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STABILITY ANALYSIS OF HIGH ORDER PHASE FITTED VARIATIONAL INTEGRATORS

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Abstract. The linear stability properties of higher order variational integration methods that use phase lag technique are investigated. Towards this purpose, at first we calculate the eigenvalues of the amplification matrix for each method. Phase fitted integrators are derived specifically for the numerical integration of systems with oscillatory solutions. A linear stability analysis shows their good behavior, when simulating these problems. Finally, we test the proposed methods in numerical examples, first with regard to their stability and secondly the behavior in long term integration is illustrated.

1 INTRODUCTION

In the present work, we investigate the stability region of high order phase fitted variational integrators using trigonometric interpolation. In the first step, discrete configurations and velocities are considered at the nodes of the time grid only (no intermediate points are taken into account), see [1, 2].

For the derivation of variational integrators, recalling discrete variational calculus, see [1], the discrete Lagrangian map $L_d : Q \times Q \to \mathbb{R}$ is defined on two copies of the configuration manifold Q, which may be considered as an approximation of a continuous action with Lagrangian $L : TQ \to \mathbb{R}$, i.e.

$$L_d(q_k, q_{k+1}) \approx \int_{t_k}^{t_{k+1}} L(q, \dot{q})dt, \tag{1}$$

in the time interval $[t_k, t_{k+1}] \subset \mathbb{R}$. The action sum $S_d : Q^{N+1} \to \mathbb{R}$, corresponding to the

Lagrangian L_d is defined as

$$S_d(\gamma_d) = \sum_{k=0}^{N-1} L_d(q_k, q_{k+1}), \tag{2}$$

with $\gamma_d = (q_0, \ldots, q_N)$ representing the discrete trajectory. The discrete Hamilton principle states that a motion γ_d of the discrete mechanical system extremizes the action sum, i.e. $\delta S_d = 0$. By differentiation and rearrangement of the terms and having in mind that both q_0 and q_N are fixed, the discrete Euler-Lagrange equations (DEL) are obtained [1]

$$D_2 L_d(q_{k-1}, q_k) + D_1 L_d(q_k, q_{k+1}) = 0, \qquad k = 1, \ldots, N-1 \tag{3}$$

where the notation $D_i L_d$ indicates the slot derivative with respect to the argument of L_d.

The definition of the discrete conjugate momentum at time steps k and $k+1$ can be computed via Legendre transforms and reads

$$p_k = -D_1 L_d(q_k, q_{k+1}), \quad p_{k+1} = D_2 L_d(q_k, q_{k+1}), \qquad k = 0, \ldots, N-1. \tag{4}$$

The above equations, also known as position-momentum form of a variational integrator, can be used when an initial condition (q_0, p_0) is known, to obtain (q_1, p_1).

2 REVIEW OF VARIATIONAL INTEGRATORS USING INTERPOLATION TECHNIQUES

To construct high order methods, we approximate the action integral along the curve segment between q_k and q_{k+1} using a discrete Lagrangian that depends only on the end points. We obtain expressions for configurations q_k^j and velocities $\dot{q}_k^j$ for $j = 0, \ldots, S-1$, $S \in \mathbb{N}$ at time $t_k^j \in [t_k, t_{k+1}]$ by expressing $t_k^j = t_k + C_k^j h$ for $C_k^j \in [0, 1]$ such that $C_k^0 = 0, C_k^{S-1} = 1$ using

$$q_k^j = g_1(t_k^j) q_k + g_2(t_k^j) q_{k+1}, \qquad \dot{q}_k^j = \dot{g}_1(t_k^j) q_k + \dot{g}_2(t_k^j) q_{k+1} \tag{5}$$

where $h \in \mathbb{R}$ is the time step. We choose functions

$$g_1(t_k^j) = \sin\left(u - \frac{t_k^j - t_k}{h} u\right)(\sin u)^{-1}, \quad g_2(t_k^j) = \sin\left(\frac{t_k^j - t_k}{h} u\right)(\sin u)^{-1} \tag{6}$$

to represent the oscillatory behavior of the solution [2, 4]. For the sake of continuity, the conditions $g_1(t_{k+1}) = g_2(t_k) = 0$ and $g_1(t_k) = g_2(t_{k+1}) = 1$ must be fulfilled. Note here that other interpolations (e.g. linear, cubic splines, e.t.c.) are possible as alternatives to (6).

