Variational Implicit-Explicit Integrators: Multiple Time Scales without Resonance Instability

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Abstract

We introduce a variational implicit-explicit (IMEX) integrator for mechanics problems with forces acting on both fast and slow time scales. This differs from traditional IMEX methods, since the splitting is done with respect to the Lagrangian rather than the Euler-Lagrange equations. This guarantees symplecticity and preservation of other geometric structures, as is well known for variational integrators, but which is not generally true for other IMEX methods.

Furthermore, we prove that our IMEX integrator eliminates the problem of numerical resonance instability, exhibited by fully explicit geometric methods such as Verlet-I/r-RESPA and asynchronous variational integrators (AVIs).

Background

Many problems in mechanics, from molecular dynamics to elasticity, require numerical integration of both fast (stiff) and slow (non-stiff) potential forces. For these highly oscillatory problems, the fast force is typically taken to be linear, while the slow force is nonlinear.

This presents a numerical challenge: to ensure stability, the fast force requires us to take small time steps, or to use an implicit integrator. This is ordinarily not too expensive, since the fast force is linear. However, it is prohibitively expensive to use such an integrator for the nonlinear slow force, since this requires a large number of function evaluations and/or a nonlinear solver.

This problem has motivated the development of various "hybrid" integrators, which treat the fast and slow forces separately. There have been two main approaches to doing this:

1. **Multiple Time Stepping:** Use an explicit integrator with a different time step size for each force. These include substepping methods, such as Verlet-I/r-RESPA, as well as asynchronous methods, such as AVIs.
2. **Implicit-Explicit (IMEX) Methods:** Use the same time step for both forces, but integrate the fast force implicitly and the slow force explicitly.

These multiple time stepping methods are all variational integrators [Lew et al., 2003], and hence they preserve geometric structures. However, it can be difficult to ensure numerical stability: it is not sufficient to choose a stable time step for the fast and slow forces individually, as *numerical resonance instability* can arise between the fast and slow scales. This danger is well-known for substepping methods [Biesiadecki and Skeel, 1993], and has been shown to arise even for asynchronous time stepping in AVIs [Fong et al., 2007].

Traditional IMEX methods, on the other hand, are generally not geometric integrators, since splitting is done at the level of the Euler-Lagrange equations rather than the Lagrangian [Crouzeix, 1980; Ascher et al., 1995].

A Variational IMEX Method

Suppose we have a Lagrangian of the form

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

where the potential energy is split into a slow component $U(q)$ and a fast component $W(q)$. Then define the following discrete Lagrangian,

$$L_d(q_0,q_1) = \frac{h}{2}\left(\frac{q_1-q_0}{h}\right)^T M \left(\frac{q_1-q_0}{h}\right) - h\left(\frac{U(q_0)+U(q_1)}{2}\right) - hW\left(\frac{q_0+q_1}{2}\right),$$

which uses the trapezoid rule for the slow potential and the midpoint rule for the fast potential.

Using the discrete Legendre transform, this generates a map $(q_0,p_0)\mapsto(q_1,p_1)$ on T^*Q, where

$$\begin{aligned} p_0 &= M\left(\frac{q_1-q_0}{h}\right) + \frac{h}{2}\nabla U(q_0) + \frac{h}{2}\nabla W\left(\frac{q_0+q_1}{2}\right)\\ p_1 &= M\left(\frac{q_1-q_0}{h}\right) - \frac{h}{2}\nabla U(q_1) - \frac{h}{2}\nabla W\left(\frac{q_0+q_1}{2}\right). \end{aligned}$$

To simplify this, we define the intermediate stage $p_{1/2} = M\left(\frac{q_1-q_0}{h}\right)$ and then rewrite the above as

$$\begin{aligned} p_{1/2} &= p_0 - \frac{h}{2}\nabla U(q_0) - \frac{h}{2}\nabla W\left(\frac{q_0+q_1}{2}\right)\\ q_1 &= q_0 + hM^{-1}p_{1/2}\\ p_1 &= p_{1/2} - \frac{h}{2}\nabla U(q_1) - \frac{h}{2}\nabla W\left(\frac{q_0+q_1}{2}\right). \end{aligned}$$

In particular, this reduces to Velocity Verlet when $\nabla W \equiv 0$ and to Midpoint Euler when $\nabla U \equiv 0$.

