

Stable, Conservative Solution Methods for Large, Stiff Hamiltonian Systems Modeling Coherent Phenomena in Nonlinear Optics and Biophysics

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1 Introduction

Introduction

The main objective of this talk is to describe a method for constructing time discretization methods for Hamiltonian systems that

- conserve the Hamiltonian (“energy”) and all quadratic and linear conserved quantities, related to affine symmetries,
- respect time reversal symmetry of the equations,
- are unconditionally stable (A-stable for the case of linear systems), and
- are of any chosen (even) order of accuracy.

The main intended applications are discretizations of dispersive nonlinear PDE’s related to NLS, and a larger class of lattice equations.

Some Notation

Vectors are indicated by bold face, as with \mathbf{y} and \mathbf{f} .

We will use the notations $D_y f$ and $\frac{\partial f}{\partial y}$ flexibly, to indicate either individual partial derivatives

$$D_k f = D_{y_k} f = \frac{\partial f}{\partial y_k},$$

gradient vectors

$$D_y f = \nabla f = \nabla_y f = \frac{\partial f}{\partial \mathbf{y}} = \left\langle \frac{\partial f}{\partial y_1} \quad \frac{\partial f}{\partial y_2} \quad \dots \right\rangle,$$

or Jacobian matrices

$$D_y \mathbf{f} = \frac{\partial \mathbf{f}}{\partial \mathbf{y}} = \left\{ \frac{\partial f_i}{\partial y_j} \right\}.$$

2 Some PDE’s and Lattice Equations of Interest

The most famous examples of the two categories are

A. The Nonlinear Schrödinger Equation [NLS]

$$i \frac{\partial z}{\partial t} + \Delta z + g(|z|^2)z = 0, \tag{1}$$

and its standard spatial discretization

B. The (Standard) Discrete Nonlinear Schrödinger Equation [DNLS]

$$i \frac{dz_n}{dt} + \kappa^2(z_{n-1} - 2z_n + z_{n+1}) + g(|z_n|^2)z_n = 0 \tag{2}$$

which can be converted to the form

$$i \frac{dz_n}{dt} + \kappa^2(z_{n-1} + z_{n+1}) + g(|z_n|^2)z_n = 0. \tag{3}$$

Some More Exotic Equations

However, suitable methods for these equations have been known since at least the 1978 work of [Strauss&Vázquez:1978], exploiting the simple single-point form of the nonlinearity.

One less familiar model of interest which introduces additional challenges to the design of a good numerical methods is Davydov's model of excitation propagation in α -helix protein from [Davydov:1971]

$$\begin{aligned} i \frac{dz_n}{dt} + \kappa^2(z_{n-3} + z_{n+3}) - \lambda^2(z_{n-1} + z_{n+1}) &= (q_{n+3} - q_{n-3})z_n, \\ m_0 \frac{d^2 q_n}{dt^2} - (q_{n-3} - 2q_n + q_{n+3}) &= |z_{n+3}|^2 - |z_{n-3}|^2 \end{aligned}$$

with

$$\kappa^2 \approx 1.4 \text{ THz}, \quad \lambda^2 \approx 2.3 \text{ THz}, \quad \omega_0 = \sqrt{1/m_0} \approx 12 \text{ THz}.$$

- The *exciton* variable z_n comes from Schrödinger's equation, and gives the probability that the C=N double bond at the n -th amino acid residue is in a rotational excited state, the only quantum mechanical excitation that is likely at biologically relevant temperatures.
- The mechanical variable q_n indicates the displacement of the n -th residue from its rest position, in the direction of the axis of the helix.
- The λ terms relate to the repulsive interaction between excitons in residues that are adjacent along the molecular backbone of residues within a helical molecular structure.
- The κ terms relate to the attractive interaction between excitons in residues that are adjacent along an almost straight *spine* of residues within a helical molecular structure: there are approximately three residues per twist of the helix.
- The remaining “mechanical” terms relate to the attractive electrostatic dipole interaction between residues adjacent along spines.

A Helical Nonlinear Schrödinger Equation with a Non-local Nonlinearity

Another system of mathematical interest is the approximation of the above on the basis that the time scale of the mechanical coupling is substantially faster than for the exciton couplings, leading to a fast and small vibration limit, equivalent to $m_0 \rightarrow 0$: the

Helical Discrete Schrödinger Equation [HDNLS]

$$\begin{aligned} i \frac{dz_n}{dt} + \kappa^2(z_{n+3} + z_{n-3}) - \lambda^2(z_{n+1} + z_{n-1}) \\ + \left(\frac{1}{2}|z_{n-3}|^2 + |z_n|^2 + \frac{1}{2}|z_{n+3}|^2 \right) z_n = 0. \end{aligned} \tag{4}$$

A Discrete Nonlinear Schrödinger Equation with a Non-local Nonlinearity

A further simplification for testing purposes is the single spine version of the above, the

Non-Local Discrete Schrödinger Equation [NLDNLS]

$$i\frac{dz_n}{dt} + \kappa^2(z_{n+1} + z_{n-1}) + \left(\frac{1}{2}|z_{n-1}|^2 + |z_n|^2 + \frac{1}{2}|z_{n+1}|^2\right)z_n = 0. \quad (5)$$

These exciton-vibration molecular chain models are interesting challenges for developing and testing numerical methods:

- They cannot be handled by some earlier approaches developed for discretizations of PDEs, due to the nonlinearity of non-local form, and
- They cannot be handled well by some other popular methods for Lagrangian and mechanical systems, such as the methods of
 - Störmer-Verlet-Newton (a.k.a. leap-frog),
 - [LaBudde, Greenspan:1976, Simo et al:1992]
 - or the locally implicit method of [Strauss&Vázquez:1978].

2.1 Hamiltonian Form

We use the general Hamiltonian form

$$\frac{d\mathbf{y}}{dt} = \mathcal{J}\nabla_{\mathbf{y}}\mathcal{H}(\mathbf{y}) = \mathcal{J}\frac{\partial\mathcal{H}}{\partial\mathbf{y}}(\mathbf{y}) \quad (6)$$

with \mathcal{J} an anti-symmetric matrix.

In the cases of interest here, \mathcal{J} is a constant matrix, but it can also be a matrix-valued function of the state variables, $\mathcal{J}(\mathbf{y})$.

Canonical (real) Hamiltonian Form

For the most familiar canonical case,

$$\mathbf{y} = \begin{bmatrix} \mathbf{q} \\ \mathbf{p} \end{bmatrix} = [q_1 \dots q_N \ p_1 \dots p_N]^T, \quad \mathcal{J} = J = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix}, \quad (7)$$

and

$$\frac{d\mathbf{q}}{dt} = \nabla_{\mathbf{p}}\mathcal{H}, \quad \frac{d\mathbf{p}}{dt} = -\nabla_{\mathbf{q}}\mathcal{H}. \quad (8)$$

Canonical Complex Hamiltonian Form

For equations of “Schrödinger type” it is convenient to use the complex form

$$\mathbf{y} = \begin{bmatrix} \mathbf{z} \\ \mathbf{z}^* \end{bmatrix}, \quad \mathcal{J} = iJ = i \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix}, \quad (9)$$

$$\frac{d\mathbf{z}}{dt} = i\nabla_{\mathbf{z}^*}\mathcal{H}, \quad \frac{d\mathbf{z}^*}{dt} = -i\nabla_{\mathbf{z}}\mathcal{H}. \quad (10)$$

Here \mathbf{z} and \mathbf{z}^* are formally independent variables, though in practice they are complex conjugates, the Hamiltonians is real in that case, and only one of the pair of equations is needed.

