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Phase Fitted Variational Integrators using Interpolation Techniques on non Regular Grids

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Abstract. The possibility of deriving a high order variational integrator that utilizes intermediate nodes within one time interval to approximate the action integral is investigated. To this purpose, we consider time nodes chosen through linear or exponential expressions and through the roots of Chebyshev polynomial of the first kind in order to approximate the configurations and velocities at those nodes. Then, by defining the Lagrange function as a weighted sum over the discrete Lagrangians corresponding to the curve segments, we apply the phase fitted technique to obtain an exponentially fitted numerical scheme. The resulting integrators are tested for the numerical simulation of the planar two body problem with high eccentricity and of the three-body orbital motion within a solar system.

Keywords: variational integrators, phase lag, Chebyshev nodes, phase-fitted methods

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INTRODUCTION AND MOTIVATION

In the general framework of geometric numerical integration variational integrators play a key role due to their symplecticity and momentum conservation properties as well as their good energy behavior [1]. One main ingredient in the derivation of variational integrators is the approximation of the action integral along a curve segment in a time interval. The number of intermediate points in a time interval increases the order of the method, see for example Refs. [1, 2, 5] where the intermediate points have been chosen to subdivide the time interval into equal subintervals. In the present work, high order variational integrators are derived that use different choices of intermediate points for the action integral approximation by employing general interpolation techniques.

According to [1], discrete Euler-Lagrange equations can be derived by following the steps of the derivation of the Euler-Lagrange equations in the time-continuous formulation of Lagrangian dynamics. To this aim, one considers approximate configurations \( q_k \approx q(t_k) \) and \( q_{k+1} \approx q(t_{k+1}) \) at the equispaced time nodes \( t_k, t_{k+1} \) with \( h = t_{k+1} - t_k \) being the time step. Let the time continuous Lagrangian \( L : TQ \to \mathbb{R} \) be defined on the tangent bundle of the configuration manifold \( Q \). In the discrete setting, a discrete Lagrangian \( L_d : Q \times Q \to \mathbb{R} \) is defined to approximate the action integral along the curve segment between \( q_k \) and \( q_{k+1} \), i.e.

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

This leads to an action sum \( S_d(\gamma_d) = \sum_{k=1}^{N-1} L_d(q_k, q_{k+1}) \), where \( \gamma_d = (q_0, \ldots, q_N) \), \( N \in \mathbb{N} \) represents the discrete trajectory. The discrete Hamilton’s principle states that a motion \( \gamma_d \) 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 are obtained

\[
D_2L_d(q_{k-1}, q_k) + D_1L_d(q_k, q_{k+1}) = 0, \quad k = 1, \ldots, N - 1
\]

where the notation \( D_iL_d \) indicates the slot derivative with respect to the \( i \)-th argument of \( L_d \), see [1].

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VARIATIONAL INTEGRATORS USING INTERPOLATION TECHNIQUES ON NON REGULAR GRIDS

In order to derive high order methods, at first we approximate the action integral along the curve segment between \( q_k \) and \( q_{k+1} \) with a discrete Lagrangian that depends only on these endpoints. To obtain appropriate expressions for the configurations \( q^j \) and velocities \( \dot{q}^j \), \( j = 0, \ldots, S-1 \) and \( S \in \mathbb{N} \), a number of time nodes \( t^j \in [t_k, t_{k+1}] \) must be defined, see Fig. 1. By choosing \( C^j \in [0, 1] \) such that

\[
C^0 = 0, \quad C^{S-1} = 1
\]  

any intermediate time node \( t^j \) can be defined by

\[
t^j = t_k + C^j h
\]

In [5] linear time nodes have been regarded by defining a partition of the interval \([0, 1]\) in equal sub intervals, i.e. \( C^j = \frac{j}{S-1} \), see Table 1. One of the goals of the present work is to explore the use of nodes on non regular grids, those resulting from the roots of the Chebyshev polynomial of first kind, known as Chebyshev nodes. According to [3], Chebyshev nodes can be defined in \([0, 1]\) by the expression

\[
C^{S-j-1} = \frac{1}{2} + \frac{1}{2} \cos \left( \frac{2j + 3}{2(S+1)} \pi \right), \quad j = 1, \ldots, S-2
\]  

Alternatively, so called exponential intermediate nodes can be computed as

\[
C^j = \frac{j}{S-1} e^{j-1-S}, \quad j = 1, \ldots, S-2
\]

Since the intermediate nodes can be fully defined from the latter equations, Eqs. (3) for \( C^0 \) and \( C^{S-1} \) must be regarded. In Table 1, the locations of the above nodes are presented for one and three internal points between \( q_k \) and \( q_{k+1} \) (i.e. \( S = 3, 5 \)).

