Implicit-explicit variational integration of highly oscillatory problems*

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The Problem: Multiple Time Scales vs. Numerical Integrators

Many systems in Lagrangian mechanics have components acting on different time scales, for example:

1. *Elasticity:* Several spatial elements of varying stiffness, resulting from irregular meshes and/or inhomogeneous materials.
2. *Planetary Dynamics:* N-body problem with nonlinear gravitational forces, arising from pairwise inverse-square potentials. Multiple time scales result from the different distances between the bodies, mass ratios, etc.
3. *Highly Oscillatory Problems:* Potential energy can be split into a "fast" linear oscillatory component and a "slow" nonlinear component. These problems are widely encountered in modeling molecular dynamics, but have also been used to model other diverse applications, for example, in computer animation.

Existing methods tend to waste too much computational effort evaluating the non-stiff forces (e.g., Störmer/Verlet, implicit midpoint) or suffer from resonance instability problems (e.g., Verlet-I/r-RESPA, AVI, many trigonometric integrators).

Can we develop geometric numerical integrators that are *stable* with respect to the stiff forces, but still *efficient* with respect to the non-stiff forces?

Review: The Discrete Lagrangian and Action Sum

Suppose we have a mechanical system on a configuration manifold Q, specified by a Lagrangian $L\colon TQ \to \mathbb{R}$. Given a set of discrete time points $t_0 < \cdots < t_N$ with uniform step size h, we wish to compute a numerical approximation $q_n \approx q\left(t_n\right),\ n = 0, \ldots, N$, to the continuous trajectory $q(t)$.

To construct a variational integrator for this problem, we define a *discrete Lagrangian* $L_h\colon Q \times Q \to \mathbb{R}$, replacing tangent vectors by pairs of consecutive configuration points, so that in some sense we have the approximation

$$L_h\left(q_n, q_{n+1}\right) \approx \int_{t_n}^{t_{n+1}} L\left(q, \dot{q}\right)\, dt.$$

Then the action integral over $[t_0, t_N]$ is approximated by the *discrete action sum*

$$S_h[q] = \sum_{n=0}^{N-1} L_h\left(q_n, q_{n+1}\right) \approx \int_{t_0}^{t_N} L\left(q, \dot{q}\right)\, dt.$$

Review: The Discrete Euler–Lagrange Equations and Legendre Transform

If we apply Hamilton's principle to this action sum, so that $\delta S_h[q] = 0$ for fixed-endpoint variations, then this yields the *discrete Euler–Lagrange equations*

$$D_1 L_h (q_n, q_{n+1}) + D_2 L_h (q_{n-1}, q_n) = 0, \qquad n = 1, \ldots, N-1,$$

where D_1 and D_2 denote partial differentiation in the first and second arguments, respectively. This defines a two-step numerical method on $Q \times Q$, mapping $(q_{n-1}, q_n) \mapsto (q_n, q_{n+1})$.

The equivalent one-step method on the cotangent bundle T^*Q, mapping $(q_n, p_n) \mapsto (q_{n+1}, p_{n+1})$, is defined by the *discrete Legendre transform*

$$p_n = -D_1 L_h (q_n, q_{n+1}), \qquad p_{n+1} = D_2 L_h (q_n, q_{n+1}),$$

where the first equation updates q, and the second updates p. Here, L_h is a *generating function* for the symplectic map $(q_n, p_n) \mapsto (q_{n+1}, p_{n+1})$.

Review: The Trapezoidal and Midpoint Discrete Lagrangians

Consider a Lagrangian of the form

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

where $Q = \mathbb{R}^d$, M is a constant $d \times d$ mass matrix, and $V \colon Q \to \mathbb{R}$ is a potential.

If we use linear interpolation of q with trapezoidal quadrature to approximate the contribution of V to the action integral, we get

$$L_h^{\text{trap}}(q_n, q_{n+1}) = \frac{h}{2}\left(\frac{q_{n+1} - q_n}{h}\right)^T M \left(\frac{q_{n+1} - q_n}{h}\right) - h\frac{V(q_n) + V(q_{n+1})}{2},$$

which we call the *trapezoidal discrete Lagrangian*. It is straightforward to see that the discrete Euler–Lagrange equations for L_h^{trap} correspond to the explicit Störmer/Verlet method.

