Stability of Asynchronous Variational Integrators

Abstract

The formulation of multiple–time–step integrators can provide substantial computational savings for mechanical systems with multiple time scales. However, the scope of these savings may be severely limited by the range of allowable time step choices. In this paper we have performed an exhaustive study of the linear stability of the fully asynchronous methods called AVI (asynchronous variational integrator), with two time steps, for essentially any combination of their values.

We have obtained approximate analytical expressions for the time step ratios that may render the scheme unstable in the case of linear equations, and verified them with extensive numerical computations. Synchronous multiple time stepping schemes such as r-RESPA show resonances when the outer step is a multiple of the effective half period of one of the fast oscillators. An elegant generalization is derived in the fully asynchronous case of AVI.

1. Introduction

Variational integrators constitute a novel paradigm for the construction of time–integration algorithms that, by design, guarantee a number of desirable and remarkable properties; see [1, 18, 20, 16, 9, 15, 11, 29, 5, 10, 14, 28, 26, 17, 12]. Chief among them are the existence of a discrete version of Noether’s theorem, the fact that every variational algorithm is automatically symplectic, and the consequent nearly perfect energy conservation properties for explicit algorithms at moderately large time steps. The distinguishing characteristic of variational integrators is that the equations that define an algorithm are the Euler–Lagrange equations of a discrete variational principle. In other words, the discrete motion is the stationary point of a functional over all discrete trajectories, termed the discrete action sum. The remarkable properties of the resulting algorithms can be directly traced back to their variational structure. These and other features of the theory of variational integrators have been thoroughly discussed in many of the previous references, in particular [11] or [16], and hence we shall skip further discussions herein.

Asynchronous Variational Integrators (AVI) are a class of variational integrators distinguished by the trait of enabling the use of different time steps for different potential energy contributions to a mechanical system. Furthermore, the time steps need not bear any integer multiple relation with each other. Their formulation and use in the context of finite element discretizations of fluids and solids can be found in [11, 12, 10].

It is well-known that multiple–time–step methods can display resonance instabilities, especially in the context of molecular dynamics simulations [2, 22, 24, 13, 4]. These resonances severely limit the relative size of the time-steps. Their effects have been somewhat mitigated in [7], but not to the extent of substantially improving the computational efficiency. When dissipative effects are included multiple–time–stepping algorithms for molecular dynamics are better exploited [21], since resonances are more effectively damped. This paper presents the first analysis of the linear stability of multiple–time–step methods when time steps with rational, and not necessarily integer, ratios are adopted.

2. Variational Derivation of AVI

To introduce the idea of variational integrators we begin by recalling the velocity Verlet (VV) integrator. Consider a system of \( N \) particles with masses \( m = (m_1, \ldots, m_N) \), positions \( x = (x_1, \ldots, x_N) \) and velocities \( v = \dot{x} = (v_1, \ldots, v_N) \) that interact according to a given potential function \( V(x) \). Their trajectories \( x(t) \) are governed by Newton’s equations of motion \( F = Ma \) where \( F = -\nabla V(x) \), \( M \) is the diagonal matrix with the particle masses along the diagonal, and \( a = \ddot{x} \). For this system the VV integrator is given by:

\[
\begin{align*}
\dot{v}^{j+1/2} &= \dot{v}^j + \frac{h}{2}M^{-1}F^j \\
\dot{x}^{j+1} &= \dot{x}^j + h\dot{v}^{j+1/2} \\
\dot{v}^{j+1} &= \dot{v}^{j+1/2} + \frac{h}{2}M^{-1}F^{j+1}
\end{align*}
\]

(1)

where \( h \) is the time step, \( t^j = jh \), \( x^j = x(t^j) \), and \( v^j = v(t^j) \).
The VV integrator is commonly used in molecular dynamics because it is easy to implement, has a low computational cost and conserves energy remarkably well. The VV integrator can also be written in a time-staggered form:

\[
\begin{align*}
x^{j+1} &= x^j + h v^{j+1/2} \\
v^{j+3/2} &= v^{j+1/2} + h M^{-1} F^{j+1}
\end{align*}
\] (2) (3)

We will now review how the staggered form of the VV integrator can be derived from a variational principle, as shown for example in [9]. This principle will be the basis of the derivation of AVI.

