wave equation

\[
\frac{d^2 \vec{w}}{dt^2} = A \vec{\nabla} a^{-1} \vec{\nabla} \cdot \vec{w}
\]

for which the initial conditions are \( \vec{w}(0) \) and \( \vec{w}'(0) \).

The exact sequence 5.1 requires that the spatial units the dependent variable in system (6.7) are \( f \sim 1 \) and \( \vec{w} \sim 1/d^2 \). At least is some applications \( a \) is a density so assume \( a \sim 1/d^3 \). If \( u_f \) are the units of \( f \) and \( u_w \) are the units of \( w \) then the two first order equation give

\[
\frac{u_w}{t} = u_A \frac{1}{d} u_f, \quad \frac{u_f}{t} = d^3 \frac{1}{d} u_w,
\]

which implies

\[ u_A = \frac{1}{d t^2}. \]

This then implies that

\[ \frac{A}{a} \sim \frac{d^2}{t^2} \]

which is required by the constant coefficient case where \( A/a = c^2 \) where \( c \) is the wave speed.

Now 6.9 become

\[ u_w = \frac{1}{t d^2} u_f, \quad u_f = t d^2 u_w. \]

Now if \( f \sim 1 \), that is \( u_f = 1 \), the \( w \sim 1/t d^2 \). On the otherhand if \( w \) is to be a velocity then \( u_w \sim d/t \) then it must be that \( u_f \sim d^3 \) and the \( df/dt \) becomes a rate of change of volume. This needs to be checked against what modelers do.

This system has a conservation law because table 5.5 imply that

\[ (a^{-1} \vec{\nabla} \cdot)^* = \vec{\nabla} \cdot (a^{-1})^* = -A \vec{\nabla} a^{-1} a = -A \vec{\nabla}, \]

so this system has the form of the equation discussed in (3.1) and consequently should have a conserved quantity given by

\[ C = \frac{||f||^2_P + ||\vec{w}||^2_S}{2} \]
This can be checked explicitly:

\[
\frac{dC}{dt} = \langle f, \frac{df}{dt} \rangle_P + \langle \vec{w}, \frac{d\vec{w}}{dt} \rangle_S
\]

\[
= \langle f, a^{-1} \nabla \cdot \vec{w} \rangle_P + \langle \vec{w}, A \vec{\nabla} f \rangle_S
\]

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

\[
= - \langle A \vec{\nabla} f, \vec{w} \rangle_S + \langle \vec{w}, A \vec{\nabla} f \rangle_S
\]

\[
= 0 .
\]

As discussed in Section 2, if \( f \) and \( \vec{w} \) are solutions of (6.7) then so are \( \frac{df}{dt} \) and \( \frac{d\vec{w}}{dt} \) and consequently the classical energy \( E \) is conserved.

To convert the Maxwell equation (6.5) to a system assume that \( \vec{v} \in H_C \) in the upper row of 5.1 and that \( \vec{w} \in H_C \) in the lower row of 5.1 then set

\[
\frac{d\vec{w}}{dt} = \vec{B}^{-1} \vec{\nabla} \times \vec{v}, \quad \frac{d\vec{v}}{dt} = -A^{-1} \vec{\nabla} \times \vec{w} .
\]

A conserved quantity is given by

\[
C = \frac{||\vec{v}||_C^2 + ||\vec{w}||_C^2}{2}
\]

because

\[
\frac{dC}{dt} = \langle \vec{v}, \frac{d\vec{v}}{dt} \rangle_C + \langle \vec{w}, \frac{d\vec{w}}{dt} \rangle_C
\]

\[
= -\langle \vec{v}, A^{-1} \vec{\nabla} \times \vec{w} \rangle_C + \langle \vec{w}, B^{-1} \vec{\nabla} \times \vec{v} \rangle_C
\]

\[
= -\langle B^{-1} \vec{\nabla} \times A^{-1} \vec{v}, \vec{w} \rangle_C + \langle \vec{w}, B^{-1} \vec{\nabla} \times \vec{v} \rangle_C
\]

\[
= -\langle B^{-1} \vec{\nabla} \times \vec{v}, \vec{w} \rangle_C + \langle \vec{w}, B^{-1} \vec{\nabla} \times \vec{v} \rangle_C
\]

\[
= 0 .
\]

Additionally,

\[
E = \frac{||\frac{d\vec{w}}{dt}||_C^2 + ||\frac{d\vec{v}}{dt}||_C^2}{2}
\]

\[
= \frac{||B^{-1} \vec{\nabla} \times \vec{v}||_C^2 + ||A^{-1} \vec{\nabla} \times \vec{w}||_C^2}{2}
\]

\[
= \frac{||\vec{\nabla} \times \vec{v}||_S^2 + ||\vec{\nabla} \times \vec{w}||_S^2}{2} .
\]
is a conserved quantity. In this case $E$ is essentially the physical energy.

Also first order systems can be made from the second order equations made from the two term second order operators $VL_1$, $VL_2$, $VL_3$ and $VL_4$ given in (5.2). However this requires three first order equations. For example, for $VL_1$, because $\vec{v} \in H_C$, let $g \in H_V$ and $\vec{u} \in H_C$

\[
\frac{dg}{dt} = \vec{\nabla} \cdot A \vec{v} \\
\frac{d\vec{u}}{dt} = B^{-1} \vec{\nabla} \times \vec{u} \\
\frac{d\vec{v}}{dt} = \vec{\nabla} a^{-1} g - A^{-1} \vec{\nabla} \times \vec{u}.
\]

For a conserved quantity set

\[
C = \left| |\vec{v}|^2_C + |\vec{u}|^2_C + |g|^2_V \right|
\]

so that

\[
\frac{dC}{dt} = \left< \vec{v}, \frac{d\vec{v}}{dt} \right>_C + \left< \vec{u}, \frac{d\vec{u}}{dt} \right>_C + \left< g, \frac{dg}{dt} \right>_V \\
= \left< \vec{v}, \vec{\nabla} a^{-1} g - A^{-1} \vec{\nabla} \times \vec{u} \right>_C + \left< \vec{u}, B^{-1} \vec{\nabla} \times \vec{v} \right>_C + \left< g, \vec{\nabla} \cdot A \vec{v} \right>_V \\
= \left< \vec{v}, \vec{\nabla} a^{-1} g \right>_C - \left< \vec{v}, A^{-1} \vec{\nabla} \times \vec{u} \right>_C + \left< A^{-1} \vec{\nabla} \times B^{-1} B \vec{u}, \vec{v} \right>_C - \left< A^{-1} A \vec{\nabla} a^{-1} g, \vec{v} \right>_V \\
= 0.
\]

As before this implies that

\[
E = \left| \left| \frac{d\vec{v}}{dt} \right|^2_C + \left| \left| \frac{d\vec{u}}{dt} \right|^2_C + \left| \frac{dg}{dt} \right|^2_V \right|
\]

\[
= \left| \left| \frac{d\vec{v}}{dt} \right|^2_C + \left| B^{-1} \vec{\nabla} \times \vec{v} \right|^2_C + \left| \vec{\nabla} \cdot A \vec{v} \right|^2_V \right|
\]

is conserved.

6.3 Standard Notation For Wave Equations in Three Dimensions

The standard notation for the Maxwell equation and the elastic wave equation are described and the connection to the notation used in this paper are discussed. Representing Maxwell’s
equations 6.10 using diagram chasing uses the center square in Figure 5.1 which is reproduced in Figure 6.1 using notation appropriate to Maxwell’s equations, that is, by setting \( A = \epsilon \) and \( B = \mu \). To make things clearer the space in the upper part of the diagram are labeled \( CU \) and \( SU \) with \( U \) for upper while the spaces in the lower row are labeled \( SD \) and \( CD \) with \( D \) for down. Maxwell’s equations can be represented using \( \vec{E} \in H_{CU}, \vec{H} \in H_{CD}, \vec{B} \in H_{SU} \) and \( \vec{D} \in H_{SD} \). The physical units for Maxwell equations are given in Table 6.1.

Diagram chasing with \( \vec{E} \in H_{CU} \) and \( \vec{H} \in H_{CD} \) gives the Maxwell equations

\[
\frac{d\vec{H}}{dt} = -\mu^{-1}\vec{\nabla} \times \vec{E}, \quad \frac{d\vec{E}}{dt} = \epsilon^{-1}\vec{\nabla} \times \vec{H}.
\]

It is also common to write the Maxwell Equations as

\[
\frac{d\vec{B}}{dt} + \vec{\nabla} \times \vec{E} = 0; \quad \frac{d\vec{D}}{dt} - \vec{\nabla} \times \vec{H} = \vec{J}.
\]  

(6.10)

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. Again the meaning of variables and their distance units are given in Table 6.1. Set \( \vec{J} = 0 \) and then eliminate \( \vec{B} \) and \( \vec{D} \) from the equation to get (6.10). This system can be written as either of two second order
equations:

\[
\frac{d^2 \vec{E}}{dt^2} = -\epsilon^{-1} \nabla \times \mu^{-1} \nabla \times \vec{E}, \quad \frac{d^2 \vec{H}}{dt^2} = -\mu^{-1} \nabla \times \epsilon^{-1} \nabla \times \vec{H}.
\]

(6.11)

The energy \( C \) can be written

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

The vector identity

\[
\nabla \cdot (\vec{E} \times \vec{H}) = (\nabla \times \vec{E}) \cdot \vec{H} - \vec{E} \cdot (\nabla \times \vec{H})
\]

can be used to see that the energy is constant.

The time derivative of \( C \) is

\[
\frac{dC}{dt} = \int_{\mathbb{R}^3} \left( \epsilon \; \frac{d\vec{E}}{dt} \cdot \vec{E} + \mu \; \frac{d\vec{H}}{dt} \cdot \vec{H} \right) dx \, dy \, dz,
\]

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

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

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

\[
= \int_{\mathbb{R}^3} \nabla \cdot \vec{S} dx \, dy \, dz,
\]

\[
= 0.
\]

The last integral is zero because it was assumed that \( \vec{E} \) and \( \vec{H} \) are zero far from the origin. Also \( \vec{S} = \vec{E} \times \vec{H} \) is called the Poynting vector which has spatial units \( 1/d^2 \). The integrand is the standard energy density confirming \( C \) is spatially dimensionless.

For the elastic wave equation for constant material properties note that there are only two second order differential operators that map vectors to vectors which are the gradient \( \nabla \times \nabla \times \) and \( \nabla \nabla \cdot \). So it is no surprise that the elastic wave equation [30] is a linear combination of these operators,

\[
\rho \frac{d^2 \vec{v}}{dt^2} = (\lambda + 2 \mu) \nabla \nabla \cdot \vec{v} - \mu \nabla \times \nabla \times \vec{v},
\]

(6.12)

where \( \mu \) and \( \lambda \) are constant scalars with spatial dimension \( 1/d \). Note that \( \mu = 0 \) produces

\[
\frac{d^2 \vec{v}}{dt^2} = \frac{\lambda}{\rho} \nabla \nabla \cdot \vec{v},
\]

(6.13)

which is a vector wave equation.