For any choice of interpolation, we define the discrete Lagrangian in the form of the weighted sum

$$L_d(q_k, q_{k+1}) = h \sum_{j=0}^{S-1} w^j L(q(t_k^j), \dot{q}(t_k^j)), \tag{7}$$

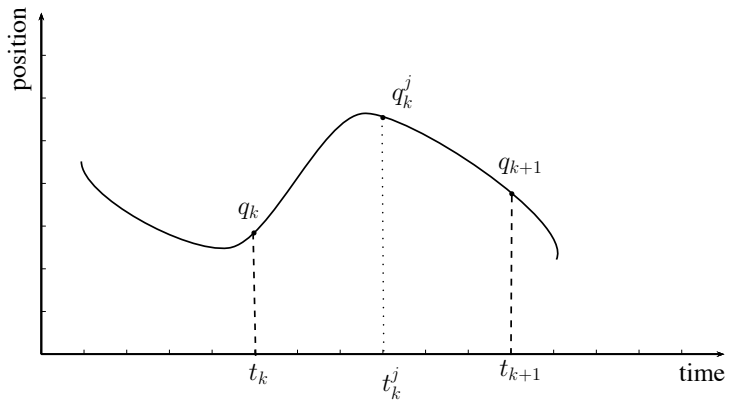

Figure 1: Intermediate time nodes $t_k^j \in [t_k, t_{k+1}]$ and corresponding configurations.

where it can be easily proved that for maximal algebraic order

$$\sum_{j=0}^{S-1} w^j (C_k^j)^m = \frac{1}{m+1}, \tag{8}$$

where $m = 0, 1, \ldots, S-1$ and $k = 0, 1, \ldots, N-1$ must hold, see [2, 4].

Applying the above interpolation technique with the trigonometric expressions (6), following the phase lag analysis of [2, 4], the parameter u can be chosen as $u = \omega h$. For problems that include a constant and known domain frequency ω (such as the harmonic oscillator) the parameter u can be easily computed. For the solution of orbital problems of the general N-body problem, where no unique frequency is given, a new parameter u must be computed by estimating the frequency of the motion of any moving point mass during the course of motion [4].

3 LINEAR STABILITY ANALYSIS

To investigate the stability properties of the proposed variational integrators, following [3, 7], we restrict ourselves to a linear stability analysis. To this end, we start by considering the harmonic oscillator

$$\ddot{q} + \omega^2 q = 0, \tag{9}$$

described by the Lagrangian

$$L(q, \dot{q}) = \frac{1}{2}\dot{q}^2 - \frac{1}{2}\omega^2 q^2, \qquad \omega \in \mathbb{R}. \tag{10}$$

Using Hamilton's equations

$$\dot{q} = p, \quad \dot{p} = -\omega^2 q \tag{11}$$

the exact solution is written as [7]

$$\begin{pmatrix} p(t) \\ q(t) \end{pmatrix} = \begin{pmatrix} \cos(\omega t) & -\omega \sin(\omega t) \\ \frac{\sin(\omega t)}{\omega} & \cos(\omega t) \end{pmatrix} \begin{pmatrix} p(0) \\ q(0) \end{pmatrix} = M_\omega \begin{pmatrix} p(0) \\ q(0) \end{pmatrix} \tag{12}$$

with $\det(M_\omega) = 1$. Since the eigenvalues of M_ω are $\lambda_{1,2} = e^{\pm i\omega t}$, we get $\mid \lambda_{1,2} \mid = 1$.