Following the usual convention in Lagrangian mechanics, the position \( x \) and velocity \( v \) will be denoted by \( q \) and \( \dot{q} \) respectively. The Lagrangian for the system defined above is given by the difference between the kinetic and potential energies:

\[
L(q, \dot{q}) = \sum_{a=1}^{N} \frac{1}{2} m_a \| \dot{q}_a \|^2 - V(q)
\]

where \( m_a \) is the mass of particle \( a \) and \( \dot{q}_a \) is the velocity of particle \( a \). The action integral for an arbitrary trajectory \( q(t) \) of the Lagrangian system is defined as the time integral of \( L \) along \( q(t) \):

\[ S(q) = \int_0^T L(q(t), \dot{q}(t)) dt \]

Lagrangian mechanics is based on Hamilton’s variational principle which states that the trajectory \( q(t) \) followed by the particles is a stationary point of the action integral \( S \). Therefore for all variations around the exact trajectory \( q + \delta q \), with fixed endpoints \( q(0) \) and \( q(T) \), we must have \( \delta S = 0 \). The Euler–Lagrange equations of this variational principle are precisely Newton’s equations of motion.

To construct a variational integrator, we begin by discretizing the time interval \([0, T]\) into a sequence of intervals \([t^j, t^{j+1}]\) with a time step \( h \). Then, the continuous-time trajectory \( q(t) \) is represented as a sequence of positions \( \{q^j\} = \{q^0, \ldots, q^M\} \) using this time discretization, the action integral can be approximated as an action sum:

\[
S_d = \sum_{j=0}^{M-1} \left( \sum_{a=1}^{N} \frac{1}{2} m_a \left| \frac{q_a^{j+1} - q_a^j}{h} \right|^2 \right) - \frac{1}{2} V(q^j) + \frac{1}{2} V(q^{j+1})
\]

We then employ a discrete analog to Hamilton’s principle to obtain the algorithm. The discrete variational principle says that \( \delta S_d = 0 \) for any variation \( \delta q \) satisfying \( \delta q^0 = 0 \) and \( \delta q^M = 0 \). The Euler–Lagrange equations of this principle are

\[
\begin{align*}
\dot{q}^{j+1/2} &= \dot{q}^{j-1/2} + h M^{-1} F^j \\
q^{j+1} &= q^j + h v^{j+1/2}
\end{align*}
\] (4) (5)

which provided that velocities at half steps are defined as

\[ q^{j+1/2} = \frac{q^{j+1} - q^j}{h} \]

are precisely the staggered form of the VV algorithm (see Eq. (2) and (3)).

An important property of variational integrators is that they are symplectic and therefore conserve energy very well (no drift) over long time scales [19, 6]. This is a key property for molecular dynamics and other problems.

To obtain an asynchronous variational integrator (AVI), we generalize the previous approximation of the action integral. We assume that the potential \( V(q) \) is written as the sum of \( K \) potentials:

\[ V(q) = \sum_{k=1}^{K} V_k(q) \]

Furthermore, we assume that the potential \( V(q) \) have different time scales associated to them, e.g. different stiffness. AVI allows for the selection of a different time step for each potential \( V_k \). As a result each inherent time scale can be resolved with the prescribed accuracy and at a lower computational cost. The action sum is now given by:

\[
S_d = \sum_{a=1}^{N} \sum_{j=0}^{M_a-1} \frac{1}{2} m_a \left( t_a^{j+1} - t_a^j \right) \left| \frac{q_a^{j+1} - q_a^j}{t_a^{j+1} - t_a^j} \right|^2 - \sum_{k=1}^{K} \sum_{l=0}^{M_k-1} \left( t_k^{l+1} - t_k^l \right) V_k(q_k^l)
\]

