Multistep Methods for Lattice QCD Simulations

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It is well-known that molecular dynamics integrators, which are used for lattice quantum chromodynamics (QCD), suffer from instabilities and possess a rather low order of the accuracy. Hence, it is highly desirable to construct a new class of geometric integrators, that overcomes these instability problems and increases the order of accuracy without increasing remarkably the computational costs.

In this paper we consider for this purpose multistep methods and give an overview of known results to systematize important knowledge for such methods being the right choice for lattice QCD simulations. At the end we try to answer the question: can multistep method be used as molecular dynamic integrators and what might be the advantage of it.

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1. Introduction

In this paper we will give a short introduction to symplectic multistep integrators, review some recent results and comment on the possible later application in lattice QCD computations.

A *geometric integrator* is a numerical method that preserves the geometric properties of the exact flow of an autonomous ordinary differential equation (ODE)

$$y' = f(y), \qquad y \in \mathbb{R}^p. \tag{1.1}$$

Especially, when solving numerically a Hamiltonian problem, it is of paramount importance that the chosen scheme retains some properties of the underlying continuous problem, like the time reversal symmetry or the area preservation property.

We consider a compatible *linear multistep methods* (LMM) with k steps of the form

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h \sum_{j=0}^{k} \beta_j f(y_{n+j}), \tag{1.2}$$

where $h = \Delta t$ denotes the time step of the grid $t_j = t_0 + jh$, and α_j, β_j are real parameters, $\alpha_j \neq 0$, and $|\alpha_0| + |\beta_0| > 0$. For an application of (1.2) we need an initial value $y_0 = y(t_0)$ as well as starting approximations $y_1, \ldots, y_{k-1}$ to $y(t_0), \ldots, y(t_{k-1})$, that are usually obtained by Runge-Kutta methods.

We recall that the LMM (1.2) is of *order s* if and only if (cf. [8])

$$\sum_{j=0}^{k} \alpha_j = 0, \quad \sum_{j=0}^{k} \alpha_j j^{\ell} = \ell \sum_{j=0}^{k} \beta_j j^{\ell-1}, \quad 1 \leq \ell \leq s, \quad \sum_{j=0}^{k} \alpha_j j^{s+1} \neq (s+1) \sum_{j=0}^{k} \beta_j j^s. \tag{1.3}$$

Furthermore, the multistep method (1.3) has the two *characteristic polynomials*

$$\rho(\xi) = \sum_{j=0}^{k} \alpha_j \xi^j, \qquad \sigma(\xi) = \sum_{j=0}^{k} \beta_j \xi^j, \tag{1.4}$$

and the LMM (1.2) is called *irreducible* if these polynomials (1.4) have no common roots.

Since the stability analysis for LMMs was difficult to establish Dahlquist [2] suggested to consider instead so-called one-leg methods that only need one evaluation of the forcing function f. The *one-leg method* (OLM) associated to the multistep method (1.2) is defined by

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = hf\left(\sum_{j=0}^{k} \beta_j y_{n+j}\right), \tag{1.5}$$

where we assume the *normalization condition* $\sigma(1) = \sum_{j=0}^{k} \beta_j = 1$. The LMMs (1.2) and OLMs (1.5) are closely related. Let $\tilde{y}$ denote the sequence of approximated values obtained from a LMM (1.2) and $\hat{y}$ be the sequence of approximated values obtained from a OLM (1.5), then we have

$$\hat{y}_j = \sum_{j=0}^{k} \beta_j \tilde{y}_{n+j}.$$

Hence the analysis of the stability for LMMs can be reduced to the stability analysis of OLMs.

