IMPLEMENTING ARBITRARILY HIGH-ORDER SYMPLECTIC METHODS VIA KRYLOV DEFERRED CORRECTION TECHNIQUE

Q.D. FENG, N.M. NIE, J.F. HUANG, Z.J. SHANG, AND Y.F. TANG

Abstract. In this paper, an efficient numerical procedure is presented to implement the Gaussian Runge-Kutta (GRK) methods (also called Gauss methods). The GRK technique first discretizes each marching step of the initial value problem using collocation formulations based on Gaussian quadrature. As is well known, it preserves the geometric structures of Hamiltonian systems. Existing analysis shows that the GRK discretization with s nodes is of order $2s$, A-stable, B-stable, symplectic and symmetric, and hence “optimal” for solving initial value problems of general ordinary differential equations (ODEs). However, as the unknowns at different collocation points are coupled in the discretized system, direct solution of the resulting algebraic equations is in general inefficient. Instead, we use the Krylov deferred correction (KDC) method in which the spectral deferred correction (SDC) scheme is applied as a preconditioner to decouple the original system, and the resulting preconditioned nonlinear system is solved efficiently using Newton-Krylov schemes such as Newton-GMRES method. The KDC accelerated GRK methods have been applied to several Hamiltonian systems and preliminary numerical results are presented to show the accuracy, stability, and efficiency features of these methods for different accuracy requirements in short- and long-time simulations.

1. Introduction

The symplectic numerical methods are specially designed for integrating Hamiltonian systems. They preserve the inherent canonical properties of the continuous Hamiltonian flows. Extensive comparative numerical experiments have shown the overwhelming superiorities of symplectic methods over nonsymplectic ones, especially in structural, global and long-time tracking capabilities and preservation of invariants (also called first integrals) [9, 16, 18, 31, 47, 48, 56]. In this paper, we focus on a special class of symplectic methods called the *Gaussian Runge-Kutta (GRK) methods* or the *Gauss methods*. The GRK methods represent a special class of collocation formulations for each time marching step using the Gaussian quadrature nodes. Previous theoretical study has shown many interesting features of the GRK methods. In particular, the GRK discretization with s Gaussian nodes is of order $2s$ (super-convergence), A-stable, B-stable, symplectic (structure preserving), and symmetric (time reversible). One refers to [31] for more details.

It is noticed that there is an order limitation to the implementations of the GRK methods. In practice, due to efficiency and stability considerations, most time integration schemes

---

2000 *Mathematics Subject Classification.* Primary 37M15, 65L06; Secondary 65B05, 65F10.

Key words and phrases. Hamiltonian system, High-order symplectic methods, Krylov Deferred Correction Technique.

This work was supported by the *Informatization Construction of Knowledge Innovation* Projects of the Chinese Academy of Sciences *“Supercomputing Environment Construction and Application”* (INF105-SCE), by the National Natural Science Foundation of China (Grant Nos. 10471145, 10571173 and 10672143), and by the Morningside Center of Mathematics, Chinese Academy of Sciences.

The third author was partially supported while he was visiting the Institute of Computational Mathematics and Scientific/Engineering Computing of the Chinese Academy of Sciences and the Morningside Center.

for general initial value problems are limited to orders of 10 or so. The fully implicit higher order GRK schemes, in spite of optimality in accuracy and flexibility in stepsize, are very inefficient to implement if directly use Newton's method and Gauss elimination as the solutions at different collocation nodes are coupled. On the other hand, the much more easily implemented schemes such as explicit higher-order Runge-Kutta or linear multistep methods are usually not structure-preserving, and require extremely small time steps due to stability restriction [2, 32]. They are not good candidates for solving complicated nonlinear problems for long time.