where \( t_k^l \) is the \( l \)th time step associated with \( V_k \). We assume that for each potential \( V_k \) the sequence \( t_k^j \) is given. Typically, a simulation time \( T \) is picked and a time step \( h_k \) is chosen such that \( T/h_k \) is an integer. Then: \( t_k^{l+1} = l h_k \). The position at time \( t_k^j \) is denoted \( q_k^j \). Using a different notation for the index, the time associated with the position of particle \( a \) at step \( j \) (\( q_a^j \)) is denoted by \( t_a^j \). Here \( M_a \) and \( M_k \) denote the total number of time steps each particle \( a \) and potential \( K \) perform, respectively. Applying the discrete form of Hamilton’s principle to the action sum, we find that (reverting to the \( x, v \) notation):

\[
\begin{align*}
x_a^{j+1} &= x_a^j + (t_a^{j+1} - t_a^j) q_a^{j+1/2} \\
v_a^{j+3/2} &= v_a^{j+1/2} + \frac{1}{m_a} (t_k^{l+1} - t_k^l) F_k(x_a^{j+1})
\end{align*}
\] (7) (8)

Since each of the potentials \( V_k \) have a different time step, a priority queue is used to determine the order in which the potentials are evaluated. The elements of this priority queue have the form \((t_k^{\text{next}}, k)\), where \( t_k^{\text{next}} \) is the next time potential \( V_k \) needs to be evaluated, with the elements sorted in ascending order with respect to \( t_k^{\text{next}} \). As a result the element at
the top gives the time of the next potential evaluation and the index of the potential that will be evaluated. Once the position and velocity have been advanced in time using Eq. (7) and (8), \( t^{\text{next}}_k \) is set to \( t^{\text{next}}_k = t^1_k + 1 \) and is pushed into the priority queue. Below is an algorithm detailing an implementation of the staggered version of AVI. An AVI algorithm similar to Eq. (1) for VV can be derived. This second formulation (not shown here) makes it more apparent that AVI is time reversible.

**Algorithm 1 Staggered AVI Algorithm**

Input: \( q^0_a, q^{1/2}_a \) and total simulation time \( T \)

Output: \( q^T_a, q^{T+1/2}_a \)

Initialization:

for \( a = 1, \ldots, N \) do

- Set the time of particle \( a \): \( \tau_a = 0 \)
- Set \( x_a = q^0_a \) and \( v_a = q^{1/2}_a \)
end for

for \( k = 1, \ldots, K \) do

- Set the time of potential \( V_k \): \( \tau_k = 0 \)
- Compute \( t^1_k \) the next time \( V_k \) is evaluated
- Push \((t^1_k, k)\) into the priority queue
end for

Integrate the system over the time interval \([0, T]\):

while the priority queue is not empty do

- Determine which potential to evaluate next by popping the top element \((t^1_k, k)\) from the priority queue
- Update the positions \( x_a \) and times \( \tau_a \) of the appropriate particles:
  \[
  x_a \leftarrow x_a + (t^1_k - \tau_a) v_a \\
  \tau_a \leftarrow t^1_k
  \]
- if \( t^1_k < T \) then
  - Update the velocities \( v_a \) and time \( \tau_k \):
    \[
    v_a \leftarrow v_a + (t^1_k - \tau_k) F_k(x_a)/m_a \\
    \tau_k \leftarrow t^1_k
    \]
  - Schedule the next potential evaluation:
    - Compute \( t^{\text{next}}_{k} = t^{1+1}_k \)
    - Push \((t^{\text{next}}_{k}, k)\) into the priority queue
end if
end while

It can be verified that AVI is a generalization of the well-known r-RESPA [27]. To this end, it is enough to choose the time steps for each potential such that \( h_{k+1}/h_k \) is an integer, for all \( k \geq 1 \).

### 3. Stability of Asynchronous Variational Integrators

Two important properties of a numerical integrator are consistency and stability. First the integrator must provide a good approximation to the exact solution of the problem. An integrator is consistent if the numerical solution approaches the exact solution as the time step \( h \to 0 \). A consistent integrator is accurate of order \( p \) if the truncation error is \( O(h^p) \). However it is not enough for an integrator to be consistent and accurate to a desired order. If the solution obtained from this integrator grows unbounded with respect to a norm when the exact solution remains bounded, the integrator is of no use. Therefore any useful integrator should be stable for certain steps \( h \).