Mixed Hamiltonian Form

For the Davydov system, a combination of the above two forms is natural, though the complex parts could as always be eliminated with the change of variables

$$\mathbf{Q} = \frac{\mathbf{z} + \mathbf{z}^*}{\sqrt{2}}, \quad \mathbf{P} = \frac{\mathbf{z} - \mathbf{z}^*}{i\sqrt{2}}. \quad (11)$$

Hamiltonians for the Above Equations

The equations above have Hamiltonian form with [using here and from now on $G' = g$ with $G(0) = 0$]

$$\mathcal{H} = \sum_n \kappa^2 (z_{n+1} - z_n)(z_{n+1}^* - z_n^*) - G(z_n z_n^*) \quad \text{for DNLS} \quad (12)$$

$$\begin{aligned} \mathcal{H} = & -\kappa^2 \sum_n (z_n^* z_{n+1} + z_n z_{n+1}^*) \\ & + \frac{1}{2} \sum_n (z_n^* z_n)(z_n^* z_n + z_{n+1}^* z_{n+1}) \end{aligned} \quad \text{for NLDNLS} \quad (13)$$

and for the Davydov system:

$$\begin{aligned} \mathcal{H} = & -\kappa^2 \sum_n (z_n z_{n+1}^* + z_{n+1} z_n^*) \\ & + \sum_n \left[\frac{p_n^2}{2m_0} + \frac{1}{2} (q_{n+1} - q_n)^2 \right] \\ & + \sum_n (q_{n+1} - q_{n-1}) z_n z_n^*. \end{aligned} \quad (14)$$

The NLS also has a Hamiltonian form using the Fréchet derivative:

$$\frac{dz}{dt} = i \frac{\delta \mathcal{H}}{\delta z^*} \quad (15)$$

with Hamiltonian functional

$$\mathcal{H}[z, z^*] = \int (\nabla z) \cdot (\nabla z^*) - G(z z^*) d\mathbf{x}. \quad (16)$$

Various end conditions can be imposed on the Hamiltonian to deal with the out-of-bounds indices $n = 0$ and $n = N + 1$ that arise, in particular:

- Homogeneous Dirichlet: $z_0 = z_{N+1} = 0$, or
- Periodic: $z_{n+N} = z_n$ (so $z_0 = z_N$ and $z_{N+1} = z_1$).

One can also consider an infinite chain: $n \in \mathbb{N}$, $z_n \rightarrow 0$ as $|n| \rightarrow \infty$.

Note that for all these equations, the Hamiltonian

1. is not in the standard form for a mechanical system, and indeed
2. does not separate as $\mathcal{H} = T(\mathbf{p}) + U(\mathbf{q})$.

Many popular conservative and symplectic numerical methods that work well for mechanical systems, such as molecular models with no quantum excitations present, rely on the latter splitting.

Conserved Charge

The equations have a conserved *charge* \mathcal{E} (also called *exciton number* or *power* depending on the physical application). This is related to the probability density of quantum mechanics, and notably, it is quadratic (like angular momentum):

$$\mathcal{E} = \sum_n z_n z_n^* \quad (17)$$

(or the counterpart $\int z z^* d\mathbf{x}$ for NLS.)

This is associated via Noether's Theorem with the linear symmetry group action $\mathbf{z} \rightarrow e^{is}\mathbf{z}$, $\mathbf{z}^* \rightarrow e^{-is}\mathbf{z}^*$.

Conserved Momentum for the Davydov System

The Davydov systems also has a conserved momentum \mathcal{P} , again (degenerately) quadratic:

$$\mathcal{P} = \sum_n p_n. \quad (18)$$

This is associated via Noether's Theorem with the symmetry group action $q_n \rightarrow q_n + s$.

2.2 Invariants (a.k.a Conserved Quantities, First Integrals)

For future reference, here are the verifications of the invariance of the conservation of these invariants.

First, for any system $dy/dt = \mathcal{J}\nabla_{\mathbf{y}}\mathcal{H}(\mathbf{y})$

$$\begin{aligned} \frac{d\mathcal{H}}{dt} &= \nabla_{\mathbf{y}}\mathcal{H} \cdot \frac{d\mathbf{y}}{dt} && \text{multivariable chain rule} \\ &= \nabla_{\mathbf{y}}\mathcal{H}(\mathbf{y}) \cdot \mathcal{J}\nabla_{\mathbf{y}}\mathcal{H}(\mathbf{y}) && \text{Hamilton's equations} \\ &= 0 && \text{from the anti-symmetry of } \mathcal{J}. \end{aligned}$$

In many any interesting mechanical systems, the Hamiltonian are invariant under a common translation of all position coordinates, $q_n \rightarrow q_n + s$.

Such a Hamiltonian can be written in terms of the translation invariant linear combinations $\Delta_{n,m} := q_n - q_m$.

This is seen in the Davydov system, where the variables q_n appear only in the translation invariant *bond-stretchings* $\Delta_n := q_{n+1} - q_n$.

Combined with the evolution equation $dp_n/dt = -\partial\mathcal{H}/\partial q_n$ this gives conservation of the (linear) momentum $\mathcal{P} = \sum_n p_n$. First,

$$\begin{aligned} \frac{d\mathcal{P}}{dt} &= \sum_n \frac{dp_n}{dt} = - \sum_n \frac{\partial\mathcal{H}}{\partial q_n} = - \sum_{n < m} \left[\frac{\partial\mathcal{H}}{\partial\Delta_{n,m}} \frac{\partial\Delta_{n,m}}{\partial q_n} + \frac{\partial\mathcal{H}}{\partial\Delta_{m,n}} \frac{\partial\Delta_{m,n}}{\partial q_n} \right] \\ &= - \sum_{n < m} \left[\frac{\partial\mathcal{H}}{\partial\Delta_{n,m}} (+1) + \frac{\partial\mathcal{H}}{\partial\Delta_{m,n}} (-1) \right]. \end{aligned}$$

For any pair of indices a and b with $a \leq b$, the term $\frac{\partial \mathcal{H}}{\partial \Delta_{a,b}}$ occurs twice: once in the first “(+1)” term; once in the second “(−1)” term.

Thus all terms pair off and cancel out, giving $\frac{d\mathcal{P}}{dt} = 0$.

Note: This is the simplest illustration of the famous relationship between continuous symmetries and conservation laws stated in Noether's Theorem, which will be discussed more below.

Phase Shift Invariance and its Invariant Quadratic Forms

Conservation of the charge can be verified directly (rather than invoking Noether's Theorem) by first noting that the state variables z_n and z_n^* appear in the Hamiltonian only through the *symmetry group quadratic combinations*

$$\pi_{n,m} = z_n z_m^*$$

which are invariant under the phase shift symmetry

$$\mathbf{z} \rightarrow e^{is} \mathbf{z}, \quad \mathbf{z}^* \rightarrow e^{-is} \mathbf{z}^*.$$

These serve the same purpose as the invariant linear forms $\Delta_{n,m}$ seen above.

Invariance of Charge

To verify invariance of the charge in time, first differentiate:

$$\begin{aligned} \frac{d\mathcal{E}}{dt} &= \sum_n \frac{d(z_n z_n^*)}{dt} \\ &= \sum_n \frac{dz_n}{dt} z_n^* + \frac{dz_n^*}{dt} z_n \\ &= i \sum_n \frac{\partial \mathcal{H}}{\partial z_n^*} z_n^* - \frac{\partial \mathcal{H}}{\partial z_n} z_n \\ &= i \sum_n \left[\sum_m \frac{\partial \mathcal{H}}{\partial \pi_{m,n}} \frac{\partial \pi_{m,n}}{\partial z_n^*} z_n^* - \sum_m \frac{\partial \mathcal{H}}{\partial \pi_{n,m}} \frac{\partial \pi_{n,m}}{\partial z_n} z_n \right] \\ &= i \sum_n \sum_m \left[\frac{\partial \mathcal{H}}{\partial \pi_{m,n}} z_n z_n^* - \frac{\partial \mathcal{H}}{\partial \pi_{n,m}} z_n^* z_m \right]. \end{aligned}$$

For any pair of indices a, b with $a \leq b$

- the term $\frac{\partial \mathcal{H}}{\partial \pi_{n,m}} z_n z_m^*$ for $m = a, n = b$ is $\frac{\partial \mathcal{H}}{\partial \pi_{b,a}} z_b z_a^*$, and
- the term $-\frac{\partial \mathcal{H}}{\partial \pi_{m,n}} z_n^* z_m$ for $m = b, n = a$ is $-\frac{\partial \mathcal{H}}{\partial \pi_{b,a}} z_a^* z_b$,

so all terms pair off and cancel, giving $\frac{d\mathcal{E}}{dt} = 0$.