Recalling that a numerical solution is asymptotically stable if the growth of the solution is asymptotically bounded, a sufficient condition for asymptotic stability is that the eigenvalues of $M_{h\omega}$ are in the unit disk of the complex plane and are simple if they lie on the unit circle. In the next subsections, we investigate the latter property for selected variational integrators.

3.1 Stability of phase fitted variational integrators

For the Lagrangian of the harmonic oscillator with frequency ω, the discrete Lagrangian (7) with trigonometric interpolation (6) reads

$$\begin{aligned} L_d(q_k, q_{k+1}) = & \frac{h}{2} \Bigg[\sum_{j=0}^{S-1} w^j \big(\dot{g}_1(t_k^j) q_k + \dot{g}_2(t_k^j) q_{k+1} \big)^2 - \\ & \omega^2 \sum_{j=0}^{S-1} w^j \big(g_1(t_k^j) q_k + g_2(t_k^j) q_{k+1} \big)^2 \Bigg]. \end{aligned} \tag{13}$$

Subsequently, the discrete Euler-Lagrange equations (3) yield the following two-step variational integrator

$$q_{k+1} + \frac{\sum_{j=0}^{S-1} w^j \left[\dot{g}_1(t_k^j)^2 + \dot{g}_2(t_k^j)^2 - \omega^2 \big(g_1(t_k^j)^2 + g_2(t_k^j)^2 \big) \right]}{\sum_{j=0}^{S-1} w^j \left[\dot{g}_1(t_k^j) \dot{g}_2(t_k^j) - \omega^2 g_1(t_k^j) g_2(t_k^j) \right]} q_k + q_{k-1} = 0. \tag{14}$$

It can be readily shown that the latter integrator is explicit for any choice of interpolation in use [8].

3.1.1 Trigonometric interpolation for $S = 2$

In the special case when no intermediate points are used, i.e. $S = 2$, $t_k^0 = t_k$ and $t_k^1 = t_{k+1}$, the coefficients C_k^j and w^j described in Section 2 take the values

$$\begin{aligned} C_k^0 &= 0, \qquad C_k^1 = 1 \\ w^0 &= \frac{1}{2}, \qquad w^1 = \frac{1}{2}. \end{aligned} \tag{15}$$

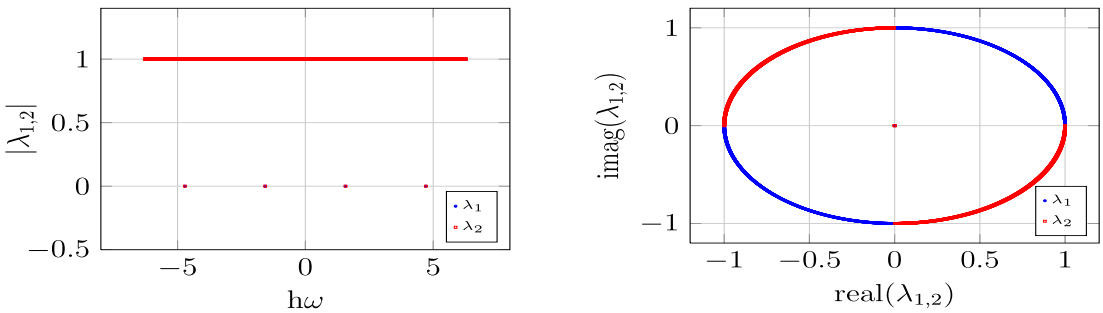

Figure 2: Modulus of the eigenvalues (16) of $M_{h,\omega}$ for the phase fitted variational integrators for $S = 2$ for $\omega h \in [-2\pi, 2\pi]$ and real and imaginary part.

Relying on the basic expressions (3) and (4) and using (5)-(14) and (15), the eigenvalues $\lambda_{1,2}$ of the matrix $M_{h,\omega}$ can be written as

$$\lambda_{1,2} = \frac{2\cos(2\omega h) + 2 \pm \sqrt{2\cos(4\omega h) - 2}}{4\cos(\omega h)}. \tag{16}$$

Since $2\cos(4\omega h) - 2 \leq 0, \forall \omega h \in \mathbb{Z}$, in order to show the stability of the resulting numerical scheme, we prove the following theorem.