In the sequel we focus on the case that the ODE (1.1) is a *linear autonomous Hamiltonian system*, i.e. $p = 2n$ (where n is the number of degrees of freedom in mechanics) and

$$y' = J^{-1}\nabla H(y), \qquad y \in \mathbb{R}^{2n}, \qquad \text{where} \quad J = \begin{pmatrix} 0 & I_n \\ -I_n & 0 \end{pmatrix}. \tag{1.6}$$

Here, $H : \mathbb{R}^{2n} \to \mathbb{R}^1$ denotes a smooth Hamiltonian function. Now we can rewrite the LMM (1.2)

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h \sum_{j=0}^{k} \beta_j J^{-1}\nabla H(y_{n+j}). \tag{1.7}$$

2. Area-Preservation and Time-Reversibility of Multistep Methods

A numerical integrator is used in a molecular dynamics step of the Hybrid Monte Carlo algorithm has to satisfy an area-preservation property, which follows from the symplecticity of the numerical method, and a time-reversibility property, which is an extension of the symmetry.

The *symmetry* is fulfilled if the coefficients of a scheme (1.2) (or (1.5)) satisfy the relations

$$\alpha_{k-j} = -\alpha_j, \qquad \beta_{k-j} = \beta_j \quad \text{for all } j = 0, 1, \ldots, k,$$

i.e.

$$\rho(\xi) \equiv -\xi^k \rho(1/\xi), \qquad \sigma(\xi) \equiv \xi^k \sigma(1/\xi).$$

They are also charaterized by having an odd number of time steps, i.e. $k = 2\nu - 1$, $\nu = 1, 2, \ldots$. This means that the numerical solutions satisfy the following reversibility requirement: whenever $y_n, \ldots, y_{n+k}$ satisfy the relation (1.2) (or (1.5)), $y_{n+k}, \ldots, y_n$ satisfy (1.2) with h replaced by $-h$. From this it follows that symmetric multistep methods are *time-reversible*.

Definition 1. *A mapping $g : \mathbb{R}^{2n} \to \mathbb{R}^{2n}$ is called symplectic (with respect to J) if*

$$\left[\frac{\partial g(y)}{\partial y}\right]^\top J \left[\frac{\partial g(y)}{\partial y}\right] \equiv J. \tag{2.1}$$

It is well-known, that the solution of the ODE (1.6) at any fixed time t^*, regarded as a function on the initial data $y(0) \in \mathbb{R}^{2n}$, (so-called *phase flow*) is a *symplectic mapping*. Hence, it is a natural task to seek for numerical methods that retain this property (in a sense to be specified later).

In the literature there exist (at least) two definitions for symplectic LMMs. Eirola and Sanz-Serna [9] considered the transformation $g : \mathbb{R}^{2nk} \to \mathbb{R}^{2nk}$, $Y_\ell \mapsto Y_{\ell+1}$, where $Y_\ell = (y_\ell^\top, \ldots, y_{\ell+k-1}^\top)^\top$, that is associated to the LMM (1.7), and obtained the following positive result.

Theorem 1 ([9]). *Assume that the OLM is symmetric and irreducible. Then the corresponding mapping $Y_\ell \mapsto Y_{\ell+1}$ is symplectic with respect to the matrix $\Lambda \otimes J$, where $\Lambda = (\lambda_{ij})$ is given by*

$$\lambda_{ij} = \sum_{m \geq 0} (\alpha_{i+m}\beta_{j+m} + \alpha_{j+m}\beta_{i+m}), \quad i \geq 0, \, j \leq k.$$

But here the symplecticity is regarded with respect to another skew symmetric matrix $\Lambda \otimes J$. We note that this symplecticity is equivalent to the preservation of quadratic first integrals, cf. [1]. For example, Ge and Feng [6] showed that the standard second order *leap-frog scheme*

$$y_{n+2} - y_n = 2hJ^{-1}\nabla H(y_{n+1}) \quad \text{is symplectic w.r.t.} \quad \begin{pmatrix} 0 & J_{2n} \\ J_{2n} & 0 \end{pmatrix} \quad \text{with} \quad \Lambda = \begin{pmatrix} 0 & 2 \\ 2 & 0 \end{pmatrix}.$$