Alternatively, if we use midpoint quadrature to approximate the integral of the potential, this yields the *midpoint discrete Lagrangian*,

$$L_h^{\text{mid}}(q_n, q_{n+1}) = \frac{h}{2}\left(\frac{q_{n+1} - q_n}{h}\right)^T M \left(\frac{q_{n+1} - q_n}{h}\right) - hV\left(\frac{q_n + q_{n+1}}{2}\right),$$

for which the resulting integrator is the implicit midpoint method.

The IMEX Discrete Lagrangian

Suppose that we have a Lagrangian of the form

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

where U is a slow potential and W is a fast potential, for the configuration space $Q = \mathbb{R}^d$.

Define the *IMEX discrete Lagrangian*

$$L_h^{\mathsf{IMEX}}(q_n, q_{n+1}) = \frac{h}{2}\left(\frac{q_{n+1} - q_n}{h}\right)^T M \left(\frac{q_{n+1} - q_n}{h}\right) - h\frac{U(q_n) + U(q_{n+1})}{2} - hW\left(\frac{q_n + q_{n+1}}{2}\right),$$

using (explicit) trapezoidal approximation for the slow potential and (implicit) midpoint approximation for the fast potential.

The discrete Euler–Lagrange equations give a two-step variational integrator on $Q \times Q$,

$$q_{n+1} - 2q_n + q_{n-1} = -h^2 M^{-1}\left[\nabla U(q_n) + \frac{1}{2}\nabla W\left(\frac{q_{n-1} + q_n}{2}\right) + \frac{1}{2}\nabla W\left(\frac{q_n + q_{n+1}}{2}\right)\right].$$

The IMEX Algorithm on T^*Q

The discrete Legendre transform for the IMEX discrete Lagrangian is

$$p_n = M\left(\frac{q_{n+1} - q_n}{h}\right) + \frac{h}{2}\nabla U\left(q_n\right) + \frac{h}{2}\nabla W\left(\frac{q_n + q_{n+1}}{2}\right),$$

$$p_{n+1} = M\left(\frac{q_{n+1} - q_n}{h}\right) - \frac{h}{2}\nabla U\left(q_{n+1}\right) - \frac{h}{2}\nabla W\left(\frac{q_n + q_{n+1}}{2}\right).$$

If we introduce the intermediate stages,

$$p_n^+ = p_n - \frac{h}{2}\nabla U\left(q_n\right), \qquad p_{n+1}^- = p_{n+1} + \frac{h}{2}\nabla U\left(q_{n+1}\right),$$

then this gives us the following impulse-type integration algorithm:

Step 1: $$p_n^+ = p_n - \frac{h}{2}\nabla U\left(q_n\right),$$ (explicit kick)

Step 2: $$\begin{cases} q_{n+1} = q_n + hM^{-1}\left(\dfrac{p_n^+ + p_{n+1}^-}{2}\right), \\ p_{n+1}^- = p_n^+ - h\nabla W\left(\dfrac{q_n + q_{n+1}}{2}\right), \end{cases}$$ (implicit midpoint)

Step 3: $$p_{n+1} = p_{n+1}^- - \frac{h}{2}\nabla U\left(q_{n+1}\right).$$ (explicit kick)

Application to Highly Oscillatory Problems

For highly oscillatory problems on $Q = \mathbb{R}^d$, we start by taking a quadratic fast potential

$$W(q) = \frac{1}{2} q^T \Omega^2 q, \qquad \Omega \in \mathbb{R}^{d \times d} \text{ symmetric and positive semidefinite.}$$

A prototypical Ω is given by the block-diagonal matrix

$$\Omega = \begin{pmatrix} 0 & 0 \\ 0 & \omega I \end{pmatrix}, \qquad \omega \gg 1,$$

where some of the degrees of freedom are subjected to an oscillatory force with constant fast frequency ω.