3 Spatial Discretization of PDE's and Lattice Systems

3.1 Discretizations of the Nonlinear Schrödinger Equation

DNLS by Discretizing the NLS Hamiltonian

Some equations of the form above arise from discretizing dispersive PDE's of Hamiltonian form, which is perhaps best done by discretizing the Hamiltonian functional itself.

For example, the 1D nonlinear Schrödinger equation

$$i \frac{\partial z}{\partial t} + \frac{\partial^2 z}{\partial x^2} + g(|z|^2)z = 0 \quad (19)$$

has Hamiltonian form

$$\frac{\partial z}{\partial t} = i \frac{\delta \mathcal{H}}{\delta z^*}, \quad \mathcal{H} = \int \left(\frac{dz}{dx} \right)^2 - G(|z|^2) dx. \quad (20)$$

Discretizing this Hamiltonian with

$$x_n := n\delta x, \quad z_n(t) \approx z(x_n, t), \quad \frac{\partial z}{\partial x}(x_n) \approx \frac{z_{n+1} - z_n}{\delta x}$$

and a suitably scaled Riemann sum gives the Hamiltonian

$$\mathcal{H} = \sum_n \frac{(z_{n+1} - z_n)}{\delta x} \frac{(z_{n+1}^* - z_n^*)}{\delta x} - G(z_n z_n^*).$$

and thus the discrete nonlinear Schrödinger equation

$$i \frac{dz_n}{dt} + \kappa^2 (z_{n-1} - 2z_n + z_{n+1}) + g(z_n z_n^*) z_n = 0$$

with $\kappa = 1/\delta x$.

3.2 More General Lattice Equations

More General Lattice Equations

This can be extended in various ways:

- to higher order accuracy in the spatial discretization
- to higher spatial dimension, and most interestingly,
- to nonlocal nonlinearities of forms like

$$\mathcal{H} = \int |\nabla z|^2 - G[z, z^*] d\mathbf{x}$$

with a nonlocal functional $G[z, z^*]$ that is invariant under the phase shift symmetry

$$z(x) \rightarrow e^{is} z(x), \quad z^*(x) \rightarrow e^{-is} z^*(x).$$

For example, $G = [(-\Delta + m^2)^{-1}(zz^*)]^2$.

This leads to interest in a general class of equations given by Hamiltonians

$$\mathcal{H} = \sum_n \sum_m (l_{nm} z_n z_m^*) + G(\mathbf{z} \mathbf{z}^*)$$

for symmetric matrix $L = \{l_{nm}\}$. Here $\mathbf{z} \mathbf{z}^*$ denotes the matrix of all products $z_n z_m^*$.

The ODEs are then a general family of *lattice nonlinear Schrödinger equations*

$$i \frac{dz_n}{dt} + \sum_m l_{nm} z_m + \sum_m g_{n,m}(\mathbf{z}, \mathbf{z}^*) z_m = 0. \quad (21)$$

3.3 Features of the Resulting ODE Systems

Features of the Resulting ODE Systems

The systems of ODE's $\frac{d\mathbf{y}}{dt} = \mathbf{f}(\mathbf{y})$ arising from such discretizations of PDEs typically have the following features:

1. The number of unknowns, N , is very large.
2. If the PDE is semi-linear or quasi-linear, the ODE system inherits an analogous property like the form

$$\frac{d\mathbf{y}}{dt} = \mathbf{f}(\mathbf{y}) = L\mathbf{y} + \mathbf{g}(\mathbf{y})$$

where L is a constant matrix and the nonlinear term $\mathbf{g}(\mathbf{y})$ is in some sense relatively small: for example, Jacobian matrix $D_{\mathbf{y}}\mathbf{g}(\mathbf{y})$ of far smaller norm than L for relevant values of \mathbf{y} .

3. The coupling between unknowns is *local*, or *predominantly local*, where
 - *local* means that the $N \times N$ Jacobian matrix $A = D_{\mathbf{y}}\mathbf{f}(\mathbf{y})$ is *banded*: the only non-zero elements A_{ij} are ones with $|i - j| \leq w$ for some *bandwidth* $w \ll N$: w is far smaller than N .
 - *predominantly local* means that the system is quasi-linear as above and the linear part L has low bandwidth w .

For example, the above spatial discretization of the nonlinear Schrödinger is quasi-linear because $\kappa = 1/\delta x \gg 1$ makes the linear term dominant, and it is local with bandwidth $w = 1$.

Some More Notation

We will focus on the time advance map for single time step, from a time t to $t + h$. Thus for a scalar variable x , a vector \mathbf{x} , and likewise for other variables like \mathbf{q} , \mathbf{p} , and \mathbf{z} :

- h or δt denotes the change in t over the time step.
- x alone without arguments denotes the value $x(t)$ at time t , typically the beginning of the current time step.
- x^+ denotes the value $x(t + h)$.

- $\delta x = x^+ - x$.
- X or $\bar{x} = \frac{x + x^+}{2}$.
- $\dot{X} = \frac{\delta x}{\delta t}$.

Note that capital letters are only used for the time averaged or approximated quantities.

Definition 1 (Symmetric Time-Stepping Method). A time stepping method is *symmetric* if the time-stepping map of step size $-h$ is the inverse of the map for step size h .

For example, the implicit midpoint method is symmetric — but no explicit one-step method is.

From now on, *we will require that all methods are symmetric*, because this is empirically seen to have desirable effects on the long-term behavior of numerical solutions, and is also convenient when constructing methods of higher order accuracy.

Symplectic Method and Discretizing Hamilton's Principle

A popular class of time discretization methods are the symplectic or variational methods, which for Hamiltonian $\mathcal{H}(\mathbf{q}, \mathbf{p})$ can be expressed in the form of a time advance map $(\mathbf{q}, \mathbf{p}) \rightarrow (\mathbf{q}^+, \mathbf{p}^+)$ given implicitly by the equations

$$\mathbf{p} = -D_1 \mathcal{L}_h(\mathbf{q}, \mathbf{q}^+), \quad \mathbf{p}^+ = D_2 \mathcal{L}_h(\mathbf{q}, \mathbf{q}^+)$$

Here \mathcal{L}_h is the generating function ensuring that the map is symplectic, and can be interpreted as a discrete approximation of the part of the action interval over time sub-interval t to $t + h$ in the Lagrangian form of the equations.

A Discrete Noether's Theorem

Noether's Theorem has a discrete analog, which says that if the above generating function \mathcal{L}_h is invariant under a continuous symmetry, then the corresponding symplectic method conserves the corresponding conserved quantity

$$I(\mathbf{q}, \mathbf{p}) = \mathbf{p} \cdot \mathbf{a}(\mathbf{q})$$

(This and most other theorems on numerical methods can be found in the book [GNI] by E. Hairer, C. Lubich and G. Wanner, herein referred to as “GNI”).

The Implicit Midpoint Method

Using the midpoint rule for quadrature as the above generating function (discrete Lagrangian) leads to the Implicit Midpoint Rule

$$\frac{\mathbf{y}^+ - \mathbf{y}}{h} = f\left(\frac{\mathbf{y} + \mathbf{y}^+}{2}\right) \quad (22)$$

This is clearly symmetric.