To analyze the stability, we will focus on systems of \( n \) first-order ODEs:

\[
\dot{x} = Ax, \quad x(0) = x_0
\]

Let \( Q \) be the propagation matrix representing the numerical integrator:

\[
x^{j+1} = Q x^j
\]

where \( \{x^0, x^1, \ldots, x^M\} \) is a time discretization of \( x(t) \). Then the integrator represented by \( Q \) is stable if and only if its eigenvalues \( \lambda_i(A) \) satisfy

\[
|\lambda_i| \leq 1.
\]

Finally, we should note that a linear stability analysis does not necessarily capture all possible instabilities. Nonlinearities can play an important role in rendering linearly stable schemes unstable, as shown in [23].

We will now use linear stability analysis to study the stability of the VV integrator, r-RESPA, and AVI. Since linear stability analysis requires writing the integrator in matrix form and determining the eigenvalues of the matrix, it can only be done analytically for small systems. The simplest example is the 1-D harmonic oscillator:

\[
\ddot{x} + \Lambda x = 0, \quad x(0) = x_0, \quad \dot{x}(0) = v_0
\]

where \( \Lambda > 0 \). Since the mass of the particle is 1 and the force is given by \( F = -\Lambda x \), the VV integrator for this problem is given by

\[
\begin{align*}
\dot{v}^j & = v^j - \frac{h}{2} \Lambda x^j \\
\dot{x}^j & = x^j + h v^{j+1/2} \\
\dot{v}^{j+1/2} & = v^{j+1/2} - \frac{h}{2} \Lambda x^{j+1}
\end{align*}
\]

or in matrix form

\[
Q_{VV} = \begin{bmatrix}
1 - \frac{h^2}{2} \Lambda & \frac{h}{2} \\
-\frac{h}{2} \Lambda \left(1 - \frac{h^2}{4} \Lambda\right) & 1 - \frac{h^2}{2} \Lambda
\end{bmatrix}
\]
It can be shown that the eigenvalues of $Q_{VV}$ are less than or equal to 1 in modulus if and only if

$$h \leq \frac{2}{\sqrt{\lambda}}$$

Next we will examine the stability of r-RESPA for the 1-D oscillator with the splitting $\Delta x = \Lambda_1 x + \Lambda_2 x$ where $\Lambda_1 \geq \Lambda_2 > 0$ and $h_2 = m h_1$. Hereafter $\Lambda_1 x$ will be referred to as the fast force and $\Lambda_2 x$ as the slow force. Assuming that $h_1$ is sufficiently small, we focus on the instabilities related to $h_2$. We begin by writing one step of r-RESPA in matrix form:

$$\begin{bmatrix} x_{j+1} \\ v_{j+1} \end{bmatrix} = V_{\text{slow}} (Q_{\text{fast}})^m V_{\text{slow}} \begin{bmatrix} x_j \\ v_j \end{bmatrix}$$

$$\equiv Q_{\text{r-RESPA}} \begin{bmatrix} x_j \\ v_j \end{bmatrix}$$

where

$$V_{\text{slow}} = \begin{bmatrix} 1 & 0 \\ \frac{h_1}{2 \Lambda_2} & 1 \end{bmatrix}$$

and

$$Q_{\text{fast}} = \begin{bmatrix} 1 - \frac{h_1^2}{2 \Lambda_1} & h_1 \\ -h_1 \Lambda_1 \left( 1 - \frac{h_1^2}{4 \Lambda_1} \right) & 1 - \frac{h_1^2}{2 \Lambda_1} \end{bmatrix}$$

Since $Q_{\text{r-RESPA}}$ is the product of matrices each with determinant 1 then $\text{det}(Q_{\text{r-RESPA}}) = 1$ so instabilities are given by $|\text{Tr}(Q_{\text{r-RESPA}})| > 2$.