We also denote the slow force $g(q) = -\nabla U(q)$ and assume, without loss of generality, that the constant mass matrix is given by $M = I$. Therefore, the nonlinear system we wish to approximate numerically is

$$\ddot{q} + \Omega^2 q = g(q).$$

IMEX as Störmer/Verlet with a Modified Mass Matrix

Applying the IMEX method to this example, we get the discrete Lagrangian

$$L_h^{\mathsf{IMEX}}(q_n, q_{n+1}) = \frac{h}{2}\left(\frac{q_{n+1}-q_n}{h}\right)^T\left(\frac{q_{n+1}-q_n}{h}\right) - h\frac{U(q_n)+U(q_{n+1})}{2} - h\left(\frac{q_n+q_{n+1}}{2}\right)^T\Omega^2\left(\frac{q_n+q_{n+1}}{2}\right),$$

and so the two-step IMEX scheme is given by the discrete Euler–Lagrange equations

$$q_{n+1} - 2q_n + q_{n-1} + \frac{h^2}{4}\Omega^2(q_{n+1}+2q_n+q_{n-1}) = h^2 g(q_n).$$

Rearranging terms, we can rewrite this as

$$\left[I + \frac{h^2}{4}\Omega^2\right](q_{n+1}-2q_n+q_{n-1}) + h^2\Omega^2 q_n = h^2 g(q_n),$$

which is equivalent to Störmer/Verlet with a modified mass matrix $I + (h\Omega/2)^2$.

The Discrete Lagrangian and Modified Mass Matrix

Proposition. *Suppose we have a Lagrangian* $L(q,\dot q) = \frac{1}{2}\dot q^T M \dot q - \frac{1}{2} q^T \Omega^2 q$ *and its corresponding midpoint discrete Lagrangian* L_h^{mid}*. Next, define the modified Lagrangian* $\widetilde{L}(q,\dot q) = \frac{1}{2}\dot q^T \widetilde{M} \dot q - \frac{1}{2} q^T \Omega^2 q$*, having the same quadratic potential but a different mass matrix* $\widetilde{M}$*, and take its trapezoidal discrete Lagrangian* $\widetilde{L}_h^{trap}$*. Then* $L_h^{mid} \equiv \widetilde{L}_h^{trap}$ *when* $\widetilde{M} = M + (h\Omega/2)^2$*.*

Proof. The midpoint discrete Lagrangian is given by

$$L_h^{\text{mid}}(q_n, q_{n+1}) = \frac{h}{2}\left(\frac{q_{n+1}-q_n}{h}\right)^T M \left(\frac{q_{n+1}-q_n}{h}\right) - \frac{h}{2}\left(\frac{q_n+q_{n+1}}{2}\right)^T \Omega^2 \left(\frac{q_n+q_{n+1}}{2}\right).$$

Now, notice that we can rearrange the terms

$$\begin{aligned}
&-\left(\frac{q_n+q_{n+1}}{2}\right)^T \Omega^2 \left(\frac{q_n+q_{n+1}}{2}\right) \\
&\qquad = \left(\frac{q_{n+1}-q_n}{2}\right)^T \Omega^2 \left(\frac{q_{n+1}-q_n}{2}\right) - \frac{1}{2} q_n^T \Omega^2 q_n - \frac{1}{2} q_{n+1}^T \Omega^2 q_{n+1} \\
&\qquad = \left(\frac{q_{n+1}-q_n}{h}\right)^T \left(\frac{h\Omega}{2}\right)^2 \left(\frac{q_{n+1}-q_n}{h}\right) - \frac{1}{2} q_n^T \Omega^2 q_n - \frac{1}{2} q_{n+1}^T \Omega^2 q_{n+1}.
\end{aligned}$$

Therefore the discrete Lagrangian can be written in the trapezoidal form

$$L_h^{\mathrm{mid}}(q_n, q_{n+1}) = \frac{h}{2}\left(\frac{q_{n+1}-q_n}{h}\right)^T \left[M + \left(\frac{h\Omega}{2}\right)^2\right]\left(\frac{q_{n+1}-q_n}{h}\right) - \frac{h}{2}\left(\frac{1}{2}q_n^T\Omega^2 q_n + \frac{1}{2}q_{n+1}^T\Omega^2 q_{n+1}\right),$$

which is precisely $\widetilde{L}_h^{\mathrm{trap}}(q_n, q_{n+1})$ when $\widetilde{M} = M + (h\Omega/2)^2$. □

Corollary. *Consider a highly oscillatory system with an arbitrary slow potential U, quadratic fast potential $W(q) = \frac{1}{2}q^T\Omega^2 q$, and constant mass matrix $M = I$, so that the Lagrangian L and IMEX discrete Lagrangian L_h^{IMEX} are defined as above. Next, take the modified Lagrangian $\widetilde{L}$ with the same potentials but different mass matrix $\widetilde{M}$. Then $L_h^{\mathit{IMEX}} \equiv \widetilde{L}_h^{\mathit{trap}}$ when $\widetilde{M} = I + (h\Omega/2)^2$.*

Analysis of Linear Resonance Stability

For a harmonic oscillator with unit mass and frequency ν, the Störmer/Verlet method is linearly stable if and only if $|h\nu| \leq 2$; for a system with constant mass m and spring constant ν^2, this condition generalizes to $h^2\nu^2 \leq 4m$.