The time-stepping method has the suggestive form

$$\dot{\mathbf{Q}} = \frac{\partial \mathcal{H}}{\partial \mathbf{P}}(\mathbf{Q}, \mathbf{P}), \quad (23)$$

$$\dot{\mathbf{P}} = -\frac{\partial \mathcal{H}}{\partial \mathbf{Q}}(\mathbf{Q}, \mathbf{P}). \quad (24)$$

Conservation of Quadratic Invariants

For a linear symmetry group $\mathbf{q} \rightarrow A(s)\mathbf{q}$, given by a matrix-valued one-parameter group $A(s)$, invariance of the Lagrangian gives invariance of the above midpoint rule discrete Lagrangian

$$\mathcal{L}_h(\mathbf{q}, \mathbf{q}^+) = h\mathcal{L}\left(\frac{\mathbf{q} + \mathbf{q}^+}{2}, \frac{\mathbf{q}^+ - \mathbf{q}}{h}\right)$$

so that for example the components of angular momenta, which are the invariants given by invariance of the Lagrangian under rotations about each coordinate axis, are also invariant under this discrete scheme.

The Störmer-Verlet (leap-frog) Method

One other basic symplectic method is given by using the trapezoid rule in the discrete Lagrangian in place of the midpoint rule. This gives

$$\begin{aligned} \mathbf{P} &= \mathbf{p} - \frac{h}{2} \frac{\partial \mathcal{H}}{\partial \mathbf{q}}(\mathbf{P}, \mathbf{q}), \\ \mathbf{q}^+ &= \mathbf{q} + \frac{h}{2} \left(\frac{\partial \mathcal{H}}{\partial \mathbf{p}}(\mathbf{P}, \mathbf{q}) + \frac{\partial \mathcal{H}}{\partial \mathbf{p}}(\mathbf{P}, \mathbf{q}^+) \right), \\ \mathbf{p}^+ &= \mathbf{p} - \frac{h}{2} \frac{\partial \mathcal{H}}{\partial \mathbf{q}}(\mathbf{P}, \mathbf{q}^+), \end{aligned} \tag{25}$$

or an alternative version with the roles of \mathbf{q} and \mathbf{p} reversed.

This method is often called the *Störmer-Verlet method*: like the midpoint method, this is second order accurate, symplectic, and time-reversal symmetric.

Historically the Störmer-Verlet method was introduced only for the case of a standard mechanical system with Lagrangian

$$\mathcal{L}(\mathbf{q}, \dot{\mathbf{q}}) = \frac{1}{2} \dot{\mathbf{q}}^T M \dot{\mathbf{q}} - U(\mathbf{q}),$$

by C. Störmer in 1903 for astronomical calculations, and independently by L. Verlet in 1967 for molecular dynamics.

However, the first publication of the method was actually by Newton, in the *Principia*!

Mechanical Systems: the Leap-Frog Method

In that case of mechanical systems, the Störmer-Verlet method can be rewritten as the explicit 2-step *leap-frog method*

$$M \frac{\mathbf{q}_{n+1} - 2\mathbf{q}_n + \mathbf{q}_{n-1}}{h^2} = -D_{\mathbf{q}}U(\mathbf{q}_n).$$

More generally, for a system with separable Hamiltonian $\mathcal{H} = T(\mathbf{p}) + U(\mathbf{q})$, this method is explicit:

$$\begin{aligned} \mathbf{P} &= \mathbf{p} - \frac{h}{2} \frac{\partial U}{\partial \mathbf{q}}(\mathbf{q}) \\ \mathbf{q}^+ &= \mathbf{q} + h \frac{\partial T}{\partial \mathbf{p}}(\mathbf{P}) \\ \mathbf{p}^+ &= \mathbf{p} - \frac{h}{2} \frac{\partial U}{\partial \mathbf{q}}(\mathbf{q}^+) \end{aligned}$$

Notes on the Störmer-Verlet/Leap-Frog Method

Since conservative and symplectic methods are typically implicit, including all symplectic Runge-Kutta methods, this explicit symplectic partitioned Runge-Kutta method is very attractive. It is thus popular for use with classical mechanics, such as in celestial mechanics and molecular biology.

On the other hand, it does not handle stiff systems well, whereas the implicit midpoint method is unconditionally stable (A-stable and B-stable).

Also, its advantages are lost with non-separable Hamiltonians, such as for discrete nonlinear Schrödinger equations.

Symplectic Methods Cannot in General Conserve Both Energy and Quadratic Invariants

There is an unfortunate limitation on all symplectic methods: *they cannot in general conserve both quadratic invariants and the energy (Hamiltonian)*.

The main reason is a theorem of [Ge,Marsden:1988] which essentially says that a symplectic method cannot also conserve energy.

More precisely, a symplectic method that also conserves energy is either

- the exact time stepping map except for shifts in time, or
- a system that decomposes into several parts of this form.

Linear systems are the exception that proves the rule: the energy is quadratic and so is conserved; the system decomposes through action-angle variables into components with one dimensional orbits that are level curves of quadratic invariant for each component.

4 Energy-Momentum Conserving Methods

Just as the derivation of variational methods is based on approximating integrals in Hamilton's Principle, an elegant approach to deriving methods that exactly conserve energy (the Hamiltonian) is to approximate the gradients appearing in the Hamiltonian equation

$$\frac{dy}{dt} = \mathcal{J} \nabla_y \mathcal{H}.$$

Again,

- conserving other invariants requires an appropriate choice of discretization, and
- there is a natural limitation to quadratic (and linear) invariants.

4.1 Energy-Momentum Methods for Central Force Mechanical Systems

[LaBudde, Greenspan:1976] introduced time discretization methods that conserve energy, angular, and linear momentum for N particle central force mechanical systems with Hamiltonian

$$\mathcal{H} = \frac{1}{2} \sum_n \frac{\|\mathbf{p}_n\|^2}{2m_n} + \sum_{m>n} U_{n,m}(\|\mathbf{q}_n - \mathbf{q}_m\|) \quad (26)$$

where now each $\mathbf{q}_n(t)$ and $\mathbf{p}_n(t)$ is a vector in \mathbb{R}^3 . The same methods were developed in a different way and then extended to continuum mechanics by Juan Simo et al, in particular in [Simo et al:1992].

However, the extensions to PDE's are essentially equivalent to first applying a suitable spatial discretization as seen above, giving a system of ODE's in the above form, and then using a time discretization equivalent to the discrete gradient method to be seen next.

Thus, details will be omitted here.

4.2 Discrete Gradient Methods

Discrete Gradient Methods

The basic idea, originating in the work of O. Gonzalez and Juan Simo [Gonzales:1996, Gonzales,Simo:1996] is to define a discrete approximation of the gradient

$$\nabla_{\mathbf{y}} f(\mathbf{y}) \approx (\tilde{\nabla}_{\mathbf{y}} f)(\mathbf{y}, \mathbf{y}^+) = \left\langle (\tilde{D}_1 f)(\mathbf{y}, \mathbf{y}^+), (\tilde{D}_2 f)(\mathbf{y}, \mathbf{y}^+), \dots \right\rangle, \quad (27)$$

giving the *discrete Hamilton's equation*

$$\frac{\delta \mathbf{y}}{\delta t} = \mathcal{J}(\tilde{\nabla}_{\mathbf{y}} \mathcal{H})(\mathbf{y}, \mathbf{y}^+). \quad (28)$$

In the case of a variable matrix $\mathcal{J}(\mathbf{y})$, one instead uses an approximation $\tilde{\mathcal{J}}(\mathbf{y}, \mathbf{y}^+)$.

The natural choice is the midpoint approximation

$$\tilde{\mathcal{J}}(\mathbf{y}, \mathbf{y}^+) = \mathcal{J}(\bar{\mathbf{y}}).$$

The approach presented here follows [LeMesurier:2012a, LeMesurier:2012b].