Linear Stability Analysis

To prove that this variational IMEX integrator does not exhibit resonance instability, we consider a simple 1D test problem. Given a particle of unit mass, let $U(q) = \frac{1}{2}\Lambda_U q^2$ and $W(q) = \frac{1}{2}\Lambda_W q^2$, so that ∇U and ∇W are both linear. After some simplification, the discrete Euler-Lagrange (DEL) equations for this system can be written

$$\left(1+\frac{h^2}{4}\Lambda_W\right)\left(\frac{q_{k+1}-2q_k+q_{k-1}}{h^2}\right) = -\left(\Lambda_U+\Lambda_W\right)q_k.$$

Therefore, this is equivalent to Verlet integration of a simple harmonic oscillator with constant

$$\Lambda = \frac{\Lambda_U+\Lambda_W}{1+\frac{h^2}{4}\Lambda_W}.$$

The stability condition for Verlet integration is $h^2\Lambda \le 4$, which is equivalent to

$$h^2\left(\Lambda_U+\Lambda_W\right) \le 4 + h^2\Lambda_W.$$

The Λ_W terms cancel, leaving $h^2\Lambda_U \le 4$, ***which is identical to the stability condition for Verlet integration of the slow scale by itself***. Therefore, because the stability conditions for the fast and slow scales essentially decouple, the variational IMEX method does not exhibit any numerical resonance instability.