Linear model problem: Let $U(q) = \frac{1}{2}q^T q$, and $W(q) = \frac{1}{2}q^T \Omega^2 q$, where $\Omega = \omega I$ for some $\omega \gg 1$, and again let $M = I$.

Theorem. *The IMEX method is linearly stable, for the system described above, if and only if $h \leq 2$ (i.e., if and only if h is a stable time step size for the slow oscillator alone).*

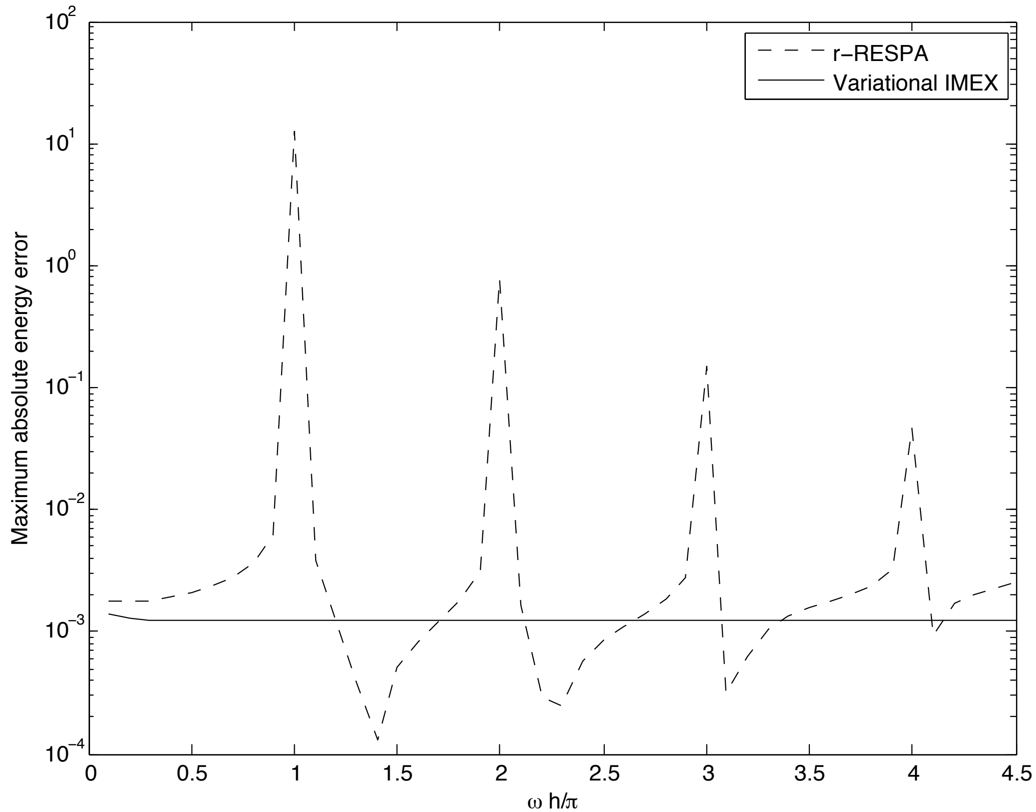
Proof. As proved in the previous section, the IMEX method for this system is equivalent to Störmer/Verlet with the modified mass matrix $I + (h\Omega/2)^2$. Now, this modified oscillatory system has constant mass $m = 1 + (h\omega/2)^2$ and spring constant $\nu^2 = 1 + \omega^2$. Therefore, the necessary and sufficient condition for linear stability is

$$h^2\left(1 + \omega^2\right) \leq 4\left(1 + \frac{h^2}{4}\omega^2\right),$$

and since the $h^2\omega^2$ terms cancel on both sides, this is equivalent to $h^2 \leq 4$, or $h \leq 2$. $\square$