To compute the trace start by defining $\theta$ such that

$$\cos \theta = 1 - \frac{h_1^2}{2 \Lambda_1}$$

$$\sin \theta = h_1 \sqrt{\Lambda_1 \left( 1 - \frac{h_1^2}{4 \Lambda_1} \right)}$$

and let

$$G = \begin{bmatrix} 1 & 0 \\ 0 & \sqrt{\Lambda_1 \left( 1 - \frac{h_1^2}{4 \Lambda_1} \right)} \end{bmatrix}$$

$$R(\theta) = \begin{bmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{bmatrix}$$

Then it can be shown that:

$$Q_{\text{fast}} = GR(\theta)G^{-1}$$

and so:

$$(Q_{\text{fast}})^m = GR(m \theta)G^{-1}$$

since $R(\theta)$ is the rotation matrix. In this formulation an effective angular frequency can be defined as $\omega_{\text{eff}} = \theta h_1$ so the effective period is given by $T_{\text{eff}} = 2 \pi / \omega_{\text{eff}} = 2 \pi h_1 / \theta$.

Using this alternative form for $Q_{\text{fast}}$ we find that

$$\text{Tr}(Q_{\text{r-RESPA}}) = 2 \left[ \cos(m \theta) - \alpha \sin(m \theta) \right]$$

where

$$\alpha = \frac{h_1^2 \Lambda_2}{2 \sqrt{\Lambda_1 \left( 1 - \frac{h_1^2}{4 \Lambda_1} \right)}}$$

Further analysis shows that instabilities occur when either

$$\tan \left( \frac{\pi h_2}{T_{\text{eff}}} \right) > \frac{1}{\alpha} > 0, \quad \text{or:}$$

$$0 > \tan \left( \frac{\pi h_2}{T_{\text{eff}}} \right) > -\alpha$$

In general $\alpha$ is small and so r-RESPA is unstable when $h_2$ is near an integer multiple of the effective half-period $T_{\text{eff}}/2$.

Last we turn our attention to the stability of the staggered AVI algorithm for the 1-D harmonic oscillator. For two time steps $h_1$ and $h_2$ a matrix $Q_{AVI}$ can be defined only if $h_2 / h_1$ is a rational number, say $p / q$ where $p$ and $q$ are integers. In that case, we see that the two potentials become synchronous at time $t = q h_2 = p h_1$. The analysis in the general case is probably quite involved. In the case where $q = 2$ and $q = 3$, the analysis was performed and the conclusion is that an instability is present whenever $q h_2$ is near an integer multiple of the effective half-period $T_{\text{eff}}/2$, thereby directly generalizing the result for AVI. We now denote $T_{1/2}(h_1) = T_{\text{eff}}(h_1)/2$.

If we assume that this holds in the general case, i.e.:

AVI is unstable whenever $q h_2$ is near an integer multiple of $T_{1/2}$

we can derive an interesting result regarding the set of all $(h_1, h_2)$ for which AVI is unstable.

Let’s consider the simpler problem of finding all the pairs $(h_1, h_2)$ such that there exists three integers $(p, q, m)$ satisfying:

$$\frac{h_2}{h_1} = \frac{p}{q}, \quad q h_2 = m T_{1/2}$$

(9)

where the Greatest Common Factor (gcf) of $p$ and $q$ is 1. If we are interested in finding the steps $h_2$ for which AVI is unstable given $h_1$, we might proceed as follows. For a given $h_1$ such that $T_{1/2}/h_1$ is rational we have:

$$\frac{T_{1/2}}{h_1} = \frac{p}{m}$$

Then for any $1 \leq q < p$ such that gcf$(p, q) = 1$ choose $h_2 = (p h_1) / q$. This approach unfortunately does not make it apparent that, in fact, the solutions $(h_1, h_2)$ of Eq. (9) lie along a set of curves. We state the key result:
**Proposition:** \((h_1, h_2)\) is a solution of Eq. (9) if and only if there exist four integers \(a, b, p\) and \(q\) such that:

\[
h_2 = \frac{b T_{1/2} h_1}{h_1 - a T_{1/2}} = \frac{p}{q} h_1
\]

Ignoring the last equation which is true almost everywhere, this result implies that \((h_1, h_2)\) lie along a family of curves parametrized by two integers \((a, b)\).