There have been many research efforts to develop higher order or even spectral schemes for initial value problems. The classical deferred and defect correction methods try to derive higher order approximations by iteratively refining the error or defect equations using lower order schemes [42, 62, 63]. In [12], Dutt *et al* introduced the spectral deferred correction (SDC) methods which use the Gaussian quadrature nodes instead of uniform ones, and the Picard integral equation formulation instead of the numerically unstable differential equation form. Extremely high-order SDC schemes (up to 30) have been tested on many initial value ODE problems. In [33], Huang *et al* noticed that the deferred and defect correction procedures are equivalent to preconditioned Neumann series expansions, in which the deferred correction schemes are applied as preconditioners to decouple the original coupled collocation formulations. Therefore, the Newton-Krylov methods can be introduced to further accelerate the convergence of the SDC methods for ODE problems, as well as to avoid the divergence of the SDC type methods for differential algebraic equations (DAEs). Numerical experiments in [33, 34] have shown that the resulting Krylov deferred correction (KDC) methods are of arbitrary order, very efficient, and can effectively eliminate the order reduction for stiff systems observed in the SDC and other initial value problem solvers. The purpose of this paper is to combine the Krylov deferred correction methods with GRK formulations, and compare the performance of different KDC accelerated initial value problem solvers. Our preliminary numerical results on several Hamiltonian systems show that for the same accuracy requirement, higher order methods are more efficient than lower order ones, and symplectic methods preserve invariants of the original system better than non-symplectic ones, hence are more stable numerically.

We want to mention that most of the fundamental building blocks in the KDC accelerated GRK methods are not new and have been studied previously. How the decoupled system can be used as a preconditioner for a couple system can be found in [38]. Detailed discussions of the KDC methods are presented in [34], and analytical properties of the GRK methods have been studied thoroughly in [31]. In this paper, these building blocks are integrated together and applied to the Hamiltonian systems, and our numerical results show that the resulting high-order symplectic methods are extremely useful tools for large-scale long-time initial value Hamiltonian system simulations.

This paper is organized as follows. In Sec. 2, we give a short introduction of symplectic methods for Hamiltonian systems. In particular, we discuss the GRK methods and their analytical properties. High-order GRK methods are traditionally considered inefficient as direct solution of the resulting discretizated system using Newton's method and Gauss elimination requires prohibitive amount of work. To improve the performance, in Sec. 3, we introduce the KDC technique, in which the spectral deferred correction (SDC) methods are used as preconditioners, and the resulting preconditioned systems are solved efficiently using Newton-Krylov schemes. Finally in Sec. 4, we present several numerical results to compare the KDC accelerated GRK methods with other solvers of different orders.

2. HAMILTONIAN SYSTEMS AND GAUSSIAN RUNGE-KUTTA METHODS

In this section, we discuss several basic concepts of the Hamiltonian systems and Gaussian Runge-Kutta methods.

2.1. **Hamiltonian Systems and Symplectic Methods.** A system of ordinary differential equations

$$\begin{cases} \dfrac{dZ}{dt} = F(Z), \quad Z \in \mathbb{R}^p, \\ Z(t_0) = Z_0 \end{cases} \tag{2.1}$$

is called a Hamiltonian system when $p = 2n$ and it takes the form

$$\begin{cases} \dfrac{dZ}{dt} = J^{-1}\nabla H(Z), \quad Z \in \mathbb{R}^{2n}, \\ Z(t_0) = Z_0 \end{cases} \tag{2.2}$$

where $J = \begin{bmatrix} \mathbf{0}_n & I_n \\ -I_n & \mathbf{0}_n \end{bmatrix}$, ∇ stands for the gradient operator, and $H : \mathbb{R}^{2n} \to \mathbb{R}^1$ is a smooth function referred to as the *Hamiltonian*.

The symplectic methods represent a special class of numerical initial value problem solvers which preserve the geometric structures of Hamiltonian systems. The mathematical definition of symplectic methods are briefly given below via the so-called step-transition operator. Interested readers are referred to [9, 16, 31] for detailed discussions of the step-transition operator as well as symplectic methods.

Definition 2.1. A numerical scheme compatible (consistent and stable) with the initial value problem in Eq. (2.2) is called symplectic if its step-transition operator $G^h : \mathbb{R}^{2n} \to \mathbb{R}^{2n}$ is symplectic , i.e.,

$$\left[\frac{\partial G^h(Z)}{\partial Z}\right]^T J \left[\frac{\partial G^h(Z)}{\partial Z}\right] = J$$

for any Hamiltonian H and sufficiently small step-size h .