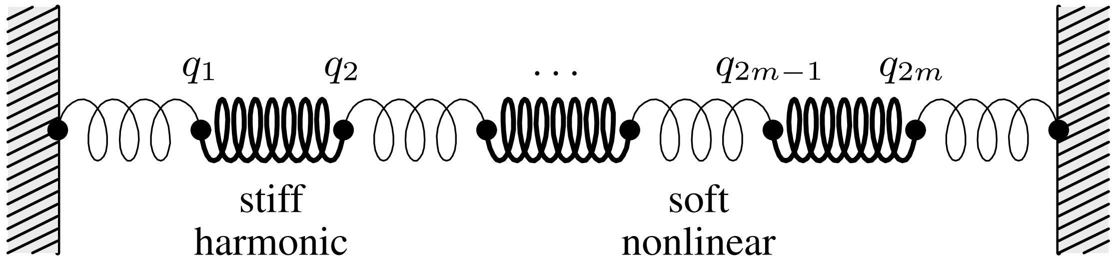
This shows that, in contrast to multiple-time-stepping methods, the IMEX method does not exhibit linear resonance instability.

Numerical Experiment: Coupled Linear Oscillators

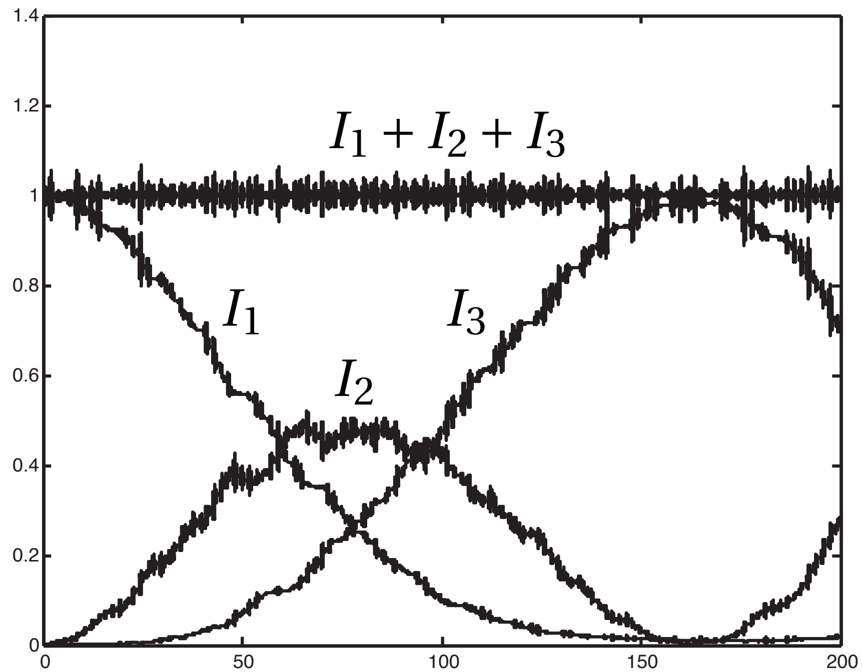


Maximum energy error of r-RESPA and variational IMEX, integrated over the time interval $[0, 1000]$ for a range of parameters ω. The r-RESPA method exhibits resonance instability near integer values of $\omega h/\pi$, while the variational IMEX method remains stable.

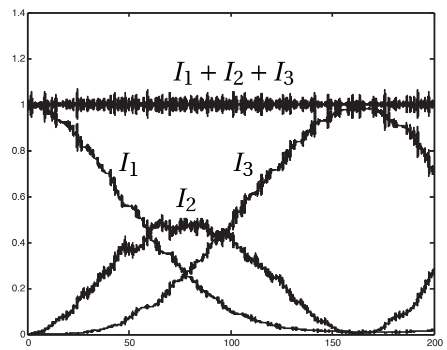
Numerical Experiment: The Fermi–Pasta–Ulam Problem



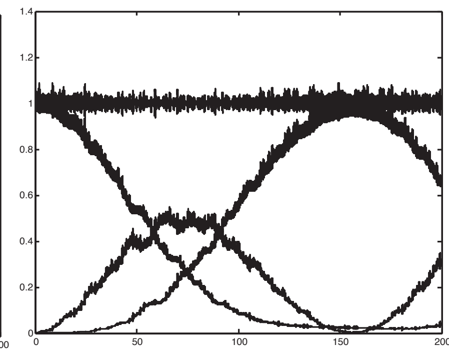
Source: Hairer, Lubich, and Wanner (2006).