From now on we will assume the natural consistency condition

$$\lim_{\mathbf{y}^+ \rightarrow \mathbf{y}} (\tilde{D}_{\mathbf{y}} f)(\mathbf{y}, \mathbf{y}^+) = D_{\mathbf{y}} f(\mathbf{y}).$$

A discrete gradient cannot simply be constructed from independently defined discrete approximations of the partial derivatives, because an important relation must be imposed on the components: all discrete gradients are required to satisfy the

Discrete (Multivariable) Chain Rule

$$\delta f = (\tilde{\nabla}_{\mathbf{y}} f)(\mathbf{y}, \mathbf{y}^+) \cdot \delta \mathbf{y}, \quad = \sum_n (\tilde{D}_n f)(\mathbf{y}, \mathbf{y}^+) \delta y_n. \quad (29)$$

A suitable discrete Jacobian $(\tilde{D}_{\mathbf{y}} \mathbf{f})(\mathbf{y}, \mathbf{y}^+)$ for a vector-valued function \mathbf{f} is then given by combining discrete gradients of each component function of \mathbf{f} .

Conservation of Energy

Conservation of energy is easily shown, by mimicking the argument used above for a (continuous time) Hamiltonian system:

$$\begin{aligned}
\frac{\delta \mathcal{H}}{\delta t} &= (\tilde{\nabla}_{\mathbf{y}} \mathcal{H})(\mathbf{y}, \mathbf{y}^+) \cdot \frac{\delta \mathbf{y}}{\delta t} \\
&= (\tilde{\nabla}_{\mathbf{y}} \mathcal{H})(\mathbf{y}, \mathbf{y}^+) \cdot \mathcal{J}(\tilde{\nabla}_{\mathbf{y}} \mathcal{H})(\mathbf{y}, \mathbf{y}^+) \\
&= 0.
\end{aligned}$$

Choosing a Discrete Gradient

There are infinitely many choices of discrete gradient satisfying this chain rule condition. (Generically: if you choose all but one component, the chain rule determines the value of that last component.)

The challenge, as with variational methods, is to choose a discrete gradient that gives *conservation of invariants*: the new strategy here is to choose a discrete gradient that allows verification of conservation by **mimicking the calculations that work for differential equations**, as was just done for conservation of energy.

There seems to be no universal way to do this, with the problem in particular being that

associativity of products cannot be respected

so that triple products cannot be handled in a canonical way.

On the other hand, there is a canonical approach if one avoids triple products, and this leads again to the familiar result that

quadratic and linear invariants can be handled,

but not in general invariants of other forms.

For a wide range of systems arising from physical problems, this is enough.

Difference Calculus for Functions of One Variable

For functions $f(x)$ of a single variable, the discrete multivariable chain rule dictates a simple and familiar difference scheme:

$$\tilde{D}_x f(x, x^+) := \begin{cases} \frac{\delta f}{\delta x}, & x^+ \neq x \\ \frac{df}{dx}(x), & x^+ = x. \end{cases} \quad (30)$$

That is, the standard centered difference approximation, with the exact derivative used when needed.

This approximation is at best second order accurate, and leads to the basic discrete gradient method being second order accurate, as for the implicit midpoint method. However, *symmetric step composition methods* can be used to construct higher order methods.

Avoiding Division By Zero

A greater problem is that this will be used with x^+ unknown, so it is unknown which of the two forms above applies.

Thus it is highly desirable (but not quite essential) to simplify the first form so as to eliminate division by δx , to get a universally valid formula.

To start with, this is possible for natural number powers with

$$\tilde{D}_x(x^r)(x, x^+) = \frac{\delta(x^r)}{\delta x} = (x)^{r-1} + (x)^{r-2}(x^+) + \cdots + (x^+)^{r-1}.$$

Linear Combinations, Compositions, and Inverses

Sums and constant factors are naturally handled by linearity, and there is a canonical choice for a *discrete chain rule* for compositions $(f \circ g)(\mathbf{x})$ with f a function of one variable:

$$\tilde{\nabla}_{\mathbf{y}}(f \circ g)(\mathbf{x}, \mathbf{x}^+) = \tilde{D}_g f(g, g^+) \tilde{\nabla}_{\mathbf{x}} g(\mathbf{x}, \mathbf{x}^+). \quad (31)$$

From this, the inverse of a function of one variable, $y = f^{(-1)}(x)$, is handled as:

$$\tilde{D}_x y = \tilde{D}_x \left(f^{(-1)} \right) (x, x^+) = \frac{1}{(\tilde{D}_y f)(y, y^+)}.$$

Combined with the above result for $f(x) = x^r$ and linearity, all elementary rational functions of one variable can be handled with a single formula, without the special “division by zero” case.

Products: A Little Thought Required at Last

For a product of two factors, the possibilities for a product rule satisfying the discrete chain rule condition include

$$\delta(fg) = \alpha(g\delta f + f^+\delta g) + (1 - \alpha)(g^+\delta f + f\delta g)$$

but the most reasonable choice is $\alpha = 1/2$, which is the only choice that has time-reversal symmetry and respects commutativity of products.

It also has the advantage of giving second order accuracy.

The Time-Symmetric Discrete Product Rule

Thus we use adopt a rule based on decomposing $\delta(fg)$ as

$$\delta(fg) = \bar{g}\delta f + \bar{f}\delta g. \quad (32)$$

That is, for a product $f(\mathbf{x})g(\mathbf{x})$, we adopt the

Discrete Product Rule

$$(\tilde{\nabla}_{\mathbf{x}}(fg))(\mathbf{x}, \mathbf{x}^+) = \bar{g}(\tilde{\nabla}_{\mathbf{x}} f)(\mathbf{x}, \mathbf{x}^+) + \bar{f}(\tilde{\nabla}_{\mathbf{x}} g)(\mathbf{x}, \mathbf{x}^+). \quad (33)$$

For Linear Systems, this is the Implicit Midpoint Rule, and so is Unconditionally Stable

For linear systems, the Hamiltonian is quadratic and so this leads to the implicit midpoint method.

Thus, any choice of discrete gradient method following these rules will have the unconditional stability of the midpoint method.

Non-Associativity of the Product Rule

For products of more than two factors, it is impossible to construct a generally applicable rule. If one applies the rule above to product uvw via the various factorizations $u(vw)$, $(uv)w$, $v(uw)$ etc., one gets different results, with different consequences for conservation of invariants.

Also, symmetrizations such as averaging over all alternatives do not necessarily give a form that respects the symmetries and conservation laws of the Hamiltonian.

This is a Calculus for Formulas, not Functions

Instead, the approach here is limited to handling conservation laws whose verification only depends on the handling of terms involving at most products of two variables — specifically, the invariant quadratic (or linear) combinations of state variables noted above.

This means that:

**the difference calculus defined here applies to formulas,
with the order of evaluation of all operations specified.**

Theorem 2. *If a Hamiltonian system (6)*

- (a) *has a collection of conserved quadratic invariants (depending only on state variables), and*
- (b) *the associated symmetry group of the Hamiltonian consists of affine transformations of the variables, and(?)*
- (c) *the Hamiltonian is “manifestly invariant” in that it can be expressed entirely in terms of quadratic combinations $\hat{y}_a(\mathbf{y})$ of the original variables that are invariant under this symmetry group*

$$\mathcal{H}(\mathbf{y}) = \hat{\mathcal{H}}(\hat{\mathbf{y}}(\mathbf{y})) \quad (34)$$

then we get a time discretization that conserves these invariants by using the discrete gradient given by applying the discrete chain rule (31) to formula (34).

A Conservative Discrete Gradient Scheme

The resulting time-stepping method is

$$\frac{\mathbf{y}^+ - \mathbf{y}}{h} = \mathcal{J}(\tilde{\nabla}_{\hat{\mathbf{y}}} \hat{\mathcal{H}})(\hat{\mathbf{y}}, \hat{\mathbf{y}}^+) \cdot (\tilde{D}_{\mathbf{y}} \hat{\mathbf{y}})(\mathbf{y}, \mathbf{y}^+). \quad (35)$$

Note:

- The choice of the discrete gradient $(\tilde{\nabla}_{\hat{\mathbf{y}}} \hat{\mathcal{H}})(\hat{\mathbf{y}}, \hat{\mathbf{y}}^+)$ in the first factor does not matter.
- The second factor $(\tilde{D}_{\mathbf{y}} \hat{\mathbf{y}})(\mathbf{y}, \mathbf{y}^+)$ is determined by the discrete product rule and linearity, through terms like

$$\tilde{D}_{y_a}(y_a y_b) = \bar{y}_b \quad (a \neq b), \quad \tilde{D}_{y_a}((y_a)^2) = 2\bar{y}_a.$$

Thus the formula for $(\tilde{D}_{\mathbf{y}} \hat{\mathbf{y}})(\mathbf{y}, \mathbf{y}^+)$ comes from the formula for the exact Jacobian $\tilde{D}_{\mathbf{y}} \hat{\mathbf{y}}(\mathbf{y})$ through the substitution $\mathbf{y} \rightarrow \bar{\mathbf{y}}$.