Numerical Comparisons

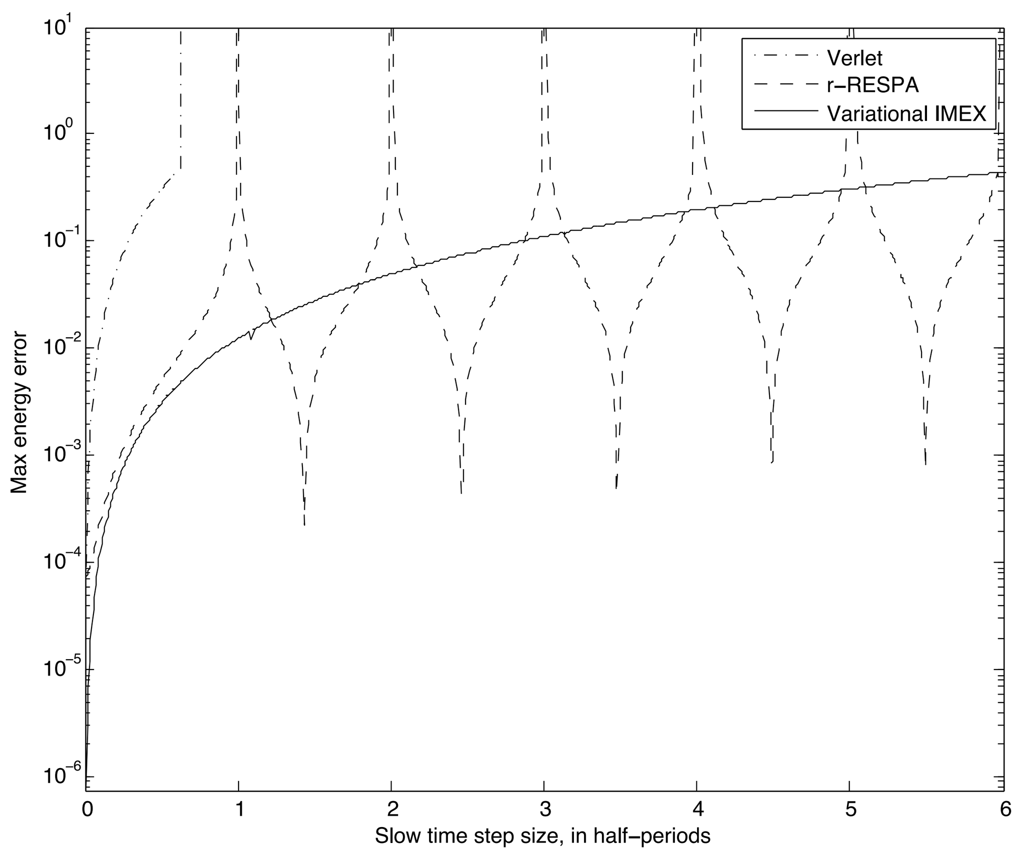

Figure 1: *Maximum energy error vs. time step size for Verlet, r-RESPA, and variational IMEX. Variational IMEX shows good energy behavior at long time steps, without the resonance instability "spikes" displayed by r-RESPA.*

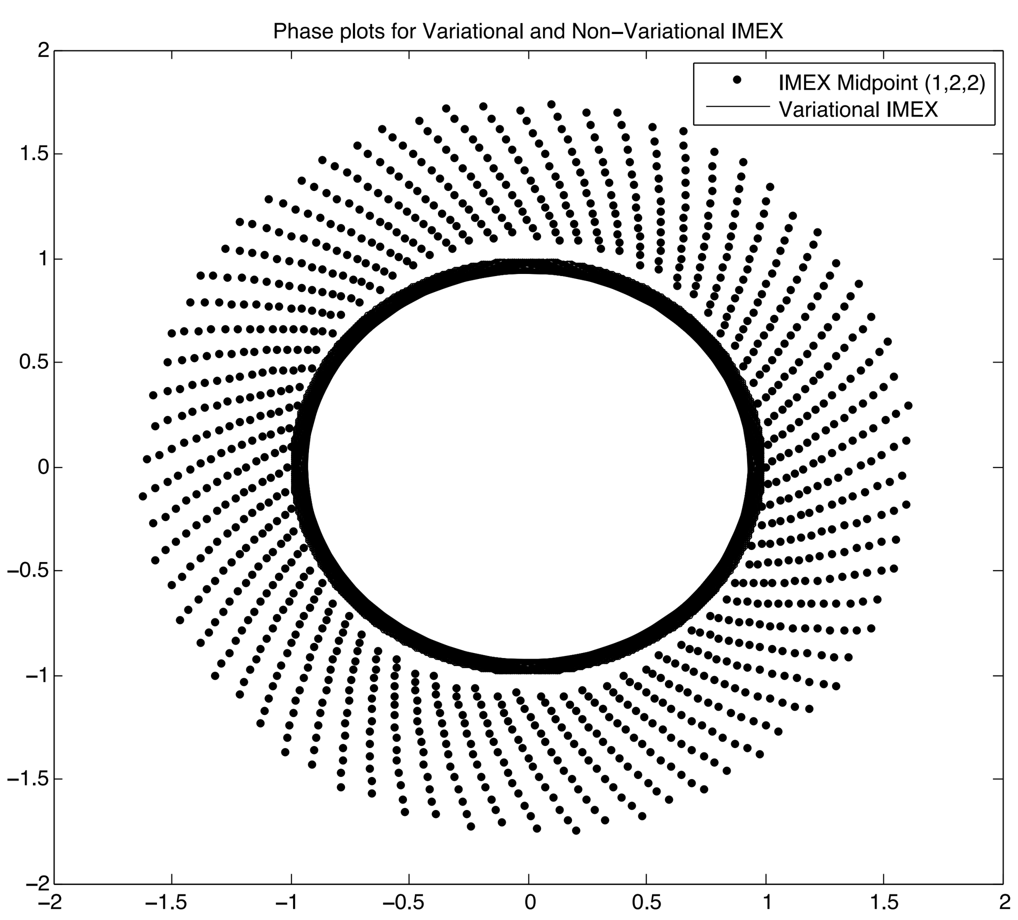

Figure 2: *Phase plot comparison for IMEX methods. The variational IMEX method is better at preserving energy and the structure of periodic orbits, while non-variational IMEX gradually gains energy and spirals outward.*

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