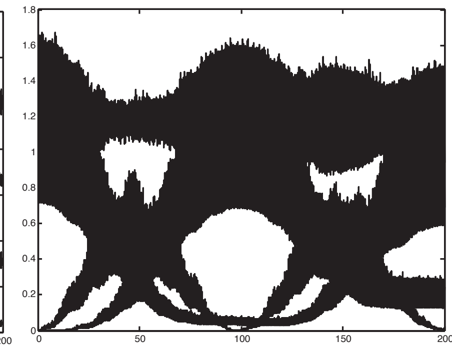
Slow energy exchange among the stiff springs.



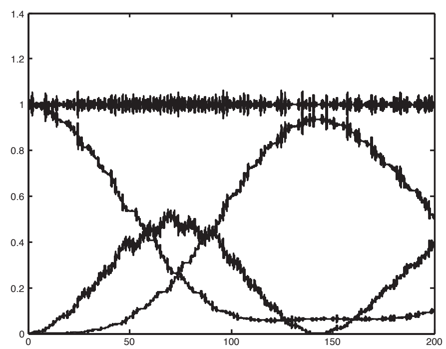
Reference solution: Störmer/Verlet with time step size $h = 0.001$.



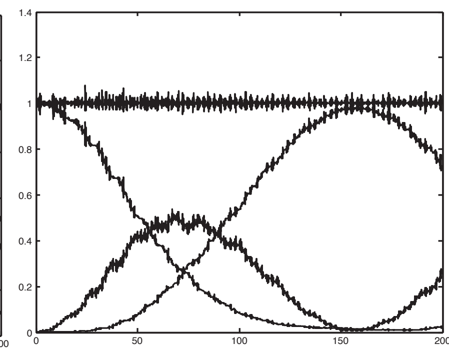
Störmer/Verlet with $h = 0.01$.



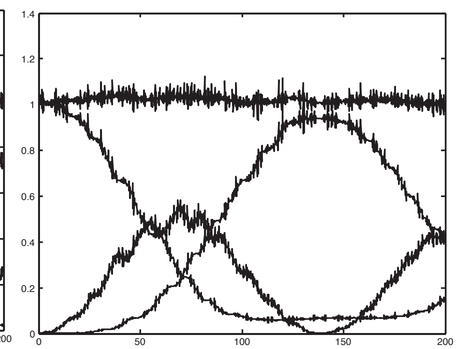
Störmer/Verlet with $h = 0.03$.



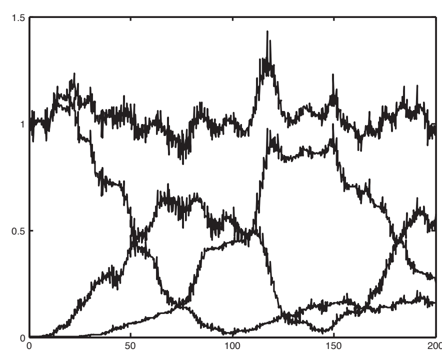
IMEX with $h = 0.03$.



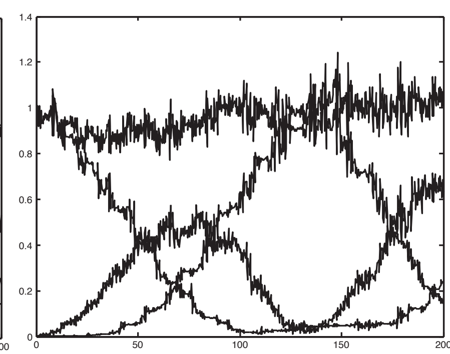
IMEX with $h = 0.1$.



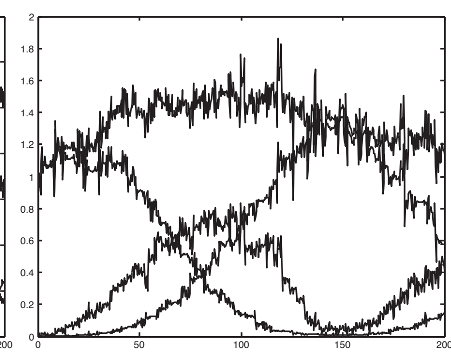
IMEX with $h = 0.15$.