Proof Idea

The main idea in the proof of this result is that for any conserved quantity $Q(\mathbf{y})$ of the ODE system that is quadratic in the state variables y_j ,

$$\frac{dQ}{dt} = D_{\mathbf{y}}Q(\mathbf{y}) \cdot \mathcal{J}D_{\hat{\mathbf{y}}}\hat{\mathcal{H}} \cdot D_{\mathbf{y}}\hat{\mathbf{y}} = 0 \quad (36)$$

and this fact does not depend on the details of the function $\hat{\mathcal{H}}$.

Why? Because any choice of $\hat{\mathcal{H}}$ gives a Hamiltonian $\mathcal{H}(\mathbf{y})$ with the required symmetry properties and thus makes Q a conserved quantity, so that the above equation is true. The result depends only on the terms $D_{\mathbf{y}}Q(\mathbf{y})$ and $D_{\mathbf{y}}\hat{\mathbf{y}}$, which are linear in the y_j .

With $\delta Q/\delta t$ for the discrete gradient scheme, the only change in these linear gradient terms is the substitution $y_j \rightarrow \bar{y}_j$, which is merely a “renaming”, and does not affect the validity of the identity:

$$\frac{\delta Q}{\delta t} = 0,$$

so $Q(\mathbf{y})$ is conserved by the time-discrete system.

Example: the LaBudde-Greenspan Method

This method can be applied to the central force particle system of Hamiltonian (26)

by rewriting each potential term as $U_{n,m} = W_{n,m}(\|q_n - q_m\|^2)$. Because then, the Hamiltonian is expressed entirely in terms of the quadratic combinations

$$\begin{aligned} \|q_n - \mathbf{q}_m\|^2 &= (q_{n,1} - \mathbf{q}_{m,1})^2 + (q_{n,2} - \mathbf{q}_{m,2})^2 + (q_{n,3} - \mathbf{q}_{m,3})^2, \\ \|\mathbf{p}_n\|^2 &= (\mathbf{p}_{n,1})^2 + (\mathbf{p}_{n,2})^2 + (\mathbf{p}_{n,3})^2 \end{aligned}$$

which are invariant under the rotational and translation symmetries associated with angular and linear momentum.

The resulting method is that of [LaBudde, Greenspan:1976] and [Simo et al:1992].

4.3 Practical Implementation: an Iterative Solution Method**A Linearly Implicit Iterative Scheme for Solving Discrete Gradient Systems**

The system of equations will be nonlinear (unless the Hamiltonian system itself is linear), so we need an iterative solution method.

The following method preserves the linear stability properties and exact momentum conservation:

- Set $\mathbf{y}^{(0)} = \mathbf{y}$ (or an approximation of \mathbf{y}^+ by some A-stable method)
- Construct successive approximations $\mathbf{y}^{(k)}$ of \mathbf{y}^+ by solving

$$\mathbf{y}^{(k+1)} - \mathbf{y} = h\mathcal{J}(\tilde{\nabla}_{\hat{\mathbf{y}}}\hat{\mathcal{H}})(\hat{\mathbf{y}}, \hat{\mathbf{y}}^{(k)}) \cdot (\tilde{D}_{\mathbf{y}}\hat{\mathbf{y}})(\mathbf{y}, \mathbf{y}^{(k+1)}). \quad (37)$$

That is, the nonlinear part $\tilde{\nabla}_{\hat{\mathbf{y}}}\hat{\mathcal{H}}$ is approximated using the current best available approximation $\mathbf{y}^{(k)}$ of \mathbf{y}^+ , while the linear terms are left in terms of the unknown $\mathbf{y}^{(k+1)}$ to be solved for.

Exact Conservation of Quadratic Invariants at Each Iteration

This equation is linear in the unknown $\mathbf{y}^{(k+1)}$, making its solution straightforward, and much as above, we have:

Theorem 3. *Each iterate $\mathbf{y}^{(k)}$ given by the above iterative scheme conserves all quadratic first integrals that are conserved by the original discrete gradient scheme (35).*

The key is again the irrelevance of the form of the approximation of $\tilde{D}_{\hat{\mathbf{y}}} \hat{\mathcal{H}}$, which is the only term that changes between the original scheme and this iterative scheme.

Unconditional Linear Stability

Another advantage of this approach to iterative solution is that it has unconditional linear stability, since for a linear system, $\tilde{D}_{\hat{\mathbf{y}}} \hat{\mathcal{H}}$ is constant, the scheme converges in a single iteration, and is the unconditionally stable implicit midpoint method.

This second order accuracy after one iteration for linear systems is seen in practice to carry over in part to mildly nonlinear systems: for various test cases, the accuracy at each iteration is about what one would expect with one more iteration of a standard explicit predictor-corrector approach.

Energy Conservation: Only in the Limit $k \rightarrow \infty$

Energy however is only conserved in the limit as the iterates $\mathbf{y}^{(k)}$ converge to \mathbf{y}^+ .

However, assuming this convergence, sufficient iterations will give energy accuracy far greater than for a scheme that does not conserve energy, such as a symplectic scheme.

Iterating until energy is accurate within rounding error is typically practical: if this take too many iterations, it is better for overall accuracy to reduce the time step size h to speed the convergence.

Handling General Elementary Function Hamiltonians

When this iterative method is applied for a non-algebraic Hamiltonian, the difficulties noted above with the definition of $(\tilde{D}_x)f(x, x^+)$ in (30) at each iteration, and this depends only on the already-known quantities y and $y^{(k)}$. Thus one knows whether to use the difference quotient form or the exact derivative at each iteration.

More carefully, the exact derivative should be used if the relevant denominator is smaller than some threshold related to rounding error.

The methods seen so far are only second order accurate in time.

Fortunately, the method of *symmetric step composition* [Creutz,Gocksch:1989, Forest:1989, Suzuki:1990, Yoshida:1990] gives a systematic way to construct methods of any higher even order while preserving all the interesting properties: conservation of quadratic invariants, time-reversal symmetry, and symplectic form.

The idea is to start with a basic symmetric time-stepping method and construct a composite step from a sequence of s basic steps, of lengths

$$\beta_1 h, \dots, \beta_s h.$$

The obvious consistency condition is that

$$\beta_1 + \dots + \beta_s = 1.$$

If in addition the basic method is of even order p then choosing the *step size factors* β_i with

$$\beta_1^{p+1} + \dots + \beta_s^{p+1} = 0$$

and the symmetry condition

$$\beta_{s+1-i} = \beta_i, \quad 1 \leq i \leq s$$

ensures that the composite step is also time-reversal symmetric, and of even order $p + 2$.

The process can then be repeated, constructing composites of composite steps to achieve arbitrarily high order.

The Triple-Jump and Suzuki Fractal Methods

The simplest such method is the *triple-jump*, with three steps:

$$\beta_1 = \beta_3 = \frac{1}{2 - 2^{1/p+1}}, \quad \beta_2 = 1 - 2\beta_1 = \frac{2^{1/p+1}}{2 - 2^{1/p+1}}.$$

Unfortunately, the steps go out of the range from t_τ to $t_{\tau+1}$, as all step size factors are greater than one in magnitude.