Theorem 3.1. *The phase fitted variational integrator using trigonometric interpolation for $S = 2$ is stable for $\omega h \neq \nu\pi + \frac{\pi}{2}, \nu \in \mathbb{Z}$.*

Proof. **1st step:** $\omega h = \nu\pi + \frac{\pi}{2}, \nu \in \mathbb{Z}$

For these values of ωh, the denominator of the eigenvalues in (16) vanishes, creating an unstable method, see Figure 2(a).

2nd case: $\omega h \neq \nu\pi + \frac{\pi}{2}, \nu \in \mathbb{Z}$

For the case when $2\cos(4\omega h) - 2 = 0$, i.e. $\omega h = \nu\pi$ (since $\omega h \neq \nu\pi + \frac{\pi}{2}, \nu \in \mathbb{Z}$), the eigenvalues (16) are

$$\lambda_{1,2} = \frac{2\cos(2\nu\pi) + 2}{4\cos(\nu\pi)} = 1. \tag{17}$$

Thus, this choice of ωh creates a stable integrator. In the case when $2\cos(4\omega h) - 2 < 0$, i.e. $\omega h \neq \nu\frac{\pi}{2}, \nu \in \mathbb{Z}$, both eigenvalues in (16) are complex numbers. The modulus of the

eigenvalues is $|\lambda_{1,2}|^2 = 1$ since

$$\begin{aligned}
|\lambda_{1,2}|^2 &= \left(\frac{2\cos(2\omega h)+2}{4\cos(\omega h)}\right)^2 + \left(\frac{\sqrt{2\cos(4\omega h)-2}}{4\cos(\omega h)}\right)^2 \\
&= \left(\frac{2\cos(2\omega h)+2}{4\cos(\omega h)}\right)^2 + \frac{|2\cos(4\omega h)-2|}{(4\cos(\omega h))^2} \\
&= \frac{4\cos^2(2\omega h)+4+8\cos(2\omega h)+2-2\cos(4\omega h)}{(4\cos(\omega h))^2} \\
&\quad \text{using } \cos(4\omega h) = 2\cos^2(2\omega h)-1 \\
&= \frac{8\cos(2\omega h)+8}{(4\cos(\omega h))^2} \\
&\quad \text{using } \cos(2\omega h) = 2\cos^2(\omega h)-1 \\
&= 1 \qquad (18)
\end{aligned}$$

□

The stability region of the phase fitted variational integrator (14) using trigonometric interpolation (6), i.e. intermediate configurations and velocities taken from (5), for $S = 2$ is shown in Figure 2. It is clear from that figure that for $\omega h \neq \nu\pi + \frac{\pi}{2}, \nu \in \mathbb{Z}$ the integrator is stable. The unstable choices of ωh are illustrated in Figures 2.

3.1.2 Trigonometric interpolation for $S = 3$

Working in a similar manner as in Section 3.1.1, for the case when one intermediate point in each time interval is used, i.e. $S = 3$ and $t_k^0 = t_k$, $t_k^1 = t_k + \frac{h}{2}$ and $t_k^2 = t_{k+1}$, the coefficients C_k^j and w^j described in Section 2 are

$$\begin{aligned}
C_k^0 &= 0, \qquad C_k^1 = \frac{1}{2}, \qquad C_k^2 = 1, \\
w^0 &= \frac{1}{6}, \qquad w^1 = \frac{1}{6}, \qquad w^2 = \frac{1}{6}. \qquad (19)
\end{aligned}$$

Again, by using the discrete Euler-Lagrange equations (3) for the discrete Lagrangian (13), the eigenvalues of the matrix $M_{h,\omega}$ can be cast in the form

$$\lambda_{1,2} = 2 + \frac{\cos^2(\omega h) - 4}{2\cos^2\left(\frac{\omega h}{2}\right)+1} \pm \frac{1}{2}\sqrt{\frac{1}{32\cos^2\left(\frac{\omega h}{2}\right)+4\cos^2(\omega h)}}\sqrt{\Delta_3(\omega,h)}. \qquad (20)$$