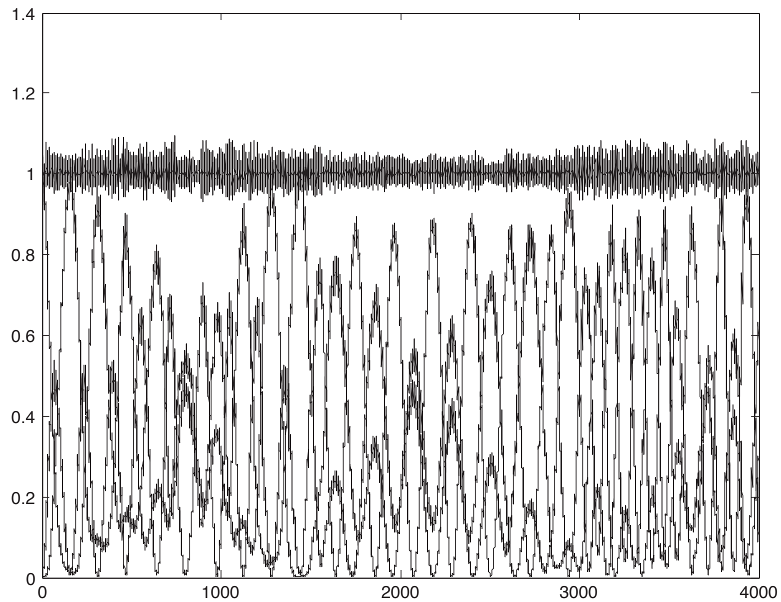
IMEX with $h = 0.2$.



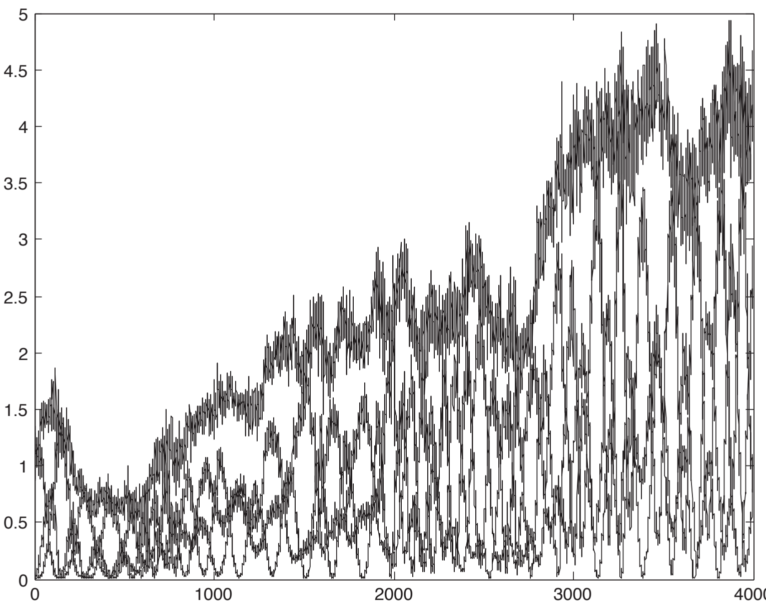
IMEX with $h = 0.25$.



IMEX with $h = 0.3$.



IMEX with $h = 0.1$



IMEX with $h = 0.3$

Numerical simulation of the FPU problem for $T = 4000$, which shows the behavior of the IMEX method on the ω^2 scale. For $h = 0.1$, we already have $h\omega = 5$, yet the oscillatory behavior and adiabatic invariant are qualitatively correct. By contrast, for $h = 0.3$, the method has begun to blow up; oscillatory coupling is a drawback of implicit midpoint methods for large time steps.

Analysis of Slow Energy Exchange

First, let us rewrite the fast oscillatory system $\ddot{q} + \Omega^2 q = 0$ as the first-order system

$$\begin{pmatrix} \Omega\dot{q} \\ \dot{p} \end{pmatrix} = \begin{pmatrix} 0 & \Omega \\ -\Omega & 0 \end{pmatrix} \begin{pmatrix} \Omega q \\ p \end{pmatrix},$$

so it follows that the exact solution satisfies

$$\begin{pmatrix} \Omega q(t+h) \\ p(t+h) \end{pmatrix} = \begin{pmatrix} \cos h\Omega & \sin h\Omega \\ -\sin h\Omega & \cos h\Omega \end{pmatrix} \begin{pmatrix} \Omega q(t) \\ p(t) \end{pmatrix}.$$

