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Deriving Numerical Techniques with Zero Phase-Lag and Derivatives for Initial Value Problems of Second Order

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Abstract. In the present we investigate the advantages of the phase lag analysis for the derivation of phase-fitted techniques on several numerical schemes. Relying on the main characteristics of the phase lag we evaluate the parameters needed firstly for Runge-Kutta methods and secondly for high order variational integration methods, so that the phase lag and its derivatives are zero. The proposed methods are tested for the solution of initial value problems on ordinary differential equations of second order, like the Hénon-Heiles model.

Keywords: Runge-Kutta methods; variational integrators; phase-lag analysis; initial value problems; orbital problems;

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INTRODUCTION

Last decades several methods have been proposed for the numerical integration of initial value problems of second order. Many of the obtained numerical methods use an optimized version of some basic numerical schemes based on phase-lag properties, see for examples Refs. [3 - 9].

From the one hand, using the above techniques, special cases of phase-fitted Runge-Kutta and Runge-Kutta-Nyström schemes have been developed [6]. Further more, numerical methods that define zero phase-lag and its derivatives have been constructed, for the solution of several physical problems, see for example Ref. [5] and references within.

On the other hand, in the general framework of geometric numerical integration, variational integrators are very popular, due to their symplectic and momentum conservation properties and their good energy behavior [7]. Since those methods are deriving using Euler-Lagrange equations to derive the second order numerical scheme, lately those methods have been combined with the phase-lag properties for the construction of phase-fitted high order variational integrators, see Ref. [8].

In this paper, a new optimized Runge-Kutta method and a new high order variational integration method are developed. Both approaches use the evaluation of the phase-lag and its first derivative based on a test equation, see Ref [9]. Preliminary results show the advantages of the proposed technique when tested for the solution of initial value problems on ordinary differential equations of second order, like the Hénon-Heiles model.

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DEVELOPMENT OF THE NEW OPTIMIZED RUNGE-KUTTA METHOD

An s -stage Runge-Kutta method has the general form

$$y_n = y_{n-1} + \sum_{i=1}^s b_i f_i,$$

where

$$f_i = hf \left(t_{n-1} + c_i h, y_{n-1} + h \sum_{j=1}^{i-1} \alpha_{ij} f_j \right), \quad i = 1, \dots, s \quad (1)$$

By applying the RK method (1) to the test equation

$$y' = i\omega y \quad (2)$$

we obtain the numerical solution

$$y_n = a_*^{n-1} y_{n-1}, \quad (3)$$

with

$$a_* = A_s(z^2) + izB_s(z^2) \quad (4)$$

where A_s, B_s are polynomials in z^2 completely determined by the parameters of the method (1).

The definition that follows is originally formulated by van der Houwen and Sommeijer [2].

Definition 1 (Phase-lag). Apply the RK method (1) to the general method (2). Then we define the phase-lag $\Phi(z) = z - \arg[a_*(z)]$. If $\Phi(z) = O(z^{q+1})$, then the RK method is said to have phase-lag order q . In addition, the quantity $a(z) = 1 - |a_*(z)|$ is called amplification error.

At this point we are going to optimize the well known third algebraic order Runge-Kutta method of Heun. The new optimized RK that will occur, is a three-stage explicit Runge-Kutta method of third algebraic order.

In order to derive the new method, we are using the following coefficients:

$$\begin{aligned} \alpha_{21} &= \frac{1}{2}, & \alpha_{31} &= 0, & \alpha_{32} &= \frac{3}{2}, \\ c_2 &= \frac{1}{3}, & c_3 &= \frac{2}{3}, & b_2 &= 0 \end{aligned} \quad (5)$$

To evaluate the variable coefficients b_1 , and b_3 , first we compute the polynomials $A_s(z^2)$ and $B_s(z^2)$ in terms of RK parameters. By substituting the parameters given above and by requiring to nullify the phase lag, we obtain the following equation

$$\Phi(z) = 0 \Rightarrow \tan(z) - \frac{z(-2/9 b_3 z^2 + b_1 + b_3)}{1 - 2/3 b_3 z^2} = 0 \quad (6)$$