Contrary, in a different second approach, Tang [10] proved a negative result for the *step-transition operator* (underlying one-step method) introduced by Feng [5] $g : \mathbb{R}^{2n} \to \mathbb{R}^{2n}$ satisfying

$$\sum_{j=0}^{k} \alpha_j g^j = h \sum_{j=0}^{k} \beta_j f \circ g^j, \tag{2.2}$$

where g^j stands for *j*-time composition $g : g \circ g \circ \cdots \circ g$. This operator characterizes the LMM (1.2) as $y_1 = g(y_0), \ldots, y_k = g(y_{k-1}) = g^k(y_0), \ldots$, e.g. for Hamiltonian systems the LMM (1.7) reads

$$\sum_{j=0}^{k} \alpha_j g^j = h \sum_{j=0}^{k} \beta_j J^{-1} (\nabla H) \circ g^j. \tag{2.3}$$

This step-transition operator g allows for a definition of symplecticity for LMMs:

Definition 2 ([10]). *The LMM* (1.7) *is symplectic if the operator g defined by* (2.3) *is symplectic, i.e.* (2.1) *holds for all Hamiltonian functions H and all sufficiently small step-sizes h.*

Theorem 2 ((Conjecture of Feng) [10]). *For a Hamiltonian system* (1.6)*, any compatible LMM (with order $s \geq 1$ of form* (1.7) *is not symplectic.*

Despite this negative result of Theorem 2, it is known that the *second order mid-point rule*

$$y_{n+1} - y_n = hJ^{-1}\nabla H\left(\frac{1}{2}(y_{n+1} + y_n)\right). \tag{2.4}$$

is a symplectic multistep method. This fact motivates to consider *generalized LMMs* of the form

$$\sum_{j=0}^{k} \alpha_j y_j = h \sum_{j=0}^{k} \beta_j J^{-1} \nabla H\left(\sum_{l=0}^{k} \gamma_{jl} y_l\right), \qquad \text{with} \quad \sum_{l=0}^{k} \gamma_{jl} = 1, \quad j = 0, \ldots, k. \tag{2.5}$$

Unfortunately, also for the scheme (2.5) the result is rather negative.

Theorem 3 ([10]). *For a Hamiltonian system* (1.6)*, if a difference scheme (with order $s \geq 1$ of the form* (2.5) *is symplectic, then it must be of order 2.*

In fact, Dai and Tang [3] showed that (2.4) is the only symplectic scheme of this form. However, following the concept of *G-stability* proposed by Dahlquist there exists another third way of transfering the definition of symplecticity to multistep methods, cf. [2].

However, recall that for integrators to be suitable for molecular dynamics integration, it is sufficient to safisfy the following *area-preservation property*.

Definition 3. *A mapping $g : \mathbb{R}^{2n} \to \mathbb{R}^{2n}$ is called area-preserving (without an orientation) if*

$$\left| \det \frac{\partial g(y)}{\partial y} \right| \equiv 1. \tag{2.6}$$

which is a slightly weaker assumption than simplecticity.