There are many ways to construct symplectic methods, including those based on the Padé approximations, generating functions, Adams, splitting, composition, and Runge-Kutta techniques. Using Cayley transform [16] or Padé approximations [17], Feng discovered that the Euler midpoint rule (GRK method with only one Gaussian node)

$$Z^{k+1} = Z^k + hF\left(\frac{Z^{k+1} + Z^k}{2}\right) \tag{2.3}$$

is second-order symplectic for any Hamiltonian system. Furthermore, the numerical scheme

$$P_m(-hJ^{-1}M)Z^{k+1} = P_m(hJ^{-1}M)Z^k \tag{2.4}$$

is $2m$th-order symplectic for a linear Hamiltonian system ($H = \frac{1}{2}Z^\top MZ$) as long as the mth-order polynomial $P_m(\lambda)$ satisfies

$$\frac{P_m(\lambda)}{P_m(-\lambda)} - \exp(\lambda) = O(\lambda^{2m+1}). \tag{2.5}$$

In [9, 17, 20], generating function techniques are discussed for the construction of arbitrarily high order symplectic methods using high-order derivatives of the Hamiltonian. In [22, 53, 61], by observing that the symplectic transformations form a group, the splitting ideas are used to construct a class of explicit symplectic methods: consider a Hamiltonian vector field which can be decomposed into several integrable pieces $H = \sum_{k=1}^{p} H_k$ with phase flows q_k^h, one can easily obtain first-order and second-order symplectic schemes for the original Hamiltonian H as in $q_p^h \circ \cdots \circ q_2^h \circ q_1^h$ and $q_1^{h/2} \circ \cdots \circ q_{p-1}^{h/2} \circ q_p^h \circ q_{p-1}^{h/2} \circ \cdots \circ q_1^{h/2}$, respectively; and, higher-order schemes can be iteratively constructed by observing that if q^h is a symplectic scheme of order p, then $q^{\alpha h} \circ q^{\beta h} \circ q^{\alpha h}$ is also symplectic with order $p+2$ when

$$\alpha = \frac{1}{2 - 2^{1/(p+1)}}, \quad \beta = -\frac{2^{1/(p+1)}}{2 - 2^{1/(p+1)}}.$$

For the classical general linear schemes, it was shown that all linear multi-step schemes are non-symplectic [29, 54], and with the exception of the trapezoid rule, all linear multi-step methods are even not conjugate-symplectic [21]. Therefore, for efficiency and stability considerations, one likes to use symplectic schemes based on the Runge-Kutta methods. The *symplectic Runge-Kutta methods* are Runge-Kutta methods

$$\begin{cases} Z^{k+1} = Z^k + h \sum\limits_{i=1}^{s} b_i F(Y_i), \\ Y_i = Z^k + h \sum\limits_{i=1}^{s} a_{ij} F(Y_j), \quad 1 \le i \le s \end{cases} \tag{2.6}$$

in which the coefficients satisfy the conditions

$$b_i b_j - b_i a_{ij} - b_j a_{ji} = 0, \quad i, j = 1, 2, \cdots, s, \tag{2.7}$$

as discussed in [40, 46, 52].

We want to mention that in general it is hard to construct symplectic schemes using (2.6) and (2.7). In the following section, we introduce a special class of symplectic Runge-Kutta methods based on the collocation formulation and Gaussian quadrature nodes.

2.2. **Collocation and Gaussian Runge-Kutta Methods.** The collocation methods are widely used for the solution of differential equations. For a general ODE initial value system in Eq. (2.1), given the stepsize h and a set of s distinct real numbers $c_1, \cdots, c_s$ with $0 \le c_j \le 1$, the collocation method searches *collocation polynomials* $\Phi(t) = [\phi_1(t), \phi_2(t), \cdots, \phi_{2n}(t)]^\top$ of degree s satisfying

$$\begin{cases} \dot{\Phi}(t_0 + c_j h) = F(t_0 + c_j h, \Phi(t_0 + c_j h)), \quad j = 1, \cdots, s. \\ \Phi(t_0) = Z_0. \end{cases} \tag{2.8}$$

The solution at $t_0 + h$ is then approximated by $Z_1 = \Phi(t_0 + h)$ [31].