Now, in these coordinates, the implicit midpoint method has the expression

$$\begin{pmatrix} I & -h\Omega/2 \\ h\Omega/2 & I \end{pmatrix} \begin{pmatrix} \Omega q_{n+1} \\ p_{n+1} \end{pmatrix} = \begin{pmatrix} I & h\Omega/2 \\ -h\Omega/2 & I \end{pmatrix} \begin{pmatrix} \Omega q_n \\ p_n \end{pmatrix}.$$

Therefore, if we take the skew matrix $A = \begin{pmatrix} 0 & \Omega \\ -\Omega & 0 \end{pmatrix}$, it follows that

$$\begin{pmatrix} \Omega q_{n+1} \\ p_{n+1} \end{pmatrix} = (I - hA/2)^{-1} (I + hA/2) \begin{pmatrix} \Omega q_n \\ p_n \end{pmatrix}.$$

Notice that the expression $(I - hA/2)^{-1} (I + hA/2) = \operatorname{cay} hA$ is the *Cayley transform*.

Implicit Midpoint and Modified Frequency

Because cay and $\exp$ are both maps from $\mathfrak{so}(2d) \to \mathrm{SO}(2d)$, the midpoint method corresponds to a *modified rotation matrix*, where Ω is replaced by $\widetilde{\Omega}$ such that

$$h\Omega/2 = \tan h\widetilde{\Omega}/2$$

This gives another interpretation of the resonance stability when $\Omega = \omega I$ and $\widetilde{\Omega} = \widetilde{\omega} I$. We always have $h\widetilde{\omega} < \pi$, since the Cayley transform maps to a rotation by π only in the limit as $h\omega \to \infty$. Therefore, we never encounter resonance points for finite $h\omega$.

We now write the variational IMEX method as the following modified impulse scheme:

Step 1: $$p_n^+ = p_n - \frac{h}{2}\nabla U\left(q_n\right),$$ (explicit kick)

Step 2: $$\begin{pmatrix} \Omega q_{n+1} \\ p_{n+1}^- \end{pmatrix} = \begin{pmatrix} \cos h\widetilde{\Omega} & \sin h\widetilde{\Omega} \\ -\sin h\widetilde{\Omega} & \cos h\widetilde{\Omega} \end{pmatrix} \begin{pmatrix} \Omega q_n \\ p_n^+ \end{pmatrix},$$ (implicit midpoint)

Step 3: $$p_{n+1} = p_{n+1}^- - \frac{h}{2}\nabla U\left(q_{n+1}\right).$$ (explicit kick)

In other words, the implicit midpoint step doesn't just "smear out" the oscillations—in fact, it *resolves* the oscillations of some modified problem. Because the propagation matrix is still special orthogonal, this does not affect the "fast" energy component.

Consistency of Slow Energy Exchange

Hairer et al. have analyzed the slow energy exchange behavior of impulse methods using *modulated Fourier expansion*. By casting IMEX as a modified impulse method, we were able to use these same techniques to prove the following theorem:

Theorem. *Let the variational IMEX method be applied to the highly oscillatory problem above, and suppose the numerical solution remains bounded. Then the ordinary differential equation [...] describing the slow energy exchange in the numerical solution, is consistent with that for [...] the exact solution; this holds up to order* $\mathcal{O}\left(\omega^{-3}\right)$.

In fact, this is *not* true for either Störmer/Verlet or implicit midpoint—so IMEX is not merely cheaper, but also better for these applications.

The only trigonometric/exponential method sharing this property is Deuflhard/impulse, which also suffers from resonance instability problems.

The most comparable integrators in this respect appear to be multi-force trigonometric methods, but these require at least twice as many force evaluations as IMEX.

Summary

The variational IMEX method is developed by splitting the discrete Lagrangian into slow (explicit) and fast (implicit) components, and applying separate quadrature rules (trapezoidal and midpoint, respectively).

For highly oscillatory problems, this is equivalent to Störmer/Verlet with a modified mass matrix. This leads to unconditional linear stability in the fast modes, and in particular, the absence of linear resonance instability.

The Fermi–Pasta–Ulam example demonstrates that the variational IMEX method does not attain its stability merely by “smoothing out” the fast frequencies, in a way that might destroy the structure of any fast-slow nonlinear coupling. Rather, despite the fact that it does not resolve the fast frequencies, the method is still capable of capturing the complex multiscale interactions seen in the FPU problem.