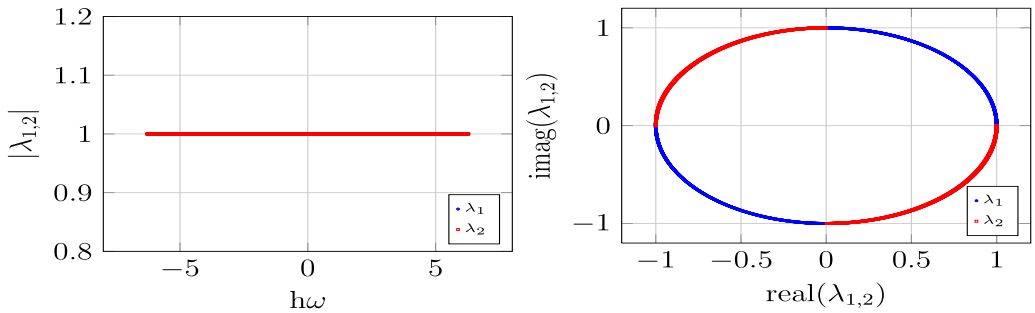

Figure 3: Modulus of the eigenvalues (20) of $M_{h,\omega}$ for the phase fitted variational integrators for $S = 3$ for $\omega h \in [-2\pi, 2\pi]$ and real and imaginary part.

The function $\Delta_3(\omega, h)$ is given by the expression

$$\Delta_3(\omega, h) = 4\cos^2(2\omega h) - 32\cos^2\left(\frac{\omega h}{2}\right) + 32\cos^2\left(\frac{3\omega h}{2}\right) + 64\cos^2(\omega h) - 68. \tag{21}$$

It is worth noting that both eigenvalues $\lambda_{1,2}$ of (20) are complex numbers for $\omega h \neq 6\nu\pi, \nu \in \mathbb{Z}$ since $\Delta_3(\omega, h) < 0$ (the period of $\Delta_3(\omega, h)$ is 6π). Furthermore, for the validity of the stability for trigonometric interpolation with $S = 3$, we prove the following theorem.

Theorem 3.2. *The phase fitted variational integrator using trigonometric interpolation for $S = 3$ is stable for any $\omega h \in \mathbb{R}$.*

Proof. **1st step:** $\omega h = 6\nu\pi, \nu \in \mathbb{Z}$

For the special case that $\omega h = 6\nu\pi$ we have $\Delta_3(\omega, h) = 0$ and, the eigenvalues in (20) lie on the unit circle, since $\lambda_{1,2} = 1$.

2nd step: $\omega h \neq 6\nu\pi, \nu \in \mathbb{Z}$

This choice of ωh leads to complex numbers for both eigenvalues of (20) which now have unity magnitude as $|\lambda_{1,2}|^2 = 1$, (the proof follows the one of Theorem 3.1). □

The degree of stability (stability region) of the phase fitted variational integrator (14) with trigonometric interpolation, for $S = 3$, is shown in Figure 3. One can conclude that for $\omega h \in \mathbb{R}$ the integrator is stable.

4 NUMERICAL SOLUTION OF HARMONIC OSCILLATOR

To illustrate the numerical convergence of the proposed variational integrators, we consider the harmonic oscillator with frequency $\omega = 1$ described by the Lagrangian (10). For concrete numerical tests, following [6], we choose the initial conditions $(q_0, p_0) =$