In [27, 59], it was shown that the collocation method is equivalent to the s-stage Runge-Kutta method

$$\begin{cases} Z_1 = Z_0 + h \sum\limits_{j=1}^{s} b_j K_j, \\ K_j = F\left(t_0 + c_j h, Z_0 + h \sum\limits_{m=1}^{s} a_{jm} K_m\right), \quad j = 1, \cdots, s, \end{cases}$$

where

$$a_{jm} = \int_0^{c_j} L_m(\tau) d\tau, \quad b_j = \int_0^1 L_j(\tau) d\tau, \tag{2.9}$$

and $L_m(\tau)$ is the *Lagrange* interpolating polynomial $L_m(\tau) = \prod\limits_{l \ne m} (\tau - c_l)/(c_m - c_l)$. Also, if the conditions

$$\sum_{j=1}^{s} b_j c_j^{k-1} = \frac{1}{k}, \quad k = 1, \cdots, p$$

hold for $p \geq s$, then the collocation formulation (and the corresponding Runge-Kutta method) has order p, the same order as the underlying quadrature formula. In this paper, instead of a discussion of general collocation methods using arbitrary collocation points, we focus on the *Gaussian Runge-Kutta (GRK) methods* based on the Gaussian quadrature nodes (zeros of the shifted Legendre polynomial $\frac{d^s}{dx^s}[x^s(x-1)^s]$). The detailed formulas of the GRK methods we implement as well as their properties are presented in the reminder of this section.

We first denote the s Gaussian nodes in the interval $[0,1]$ as $c_1, c_2, \cdots, c_s$, and define the derivatives $\dot{\Phi}(t)$ of $\Phi(t)$ at the Gaussian nodes as the new unknown $\boldsymbol{\Psi}$ as in

$$\boldsymbol{\Psi} = \begin{pmatrix} \overrightarrow{\dot{\phi}}_1 \\ \vdots \\ \overrightarrow{\dot{\phi}}_i \\ \vdots \\ \overrightarrow{\dot{\phi}}_{2n} \end{pmatrix} = \begin{pmatrix} \left[\dot{\phi}_1(t_0+c_1h), \cdots, \dot{\phi}_1(t_0+c_sh)\right]^\top \\ \vdots \\ \left[\dot{\phi}_i(t_0+c_1h), \cdots, \dot{\phi}_i(t_0+c_sh)\right]^\top \\ \vdots \\ \left[\dot{\phi}_{2n}(t_0+c_1h), \cdots, \dot{\phi}_{2n}(t_0+c_sh)\right]^\top \end{pmatrix}. \tag{2.10}$$

Next, notice that

$$\phi_i(t_0+c_jh) = [Z_0]_i + \int_{t_0}^{t_0+c_jh} \dot{\phi}_i(t)dt = [Z_0]_i + h\int_0^{c_j} \dot{\phi}_i(t_0+\tau h)d\tau, \quad j = 1, \cdots, s \tag{2.11}$$

where $[Z_0]_i$ is the ith component of the initial value vector Z_0, we can construct the approximating Legendre polynomial of $\dot{\phi}_i(t)$ by calculating its coefficients using Gaussian quadrature, and integrate the interpolating polynomial exactly to get

$$\boldsymbol{\Phi} = \begin{pmatrix} \overrightarrow{\phi_1} \\ \vdots \\ \overrightarrow{\phi_i} \\ \vdots \\ \overrightarrow{\phi_{2n}} \end{pmatrix} = \begin{pmatrix} [\phi_1(t_0+c_1h), \cdots, \phi_1(t_0+c_sh)]^\top \\ \vdots \\ [\phi_i(t_0+c_1h), \cdots, \phi_i(t_0+c_sh)]^\top \\ \vdots \\ [\phi_{2n}(t_0+c_1h), \cdots, \phi_{2n}(t_0+c_sh)]^\top \end{pmatrix} \tag{2.12}$$