If

\[
a = \sqrt{\frac{(\lambda + 2 \mu)}{\rho}}, \quad b = \sqrt{\frac{\mu}{\rho}}
\]

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then, like for $c$ in the scalar wave equation, $a$ and $b$ have units $d$, so the elastic wave equation (6.12) can be written in dimensionless form as

$$\frac{d^2 \vec{v}}{dt^2} = a^2 \vec{\nabla} \cdot \vec{v} - b^2 \vec{\nabla} \times \vec{\nabla} \times \vec{v}.$$  (6.14)

This equation can be converted to a system of three dimensionless first order equations:

$$\frac{d \vec{g}}{dt} = a \vec{\nabla} \cdot \vec{v} ;$$
$$\frac{d \vec{u}}{dt} = b \vec{\nabla} \times \vec{v} ;$$
$$\frac{d \vec{v}}{dt} = a \vec{\nabla} g - b \vec{\nabla} \times \vec{u} .$$

The quantity

$$C = \frac{||\vec{v}||^2 + ||\vec{u}||^2 + ||g||^2}{2} ,$$

is conserved because

$$\frac{dC}{dt} = \langle \frac{d \vec{v}}{dt}, \vec{v} \rangle + \langle \frac{d \vec{u}}{dt}, \vec{u} \rangle + \langle \frac{d \vec{g}}{dt}, \vec{g} \rangle$$
$$= \langle a \vec{\nabla} g - b \vec{\nabla} \times \vec{u}, \vec{v} \rangle + \langle b \vec{\nabla} \times \vec{v}, \vec{u} \rangle + \langle a \vec{\nabla} \cdot \vec{v}, \vec{g} \rangle$$
$$= a \langle \vec{\nabla} g, \vec{v} \rangle - b \langle \vec{\nabla} \times \vec{u}, \vec{v} \rangle + b \langle \vec{\nabla} \times \vec{v}, \vec{u} \rangle + a \langle \vec{\nabla} \cdot \vec{v}, \vec{g} \rangle$$
$$= a \langle \vec{g}, \vec{\nabla} \cdot \vec{v} \rangle - b \langle \vec{\nabla} \times \vec{u}, \vec{v} \rangle + b \langle \vec{\nabla} \times \vec{v}, \vec{u} \rangle + a \langle \vec{\nabla} \cdot \vec{v}, \vec{g} \rangle$$
$$= 0$$

Table 6.2: 3D Quantities and their spatial units.
The general elastic wave equations does not fit into the diagram chasing. This discussion is based on [15] and a summary of the notation is given in Table 6.2. When there are no external forces the general elastic wave equation in a material with spatially variable properties is given by Newton’s law applied to the displacements of the material:

$$\rho \frac{d^2 u_i}{dt^2} = \sum_{j=1}^{3} \frac{d\sigma_{i,j}}{dx_j}, \quad 1 \leq i \leq 3 \quad (6.15)$$

where $t$ is time, $\vec{u} = \vec{u}(\vec{x}, t)$, are the displacements of the material, $\rho = \rho(\vec{x})$ is the density of the material, and $\sigma = \sigma(\vec{x})$ is the symmetric stress tensor:

$$\sigma_{i,j} = \sum_{k,l=1}^{3} C_{k,l,i,j} e_{k,l}.$$  

The strains are

$$e_{i,j} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$$

which are dimensionless. The material properties other than density are given by the $C_{k,l,i,j}$ where $C = C(\vec{x})$ and where $C$ has the symmetries $C_{k,l,i,j} = C_{l,k,i,j} = C_{k,l,j,i}$. Consequently $C$ has only 21 independent entries [15]. However the most general second order wave equations generated by diagram chasing 5.2 have only 13 independent entries. Even if the matrices in 5.2 are not assumed symmetric there are only 19 parameters.
7 Mimetic 3D Discretizations

This discussion and notation will follow that in [46]. 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 the focus will be on applying mimetic methods to physical problems by adding a time variable and its discretization, adding inhomogeneous and anisotropic material properties and focus on how to use physical spatial and time units to correctly discretize physical problems. Historically, this type of discretization appeared in the Yee grid for Maxwell’s equations [62] which will be discussed in Section 8.3. This section finishes by describing simulation programs used to test the results presented here.

A possible difficulty is that to derive conserved quantities the discrete versions of $a$ and $a^{-1}$, $b$ and $b^{-1}$, $A$ and $A^{-1}$ and $B$ and $B^{-1}$ must be exact inverses of each other, see 6.2. This is trivial for $a$ and $b$ and also for diagonal $A$ and $B$. The non-diagonal case is important and has not yet been resolved.
Table 7.1: Notation for the indices of the nodes and the center points of the edges, faces and cells in the primal and dual grids where $-\infty < i, j, k < \infty$.

| primal      | dual          |
|-------------|---------------|
| nodes       | $(i \Delta x, j \Delta y, k \Delta z)$ | cells |
| edges       | $(i \Delta x, j \Delta y, k \Delta z)$ | faces |
|             | $(i + \frac{1}{2}) \Delta x, j \Delta y, (k + \frac{1}{2}) \Delta z)$ |
| faces       | $(i \Delta x, (j + \frac{1}{2}) \Delta y, k \Delta z)$ | edges |
|             | $(i + \frac{1}{2}) \Delta x, j \Delta y, (k + \frac{1}{2}) \Delta z)$ |
|             | $(i + \frac{1}{2}) \Delta x, (j + \frac{1}{2}) \Delta y, k \Delta z)$ |
| cells       | $(i + \frac{1}{2}) \Delta x, (j + \frac{1}{2}) \Delta y, (k + \frac{1}{2}) \Delta z)$ | nodes |
| primal      | dual          |

Table 7.2: Notation for the primal and dual, scalar and vector fields where $-\infty < i, j, k < \infty$.

| units | primal      | dual          | units |
|-------|-------------|---------------|
| 1     | $s_{i,j,k}$ | $d^*_{i,j,k}$ | $1/d^3$ |
| $1/d$ | $tx_{i+\frac{1}{2},j,k}$ | $nx^*_{i+\frac{1}{2},j,k}$ | $1/d^2$ |
|       | $ty_{i,j+\frac{1}{2},k}$ | $ny^*_{i,j+\frac{1}{2},k}$ |
|       | $tz_{i,j,k+\frac{1}{2}}$ | $nz^*_{i,j,k+\frac{1}{2}}$ |
| $1/d^2$ | $nx^*_{i,j+\frac{1}{2},k+\frac{1}{2}}$ | $tx^*_{i,j+\frac{1}{2},k+\frac{1}{2}}$ | $1/d$ |
|       | $nz^*_{i,j+\frac{1}{2},k+\frac{1}{2}}$ | $ty^*_{i,j,k+\frac{1}{2}}$ |
|       | $nz^*_{i,j,k+\frac{1}{2}}$ | $tz^*_{i,j,k+\frac{1}{2}}$ |
| $1/d^3$ | $d_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}$ | $s^*_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}$ | $1$ |
| units | primal      | dual          | units |

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Mimetic discretizations use primal and dual spatial grids as shown in Figure 7.1 and the notation for the nodes, edges, faces and cells of the grid are given in Table 7.1 while the notation for scalar and vector fields are given in Table 7.2. It is important that the components of vector fields are not located at the same points in the grid. All scalar and vector fields are defined on all of space are assumed to converge to zero far from the origin. To start all of the grids and all of the scalar and vector functions will all of three dimensional space.

There two types of scalar fields and also two type of vector fields on both the primal and dual grids. On the primal grid there are scalar fields \( s \) that do not have a spatial dimension, vector fields \( \vec{t} \) (for tangent) that have spatial dimension \( 1/d \), vector fields \( \vec{n} \) (for normal) that have units \( 1/d^2 \), and scalar fields with spatial dimension \( 1/d^3 \) (as in densities) while the dual grid has the same types of fields labeled with a superscript star as in \( s^\star \). Note that at each point in the grid there is a value from both the primal and dual fields. The spatial dimensions of these fields are different so they are really different fields.

7.2 The Discrete Double Exact Sequences

This section describes the discrete double exact sequences shown in Figure 7.2. This begins with a description of the discrete difference operators gradient, curl and divergence on the primal and dual grids. Next the star or multiplication operators that describe material properties are discretized.

7.2.1 Difference Operators

The discrete gradient \( \mathcal{G} \), curl or rotation \( \mathcal{R} \) and divergence \( \mathcal{D} \) are difference operators on discrete 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 \( k \rightarrow k + 1/2 \) in the formulas for the primal grid.

**The Gradient:** If \( s \in S_N \) is a discrete scalar field, then its gradient \( \mathcal{G}s = (\mathcal{G}sx, \mathcal{G}sy, \mathcal{G}sz) \in \mathbb{R}^3 \).
\( V_\varepsilon \) is an edge vector field:

\[
\begin{align*}
G_{sx_{i,j,k}} & \equiv \frac{s_{i+1,j,k} - s_{i,j,k}}{\Delta x}; \\
G_{sy_{i,j,k}} & \equiv \frac{s_{i,j+1,k} - s_{i,j,k}}{\Delta y}; \quad (7.1) \\
G_{sz_{i,j,k}} & \equiv \frac{s_{i,j,k+1} - s_{i,j,k}}{\Delta z}.
\end{align*}
\]

**The Curl:** If \( \vec{t} = (tx, ty, tz) \in V_\varepsilon \) is a discrete edge vector field, then its curl \( R\vec{t} \in \mathcal{V}_\varepsilon \) is a discrete face vector field:

\[
\begin{align*}
R_{tx_{i,j,k}} & \equiv \frac{tz_{i,j,k+1} - tz_{i,j,k}}{\Delta y} - \frac{ty_{i,j,k+1} - ty_{i,j,k}}{\Delta z}; \\
R_{ty_{i,j,k}} & \equiv \frac{tx_{i,j,k+1} - tx_{i,j,k}}{\Delta z} - \frac{ty_{i,j,k+1} - ty_{i,j,k}}{\Delta x}; \quad (7.2) \\
R_{tz_{i,j,k}} & \equiv \frac{ty_{i,j,k+1} - ty_{i,j,k}}{\Delta x} - \frac{tx_{i,j,k+1} - tx_{i,j,k}}{\Delta y}.
\end{align*}
\]

**The Divergence:** If \( \vec{n} = (nx, ny, nz) \in \mathcal{V}_\varepsilon \) is a discrete face vector field, then its divergence \( D\vec{n} \in \mathcal{S}_C \) is a cell scalar field:

\[
\begin{align*}
D\vec{n}_{i,j,k} & \equiv \frac{nx_{i,j,k+1} - nx_{i,j,k}}{\Delta x} + \frac{ny_{i,j,k+1} - ny_{i,j,k}}{\Delta y} + \frac{nz_{i,j,k+1} - nz_{i,j,k}}{\Delta z}; \quad (7.3)
\end{align*}
\]

**The Star Gradient:** If \( s^* \in \mathcal{S}_{N^*} \) is a discrete star scalar field then its star gradient \( G^* s^* \in V_{\varepsilon^*} \) is a star edge vector field:

\[
\begin{align*}
G^* s^*_{x_{i,j,k}} & \equiv \frac{s^*_{i+1,j,k} - s^*_{i-1,j,k}}{\Delta x}; \\
G^* s^*_{y_{i,j,k}} & \equiv \frac{s^*_{i,j+1,k} - s^*_{i,j-1,k}}{\Delta y}; \quad (7.4) \\
G^* s^*_{z_{i,j,k}} & \equiv \frac{s^*_{i,j+1,k} - s^*_{i,j-1,k}}{\Delta z}.
\end{align*}
\]