<table>
<thead>
<tr>
<th>Number of nodes ( S )</th>
<th>Linear nodes</th>
<th>Chebyshev nodes</th>
<th>Exponential nodes</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>([0, 0.5, 1])</td>
<td>([0, 0.3087, 1])</td>
<td>([0, 0.1839, 1])</td>
</tr>
<tr>
<td>5</td>
<td>([0, 0.25, 0.5, 0.75, 1])</td>
<td>([0, 0.1464, 0.3706, 0.6294, 1])</td>
<td>([0, 0.0124, 0.0677, 0.2759, 1])</td>
</tr>
</tbody>
</table>

With the above the configuration and velocity at any intermediate time node \( t^j \) is obtained by the expressions

\[
q^j = g_1(t^j)q_k + g_2(t^j)q_{k+1}, \quad \dot{q}^j = \dot{g}_1(t^j)q_k + \dot{g}_2(t^j)q_{k+1}
\]

The functions \( g_1(t^j) \) and \( g_2(t^j) \) are chosen according to the type of interpolation we consider. For the sake of continuity, the conditions \( g_1(t_{k+1}) = g_2(t_k) = 0 \) and \( g_1(t_k) = g_2(t_{k+1}) = 1 \) is required.

For any choice of interpolation, one can define the discrete Lagrangian by a weighted sum of the form

\[
L_d(q_k, q_{k+1}) = h \sum_{j=0}^{S-1} w_j L(g_1(t^j)q_k + g_2(t^j)q_{k+1}, \dot{g}_1(t^j)q_k + \dot{g}_2(t^j)q_{k+1})
\]
As can be easily proved, for maximal algebraic order it must hold \( \sum_{j=0}^{S-1} w_j (C^j)^m = 1/(m+1) \), where \( m = 0, 1, \ldots, S-1 \), see Ref. [5]. In our applications, we concentrate on interpolation techniques using trigonometric functions of Ref. [5], i.e. 
\[
    g_1(t^j) = \frac{\sin \left( u - \frac{t^j}{h} \right)}{\sin u}, \quad g_2(t^j) = \frac{\sin \left( \frac{t^j}{h} - u \right)}{\sin u}
\]
for \( u = \in \mathbb{R} \setminus \{k\pi, k \in \mathbb{Z}\} \). For the evaluation of the parameter \( a \) the phase lag technic is used (see Appendix).

**PLANAR TWO BODY PROBLEM**

To investigate the effect of different interpolations in the discrete Lagrangian (7), we consider the planar two-body problem, see e.g. Ref. [4]. By choosing one of the bodies (the heavier) as the center of our coordinate system, the motion remains planar. Denoting the position of the second body by \( q = (q_1, q_2)^T \), the Lagrangian of the system (assuming the masses of the bodies and the gravitational constant are equal to 1) takes the form
\[
    L(q, \dot{q}) = \frac{1}{2} \dot{q}^2 + \frac{1}{|q|}
\]
As initial conditions (position and velocity) we assume \( q = (1 - \varepsilon, 0)^T \) and \( \dot{q} = (0, \sqrt{(1 + \varepsilon)/(1 - \varepsilon)})^T \) where \( \varepsilon \) is the eccentricity of the orbit.

**FIGURE 2.** Energy evolution for the planar two body problem using \( S = 5 \) and time step \( h = 0.01 \) for the time nodes of Table 1. (a): \( \varepsilon = 0.8 \) using Chebyshev nodes (b): \( \varepsilon = 0.9 \) using exponential nodes.

For the numerical test, we consider high eccentricity orbits, i.e. \( \varepsilon \geq 0.8 \). First, we monitor the evolution of kinetic, potential and total energy in Fig. 2a for the integrator based on the Chebyshev intermediate nodes in Eq. (4) and in Fig. 2b for the intermediate exponential nodes given in Eq. (5). For both integrators the resulting total energy is preserved as expected, even for high eccentricities.

We then check the resulting position error, taken as the norm of the exact minus the calculated position, for the time nodes derived for \( S = 3 \), see Table 1. For the different choices of nodes, in Fig. 3a the error in position is illustrated for the two body problem with \( \varepsilon = 0.8 \) and \( h = 0.01 \), while in Fig. 3b the total energy error (norm of the calculated minus the initial energy) for the same problem is shown. The behavior of the errors is similar for the three choices of intermediate nodes. In particular it must be observed that the choice of linear nodes yields the smallest energy error while it performs worst in the position error and vice versa do the exponential nodes. At this point, we can not explain this behavior, this will be subject to future investigation. Last, we test the integrator derived using

**FIGURE 3.** Planar two body problem with eccentricity \( \varepsilon = 0.85 \), using \( S = 3 \) and time step \( h = 0.01 \) for the time nodes of Table 1. (a): Norm of the position error (b): Norm of the total energy error.

Chebyshev time nodes introduced in Eq. (4) for eccentricity \( \varepsilon = 0.8 \), for \( S = 5 \) and time step \( h = 0.01 \). The calculated
norm of the position error (calculated as in the previous figures) is plotted in Fig. 4 together with the errors obtained using the Matlab ode solvers ode45, ode23 and ode113 and the Störmer-Verlet algorithm, see Ref. [4]. Here, the two structure preserving schemes (Störmer-Verlet and the variational integrator with Chebyshev nodes) show a better energy behavior, as expected.