at the Gaussian nodes. Notice that this procedure represents a linear mapping from the derivatives $\overrightarrow{\dot{\phi}}_i = [\dot{\phi}_i(t_0+c_1h), \cdots, \dot{\phi}_i(t_0+c_sh)]^\top$ to the values $\overrightarrow{\phi}_i = [\phi_i(t_0+c_1h), \cdots, \phi_i(t_0+c_sh)]^\top$, i.e., $\overrightarrow{\phi_i} = \overrightarrow{[Z_0]_i} + hA\overrightarrow{\dot{\phi}}_i$ where $\overrightarrow{[Z_0]_i} = [[Z_0]_i, \cdots, [Z_0]_i]$ has dimension s, A is the spectral integration matrix independent of h as discussed in [12], and can be accurately precomputed using tools such as *Mathematica*. In the following, we symbolically represent the corresponding mapping from $\boldsymbol{\Psi}$ to $\boldsymbol{\Phi}$ as $\boldsymbol{\Phi} = \mathbf{Z}_0 + h\mathcal{A}\boldsymbol{\Psi}$ with

$$\mathbf{Z}_0 = \begin{pmatrix} \overrightarrow{[Z_0]_1} \\ \vdots \\ \overrightarrow{[Z_0]_i} \\ \vdots \\ \overrightarrow{[Z_0]_{2n}}, \end{pmatrix} \tag{2.13}$$

and $\mathcal{A}$ is a block diagonal matrix of size $2ns \times 2ns$ with its diagonal blocks the spectral integration matrix A

$$\mathcal{A} = \begin{pmatrix} A & 0 & \cdots & 0 \\ 0 & A & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & A \end{pmatrix}.$$

The collocation formulation to be solved then becomes

$$\boldsymbol{\Psi} = \begin{pmatrix} \overrightarrow{\dot{\phi}_1} \\ \vdots \\ \overrightarrow{\dot{\phi}_i} \\ \vdots \\ \overrightarrow{\dot{\phi}_{2n}} \end{pmatrix} = \begin{pmatrix} \overrightarrow{F_1}(\boldsymbol{\Phi}) \\ \vdots \\ \overrightarrow{F_i}(\boldsymbol{\Phi}) \\ \vdots \\ \overrightarrow{F_{2n}}(\boldsymbol{\Phi}) \end{pmatrix} = \boldsymbol{F}(\boldsymbol{\Phi}) = \boldsymbol{F}(\mathbf{Z}_0 + h\mathcal{A}\boldsymbol{\Psi}), \tag{2.14}$$

or more succinctly,

$$\boldsymbol{M}(\boldsymbol{\Psi}) = \mathbf{0}, \tag{2.15}$$

In the formula,

$$\overrightarrow{F_i}(\boldsymbol{\Phi}) = \begin{pmatrix} F_i(\Phi_1) \\ \vdots \\ F_i(\Phi_s) \end{pmatrix}, \tag{2.16}$$

F_i is the i_{th} component of F, and

$$\Phi_i = \begin{pmatrix} \phi_1(t_0 + c_i h) \\ \vdots \\ \phi_{2n}(t_0 + c_i h) \end{pmatrix}.$$

We want to mention that the GRK formulation has been extensively studied previously and many of its interesting analytical properties have been revealed as in the following theorem [14, 15, 46, 58].

Theorem 2.2. *For the Hamiltonian system in Eq. (2.2), the Gaussian Runge-Kutta method with s nodes is of order $2s$ (super convergence), A-stable, B-stable, symplectic (structure preserving), and symmetric (time reversible).*

Unfortunately, as the solutions at different collocation points are coupled in the resulting algebraic system (mostly nonlinear), its direct solution using Newton' method and Gauss elimination requires prohibitive amount of work. In next section, we introduce the newly developed Krylov deferred correction technique to improve the efficiency in solving the GRK formulations.

We want to mention that the preservation of the geometric structures by symplectic methods has a profound implication in dynamics. Although symplectic methods may not preserve analytical invariants exactly, they do preserve them very well in a generalized sense. When a symplectic method applies to an integrable or a nearly integrable Hamiltonian system, most of the invariant tori of the system can be preserved if the step size of the method is sufficiently small [31, 49, 50]. These invariant tori are the level sets of the numerical invariants of the symplectic method applied to the system [49]. These numerical invariants are well defined in a Cantor set, with large Lebesgue measure, of the phase space and approximate the exact invariants of the system with order of accuracy equal to that of the method [49]. Backward error analysis shows that the numerical orbits of a symplectic method approximate the exact orbits of some perturbed Hamiltonian system very well during a very long interval of iteration steps (exponentially long in $1/h$ where h is the step size) [31]. For the GRK methods, assuming the discretized collocation formulation is solved exactly, it has been proven that all the quadratic invariants are exactly preserved in the numerical simulation [19, 31]. Non-quadratic invariants, as we will show later, are usually not exactly preserved and, as remarked above, can still be used as measures of the solution error in the numerical simulation when analytical formulas are not available.