**The Star Curl:** If \( \vec{t}^* = (tx^*, ty^*, tz^*) \in \mathcal{S}_{C^*} \) is a discrete star edge vector field then its curl
\( R^* i^* \in V_F \) is a discrete star face vector field:

\[
R^* t^* x_{i+\frac{1}{2},j,k} \equiv \frac{t^*_{i+\frac{1}{2},j+\frac{1}{2},k} - t^*_{i+\frac{1}{2},j-\frac{1}{2},k}}{\Delta y} - \frac{t^*_{i+\frac{1}{2},j,k+\frac{1}{2}} - t^*_{i+\frac{1}{2},j,k-\frac{1}{2}}}{\Delta z} ;
\]

\[
R^* t^* y_{i,j+\frac{1}{2},k} \equiv \frac{t^*_{i+\frac{1}{2},j,k+\frac{1}{2}} - t^*_{i+\frac{1}{2},j,k-\frac{1}{2}}}{\Delta z} - \frac{t^*_{i+\frac{1}{2},j+\frac{1}{2},k} - t^*_{i+\frac{1}{2},j-\frac{1}{2},k}}{\Delta x} ;
\]

\[
R^* t^* z_{i,j,k+\frac{1}{2}} \equiv \frac{t^*_{i+\frac{1}{2},j,k+\frac{1}{2}} - t^*_{i+\frac{1}{2},j,k-\frac{1}{2}}}{\Delta y} + \frac{t^*_{i,j,k+\frac{1}{2}} - t^*_{i,j,k-\frac{1}{2}}}{\Delta y} .
\]

The Star Divergence: If \( \vec{n}^* = (nx^*, ny^*, nz^*) \in V_F \) 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

\[
D^* \vec{n}^*_{i,j,k} \equiv \frac{nx^*_{i+\frac{1}{2},j,k} - nx^*_{i-\frac{1}{2},j,k}}{\Delta x} + \frac{ny^*_{i,j+\frac{1}{2},k} - ny^*_{i,j-\frac{1}{2},k}}{\Delta y} + \frac{nz^*_{i,j,k+\frac{1}{2}} - nz^*_{i,j,k-\frac{1}{2}}}{\Delta z} .
\]

The second order accuracy of the difference operators is confirmed in TestAccuracy3.m.

### 7.2.2 Mimetic Properties of Difference Operators

If \( c \) is a constant scalar field then a direct computation [46] shows that:

\[
G c \equiv 0 , \quad R G \equiv 0 , \quad D R \equiv 0 , \quad G^* c \equiv 0 , \quad R^* G^* \equiv 0 , \quad D^* R^* \equiv 0 .
\]

The code TestMimetic.m shows that these relationships are satisfied up to a small multiple of \( \varepsilon \). These properties are summarized by saying that the discretization is exact or that the sequences in Figure 7.2 are exact, see [46] for a proof that the diagram is exact.

### 7.2.3 Discrete Star or Multiplication Operators

The star operators are multiplication operators that model the material properties and are given by two positive scalar functions \( a = a(x, y, z) \) and \( b = b(x, y, z) \) and two \( 3 \times 3 \) matrix functions \( A = A(x, y, z) \) and \( B = B(x, y, z) \) that are symmetric and positive definite. The spatial dimensions of \( a \) and \( b \) must be \( 1/d^3 \) while for \( A \) and \( B \) must be \( 1/d \).

If \( s \in S_N \) and \( d^* = a s \in S_C^* \) and

\[
a_{i,j,k} = a(i \Delta x, j \Delta y, k \Delta z)
\]

then

\[
d^*_{i,j,k} = a_{i,j,k} s_{i,j,k} .
\]
If $s^* \in S_{N^*}$ and $d = b s^* \in S_C$, and
\[
 b_{i,j,k} = b(i \Delta x, j \Delta y, k \Delta z)
\]
then
\[
d_{i + \frac{1}{2}, j + \frac{1}{2}, k + \frac{1}{2}} = b_{i + \frac{1}{2}, j + \frac{1}{2}, k + \frac{1}{2}} \in S_{i + \frac{1}{2}, j + \frac{1}{2}, k + \frac{1}{2}}.
\]
The assumption that $a$ and $b$ are not zero implies that these star operators are invertible.

The discretization of $A$, $B$, $A^{-1}$ and $B^{-1}$ is more complicated except for when these matrices are diagonal. For example let
\[
 A = \begin{bmatrix}
 A_{xx} & A_{xy} & A_{xz} \\
 A_{yx} & A_{yy} & A_{yz} \\
 A_{zx} & A_{zy} & A_{zz}
 \end{bmatrix},
\]
where $A$ is symmetric, positive definite, and the entries in $A$ are functions of $(x, y, z)$. For $\tilde{t} \in V_c$, $\tilde{\eta}^* = A \tilde{t} \in S_{N^*}$ is given by
\[
\begin{align*}
 nx^*_{i + \frac{1}{2}, j, k} &= A_{xx} x_{i + \frac{1}{2}, j, k} + A_{xy} y_{i + \frac{1}{2}, j, k} + A_{xz} z_{i + \frac{1}{2}, j, k} + A_{yx} x_{i + \frac{1}{2}, j, k} + A_{yy} y_{i + \frac{1}{2}, j, k} + A_{yz} z_{i + \frac{1}{2}, j, k} + A_{zx} x_{i + \frac{1}{2}, j, k} + A_{zy} y_{i + \frac{1}{2}, j, k} + A_{zz} z_{i + \frac{1}{2}, j, k}, \\
 ny^*_{i, j + \frac{1}{2}, k} &= A_{yx} y_{i, j + \frac{1}{2}, k} + A_{yy} y_{i, j + \frac{1}{2}, k} + A_{yz} y_{i, j + \frac{1}{2}, k} + A_{zx} x_{i, j + \frac{1}{2}, k} + A_{zy} y_{i, j + \frac{1}{2}, k} + A_{zz} z_{i, j + \frac{1}{2}, k} + A_{zx} x_{i, j + \frac{1}{2}, k} + A_{zy} y_{i, j + \frac{1}{2}, k} + A_{zz} z_{i, j + \frac{1}{2}, k}, \\
 nz^*_{i, j, k + \frac{1}{2}} &= A_{zx} z_{i, j, k + \frac{1}{2}} + A_{zy} z_{i, j, k + \frac{1}{2}} + A_{zz} z_{i, j, k + \frac{1}{2}}.
\end{align*}
\]
To maintain second order accuracy the values with an over bar are given by average values:
\[
\begin{align*}
 \overline{t x}_{i, j, k} &= \frac{tx_{i-\frac{1}{2}, j, k} + tx_{i+\frac{1}{2}, j, k} + tx_{i-\frac{1}{2}, j+1, k} + tx_{i+\frac{1}{2}, j+1, k}}{4}; \\
 \overline{t y}_{i, j, k} &= \frac{ty_{i-\frac{1}{2}, j+\frac{1}{2}, k} + ty_{i+\frac{1}{2}, j+\frac{1}{2}, k} + ty_{i-\frac{1}{2}, j+1, k} + ty_{i+\frac{1}{2}, j+1, k}}{4}; \\
 \overline{t z}_{i, j, k} &= \frac{tz_{i-\frac{1}{2}, j, k} + tz_{i+\frac{1}{2}, j, k} + tz_{i-\frac{1}{2}, j+1, k} + tz_{i+\frac{1}{2}, j+1, k}}{4};
\end{align*}
\]
There are similar formulas for multiplication by $B$, $A^{-1}$ and $B^{-1}$.

### 7.3 Discrete Inner Products
To study conserved quantities an inner product is needed for each of the eight linear spaces in the dual exact sequences Figure (7.2). The inner products will be defined in terms of four
symmetric bilinear forms as in 5.3. As in the continuum, an important property of the inner products is that they need to be symmetric, positive definite and importantly dimensionless.

Set \( \Delta V = \Delta x \Delta y \Delta z \). If \( s \in S_{N^*} \) and \( d^* \in S_{C^*} \) then

\[
\langle \langle s, d \rangle \rangle = \sum s_{i,j,k} d_{i,j,k}^* \Delta V .
\]

If \( \vec{t} \in V_{E} \) and \( \vec{n}^* \in V_{F^*} \) then

\[
\langle \langle \vec{t}, \vec{n}^* \rangle \rangle = \left( \sum tx_{i+\frac{1}{2},j,k} nx_{i,\frac{j+\frac{1}{2},k}+1} + \sum ty_{i,j+\frac{1}{2},k} ny_{i,j,\frac{k+\frac{1}{2}}{2}} + \sum tz_{i,j,k+\frac{1}{2}} n^*_{i,j,k+\frac{1}{2}} \right) \Delta V .
\]

If \( \vec{n} \in V_{E} \) and \( \vec{t} \in V_{F} \) then

\[
\langle \langle \vec{n}, \vec{t} \rangle \rangle = \left( \sum nx_{i,j+\frac{1}{2},k+\frac{1}{2}} tx_{i,j+\frac{1}{2},k+\frac{1}{2}} + \sum ny_{i+j,k+\frac{1}{2}} ty_{i,\frac{j+\frac{1}{2},k}+1} + \sum nz_{i,j,k+\frac{1}{2}} t^*_{i,j,k+\frac{1}{2}} \right) \Delta V .
\]

If \( g \in S_{C} \) and \( f^* \in S_{N^*} \) then

\[
\langle \langle g, f^* \rangle \rangle = \sum g_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} f^*_{i+\frac{1}{2},j+\frac{1}{2},k+1} \Delta V .
\]

The eight inner products are given by the bilinear forms.

If \( s1, s2 \in S_{N} \) then \( \langle s1, s2 \rangle_{N} = \langle \langle a s1, s2 \rangle \rangle \).

If \( t1, t2 \in V_{E} \) then \( \langle \langle t1, t2 \rangle \rangle_{E} = \langle \langle A t1, t2 \rangle \rangle \).

If \( n1, n2 \in V_{F} \) then \( \langle \langle n1, n2 \rangle \rangle_{F} = \langle \langle B^{-1} n1, n2 \rangle \rangle \).

If \( d1, d2 \in S_{C} \) then \( \langle d1, d2 \rangle_{C} = \langle \langle b^{-1} d1, d2 \rangle \rangle \).

If \( s1^*, s2^* \in S_{N^*} \) then \( \langle s1^*, s2^* \rangle_{N^*} = \langle \langle b s1^*, s2^* \rangle \rangle \).

If \( t1^*, t2^* \in V_{E^*} \) then \( \langle \langle t1^*, t2^* \rangle \rangle_{E^*} = \langle \langle B t1^*, t2^* \rangle \rangle \).

If \( n1^*, n2^* \in V_{F^*} \) then \( \langle \langle n1^*, n2^* \rangle \rangle_{F^*} = \langle \langle A^{-1} n1^*, n2^* \rangle \rangle \).

If \( d1^*, d2^* \in S_{C^*} \) then \( \langle d1^*, d2^* \rangle_{C^*} = \langle \langle a^{-1} d1^*, d2^* \rangle \rangle \).