For example, with $p = 2$ as for the midpoint method, $\beta_1 \approx 1.35$ and $\beta_2 \approx -1.70$.

Thus a better approach is the five-step *Suzuki fractal method*, where all $|\beta_i| < 1$:

$$\beta_1 = \beta_2 = \beta_4 = \beta_5 = \frac{1}{4 - 4^{1/p+1}}, \quad \beta_3 = 1 - 4\beta_1 = \frac{4^{1/p+1}}{4 - 4^{1/p+1}}.$$

For $p = 2$, the factors are $\beta_1 \approx 0.41$, $\beta_2 \approx -0.66$.

5 Numerical Results

We conclude with a few numerical results, to first test the method, and then make one novel observation about continuum limits of DNLS equations.

5.1 Testing With The Non-Locally Nonlinear DNLS

Testing With The Non-Locally Nonlinear DNLS

For a comparison of the discrete gradient method to the popular symplectic implicit midpoint method, illustrating some advantages for the discrete gradient method in preserving qualitative features of solutions, the equations solved are the nonlocal discrete nonlinear Schrödinger equation (5)

As mentioned before, a continuum limit approximation of assuming slow variation along the chain leads to the cubic focusing nonlinear Schrödinger equation

$$i \frac{\partial z}{\partial t} + \frac{\partial^2 z}{\partial x^2} + 2|z|^2 z = 0$$

with solutions including the hyperbolic secant solitons

$$\psi(t, x) = A \operatorname{sech}(A(x - vt)) \exp \left[-\frac{i}{2}(vx - (v^2/4 - A^2)t) \right].$$

so initial data is chosen to see how closely solutions of the DNLS system resemble these solitons. Specifically, initial data is of the form above except of double the height, so that in NLS a soliton plus other radiation is expected to develop.

However, accuracy is tested without relying on the continuum limit, but comparing to an effectively exact solution computed by using time step so small that further reduction produces no visible change, and the results agree between methods.

5.2 A Different Continuum Limit for the Helical DNLS Model

Results for Helical DNLS Model

The final numerical results are for Helical DNLS Model with impulsive initial data at one end of the molecular chain,

$$z_1(0) = 1, \quad z_n(0) = 0 \text{ for } n > 1.$$

Results for Helical DNLS Model

The final numerical results show that with impulsive initial data at one end of the molecular chain, the Helical discrete nonlinear Schrödinger equation model does not produce pulses resembling sech solitons, but instead pulses with a different possible continuum limit for $i^n z_n(t)$.

The corresponding PDE approximation is then a “complex nonlinear Airy PDE”

$$\frac{\partial z}{\partial t} = \frac{\partial^3 z}{\partial x^3} + 2i|z|^2 z.$$

Question: Does any one here know anything about solutions of this equation?!

6 Some Plans and Questions

1. Implement the fourth-order Gauss method, a fourth order symplectic diagonally implicit Runge-Kutta method, and the two fourth order discrete gradient methods given by the triple jump and Suzuki fractal methods for this system, and repeat the comparisons made here.
2. Study other systems, such as 2D lattice equations from models of thin bio-molecular films, and multiple-core fiber optics models.
3. Add small dispersion while retaining correct conservation of charge and accurate evolution of energy. (E.g. split-step approaches.)
4. Add fixed pattern noise and stochastic terms.
5. Find out about the new continuum limit equation

$$\frac{\partial z}{\partial t} = \frac{\partial^3 z}{\partial x^3} + 2i|z|^2 z.$$

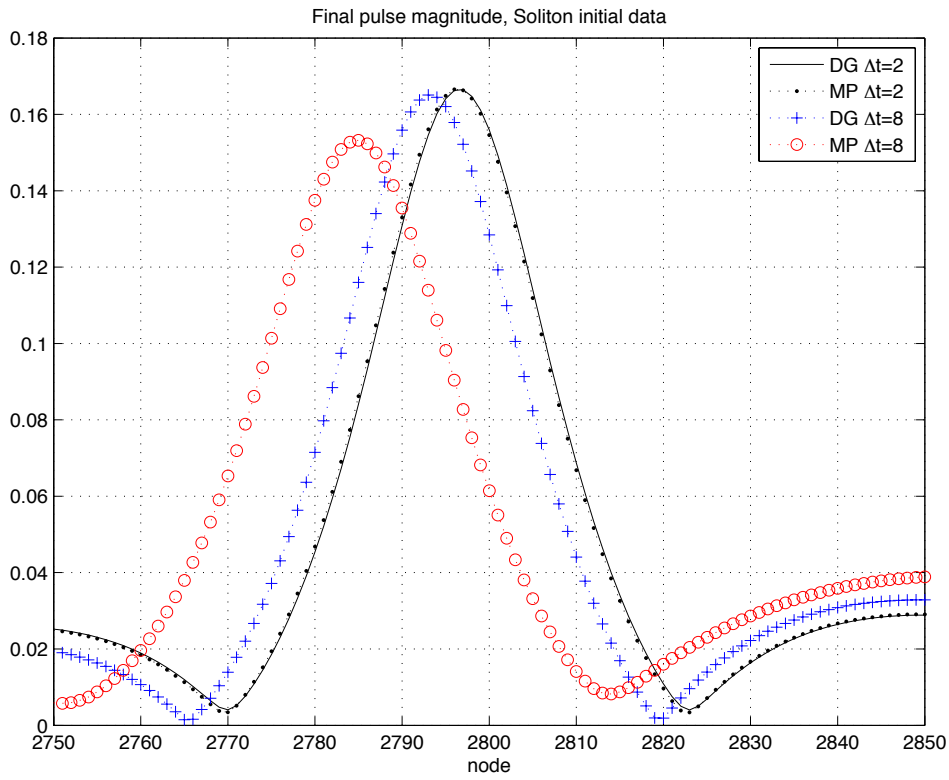


Figure 1: NLDNLS, $A = 2$: $|z_n|$ at time $t = 40000$.

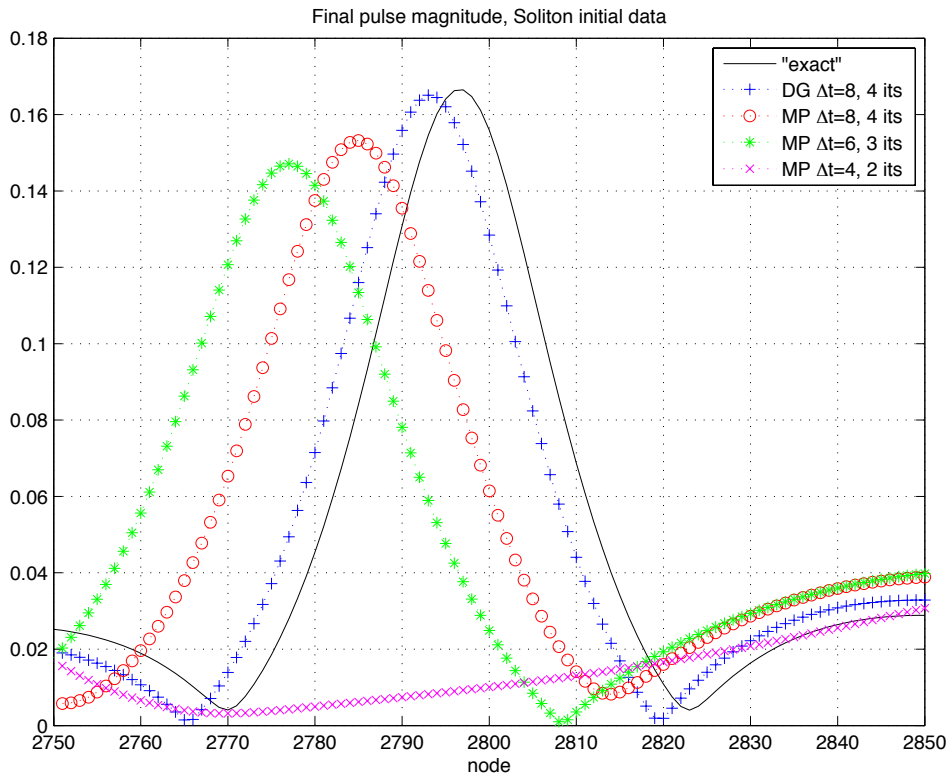


Figure 2: NLDNLS, $A = 2$: $|z_n|$ at time $t = 40000$, methods of roughly equal time cost.