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3. Numerical Experiments

We consider a model of a *simple harmonic oscillator (SHO)* with the Hamiltonian

$$H(p,q) = \frac{1}{2}p^2 + \frac{1}{2}w^2q^2 \tag{3.1}$$

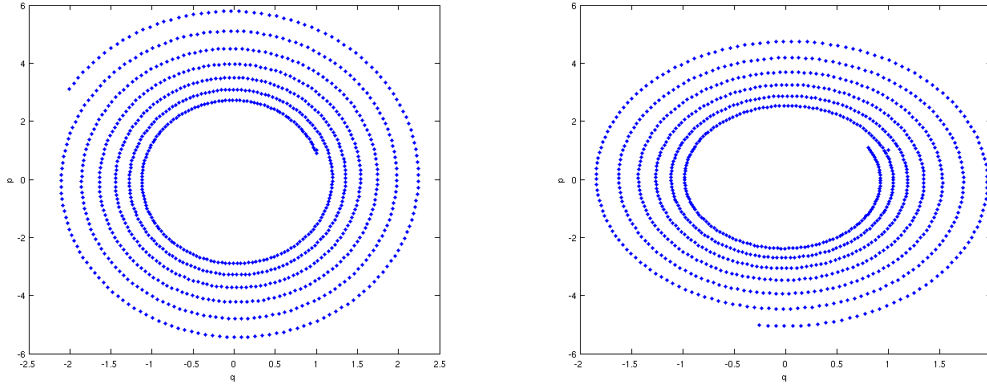to investigate the stability behavior of solutions for this system by *G*-symplectic multistep methods.

Figure 1: Solutions of the SHO; explicit Euler method with step size $h = 0.1$, initial value $(p_0, q_0) = (0,1)$; implicit Euler method with step size $h = 0.1$, initial value $(p_0, q_0) = (0,1)$.

We choose the three *G*-symplectic methods and show the corresponding numerical solution of the SHO problem (3.1). The first method is a *4-step explicit method*

$$y_{n+3} - y_{n+2} + y_{n+1} - y_n = \frac{h}{2}\left(f_{n+2} + f_{n+1}\right). \tag{3.2}$$

The second method is a *predictor-corrector method*

$$
\begin{aligned}
y_{n+4} - y_{n+3} &= \frac{h}{24}\left(55f_{n+3} - 59f_{n+2} + 37f_{n+1} - 9f_n\right) &&\text{as a predictor}\\
y_{n+4} - y_{n+3} &= \frac{h}{24}\left(9f_{n+4} + 19f_{n+3} - 5f_{n+2} + f_{n+1}\right) &&\text{as a corrector,}
\end{aligned}
\tag{3.3}
$$

using the explicit method to compute f_{n+4} of the implicit one. Finally, we consider a *partitioned method*, where for each equation of the system of SHO we apply a different multistep method:

$$
\begin{aligned}
y_{n+3} - y_{n+2} + y_{n+1} - y_n &= h\left(f_{n+2} + f_{n+1}\right),\\
y_{n+3} - y_{n+1} &= 2h\left(f_{n+2} + f_{n+1}\right).
\end{aligned}
\tag{3.4}
$$

Figures 2, 3, 4 show (from left to right) the numerical solutions obtained by the corresponding multistep methods (3.2) - (3.4) and their long-time behavior ($n = 1000000$ time steps).
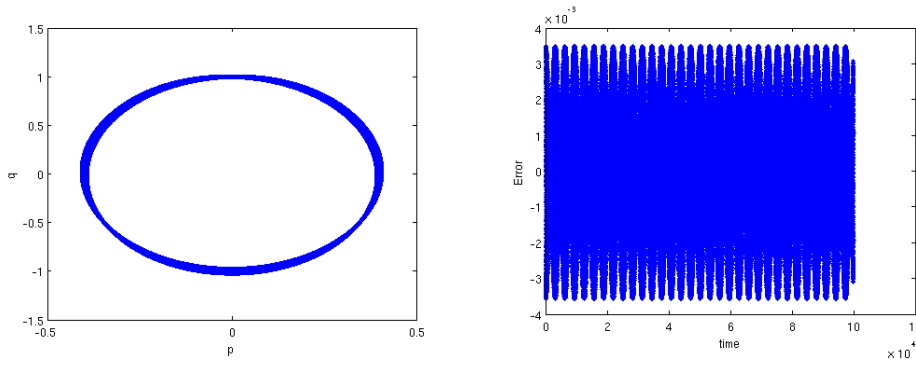
Figure 2: Solution of the SHO by the 4-step explicit method (3.2); with step size $h = 0.1$, initial value $(p_0, q_0) = (0, 1)$; the error of the computed solution of the method (3.2) to exact solution.
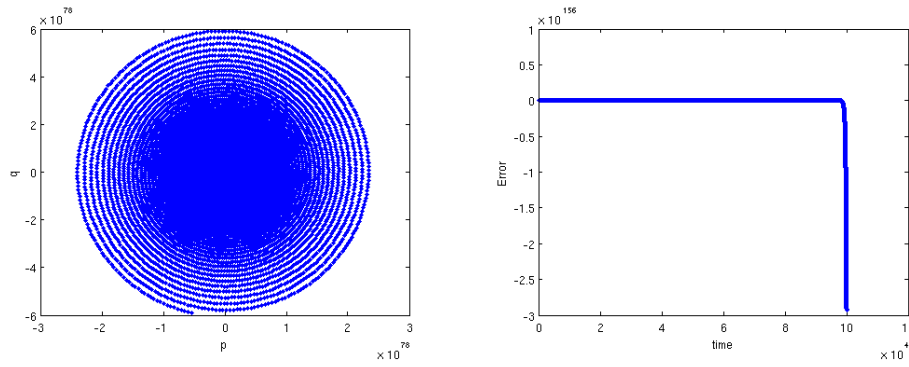