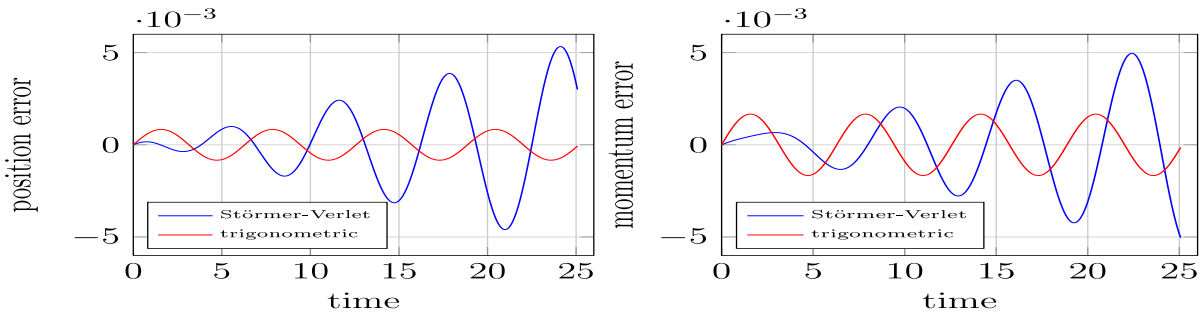

Figure 4: Harmonic oscillator with $\omega = 1$, using $h = 0.05$ and $S = 3$. (a): Errors in position and (b) errors in momentum for the Störmer-Verlet [5] and the trigonometric interpolation method with $u = \omega h$.

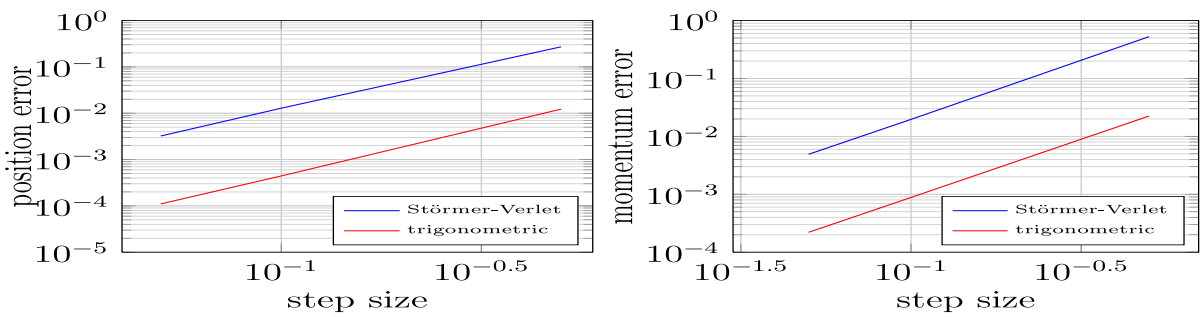

Figure 5: Harmonic oscillator with $\omega = 1$ and $S = 3$. Global errors of (a): the position and (b): the momentum using three step sizes h for the Störmer-Verlet [5] and the trigonometric interpolation method with $u = \omega h$.

$(2, 1)$ and the time interval $[0, 25]$. In Figures 4(a) and 4(b) the evolution of the errors in the position q and the momentum p are plotted for the Störmer-Verlet [5] and the trigonometric interpolation method with $S = 3$ ($u = \omega h$). From the comparison one can see that the errors using the trigonometric interpolation are much smaller (also bounded for all the integration time) than those obtained by using Störmer-Verlet method of [5].

As a further test, the global errors for the position and momentum components at $t = 3$ for time steps $h \in \{0.05, 0.1, 0.5\}$ are compared in Figure 5 to the Störmer-Verlet method [5] for the case of the harmonic oscillator. Evidently, while both methods are of the same order, for all the step sizes tested, smaller errors in position and momentum result when trigonometric interpolation for $u = \omega h$ is employed.

5 CONCLUSIONS

In the present paper, linear stability properties of higher order variational integration methods that use the phase lag technique are presented. Calculating the eigenvalues of the amplification matrix for thee example of a harmonic oscillator shows that the methods are stable for a wide range of parameters. Finally, testing the proposed methods concerning

position error and energy conservation on long integration of oscillatory problems, show good behavior of the proposed simulation technique.

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