### 7.4 Adjoint Operators

The derivation of the adjoints of the discrete operators in the discrete exact sequences shown in Figure 7.2 are similar to the derivation for the continuum the adjoint operators defined in Section 5.5. Again note that the discrete operators are not mapping of a space into itself. Some of the adjoints can easily be guessed by diagram chasing using 7.2:

\[
\begin{align*}
G^* &= -a^{-1} D^* A \\
\mathcal{R}^* &= +A^{-1} \mathcal{R}^* B^{-1} \\
D^* &= -B G^* b^{-1} \\
A^* &= A^{-1} \\
a^* &= a^{-1}
\end{align*}
\]

\[
\begin{align*}
G^{**} &= -b^{-1} D B, \\
\mathcal{R}^{**} &= +B^{-1} \mathcal{R} A^{-1}, \\
D^{**} &= -A G a^{-1}, \\
B^* &= B^{-1}, \\
b^* &= b^{-1}.
\end{align*}
\] (7.10)
When working with systems of first order wave equation adjoints of products of operators will be needed. For example (5.4) gives
\[(A\mathcal{G})^* = \mathcal{G}^* A^* = -a^{-1} \mathcal{D}^* AA^{-1} = -a^{-1} \mathcal{D}^* .\]

Also
\[(a^{-1} \mathcal{D}^*)^* = -A\mathcal{G} a^{-1} a = -A\mathcal{G} .\]

Consequently
\[(a^{-1} \mathcal{D}^* A\mathcal{G})^* = (A\mathcal{G})^* (a^{-1} \mathcal{D}^*)^* = a^{-1} \mathcal{D}^* A\mathcal{G} ,\]

so this operator is self adjoint. In terms of inner products, if \(s \in S_N\) and \(\vec{n}^* \in V_{\mathcal{F}^*}\) then
\[\langle A\mathcal{G} s, \vec{n}^* \rangle_{\mathcal{F}^*} = -\langle s, a^{-1} \mathcal{D}^* \vec{n}^* \rangle_N .\]

In addition
\[\langle (a^{-1} \mathcal{D}^* A\mathcal{G}) f, f \rangle_N = -\langle A\mathcal{G} f, A\mathcal{G} f \rangle_{\mathcal{F}^*} \leq 0 ,\]

so this operator is negative.

### 7.5 Testing the Differential Operators

Test show that the differential operators gradient, curl and divergence are second order accurate and that the curl of the gradient and the divergence of the curl are zero up to a small multiple of machine epsilon. The exactness is tested using TestZero3.m and the accuracy is tested using TestAccuracy3.m which depends on ConvergenceRate.m. The grids are generated using Grids3.m and the differential operators are given by Grad3.m, Curl3.m and Div3.m. The scalar and vector fields used for the tests are given by FieldScalarPrimal3.m, FieldTangentPrimal3.m, FieldGradientPrimal3.m, FieldNormalPrimal3.m, FieldCurlPrimal3.m, FieldDensityPrimal3.m, FieldDivergenceDual3.m.

Note that there are no star differential operators listed. This is because only uniform grids are used so the code for the star operators is the same as for the non-star operators.
8 Discretizing Wave Equations in 3D

The results in Section 7 will be used to discretize the three dimensional scalar wave equation and Maxwell’s wave equation in three dimensions.

A technical detail in the simulation code is given the spatial discretization how can one choose a reasonable time step. The estimates in [32] were helpful.

8.1 The Scalar Wave Equation

The second order scalar wave equation (6.3) can be written as as first order system as in (6.7). But here the notation will be changed to match that in Section 7:

\[
\frac{\partial s}{\partial t} = a^{-1} \vec{\nabla} \cdot \vec{v}, \quad \frac{\partial \vec{v}}{\partial t} = A \vec{\nabla} s,
\]

with \( s \in H_P \) and \( \vec{v} \in H_S \). This system will be discretized using the operators described in Section 7 so now let \( s \in S_N \) and \( \vec{v} \in V_F \) and then the leapfrog discretization is

\[
\frac{s^{n+1} - s^n}{\Delta t} = a^{-1} \mathcal{D}^* v^{n+\frac{1}{2}}, \quad \frac{v^{n+\frac{1}{2}} - v^{n-\frac{1}{2}}}{\Delta t} = A \mathcal{G} s^n.
\] (8.1)

If \( s^0 \) and \( v^{\frac{1}{2}} \) are given then the leapfrog scheme for \( n \geq 0 \) is

\[
s^{n+1} = s^n + \Delta t a^{-1} \mathcal{D}^* v^{n+\frac{1}{2}}, \quad v^{n+\frac{3}{2}} = v^{n+\frac{1}{2}} + \Delta t A \mathcal{G} s^{n+1}.
\]

If \( s^0 \) and \( v^0 \) are given then a second order accurate value for \( v^{\frac{1}{2}} \) is given by the Taylor series

\[
v^{\frac{1}{2}} = v(\Delta t/2)
\]

\[
= v(0) + v'(0) \frac{\Delta t}{2} + \frac{v''(0)}{2} \left( \frac{\Delta t}{2} \right)^2
\]

\[
= v(0) + A \vec{\nabla} s(0) \frac{\Delta t}{2} + \frac{A \vec{\nabla} s'(0)}{2} \left( \frac{\Delta t}{2} \right)^2
\]

\[
= v(0) + A \vec{\nabla} s(0) \frac{\Delta t}{2} + \frac{1}{2} A \vec{\nabla} a^{-1} \vec{\nabla} \cdot \vec{v}(0) \left( \frac{\Delta t}{2} \right)^2
\] (8.2)

The discretization of the first order system gives a discretization of the second order scalar wave equation (6.3) as

\[
\frac{s^{n+1} - 2 s^n + s^{n-1}}{\Delta t^2} = a^{-1} \mathcal{D}^* A \mathcal{G} s^n,
\] (8.3)

and as discussed in Section 6 on continuum wave equations. This is also a discretization of the vector wave equation

\[
\frac{v^{n+\frac{3}{2}} - 2 v^{n+\frac{1}{2}} + v^{n-\frac{1}{2}}}{\Delta t^2} = A \mathcal{G} a^{-1} \mathcal{D}^* v^{n+\frac{1}{2}}.
\] (8.4)
The results in Section 3 give two conserved quantities for the discretization. To see this using (3.8) and (3.6) set $A$ to $a^{-1} D^*$, $A^x$ to $-A G$, $g^{n + \frac{1}{2}}$ to $v^{n + \frac{1}{2}}$ and $f^n$ to $s^n$ to get the conserved quantities

$$C^n = ||s^n||_N^2 + \left\| \frac{v^{n + 1/2} + v^{n - 1/2}}{2} \right\|^2_{\mathcal{F}^*} - \frac{\Delta t^2}{4} ||A G s^n||_{\mathcal{F}^*}^2, \quad (8.5)$$

$$C^{n + 1/2} = ||v^{n + 1/2}||_{\mathcal{F}^*}^2 + \left\| \frac{s^{n + 1} + s^n}{2} \right\|^2_N - \frac{\Delta t^2}{4} ||a^{-1} D^* v^{n + 1/2}||_N^2. \quad (8.6)$$

These formulas agree with those derived in detail in Appendix B.

8.2 Testing the Wave Equation Codes

The test were done in stages, first for trivial material properties with Wave3DTMP.m. For this code the energies $C_n$ and $C_{n + 1/2}$ are constant to a small multiple of $\text{e}ps$ and the solutions are again forth order accurate for the example tested.

Currently working on Wave3DGMP.m to model more complex material properties. Can do constant $a$ and constant diagonal $A$.

8.3 Maxwell’s Equations

This is to be redone. xxx

Assume that $\vec{E} \in V_\varepsilon$ and $\vec{H} \in V_{\varepsilon^*}$, so that, using the notation in the previous sections, the Maxwell system 6.10 will be discretized as

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

where in Exact Sequence diagram (7.2) $A = \epsilon$ and $B = \mu$. Here $\epsilon$ and $\mu$ can be symmetric positive definite matrices. If $\vec{E} = (Ex, ER, Ez)$ and $\vec{H} = (Hx, Hy, Hz)$ then Table 7.1 shows that $Ex$ and $Hx$ are indexed as

$$Ex_{i + \frac{1}{2}, j, k}, \quad Hx_{i, j + \frac{1}{2}, k + \frac{1}{2}}$$

just as in Yee’s paper [62]. If $\vec{E}^0$ and $\vec{H}^\frac{1}{2}$ are given then the leapfrog scheme for $n \geq 0$ is

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

Using a similar argument, it is easy to see that

$$C_{n + 1/2} = \left\| \frac{\vec{E}^{n + 1} + \vec{E}^n}{2} \right\|^2_{\mathcal{E}} + \left\| \vec{H}^{n + 1/2} \right\|^2_{\mathcal{E}^*} - \frac{\Delta t^2}{4} \left\| \epsilon^{-1} \mathcal{R}^* \vec{H}^{n + 1/2} \right\|^2_{\mathcal{E}}.$$
is a conserved quantity and that
\[ C_{n+1/2} \geq \left\| \frac{\vec{E}^n + \vec{E}^{n+1}}{2} \right\|_\varepsilon^2 + \left( 1 - \frac{\Delta t^2}{4} \left\| \epsilon^{-1} \mathcal{R}^* \right\|_\varepsilon^2 \right) \left\| \frac{\vec{H}^{n+1/2}}{2} \right\|_\varepsilon^2. \]

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

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

is a conserved quantity and
\[ \left\| C_n \right\| \geq \left( 1 - \frac{\Delta t^2}{4} \left\| \mu^{-1} \mathcal{R} \right\|_\varepsilon^2 \right) \left\| \vec{E}^n \right\|_\varepsilon^2 + \left\| \frac{\vec{H}^{n+1/2} + \vec{H}^{n-1/2}}{2} \right\|_{\mathcal{F}^*}^2. \]

So \( \left\| C_n \right\| \) is positive for sufficiently small \( \Delta t \) if \( \left\| \mu^{-1} \mathcal{R} \vec{E}^n \right\|_\varepsilon \) is finite. Also, these formulas agree with those derived in detail in Appendix B.

The codes \texttt{Maxwell.m} and \texttt{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 Implementation in 2D

The goal is to illustrate how scalar and vector functions are discretized in 2D and then show how the gradient and divergence are discretized. This will provide some intuition on how to discretize functions and differential operators in 3D. For 3D the primal and dual grids are shown in Figure 7.1 and described in Table 7.1. In some ways the 2D discretization is more complicated than the 3D because in 3D cells have edges and faces while in 2D the edge of a cell can correspond to either an edge or a face in 3D.

The implementation of mimetic finite difference discretizations in a bounded region can be annoying due to the two staggered grids and indices that contain a half. Additionally, the components of vector fields are discretized at different points. There are also problems at the boundary that the star operators will be used fix. Initially the star operators will be trivial, except at the boundary. The simulation region will be the unit square.

For 3D a detailed description of the mimetic discretization is given in Section 7. In particular the left most box in Figure 7.2 will be used for the 2D discretization.

To facilitate programming, all indices are integers greater than zero, for example \( i \geq 1 \) and \( j \geq 1 \).

9.1 2D Exact solution

\[
\begin{align*}
    s &= \sqrt{m^2 + n^2} \\
    u(x, y, t) &= \cos(cs\pi t) \sin(m\pi x) \sin(n\pi y) \\
    v(x, y, t) &= \frac{1}{s} \sin(cs\pi t)(m \cos(m\pi x) \sin(n\pi y), n \sin(m\pi x), \cos(n\pi y))
\end{align*}
\]

9.2 The 2D primal and dual grids

Let \( N_x, N_y \) be positive integers and then set \( dx = 1/N_x, dy = 1/N_y \). The primal grid nodes (cell corners) are given by

\[
(xp(i, j), yp(i, j)) = ((i - 1) dx, (j - 1) dy), \quad 1 \leq i \leq N_x + 1, 1 \leq j \leq N_y + 1,
\]

and the dual grid nodes are given by

\[
(xd(i, j), yd(i, j)) = ((i - 1/2) dx, (j - 1/2) dy), \quad 1 \leq i \leq N_x, 1 \leq j \leq N_y.
\]

Note that in the primal grid \( N_x \) is the number of cells in \( x \) direction and \( N_y \) is the number of cells in the \( y \) direction. For \( N_x = 4 \) and \( N_y = 5 \) the positions of scalar and vector function on the primal and dual grids are illustrated in Figures 9.1 and 9.2, see FigurePrimalDual2.m. Compare these to Figure 7.1 for a 3D grid.