Figure 3: Solution of the SHO by the predictor-corrector method (3.3) with step size $h = 0.1$, initial value $(p_0, q_0) = (0, 1)$; the error of the computed solution of the method (3.3) to exact solution.
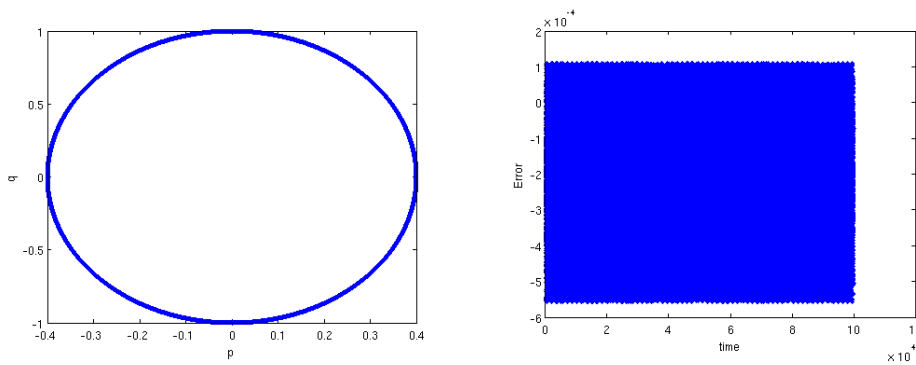

Figure 4: Solution of the SHO by the partitioned method (3.4) with step size $h = 0.1$, initial value $(p_0, q_0) = (0, 1)$; the error of the computed solution of the method (3.4) to exact solution.

The method (3.2) shows quite stable behavior for the numerical solution of the SHO, but further considerations show that increasing the number of steps lead us to oscillations and symplecticity of the solutions will be destroyed. But for the short term problems the method behavior is suitable. The method (3.3) collapses after some time and the error of this method grows exponentially, but still for short time period it gives the proper results and the symplectic property is

satisfied. The last method (3.4) yields the best results, its numerical solutions behave symplectic even during long time, it conserves the energy of system properly and this class of partitioned multistep method, according to [8], gives the correct results even for the long time integrations.

4. Conclusion and Outlook

In spite of the collected negative results, the numerical experiments showed that the short-time behavior of the multistep methods is rather promising. The main advantage of multistep method is that the high-order version of such methods can be easily obtained by one function evaluation per time step and it, consequently, will increase the accuracy of computations.

Despite these predominant negative statements, we recall that in lattice QCD simulations one solely needs an area-preserving integrator which is a slightly weaker assumption than the discussed symplecticity. In a forthcoming paper we will investigate, following an idea of Hairer [7], a *projected LMM* that conserves the Hamiltonian and hence makes the *acceptance step* in the hybrid Monte Carlo simulations obsolete. This feature is especially interesting for small lattice spacings.

Acknowledgments

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