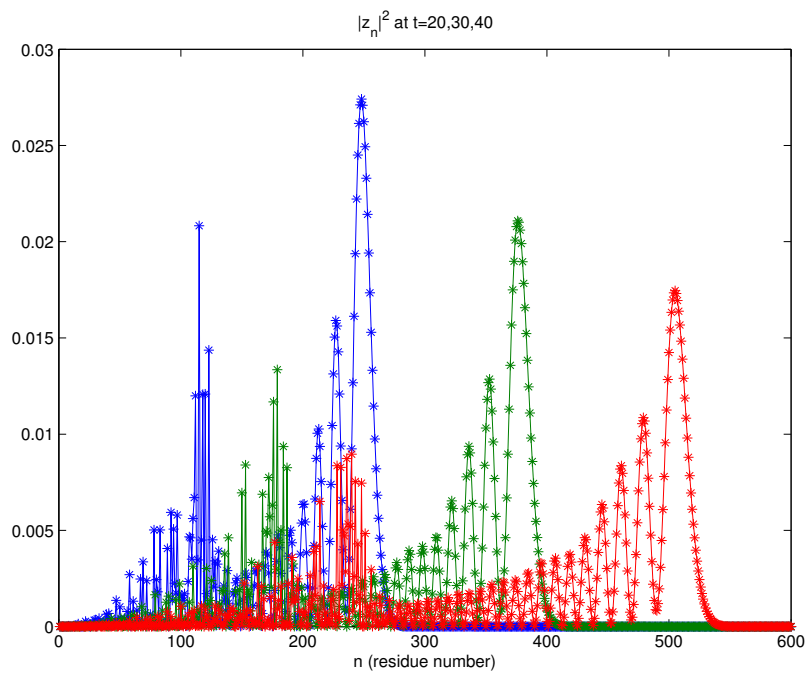


Figure 3: HDNLS: $|z_n|^2$ at time $t = 20, 30, 40$.

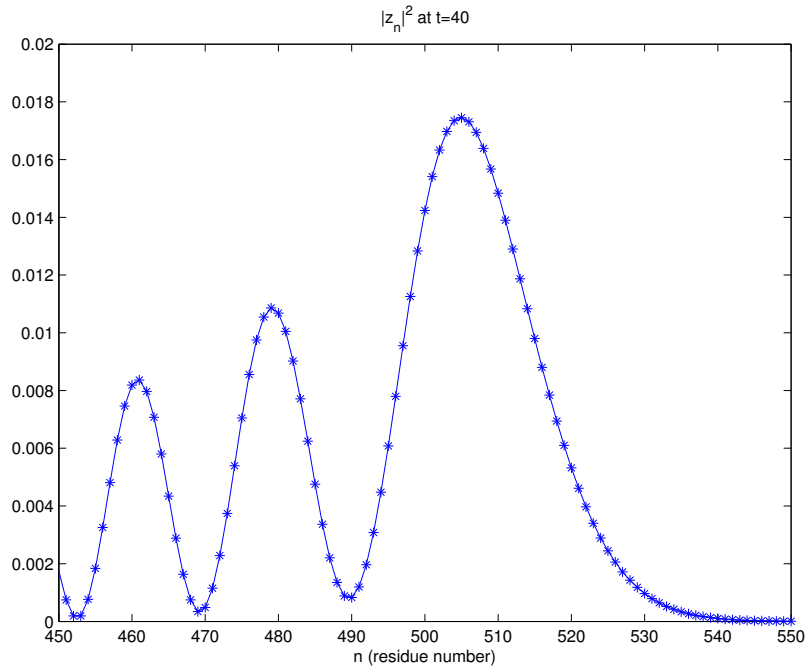


Figure 4: HDNLS: $|z_n|^2$ at time $t = 20, 30, 40$, near main pulse — a continuum limit?

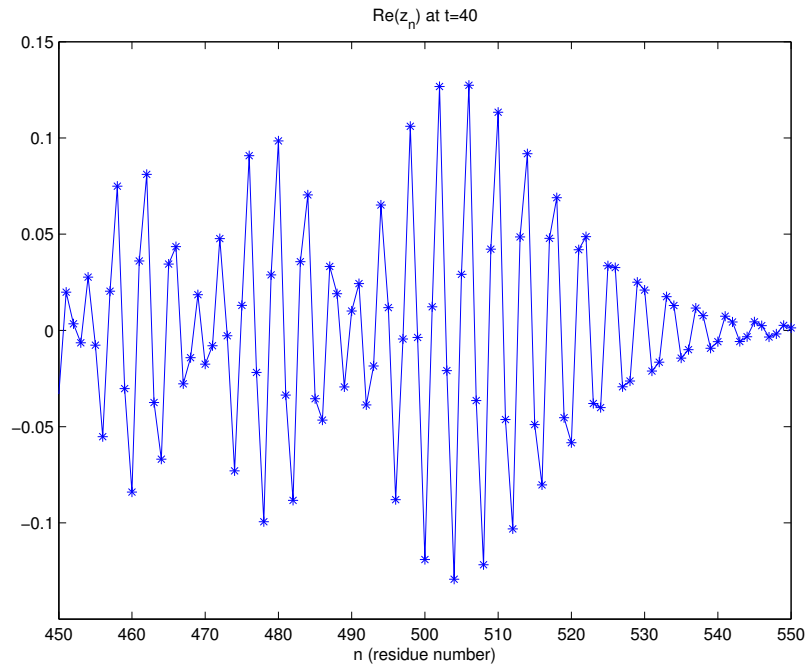


Figure 5: HDNLS: $\text{Re}(z_n)$ at time $t = 40$ — no continuum limit!

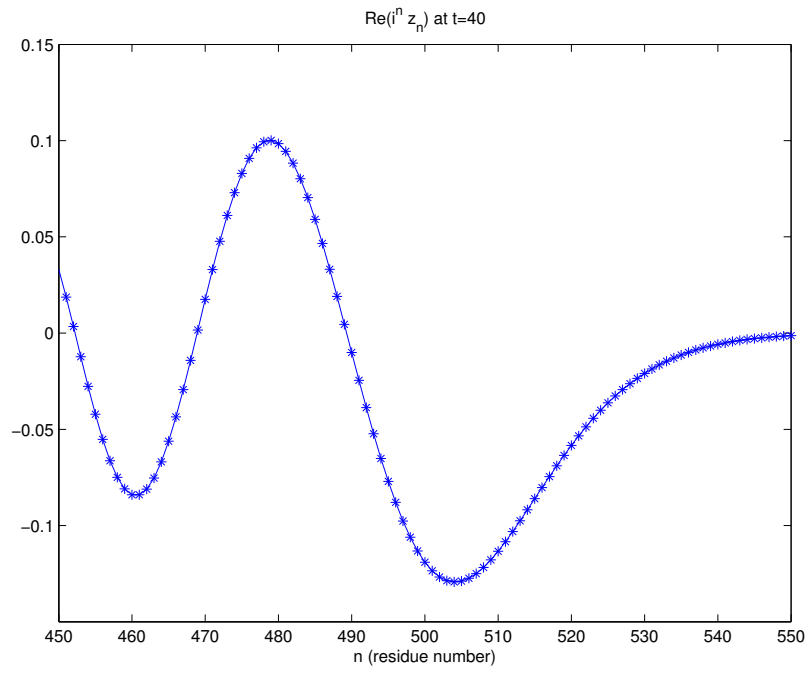


Figure 6: HDNLS: $\text{Re}(i^n z_n)$ at time $t = 40$: — maybe a continuum limit now.

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