Important points are that a primal grid cell center is given by a dual grid node and the dual grid centers are given by given by the interior primal grid nodes. Additionally the location of dual grid tangent vectors are the same as the location of the primal grid interior.
Figure 9.1: 2D primal grid tangent and normal vector fields, $N_x = 4, N_y = 5$

Figure 9.2: 2D dual grid tangent and normal vector fields, $N_x = 4, N_y = 5$
normal vectors and the position of the dual grid normal vectors are the same as the position of the interior grid tangent vectors. On the boundary of the primal grid the positions of points and vectors do not correspond to anything in the dual grid. As will be seen this is important for representing boundary conditions for partial differential equations.

9.3 Discretizing continuum functions on the 2D grids

Scalar functions will be discretized at either the nodes (corners) or cell centers of the primal and dual grids while vector fields will be discretized at the centers of the edges of the cells as illustrated in Figures 9.1 and 9.2 for grids in a region that is a unit square (see FigureDetailsPrimalDual2.m). There are a total of eight types of discretized functions. In the text, function names on the primal grid have a \( p \) appended as in \( f_p \) while functions on the dual grid have a \( d \) appended as in \( f_d \). In the figures which grid the functions are on is clear.

For the primal grid there are four cases. A scalar function \( f(x, y) \) with spatial weight 1 is discretized at primal cell nodes:

\[
f_p(i, j) = f(xp(i), yp(j)), \quad i \leq Nx + 1, \quad j \leq Ny + 1. \tag{9.1}
\]

A scalar function \( g(x, y) \) with spatial weights \( 1/d^3 \) is discretized at primal grid cell centers:

\[
g_p(i, j) = g(xd(i), yd(j)), \quad i \leq Nx, \quad j \leq Ny. \tag{9.2}
\]

A vector function \( (tx(x, y), ty(x, y)) \) with spatial weight \( 1/d \) (tangent on primal grid) is discretized at cell edge centers:

\[
txp(i, j) = tx(xd(i), yp(j)), \quad i \leq Nx, \quad j \leq Ny + 1; \tag{9.3}
\]

\[
typ(i, j) = ty(xp(i), yd(j)), \quad i \leq Nx + 1, \quad j \leq Ny. \tag{9.4}
\]

A vector function \( (nx(x, y), ny(x, y)) \) with spatial weight \( 1/d^2 \) (normal on primal grid) is also discretized at cell edge centers:

\[
nxp(i, j) = nx(xp(i), yd(j)), \quad i \leq Nx + 1, \quad j \leq Ny; \tag{9.5}
\]

\[
nyp(i, j) = ny(xd(i), yp(j)), \quad i \leq Nx, \quad j \leq Ny + 1. \tag{9.6}
\]

For the dual grid there are also four cases. A scalar function \( f(x, y) \) with spatial weight 1 is discretized at the dual cell nodes:

\[
fd(i, j) = f(xd(i), yd(j)), \quad i \leq Nx, \quad j \leq Ny. \tag{9.7}
\]

A scalar function \( g(x, y) \) with spatial weights \( 1/d^3 \) is discretized at dual grid cell centers:

\[
gd(i, j) = g(xp(i + 1), yp(j + 1)), \quad i \leq Nx - 1, \quad j \leq Ny - 1. \tag{9.8}
\]
Figure 9.3: Scalar and vector fields on the primal grid.
Figure 9.4: Scalar and vector fields on the dual grid,
A vector function \((tx(x,y), ty(x,y))\) with spatial weight \(1/d\) (tangent on dual grid) is discretized at cell edge centers:

\[
    t_{xd}(i,j) = tx(xp(i+1), yp(j)), \quad i \leq Nx - 1, \quad j \leq Ny; \quad (9.9)
\]

\[
    t_{yd}(i,j) = ty(xd(i), yp(j+1)), \quad i \leq Nx, \quad j \leq Ny. \quad (9.10)
\]

A vector function \((nx(x,y), ny(x,y))\) with spatial weight \(1/d^2\) (normal on the dual grid) is discretized at cell face centers:

\[
    n_{xd}(i,j) = nx(xd(i), yp(j+1)), \quad i \leq Nx, \quad j \leq Ny - 1; \quad (9.11)
\]

\[
    n_{yd}(i,j) = ny(xp(i+1), yp(j)), \quad i \leq Nx - 1, \quad j \leq Ny. \quad (9.12)
\]

Examples of 2D scalar and vector fields can be generated using ScalarField2p.m, ScalarField2d.m, TangentField2p.m, TangentField2d.m, NormalField2p.m, NormalField2d.m, DensityField2p.m, DensityField2d.m and tested using TestFields2pd.m

### 9.4 The Star Operators

For simplicity the discussion of star operators will begin for material properties that are constant. These star operators will map quantities defined on the primal grid to the dual grid while their inverses do the opposite. For constant and isotropic materials the star operators are multiplication by a constant for quantities that are defined at the same point in the grids. For scalar variables this is done by multiplication by a constant \(a > 0\) with spatial dimension \(1/d^3\). For vectors a constant diagonal matrix

\[
    A = \begin{bmatrix}
    A_{11} & 0 \\
    0 & A_{22}
    \end{bmatrix}
\]

with \(A_{11} > 0\) and \(A_{22} > 0\) spatial dimension \(1/d\) will be used. If \(A_{11} \neq A_{22}\) then there is a simple anisotropy. Away from the boundaries of the region, the two star operators are inverses of each other. For boundary value problems, the mismatch between the sizes of the primal and dual grids will be used to represent the boundary conditions. The star operators will be given in pairs that are essentially inverse of each other, first the mapping from the primal grid to the dual grid and then the inverse.

If \(gd = *fp\) then

\[
    gd(i,j) = a fp(i+1, j+1), \quad 1 \leq i \leq Nx - 1, \quad 1 \leq j \leq Ny - 1. \quad (9.13)
\]

If \(fp = *gd\) then

\[
    fp(i,j) = \frac{1}{a} gd(i-1, j-1), \quad 2 \leq i \leq Nx, \quad 2 \leq j \leq Ny. \quad (9.14)
\]

In this case \(fp\) is not defined on the boundary of the primal grid.
If \( fd = \star gp \) then
\[
\begin{align*}
    gp(i, j) &= afd(i, j), \quad 1 \leq i \leq N_x, \quad 1 \leq j \leq N_y.
\end{align*}
\]
(9.15)

If \( gp = \star fd \) then
\[
\begin{align*}
    gp(i, j) &= \frac{1}{a} fd(i, j), \quad 1 \leq i \leq N_x, \quad 1 \leq j \leq N_y.
\end{align*}
\]
(9.16)

If \((txd,tyd) = \star (nxp,nyp)\) then
\[
\begin{align*}
    txd(i, j) &= \frac{1}{A_{11}} nxp(i + 1, j), \quad 1 \leq i \leq N_x - 1, \quad 1 \leq j \leq N_y.
    \\
tyd(i, j) &= \frac{1}{A_{22}} nyp(i, j + 1), \quad 1 \leq i \leq N_x, \quad 1 \leq j \leq N_y - 1.
\end{align*}
\]
(9.17)

If \((nxp,nyp) = \star (txd,tyd)\) then
\[
\begin{align*}
    nxp(i, j) &= A_{11} txd(i - 1, j), \quad 2 \leq i \leq N_x, \quad 1 \leq j \leq N_y.
    \\
nyp(i, j) &= A_{22} tyd(i, j - 1), \quad 1 \leq i \leq N_x, \quad 2 \leq j \leq N_y.
\end{align*}
\]
(9.18)

If \((nxd,nyd) = \star (txp,typ)\) then
\[
\begin{align*}
    nxd(i, j) &= A_{11} txp(i, j + 1), \quad 1 \leq i \leq N_x, \quad 1 \leq j \leq N_y - 1.
    \\
    nyp(i, j) &= A_{22} typ(i + 1, j), \quad 1 \leq i \leq N_x - 1, \quad 1 \leq j \leq N_y.
\end{align*}
\]
(9.19)

If \((txp,typ) = \star (nxd,nyd)\) then
\[
\begin{align*}
    txp(i, j) &= \frac{1}{A_{11}} nxd(i, j - 1), \quad 1 \leq i \leq N_x, \quad 2 \leq j \leq N_y.
    \\
typ(i, j) &= \frac{1}{A_{22}} nyd(i - 1, j), \quad 2 \leq i \leq N_x, \quad 1 \leq j \leq N_y.
\end{align*}
\]
(9.20)

### 9.5 2D Differential Operators

The 2D discrete differential operators are the gradient and divergence which are given by \texttt{Grad2p.m} and \texttt{Grad2d.m} and \texttt{Div2p.m} and \texttt{Div2d.m}. All the differential operators use centered differences. The operators on the primal and dual grids differ in their indexing. The programs \texttt{TestGradDiv2p.m} and \texttt{TestGradDiv2d.m} show that the gradient and divergence operators are second order accurate on the primal and dual grids.

### 9.6 Scalar Wave Equation

The discretization of the 2D scalar wave equation is the same as the discretization of 3D scalar wave equation given in (8.1) and has been implemented in \texttt{Wave2D.m}. The wave equation is written as a first order system of differential equations that are discretized using
staggered space-time grids and \texttt{Grad2p} and \texttt{Div2d}. In general the approximate solutions of the discrete wave equation are second order accurate. For some cases the solutions are fourth order accurate and there is at least one example where the solution is exact (set \(m1 = n1 = 1\) and eliminate the \(m2, n2\) part of the test solution to see this). Both conservation laws are constant to at least 1 part in \(10^{15}\) when the star operator is trivial.

What star was used in \texttt{Wave2D.m}? See (9.19).

### 9.7 Boundary Conditions

The needs a rewrite.

Figures 9.3 and 9.4 illustrates the position of the scalar field \(f\) and the scalar function \(g\) which is the Laplacian of \(f\), that is the divergence of the gradient of \(f\). It also illustrates the positions of the boundary conditions which must specify \(g\) on the boundary:

\[
\begin{align*}
g_{1,j}, & \ 1 \leq j \leq Ny + 1 \\
g_{Nx+1,j}, & \ 1 \leq j \leq Ny + 1 \\
g_{i,1}, & \ 1 \leq i \leq Nx + 1 \\
g_{i,Ny+1}, & \ 1 \leq i \leq Nx + 1 .
\end{align*}
\]

Note that the values of \(g\) are defined twice at the corner points of the region: \((1, 1); (1, Ny+1); (Nx+1, 1)\) and \((Nx+1, Ny+1)\). In fact in standard discrete boundary value problems these values of \(g\) are not needed and can be assigned any value. On the other hand creating a data structure that doesn’t have these values creates a programming mess. The figures were generated using \texttt{Figure2DDiv.m}, \texttt{Figure2DGrad.m} and \texttt{Figure2DLap.m}.