3. Krylov Deferred Correction Techniques

To solve the nonlinear system in Eq. (2.15), classical Newton's method can be employed to iteratively refine the approximate solution using

$$\mathbf{\Psi}^{[n+1]} = \mathbf{\Psi}^{[n]} - \boldsymbol{\delta}^{[n]} \tag{3.1}$$

where $\boldsymbol{\delta}^{[n]}$ solves the linear approximation of the error equation given by

$$J_{\boldsymbol{M}}\left(\mathbf{\Psi}^{[n]}\right) \boldsymbol{\delta}^{[n]} = \boldsymbol{M}\left(\mathbf{\Psi}^{[n]}\right), \tag{3.2}$$

and $J_{\boldsymbol{M}}\left(\mathbf{\Psi}^{[n]}\right)$ is the Jacobian of $\boldsymbol{M}(\mathbf{\Psi})$ at $\mathbf{\Psi}^{[n]}$. As $J_{\boldsymbol{M}}\left(\mathbf{\Psi}^{[n]}\right)$ is in general a dense matrix, solving Eq. (3.2) using direct Gaussian elimination requires prohibitive $O((2ns)^3)$ operations, which becomes extremely expensive for large s. Therefore, most existing implementations of the GRK methods are limited to order up to 10 ($s = 5$) or so.

An alternative class of methods for solving Eq. (3.2) iteratively searches the optimal solution in the Krylov subspace defined by

$$\mathcal{K}_k\left(J_{\boldsymbol{M}}, \boldsymbol{M}\left(\mathbf{\Psi}^{[n]}\right)\right) = \left\{\boldsymbol{M}\left(\mathbf{\Psi}^{[n]}\right), J_{\boldsymbol{M}}\boldsymbol{M}\left(\mathbf{\Psi}^{[n]}\right), \cdots, J_{\boldsymbol{M}}^{k-1}\boldsymbol{M}\left(\mathbf{\Psi}^{[n]}\right)\right\}. \tag{3.3}$$

Consider the case where the Jacobian matrix is of the form

$$J_{\boldsymbol{M}}\left(\mathbf{\Psi}^{[n]}\right) = \pm I - C, \tag{3.4}$$

and most eigenvalues of C are clustered at 0. As the numerical rank of the corresponding Krylov subspace is low, it is not hard to see that the solution converges to a prescribed accuracy after a few *Krylov iterations* and the resulting Krylov subspace method can be extremely efficient. Further notice that to solve the nonlinear equation (2.15), it is not necessary to solve Eq. (3.2) exactly during each Newton iteration, therefore the Newton iteration can be resumed once the residual in Eq. (3.2) is reduced by a prescribed factor in the Krylov subspace methods. The resulting methods are usually referred to as the *Newton-Krylov methods* [36, 37, 45]. In summary, an efficient implementation of the Newton-Krylov method requires

(a) the Jacobian matrix of the nonlinear system be close to the identity matrix I and hence well-conditioned, and
(b) an efficient procedure to compute the matrix vector product $J_{\boldsymbol{M}}\boldsymbol{M}(\mathbf{\Psi}^{[n]})$.

For (a), a common practice to derive well-conditioned system is to introduce preconditioners to the original equation. Traditionally, the inverse of a sparse matrix close to the original system has been widely used as preconditioner in numerical linear algebra. More recent results include integral operators as preconditioners which can be applied efficiently to any vector using fast convolution algorithms such as the fast multipole methods or the precorrected FFT [26, 44]. In this paper, we utilize the Krylov deferred correction technique which uses a lower order explicit or implicit method to precondition the higher order implicit GRK formulations and decouple the equation at different collocation nodes. Similar to deferred or defect correction schemes, we first assume a provisional solution to the collocation formulation (2.15) is derived using a low order marching scheme (such as the forward Euler or low order Runge-Kutta methods) and denote it by