THREE BODY PROBLEM

In the last section, we consider the modified solar system with two planets, see Ref. [4], which is described by the Lagrange function

\[ L(q, \dot{q}) = \frac{1}{2} \sum_{i=1}^{3} m_i \dot{q}_i^2 + \sum_{i=1, i \neq j}^{3} \frac{m_i m_j}{||q_i - q_j||} \]  

With masses \( m_1 = 1, m_2 = m_3 = 10^{-2} \), initial configurations \( q_1 = (0, 0), q_2 = (1, 0), q_3 = (4, 0) \) and initial velocities \( \dot{q}_1 = (0, 0), \dot{q}_2 = (0, 1), \dot{q}_3 = (0, 0.5) \) the resulting motion of the two planets is nearly circular with periods close to \( 2\pi \) and \( 14\pi \) respectively, see Ref. [4]. Again, we use linear, Chebychev and exponential intermediate nodes in the discrete Lagrangian (7). The total energy evolution, using \( S = 3 \) and time step \( h = 0.01 \) is shown in Fig. 5 for the three choices of intermediate nodes. In contrast to the two body example, here the exponential nodes yield the best energy behavior while the linear nodes lead to the largest amplitude of oscillation.

SUMMARY AND CONCLUSIONS

The derivation of phase fitted variational integrators using interpolation techniques that use discrete Lagrangian defined on non regular grids is investigated. Numerical problems which have been tested, i.e. the special case of the planar two body with high eccentricity and the three body solar system model.

The preliminary results concerning position error and energy conservation for these problems show good behavior of the proposed simulation technique. A further investigation is on the way to elaborate the selection of the time nodes.

Appendix

The features of the phase fitting technique become obvious in its application to first order ordinary differential equations, as e.g. in the problem \( \frac{dy(t)}{dt} = i\omega y(t) \), \( y(0) = 1 \) which has the exact (oscillatory type) solution: \( y(t) = e^{i\omega t} \).
A numerical map $\tilde{\Phi}(h)$, when applied to a set of known past values, produces a numerical estimation $\tilde{y}(t+h)$. By calculating the fraction of the estimated divided by the exact solution given by

$$\frac{\tilde{y}(t+h)}{y(t+h)} = \alpha(\omega h)e^{-i(\omega h)} , \quad (11)$$

one obtains the phase lag $\ell(\omega h)$ of the numerical map $\tilde{\Phi}(h)$. The goal of the phase fitting technique is to minimize the phase lag while simultaneously forcing $\alpha(\omega h)$ to approach unity as closely as possible, see Refs. [8, 9, 10].

Following the procedure of Ref. [7] we consider a harmonic oscillator with frequency $\omega$, the motion of which is described by the Lagrange function $L(q, \dot{q}) = \frac{1}{2}q^2 - \frac{1}{2}\omega^2 \dot{q}^2$. Under these circumstances, the expression of the discrete Lagrangian, Eq. (7) can be obtained. By inserting the resulting Lagrangian to Eqs. (2) we get the two step variational phase lag while simultaneously forcing $\Lambda(\omega, h)$ to approach unity as closely as possible, see Ref. [6].

$$\sum_{j=1}^{S} w_j \left[ \dot{g}_1(t^j)^2 + \dot{g}_2(t^j)^2 - \omega^2 (g_1(t^j)^2 + g_2(t^j)^2) \right] \quad \quad \sum_{j=1}^{S} w_j \left[ \dot{g}_1(t^j)\dot{g}_2(t^j) - \omega^2 g_1(t^j)g_2(t^j) \right] q_k + q_{k-1} = 0. \quad (12)$$

The latter is equal to that of Ref. [5] in the case when $g_1$ and $g_2$ are given by Eq. (8). The phase lag of the method for the initial positions $q(0) = \dot{q}_0$, $q(h) = \dot{q}_1$ has the form

$$\frac{\dot{q}_2}{q(2h)} = \frac{\Lambda(u, \omega, h)\dot{q}_1 + \dot{q}_0}{\dot{q}_0 - 2\cos(\omega h)\dot{q}_1}$$

where

$$\Lambda(u, \omega, h) = \frac{\sum_{j=1}^{S} w_j \left[ \dot{g}_1(t^j)^2 + \dot{g}_2(t^j)^2 - \omega^2 (g_1(t^j)^2 + g_2(t^j)^2) \right]}{\sum_{j=1}^{S} w_j \left[ \dot{g}_1(t^j)\dot{g}_2(t^j) - \omega^2 g_1(t^j)g_2(t^j) \right]} \quad (13)$$

It is clear that for exponentially fitted methods

$$\Lambda(u, \omega, h) = -2\cos(\omega h) \quad (14)$$

must hold. For particle motion in three dimensions, it can be shown that for the case of variational integrators using trigonometric functions $g_1(t^j)$ and $g_2(t^j)$, the phase lag is zero for $u = \omega h$. For the numerical solution of orbital problems, the estimation of the parameter $\omega$ can be obtained by calculating the angular velocity $\omega(t) = \sqrt{\frac{\dot{q}(t)^2 + \dot{q}(t)^2}{|\dot{q}(t)|^2}}$ for the generalized configuration $q(t)$ of particles motion, see also Ref. [6].

REFERENCES