The typical boundary condition is of mixed or Robin type, that is,

\[
\alpha \vec{n} \cdot \vec{v} + \beta f = \gamma ,
\]

which in the discrete setting becomes

\[
\begin{align*}
\text{at } y = 0 & \quad \alpha_{1,j} v_{y_{1,j}} + \beta_{1,j} g_{1,j} = \gamma_{1,j} ; \\
\text{at } y = 1 & \quad \alpha_{Nx+1,j} v_{y_{Nx+1,j}} + \beta_{Nx+1,j} g_{Nx+1,j} = \gamma_{Nx+1,j} ; \\
\text{at } x = 0 & \quad \alpha_{i,1} v_{y_{i,1}} + \beta_{i,1} g_{i,1} = \gamma_{i,1} ; \\
\text{at } x = 1 & \quad \alpha_{i,Ny+1} v_{y_{i,Ny+1}} + \beta_{i,Ny+1} g_{i,Ny+1} = \gamma_{i,Ny+1} .
\end{align*}
\]

These equations can be trivially solved for \(g_{1,1}, g_{i,Ny+1}, g_{1,j}, g_{Nx+1,j}\) which could give two different values of \(f\) for the corner points. In the typical explicit time stepping algorithms for wave equations, these values are never used.

Check this, probably not correct. For Dirichlet boundary conditions the program \texttt{Wave2D.m} confirms that the solution of the 2D wave equation is second order accurate while the program \texttt{Wave2DExact.m} illustrates some cases where the solutions are accurate up to some small multiple of \(\epsilon_{\text{ps}}\).
References

[1] Donu Arapura. Introduction to differential forms. https://www.math.purdue.edu/~dvb/preprints/diffforms.pdf. Accessed: 2017-01-06.

[2] Douglas Arnold, Richard Falk, and Ragnar Winther. Finite element exterior calculus: from hodge theory to numerical stability. Bulletin of the American mathematical society, 47(2):281–354, 2010.

[3] Pavel B. Bochev and James M. Hyman. Principles of mimetic discretizations of differential operators. In Douglas N. Arnold, Pavel B. Bochev, Richard B. Lehoucq, Roy A. Nicolaides, and Mikhail Shashkov, editors, Compatible Spatial Discretizations, pages 89–119, New York, NY, 2006. Springer New York.

[4] F. Brezzi, A. Buffa, and G. Manzini. Mimetic scalar products of discrete differential forms. Journal of Computational Physics, 257, Part B:1228 – 1259, 2014. Physics-compatible numerical methods.

[5] Franco Brezzi, Konstantin Lipnikov, and Valeria Simoncini. A family of mimetic finite difference methods on polygonal and polyhedral meshes. Mathematical Models and Methods in Applied Sciences, 15(10):1533–1551, 2005.

[6] Francesco Capuano. Development of high-fidelity numerical methods for turbulent flows simulation. PhD thesis, Universitá degli Studi di Napoli Federico II, Napoli, Italy, 2015.

[7] Wenbin Chen, Xingjie Li, and Dong Liang. Energy-conserved splitting ftdt methods for maxwell’s equations. Numerische Mathematik, 108(3):445–485, 2008.

[8] Andrew J. Christlieb, James A. Rossmanith, and Qi Tang. Finite difference weighted essentially non-oscillatory schemes with constrained transport for ideal magnetohydrodynamics, Mar. 2014. 1309.3344 [math.NA].

[9] Armando Coco and Giovanni Russo. Finite-difference ghost-point multigrid methods on cartesian grids for elliptic problems in arbitrary domains. Journal of Computational Physics, 241:464 – 501, 2013.

[10] F. Collino, T. Fouquet, and P. Joly. Conservative space-time mesh refinement methods for the {FD}{TD} solution of maxwell’s equations. Journal of Computational Physics, 211(1):9 – 35, 2006.

[11] E. R. Crain. Electromagnetic concepts - maxwell’s equations. https://www.spec2000.net/06-electromag.htm. Accessed: 2017-08-3.

[12] Lourenco Beirao da Veiga, Luciano Lopez, and Giuseppe Vacca. Mimetic finite difference methods for hamiltonian wave equations in 2d. Computers and Mathematics with Applications, 74:1123–1141, September 2017.
[13] Paul Dawkins. The wave equation - pauls online math notes, 2010. Department of Mathematics, Lamar University.

[14] Robert D. Engle, Robert D. Skeel, and Matthew Drees. Monitoring energy drift with shadow hamiltonians. *Journal of Computational Physics*, 206(2):432 – 452, 2005.

[15] John T Etgen. Finite-difference elastic anisotropic wave propagation. http://sepwww.stanford.edu/public/docs/sep56/56_03.pdf. Accessed: 2017-07-3.

[16] John T. Etgen and Michael J. O’Brien. Computational methods for large-scale 3d acoustic finite-difference modeling: A tutorial. *GEOPHYSICS*, 72(5):SM223–SM230, 2007.

[17] David C. Del Rey Fernández, Jason E. Hicken, and David W. Zingg. Review of summation-by-parts operators with simultaneous approximation terms for the numerical solution of partial differential equations. *Computers and Fluids*, 95(Supplement C):171 – 196, 2014.

[18] Jason Gans and David Shalloway. Shadow mass and the relationship between velocity and momentum in symplectic numerical integration. *Phys. Rev. E*, 61:4587–4592, Apr 2000.

[19] LiPing Gao and Bo Zhang. Optimal error estimates and modified energy conservation identities of the adi-fdtd scheme on staggered grids for 3d maxwell’s equations. *Science China Mathematics*, 56(8):1705–1726, 2013.

[20] Z. Gao and J. Wu. A second-order positivity-preserving finite volume scheme for diffusion equations on general meshes. *SIAM Journal on Scientific Computing*, 37(1):A420–A438, 2015.

[21] Marc Gerritsma, Artur Palha, Varun Jain, and Yi Zhang. Mimetic spectral element method for anisotropic diffusion, Feb. 2018. arXiv:1802.04597v1 [math.NA].

[22] Ernst Hairer. Numerical geometric integration. http://www.dmae.upct.es/~amat/simplecticos2.pdf. Accessed: 2016-08-28.

[23] Ernst Hairer, Christian Lubich, and Gerhard Wanner. *Geometric Numerical Integration*, Structure-Preserving Algorithms for Ordinary Differential Equations, Second Edition. Springer Series in Computational Mathematics, Springer-Verlag Berlin Heidelberg, 2005.

[24] J. Hyman, J. Morel, M. Shashkov, and S. Steinberg. Locally conservative numerical methods for flow in porous media. *Journal of Computational Geosciences*, 6:333–352, 2002.
[25] James Hyman, Mikhail Shashkov, and Stanly Steinberg. The numerical solution of diffusion problems in strongly heterogeneous non-isotropic materials. *Journal of Computational Physics*, 132(1):130 – 148, 1997.

[26] James M. Hyman, J. Morel, Mikhail J. Shashkov, and Stanly Steinberg. Mimetic finite difference methods for diffusion equations. *Comput. Geosci.*, 6(3):333–352, 2002. LA-UR-01-2434.

[27] James M. Hyman and Mikhail Shashkov. Adjoint operators for the natural discretizations of the divergence, gradient, and curl on logically rectangular grids. *APPL. NUMER. MATH*, 25:413–442, 1997.

[28] J.M. Hyman and M. Shashkov. Natural discretizations for the divergence, gradient, and curl on logically rectangular grids. *Computers & Mathematics with Applications*, 33(4):81 – 104, 1997.

[29] J.M. Hyman and M. Shashkov. Mimetic finite difference methods for maxwell’s equations and the equations of magnetic diffusion. *PIER*, 32:89–121, 2001.

[30] Heiner Igel. The elastic wave equation. https://www.geophysik.uni-muenchen.de/~igel/Lectures/Sedi/sedi_weq.pdf. Accessed: 2017-07-4.

[31] Barry Koren, Rémi Abgrall, Pavel Bochev, Jason Frank, and Blair Perot. Physics-compatible numerical methods. *Journal of Computational Physics*, 257, Part B:1039 –, 2014. Physics-compatible numerical methods.

[32] Larry R. Lines, Raphael Slawinski, and R. Phillip Bording. A recipe for stability of finite-difference wave-equation computations. *Geophysics*, 64(3):967–969, 1999.

[33] K. Lipnikov, L. Beirao da Veiga, and G. Manzini. *The Mimetic Finite Difference Method for Elliptic PDEs*. Springer, New York, 2014.

[34] Konstantin Lipnikov, Gianmarco Manzini, and Mikhail Shashkov. Mimetic finite difference method. *Journal of Computational Physics*, 257, Part B:1163 – 1227, 2014. Physics-compatible numerical methods.

[35] Mamdouh S. Mohamed, Anil N. Hirani, and Ravi Samtaney. Discrete exterior calculus discretization of incompressible navier–stokes equations over surface simplicial meshes. *Journal of Computational Physics*, 312:175 – 191, 2016.

[36] Y. Morinishi, T.S. Lund, O.V. Vasilyev, and P. Moin. Fully conservative higher order finite difference schemes for incompressible flow. *Journal of Computational Physics*, 143(1):90 – 124, 1998.

[37] Jan Nordström and Tomas Lundquist. Summation-by-parts in time. *Journal of Computational Physics*, 251(Supplement C):487 – 499, 2013.
[38] J.F. Nye. *Physical Properties of Crystals: Their representation by tensors and matrices.* Oxford University Press, London, England, 1960.

[39] Peter J. Olver. Numerical analysis lecture notes. [Online; accessed 25-Oct-2016].

[40] Artur Palha and Marc Gerritsma. A mass, energy, enstrophy and vorticity conserving (meevc) mimetic spectral element discretization for the 2d incompressible navier-stokes equations, Apr. 2016. arXiv:1604.00257 [math.NA].

[41] Artur Palha, Pedro Pinto Rebelo, René Hiemstra, Jasper Kreeft, and Marc Gerritsma. Physics-compatible discretization techniques on single and dual grids, with application to the poisson equation of volume forms. *Journal of Computational Physics*, 257, Part B:1394 – 1422, 2014. Physics-compatible numerical methods.

[42] J. Blair Perot. Discrete conservation properties of unstructured mesh schemes. *Annual Review of Fluid Mechanics*, 43(1):299–318, 2011.

[43] J. Blair Perot and Christopher J. Zusi. Differential forms for scientists and engineers. *Journal of Computational Physics*, 257, Part B:1373 – 1393, 2014. Physics-compatible numerical methods.

[44] Roger Peyret and Thomas D. Taylor. *Computational Methods for Fluid Flow*. Springer-Verlag, New York, 1983.

[45] G.R.W. Quispel and D.I. McLaren. A new class of energy-preserving numerical integration methods. *Journal of Physics A: Mathematical and Theoretical*, 41(4):045206, 2008. Stan: methods probably implicit.

[46] Nicolas Robidoux and Stanly Steinberg. A discrete vector calculus in tensor grids. *CMAM*, 11:23–66, 2011.

[47] Rick Salmon. A general method for conserving energy and potential enstrophy in shallow-water models. *JAS*, 73(6):515–531, 2007.

[48] Eduardo Sanchez, Christopher Paolini, Peter Blomgren, Jose Castillo, Martin Berzins, and S. Jan Hesthaven. *Spectral and High Order Methods for Partial Differential Equations ICOSAHOM 2014: Selected papers from the ICOSAHOM conference, June 23-27, 2014, Salt Lake City, Utah, USA*, chapter Algorithms for Higher-Order Mimetic Operators, pages 425–434. Springer International Publishing, Cham, 2015. Kirby, M. Robert.

[49] B. Sanderse. Energy-conserving runge–kutta methods for the incompressible navier–stokes equations. *Journal of Computational Physics*, 233:100 – 131, 2013.

[50] R. Schuhmann and T. Weiland. Conservation of discrete energy and related laws in the finite integration technique. *PIER*, 32:301–316, 2001.