$$\boldsymbol{\Psi}^{[0]} = \begin{bmatrix} \overrightarrow{\psi_1}^{[0]} \\ \vdots \\ \overrightarrow{\psi_{2n}}^{[0]} \end{bmatrix},$$

where the vectors represent the solutions for each component at different collocation nodes as given by

$$\overrightarrow{\psi_i}^{[0]} = \begin{bmatrix} \psi_i^{[0]}(t_1) \\ \vdots \\ \psi_i^{[0]}(t_s) \end{bmatrix}, \quad i = 1, \cdots, 2n.$$

As Gaussian nodes are used as the interpolation points, we can calculate the coefficients of the degree $s-1$ interpolating polynomials

$$\Psi^{[0]}(t) = \begin{bmatrix} \psi_1^{[0]}(t) \\ \vdots \\ \psi_{2n}^{[0]}(t) \end{bmatrix}$$

using Gaussian quadratures and fast Legendre transform [13], and define the error as

$$\overrightarrow{\delta}(t) = \begin{bmatrix} \delta_1(t) \\ \vdots \\ \delta_{2n}(t) \end{bmatrix} = \begin{bmatrix} \psi_1(t) \\ \vdots \\ \psi_{2n}(t) \end{bmatrix} - \begin{bmatrix} \psi_1^{[0]}(t) \\ \vdots \\ \psi_{2n}^{[0]}(t) \end{bmatrix}. \tag{3.5}$$

The discretized error equation is then simply

$$\boldsymbol{\delta} = \boldsymbol{F}\left(\mathbf{Z}_0 + h\boldsymbol{\mathcal{A}}\boldsymbol{\Psi}^{[0]} + h\boldsymbol{\mathcal{A}}\boldsymbol{\delta}\right) - \boldsymbol{\Psi}^{[0]}, \tag{3.6}$$

where $\boldsymbol{\delta} = (\delta_1(t_1), \cdots, \delta_1(t_s), \cdots, \delta_{2n}(t_1), \cdots, \delta_{2n}(t_s))^\top$.

Next, similar to the deferred correction schemes, a low order method can be used to solve the error equation. In [33], it was shown that the low order method is equivalent to applying a lower triangular matrix to approximate the integral operator and the spectral integration matrix A, in particular, the forward Euler's method is equivalent to the rectangular rule using left end-point and the backward Euler's method the rectangular rule using the right end-point. Hence the low order method solves the discretized system

$$\tilde{\boldsymbol{\delta}} = \boldsymbol{F}\left(\mathbf{Z}_0 + h\boldsymbol{\mathcal{A}}\boldsymbol{\Psi}^{[0]} + h\tilde{\boldsymbol{\mathcal{A}}}\tilde{\boldsymbol{\delta}}\right) - \boldsymbol{\Psi}^{[0]}, \tag{3.7}$$

where $\tilde{\boldsymbol{\mathcal{A}}}$ is the low order approximation of the spectral integration operator $\boldsymbol{\mathcal{A}}$ and $\tilde{\boldsymbol{\delta}}$ the low order approximation of the error $\boldsymbol{\delta}$. We can succinctly write Eq. (3.7) as an explicit function

$$\tilde{\boldsymbol{\delta}} = \widetilde{\boldsymbol{M}}\left(\boldsymbol{\Psi}^{[0]}\right). \tag{3.8}$$

Notice that when $\boldsymbol{\Psi}^{[0]}$ solves the GRK collocation formulation in Eq. (2.15), we have $\tilde{\boldsymbol{\delta}} = 0$. Therefore, solving Eq. (2.15) is equivalent to finding the zero of $\widetilde{\boldsymbol{M}}$. Using the implicit function theorem, the Jacobian of $\widetilde{\boldsymbol{M}}$ can be easily derived as

$$\boldsymbol{J}_{\widetilde{\boldsymbol{M}}} = \frac{\partial \tilde{\boldsymbol{\delta}}}{\partial \boldsymbol{\Psi}^{[0]}} = -\left(\boldsymbol{\mathcal{I}} - h\boldsymbol{J}_{\boldsymbol{F}}\tilde{\boldsymbol{\mathcal{A}}}\right)^{-1}\left(\boldsymbol{\mathcal{I}} - h\boldsymbol{J}_{\boldsymbol{F}}\boldsymbol{\mathcal{A}}\right).$$