**Proof:** Assume that \((h_1, h_2)\) is a solution of Eq. (9). Then, we can find \(a\) and \(b\) such that \(a p + b q = 1\). Consequently:

\[
am p + b m q = m, \Rightarrow am h_2^2 + bm = \frac{h_2}{T_{1/2}}
\]

We can solve for \(h_2\) and:

\[
h_2 = \frac{(bm)(T_{1/2}) h_1}{h_1 - (am)(T_{1/2})}
\]

Let’s now assume that there exist \(a\) and \(b\) such that:

\[
h_2 = \frac{b T_{1/2} h_1}{h_1 - a T_{1/2}}
\]

Let’s further assume that \(h_2/h_1 = p/q\). These last two equations imply that:

\[
q h_2 = p h_1 = (ap + bq) T_{1/2}.
\]

\(\Box\)

In the next section, we plot the set of all points \((h_1, h_2)\) such that AVI is unstable and confirm that indeed these points lie along a family of curves.

**4. Numerical Results: Stability of AVI**

To study the stability of AVI we begin by rewriting the ODE for the harmonic oscillator as a system of first-order ODEs:

\[
\begin{align*}
\dot{x} &= v \\
\dot{v} &= -(\Lambda_1 + \Lambda_2)x
\end{align*}
\]

In order to use the linear stability analysis from before, the numerical scheme is written as

\[
x^{j+1} = Q_{AVI} x^j
\]

for some propagation matrix \(Q_{AVI}\). The eigenvalues of \(Q_{AVI}\) are numerically computed. If their modulus is larger than 1, the time steps \((h_1, h_2)\) are unstable.

In this simulation, pairs of time steps are selected such that they are both integer multiples of a given grid spacing \(h = 0.0005\). We take \(\lambda_1 = \pi^2\), \(\lambda_2 = \pi^2/25\), \(h \leq h_1 \leq 2/\pi\), and \(h_1 \leq h_2 \leq 3.5\). If the propagation matrix \(Q_{AVI}\) for a given pair of time steps \((h_1, h_2)\) has a spectral radius greater than 1, the pair is marked by a point. Fig. 1 shows the time step pairs in the domain \([h, 2/\pi] \times [h, 3.5]\) for which the AVI algorithm is unstable.

This figure confirms the theoretical analysis of the previous section. The points \((h_1, h_2)\) lie along lines which are parametrized by the integers \(a\) and \(b\) of Eq. (10). The thick solid lines correspond to \(a = 0\) (r-RESPA case), the dotted lines to \(a = 1\), the dashed lines to \(a = 2\), and the thin solid lines to \(a = -1\).

**5. Conclusion**

We studied the stability of AVI integrators and showed that results derived for the synchronous r-RESPA family of integrators can be generalized to asynchronous integrators such as AVI. One key result is that for a system of two 1D springs with different stiffnesses an instability is observed when the time steps \((h_1, h_2)\) lie along a family of lines parametrized by two integers.

This analysis however only covers the linear case. Nonlinear stability analysis are much more challenging but some results can be obtained for example in the vicinity of stable equilibrium points (e.g. Skeel et al.[25]).

The authors note that classical techniques such as MOLLY [8] to stabilize multiple time stepping schemes are applicable to AVI as well and should lead to significant improvements. In the context of molecular dynamics, formulations based on Langevin equations are attractive as they naturally generate trajectories at constant temperature and are known to stabilize multiple time stepping integrators (see [3] for example).

**References**


Figure 1. AVI stability plot. $h_1$ is on the $x$ axis. $h_2$ is on the $y$ axis. Left plot: each unstable pair $(h_1, h_2)$ is shown with a dot. Right plot: the theoretical prediction given by $h_2 = (bT_1/2 h_1)/(h_1 - a T_1/2)$ for some pairs of $a$ and $b$ is shown. The matching with the numerical results is excellent.