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[51] M. Shashkov. SIAM featured minisymposium: Physics-compatible numerical methods, 2015. [Online; accessed 27-May-2016].

[52] Ari Stern, Yiyeng Tong, Mathieu Desbrun, and Jerrold E. Marsden. Geometric computational electrodynamics with variational integrators and discrete differential forms. In Dong Eui Chang, Darryl D. Holm, George Patrick, and Tudor Ratiu, editors, *Geometry, mechanics, and dynamics*, volume 73 of *Fields Institute Communications*, pages 437–475. Springer, New York, 2015.

[53] Molei Tao. Explicit symplectic approximation of nonseparable hamiltonians: Algorithm and long time performance. *Phys. Rev. E*, 94:043303, Oct 2016.

[54] Mark A. Taylor and Aimé Fournier. A compatible and conservative spectral element method on unstructured grids. *Journal of Computational Physics*, 229(17):5879 – 5895, 2010.

[55] F. L. Teixeira. Random lattice gauge theories and differential forms, Aug. 2013. arXiv:1304.3485v2 [math-ph].

[56] Enzo Tonti. Why starting from differential equations for computational physics? *Journal of Computational Physics*, 257, Part B:1260 – 1290, 2014. Physics-compatible numerical methods.

[57] Bas [van ’t Hof] and Mathea J. Vuik. Symmetry-preserving finite-difference discretizations of arbitrary order on structured curvilinear staggered grids. *Journal of Computational Science*, 36:101008, 2019.

[58] Andy T.S. Wan, Alexander Bihlo, and Jean-Christophe Nave. The multiplier method to construct conservative finite difference schemes for ordinary and partial differential equations. *SIAM Journal on Numerical Analysis*, 54(1):86–119, 2016.

[59] Siyang Wang and Gunilla Kreiss. Convergence of summation-by-parts finite difference methods for the wave equation. *Journal of Scientific Computing*, 71(1):219–245, Apr 2017.

[60] Yushun Wang Wenjun Cai, Chaolong Jiang. Structure-preserving algorithms for the two-dimensional sine-gordon equation with neumann boundary conditions, Sep. 2018. arXiv:1809.02704v1 [math.NA].

[61] Wikipedia. Finite-difference time-domain method, 2016. [Online; accessed 22-May-2016].

[62] K. S. Yee. Numerical solution of initial boundary value problems involving Maxwell’s equations in isotropic media. *IEEE Transactions of Antennas and Propagation*, AP-14(3):302–307, 1966.
A Energy Preserving Discretizations of the Harmonic Oscillator

Here the well-known fact that the Crank-Nicholson discretization conserves the discrete analog of the energy for the harmonic oscillator is shown. It is also shown that the methods introduced in [58] 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 (2.7):

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

This gives a discretization of the second order differential equation:

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

Then

$$C_{n+1}^2 - C_n^2 = \frac{1}{2} (v_{n+1} + v_n) (v_{n+1} - v_n) + \frac{1}{2} (u_{n+1} + u_n) (u_{n+1} - u_n)$$

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

so $C_n$ is conserved. Write the system as

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

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

so 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

Following the discussion in [58] it is easy to show that the only reasonable discretization that conserves the simple conservation law (2.7) is equivalent to the Crank-Nicholson discretization. First compute using (2.7) that

$$C_{n+1}^2 - C_n^2 = (u_{n+1} - u_n) (u_n + u_{n+1}) + \left( v_{n+\frac{3}{2}} - v_{n-\frac{1}{2}} \right) \frac{v_{n-\frac{1}{2}} + 2v_{n+\frac{1}{2}} + v_{n+\frac{3}{2}}}{4}.$$  

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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 its conserved quantity to the Crank-Nicholson scheme along with its conserved quantity.
B Details for Discrete Conserved Quantities

B.1 Scalar Wave

As before a second order discrete equation and a second order average will be needed

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

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

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

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

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

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

To find a conserved quantity let

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

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

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

As before compute:

\[
C_{1n+1/2} - C_{1n-1/2} = \left\langle \frac{u^{n+1} + 2u^n + u^{n-1}}{4}, u^{n+1} - u^{n-1} \right\rangle_N
\]

\[
= \left\langle u^n + \frac{\Delta t^2 a^{-1} D^* A G u^n}{4}, u^{n+1} - u^{n-1} \right\rangle_N
\]

\[
= \left\langle u^n, u^{n+1} - u^{n-1} \right\rangle_N + \frac{\Delta t^2}{4} \left\langle a^{-1} D^* A G u^n, u^{n+1} - u^{n-1} \right\rangle_N;
\]

Using the adjoint equation \( v^\star \) gives

\[
C_{2n+1/2} - C_{1n-1/2} = \left\langle v^{n+1/2} + v^{n-1/2}, v^{n+1/2} + v^{n-1/2} \right\rangle_{F^*}
\]

\[
= \left\langle v^{n+1/2} + v^{n-1/2}, \Delta t A G u^n \right\rangle_{F^*}
\]

\[
= -\Delta t \left\langle a^{-1} D^* v^{n+1/2} + a^{-1} D^* v^{n-1/2}, u^n \right\rangle_N
\]

\[
= -\Delta t \left\langle u^{n+1} - u^{n-1}, \Delta t \right\rangle_{N}
\]

\[
= -\left\langle u^n, u^{n+1} - u^{n-1} \right\rangle_N;
\]
Also
\[ C_{n+1/2} - C_{n-1/2} = \Delta t^2 \left\langle a^{-1} D^* v^{n+1/2} - a^{-1} D^* v^{n-1/2}, a^{-1} D^* v^{n+1/2} + a^{-1} D^* v^{n-1/2} \right\rangle_N \]
\[ = \Delta t^2 \left\langle a^{-1} D^* (v^{n+1/2} - v^{n+1/2}), u^{n+1} - u^{n-1} \right\rangle_N / \Delta t \]
\[ = \Delta t^2 \left\langle -\Delta t a^{-1} D^* - A \mathcal{G} u^n, u^{n+1} - u^{n-1} \right\rangle_N \]
\[ = \Delta t^2 \left\langle a^{-1} D^* A \mathcal{G} u^n, u^{n+1} - u^{n-1} \right\rangle_N . \]

Consequently \( C = C_1 + C_2 - C_3/4 \) is a conserved quantity:
\[ C_{n+1/2} = \left\| \frac{u^{n+1} + u^n}{2} \right\|^2 + \left\| v^{n+1/2} \right\|^2 - \frac{\Delta t^2}{4} \left\| a^{-1} D^* v^{n+1/2} \right\|^2 . \]

This implies that
\[ C_{n+1/2} \geq \left\| \frac{u^{n+1} + u^n}{2} \right\|^2 + \left( 1 - \frac{\Delta t^2}{4} \left\| a^{-1} D^* \right\|^2 \right) \left\| v^{n+1/2} \right\|^2 . \]

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

Next look for an analog \( C_n \) of the scalar conserved quantity
\[ C_{1n} = \left\| \frac{v^{n+1/2} + v^{n-1/2}}{2} \right\|^2 ; \]
\[ C_{2n} = \left\| v^n \right\|^2_N ; \]
\[ C_{3n} = \Delta t^2 \left\| A \mathcal{G} u^n \right\|^2_x . \]

First compute
\[ C_{1n+1} - C_{1n} = \left\langle \frac{v^{n+3/2} + 2 v^{1/2} + v^{n-1/2}}{4} - v^{n+3/2} - v^{n-1/2}, v^{n+3/2} - v^{n-1/2} \right\rangle_x \]
\[ = \left\langle v^{n+1/2}, v^{n+3/2} - v^{n-1/2} \right\rangle_x + \frac{\Delta t^2}{4} \left\langle A \mathcal{G} a^{-1} D^* v^{n+1/2} - v^{n+3/2} - v^{n-1/2}, v^{n+3/2} - v^{n-1/2} \right\rangle_x . \]

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

\[ C_{3n+1} - C_{3n} = \Delta t^2 \langle A \mathcal{G} u^{n+1} - A \mathcal{G} u^n, A \mathcal{G} u^{n+1} + A \mathcal{G} u^n \rangle_{F^*} \]

\[ = \Delta t^2 \left\langle A \mathcal{G} u^{n+1} - A \mathcal{G} u^n, \frac{v^{n+3/2} - v^{n-1/2}}{\Delta t} \right\rangle_{F^*} \]

\[ = \Delta t^2 \left\langle \Delta t A \mathcal{G} a^{-1} D^* v^{n+1/2}, \frac{v^{n+3/2} - v^{n-1/2}}{\Delta t} \right\rangle \]

\[ = \Delta t^2 \left\langle A \mathcal{G} a^{-1} D^* v^{n+1/2}, v^{n+3/2} - v^{n-1/2} \right\rangle. \]

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

\[ C_n = ||u^n||^2 - \frac{\Delta t^2}{4} ||A \mathcal{G} u^n||^2 + \left| \left| \frac{v^{n+1/2} + v^{n-1/2}}{2} \right| \right|^2. \]

This implies that

\[ ||C_n|| \geq \left( 1 - \frac{\Delta t^2}{4} ||A \mathcal{G}||^2 \right) ||u^n||^2 + \left| \left| \frac{v^{n+1/2} + v^{n-1/2}}{2} \right| \right|^2, \]

so \( ||C_n|| \) is positive for sufficiently small \( \Delta t \) if \( ||A \mathcal{G} u^n|| \) is finite.

### B.2 Maxwell

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

\[ \frac{\vec{E}^{n+1} - 2 \vec{E}^n + \vec{E}^{n-1}}{\Delta t^2} = -\epsilon^{-1} \mathcal{R}^* \mu^{-1} \mathcal{R} \vec{E}^n \]

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

To find a conserved quantity \( C_{n+1/2} \) let

\[ C_{1n+1/2} = \left| \left| \frac{\vec{E}^{n+1} + \vec{E}^n}{2} \right| \right|_{\mathcal{E}}, \]

\[ C_{2n+1/2} = \left| \left| \vec{H}^{n+1/2} \right| \right|_{\mathcal{E}^*}, \]

\[ C_{3n+1/2} = \Delta t^2 \left| \left| \epsilon^{-1} \mathcal{R}^* \vec{H}^{n+1/2} \right| \right|_{\mathcal{E}}. \]
As before compute:

\[
C_{1_{n+1/2}} - C_{1_{n-1/2}} = \left\langle \frac{E_{n+1} + 2E_n + E_{n-1}}{4}, E_{n+1} - E_{n-1} \right\rangle \varepsilon
\]

\[
= \left\langle E_n - \frac{\Delta t^2}{4} \epsilon^{-1} \mathcal{R} \mu^{-1} \mathcal{R} E_n, E_{n+1} - E_{n-1} \right\rangle \varepsilon;
\]

\[
= \left\langle E_n, E_{n+1} - E_{n-1} \right\rangle \varepsilon - \frac{\Delta t^2}{4} \left\langle \epsilon^{-1} \mathcal{R} \mu^{-1} \mathcal{R} E_n, E_{n+1} - E_{n-1} \right\rangle \varepsilon;
\]