From the latter equation we can obtain the first derivative of phase-lag. If we vanish the resulting first derivative of phase-lag, we get the expression

$$\begin{aligned} \Phi'(z) &= 0 \Rightarrow \\ 1 + (\tan(z))^2 - \frac{-2/9 b_3 z^2 + b_1 + b_3}{1 - 2/3 b_3 z^2} + 4/9 \frac{b_3 z^2}{1 - 2/3 b_3 z^2} - 4/3 \frac{z^2 (-2/9 b_3 z^2 + b_1 + b_3) b_3}{(1 - 2/3 b_3 z^2)^2} &= 0 \end{aligned} \quad (7)$$

From Eqs. (6) and (7) we derive a system of two equations. Solving this system we obtain the coefficients b_1 and b_3 , which are fully depended from the product of the step-length h and the frequency w .

HIGH ORDER PHASE FITTED VARIATIONAL INTEGRATORS

Following the definitions of Marsden and West [7], we can obtain high order variational integrators (of order S) using approximations for intermediate positions q^j and velocities $\dot{q}^j$ for each adjacent pair (q_k, q_{k+1}) , for $k = 0, \dots, N$. We can then define the discrete Lagrangian by the expression of Ref. [8], i.e.

$$L_d(q_k, q_{k+1}) = h \sum_{j=0}^{S-1} w_j L(q^j, \dot{q}^j), \quad (8)$$

For the above approximations, we can now adopt a new interpolation scheme based on hyperbolic functions.

Using expressions of $\cosh$ at intermediate time nodes, i.e. at time $t^j = t_k + c^j h$, where $t^j \in [t_k, t_{k+1}]$ (see Ref. [8]) we can define approximations of the form

$$\begin{aligned} q^j &= (1 - c^j) \cosh(c^j U) q_k + c^j \cosh(c^j U - U) q_{k+1} \\ \dot{q}^j &= -(\cosh(c^j U) - (1 - c^j) \sinh(c^j U)) q_k + (\cosh(c^j U - U) + c^j \sinh(c^j U - U)) q_{k+1} \end{aligned} \quad (9)$$

For the coefficients c^j and w_j see [8].

By applying the Lagrangian of Eq. (8) in the discrete Euler-Lagrange equations, see Ref. [7]

$$D_1 L_d(q_k, q_{k+1}) + D_2 L_d(q_{k-1}, q_k) = 0, \quad k = 1, \dots, N-1 \quad (10)$$

we can derive the numerical map for any choice of the continuous Lagrangian L . The notation $D_i L_d$ indicates the slot derivative with respect to the i -th argument of L_d .

To evaluate the parameter U of Eqs. (9) we can now use the phase lag technique described above, to derive exponential numerical map, see [9]. It can be shown that even for numerical methods derived using high order phase fitted variational integrators, the parameter U depends only on the product of the step-length h and the frequency ω .

NUMERICAL TESTS

We consider the Hénon-Heiles problem, which can be expressed as a function of two spatial coordinates q_1 and q_2 and the two momenta p_1 and p_2 with the Hamiltonian (see Ref. [1])

$$H = \frac{1}{2}(p_1^2 + p_2^2) + \frac{1}{2}(q_1^2 + q_2^2) + q_1^2 q_2 - \frac{1}{3} q_2^3 \quad (11)$$

For the above the corresponding second order system of differential equations

$$\begin{aligned} \ddot{q}_1 &= -q_1 - 2q_1 q_2 \\ \ddot{q}_2 &= -q_2 - q_1^2 + q_2^2 \end{aligned} \quad (12)$$

has solutions with nontrivial properties depending on the initial conditions [1]. For given initial values, the solution stays there and moves somehow like a mass point gliding on this surface of Fig. 1, see also Ref. [1].

FIGURE 1. Potential of the Hénon-Heiles model described by Eq. (11)

Numerical results can be now obtained using the numerical techniques with zero phase-lag and derivatives, as described above.

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