Using the adjoint equation \( \ldots \) gives

\[
C_{2_{n+1/2}} - C_{1_{n-1/2}} = \left\langle \tilde{H}_{n+1/2} + \tilde{H}_{n-1/2}, \tilde{H}_{n+1/2} - \tilde{H}_{n-1/2} \right\rangle_{\mathcal{F}^*}
\]

\[
= \left\langle \tilde{H}_{n+1/2} + \tilde{H}_{n-1/2}, - \Delta t \mu^{-1} \mathcal{R} E_n \right\rangle_{\mathcal{F}^*}
\]

\[
= -\Delta t \left\langle \epsilon^{-1} \mathcal{R} \tilde{H}_{n+1/2} + \epsilon^{-1} \mathcal{R} \tilde{H}_{n-1/2}, E_n \right\rangle \varepsilon
\]

\[
= -\Delta t \left\langle \frac{\tilde{E}_{n+1} - \tilde{E}_{n-1}}{\Delta t}, \varepsilon \right\rangle E_n \varepsilon
\]

\[
= -\left\langle \tilde{E}_n, \tilde{E}_{n+1} - \tilde{E}_{n-1} \right\rangle \varepsilon;
\]

Also

\[
C_{3_{n+1/2}} - C_{1_{n-1/2}} = \Delta t^2 \left\langle \epsilon^{-1} \mathcal{R} \tilde{H}_{n+1/2} - \epsilon^{-1} \mathcal{R} \tilde{H}_{n-1/2}, \epsilon^{-1} \mathcal{R} \tilde{H}_{n+1/2} + \epsilon^{-1} \mathcal{R} \tilde{H}_{n-1/2} \right\rangle \varepsilon
\]

\[
= \Delta t^2 \left\langle \epsilon^{-1} \mathcal{R} \left( \tilde{H}_{n+1/2} - \tilde{H}_{n-1/2} \right), \frac{\tilde{E}_{n+1} - \tilde{E}_{n-1}}{\Delta t} \right\rangle \varepsilon
\]

\[
= \Delta t^2 \left\langle -\Delta t \epsilon^{-1} \mathcal{R} \mu^{-1} \mathcal{R} E_n, \frac{\tilde{E}_{n+1} - \tilde{E}_{n-1}}{\Delta t} \right\rangle \varepsilon
\]

\[
= -\Delta t^2 \left\langle \epsilon^{-1} \mathcal{R} \mu^{-1} \mathcal{R} E_n, \tilde{E}_{n+1} - \tilde{E}_{n-1} \right\rangle \varepsilon.
\]

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

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

This implies that

\[
C_{n+1/2} \geq \left\| \frac{E_{n+1} + E_n}{2} \right\|_{\varepsilon}^2 + \left( 1 - \frac{\Delta t^2}{4} \left\| \epsilon^{-1} \mathcal{R} \right\|_{\varepsilon^*}^2 \right) \left\| \tilde{H}_{n+1/2} \right\|_{\varepsilon^*}^2.
\]
So \( C_{n+1/2} \geq 0 \) for \( \Delta t \) sufficiently small provided \( \| \epsilon^{-1} \mathcal{R}^* \| \) is finite.

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

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

First compute

\[
C_{1n+1} - C_{1n} = \left\langle \frac{\bar{H}^{n+3/2} + 2 \bar{H}^{n+1/2} + \bar{H}^{n-1/2}}{4}, \bar{H}^{n+3/2} - \bar{H}^{n-1/2} \right\rangle_{\mathcal{F}^*}
\]
\[
= \left( \bar{H}^{n+1/2}, \bar{H}^{n+3/2} - \bar{H}^{n-1/2} \right)_{\mathcal{F}^*} + \frac{\Delta t^2}{4} \left\langle \mu^{-1} \mathcal{R} \epsilon^{-1} \mathcal{R}^* \bar{H}^{n+1/2}, \bar{H}^{n+3/2} - \bar{H}^{n-1/2} \right\rangle_{\mathcal{F}^*}.
\]

Using the adjoint equation xxx gives

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

Also

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

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

\[
C_n = \left\| \bar{E}^n \right\|_{\varepsilon}^2 - \frac{\Delta t^2}{4} \left\| \mu^{-1} \mathcal{R} \bar{E}^n \right\|_{\mathcal{F}^*}^2 + \left\| \frac{\bar{H}^{n+1/2} + \bar{H}^{n-1/2}}{2} \right\|_{\mathcal{F}^*}^2.
\]
This implies that
\[ ||C_n|| \geq (1 - \frac{\Delta t^2}{4} ||\mu^{-1}\mathcal{R}||^2) \left( ||\vec{E}^n||^2 + \left|\left| \frac{\tilde{H}^{n+1/2} + \tilde{H}^{n-1/2}}{2} \right|\right|^2 \right), \]
so \( ||C_n|| \) is positive for sufficiently small \( \Delta t \) if \( ||\mu^{-1}\mathcal{R} \vec{E}^n|| \) is finite.

The codes \texttt{Maxwell.m} and \texttt{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.
C Conservation Laws and Positive Solutions

Do a search on "Positivity-Preserving" for diffusion equations.

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 [44] (equations 1.5, 1.6 and 1.7) can be put into this form. To provide some insight into discretizing such conservation laws, two important but simple cases will be considered. For a similar discussion see Chapter 11 in [39]. Also [21] develop mimetic methods for anisotropic 2D diffusion. For positivity preserving for the 3D heat equation see [20].

C.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 primal 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 a primal grid is chosen then 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
\[ \Delta x \rho_{i+\frac{1}{2}}^{n+3/2} = \Delta x \rho_{i+\frac{1}{2}}^{n+1/2} + \Delta t v_i \rho_{i-\frac{1}{2}}^{n+1/2} - \Delta t v_{i+1} \rho_{i+\frac{1}{2}}^{n+1/2}. \]

Rewrite this as
\[ \frac{\rho_{i+\frac{1}{2}}^{n+3/2} - \rho_{i+\frac{1}{2}}^{n+1/2}}{\Delta t} + \frac{v_{i+1} \rho_{i+\frac{1}{2}}^{n+1/2} - v_i \rho_{i-\frac{1}{2}}^{n+1/2}}{\Delta x} = 0, \]

to see that the discretization is a first order approximation of the differential equation. As an update of the density the equation becomes
\[ \rho_{i+\frac{1}{2}}^{n+3/2} = \rho_{i+\frac{1}{2}}^{n+1/2} + \frac{\Delta t}{\Delta x} v_i \rho_{i-\frac{1}{2}}^{n+1/2} - \frac{\Delta t}{\Delta x} v_{i+1} \rho_{i+\frac{1}{2}}^{n+1/2}. \]

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 consider \( v \) rather than \( \rho \).

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

Figure C.1: A: Left transport of a square wave \( v \frac{\Delta t}{\Delta x} = -1 \). B: Right transport of a square wave with \( v = 0.4167 \). (See `Transport.m`)
solution as follows:

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

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

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

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 \(v_i \frac{\Delta t}{\Delta x} = \pm 1\) it gives an exact solution of solution as shown in Figure C.1. 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 with out 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.
C.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 and \( D = D(x) \geq 0 \) 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

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

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.
D Other Stuff

To be revised.

The paper [57] extends mimetic methods in 2D to curvilinear grids for several linear wave equations.

Section 6 reviews some continuum wave equations in 3 dimensions when the material properties are constant. The main issue is understanding the role of the spatial dimension for distance $d$ plays in the partial differential equations. The scalar and vector wave equations, the elastic wave equation [16] and Maxwell’s equations are introduced and a conserved quantity is given for each equation. See [62] [10] for a related explicit scheme for Maxwell equation.

In Section 5 continuum second order differential operators for anisotropic and inhomogeneous materials are introduced. The main idea is to use the notion of a double exact sequence and diagram chasing to define a large class of second order spatial differential operators that can be used to define wave equations. This idea is motivated by the exact sequences used in differential geometry. A knowledge of differential forms is not required for understanding this material but can be helpful [1]. A discrete double exact sequence is critical for the discussion of discretizations using staggered grids. Importantly, the discrete double exact sequence cannot be reduced to a single sequence. The paper [41], Figure 9, uses a double exact sequence that is called a De Rham complex.

Additionally, weighted inner products for scalar and vector functions are introduced and used to define adjoint operators and to show that the second order operators are either positive or negative. The main difference between the discussion here and that in [46] is the introduction of variable material properties. This discussion depends heavily on the spatial units of the dependent variables, the differential operators, and the material properties.

In Section 6 the second order differential operators defined in the previous section are combined with a second time derivative to define several types of wave equations with variable material properties. The second order equations are written as a first order system that has properties similar to the systems studied earlier. This then gives an automatic definition of a conserved quantity. At the end of the section Maxwell’s equations and the general elastic wave equations examples are studied.

The material below to be revised soon! In Section 7 primal and dual staggered grids in 3D are introduced. These grids are the same as those introduce by Yee [62] in 1966 to discretize Maxwell’s equations. Consequently there are two types of discrete scalar fields and two types of discrete vector fields. The differential operators divergence, gradient and curl are discretized as in [46]. Because two grids are used there are two discrete version of each of the first order discrete operators divergence $\nabla \cdot$, curl $\nabla \times$ and gradient $\nabla$. Additionally it is shown how to discretize the material properties. This section continues by defining discrete inner products and adjoint operators critical for understanding important properties of the discrete operators. Note that the paper [35] also used a dual grid differential form method to discretize the Navier-Stokes Equations. For an introduction to the relationship of vector calculus to differential forms see the notes [1].
In Section 8.3 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.

For isotropic and homogeneous materials, simulations show that the three dimensional scalar wave equation and Maxwell’s equations without sources the approximate energy 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.

Should section 10 be an appendix?

D.1 Notes

This will be revised.

For the latest, see the minisymposium at a recent SIAM meeting [51]. For more information on steady state problems see [33]. For an idea of the difficulties encountered in discretizing Maxwell’s equations see [8]. Others have used approximate quantities to study time discretizations [23, 22, 14, 18, 45]. It appears that most of the energy preserving methods are implicit, but by introducing additional variables, explicit methods that conserve a modified energy are discussed in [53].

One complexity of mimetic spatial discretizations is caused by having primal and dual grids. This is leads to there being a primal gradient, curl, and divergence and dual gradient, curl and divergence. The dual operators are labeled with a star $\star$. This complexity was already present in the paper by Yee [62] which has evolved into the FDTD discretization method [61].

There are several minor problems caused by writing wave equations as a second order differential equations or as a system of two first order equations. For example second order equations are not exactly equivalent to first order system. 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 and vice versa. Additionally, because the equations studied are linear, if they conserve some quantity, they will conserve infinitely many quantities and thus there are choices in what conserved quantity to study. For the first order system there is a natural primitive conserved quantity.

This paper was inspired by the papers [58] and [62]. We note that in [50] (see equation (45)) the same stability constraint was found as the one in this paper for conserving the classical energy by modifying the discretization of Maxwell’s equations. In [19] an implicit (ADI) method is developed that has a modified energy that is similar to the one used here but the added term is positive while the added term here is negative. For a finite element approach that produce many of the same results that as in this paper see [54, 4].

The paper [49] gives an overview of energy conserving methods for Navier-Stokes equations and develops some implicit Runge-Kutta methods for doing this. The thesis [6] addresses energy conservation for turbulent flows. For a differential forms approach to discretization see [43, 55] and additionally for multisymplectic time integration approach to
Maxwell’s equations see [52]. For two dimensional problems see [7, 42, 40, 47, 12, 36, 27, 28].

The papers [56, 58] take a novel approach to finding discrete models. For a finite-element approach to vector wave equations see Section 2.3.2 of [2].

For higher order mimetic methods, see [48].

Others have used summation by parts to obtain mimetic like discretizations [59, 17, 37].

It would be very interesting to extend the methods described here to nonlinear partial differential equations [60].