As both $h\tilde{\mathcal{A}}$ and $h\mathcal{A}$ are approximations of the integral operator, it is not surprising that for reasonable small h, the two matrices are close and the Jacobian matrix $\boldsymbol{J}_{\widetilde{\boldsymbol{M}}}$ is hence very close to $-\boldsymbol{I}$, i.e., the preconditioned equation

$$\widetilde{\boldsymbol{M}}\left(\boldsymbol{\Psi}^{[0]}\right) = 0$$

is better conditioned, hence the Newton-Krylov methods quickly converge to the prescribed accuracy requirement. For comparison, the Jacobian of $\boldsymbol{M}$ is given by

$$\boldsymbol{J}_{\boldsymbol{M}} = h\boldsymbol{J}_{\boldsymbol{F}}\mathcal{A} - \boldsymbol{I}.$$

As for (b), one can either formulate the Jacobian matrix of $\widetilde{\boldsymbol{M}}$ explicitly if possible, or apply the Jacobian free technique where the matrix vector product is approximated by a forward difference formula, i.e., for any vector v, $J_{\widetilde{\boldsymbol{M}}}(x)v$ is approximated by

$$D_\tau\widetilde{\boldsymbol{M}}(x : v) = \frac{\widetilde{\boldsymbol{M}}(x + \tau v) - \widetilde{\boldsymbol{M}}(x)}{\tau}$$

for some properly chosen parameter τ [37]. Notice that the evaluation of $\widetilde{\boldsymbol{M}}$ is simply one low order solution of the error equation and hence can be very efficient. Our numerical experiments show that the Jacobian free techniques are more efficient during each Krylov iteration, while the explicit formula utilizing the analytical Jacobian matrix provides better convergence behavior in the Newton-Krylov methods because of its improved accuracy. The implementation details of the Newton-Krylov methods are still being studied by the authors and results will be reported in the future.

Finally in this section, we want to mention that most of the techniques we use have been studied previously. Hence many of the technical details are neglected in this paper and we refer interested readers to [36, 37] for further discussions of the Newton-Krylov techniques, to [38] for an interesting summary of existing Jacobian free Newton-Krylov methods, to [12, 13] for the spectral deferred correction methods and how the spectral integration matrix and error equation are computed, and to [33, 34] for a detailed discussion of the Krylov deferred correction methods for general differential algebraic equations.

4. Numerical Results

In this section, we study the performance of the GRK methods with different orders, and compare the symplectic methods with non-symplectic ones in efficiency and invariant preservation.

4.1. **Hamiltonian Systems.** Our numerical experiments focus on three Hamiltonian systems: the harmonic oscillator, Kepler motion, and geodesic flow on ellipsoid, which represent the linear, semi-linear and non-linear Hamiltonian systems, respectively.

Harmonic Oscillator

The harmonic oscillator is a simple linear Hamiltonian system which describes the motion of a mass point controlled by an elastic spring. It is given by the equations

$$\frac{dp}{dt} = -q$$
$$\frac{dq}{dt} = p,$$

where the Hamiltonian function is defined as $H = \frac{1}{2}(p^2 + q^2)$.

Kepler Motion

The Kepler motion is a semi-linear Hamiltonian system modeling the movement of celestial bodies. It is usually given by

$$\begin{aligned} \dot p_1 &= -\frac{q_1}{(q_1^2+q_2^2)^{3/2}}, \quad \dot q_1 = p_1, \\ \dot p_2 &= -\frac{q_2}{(q_1^2+q_2^2)^{3/2}}, \quad \dot q_2 = p_2, \end{aligned}$$

where the Hamiltonian function is defined as $H = \frac{1}{2}(p_1^2 + p_2^2) - 1/\sqrt{q_1^2+q_2^2}$. For this system, both the Hamiltonian and angular momentum $L = q_1p_2 - q_2p_1$ are invariants.

As the orbit of the Kepler motion is an ellipse, we choose the initial values $p_1(0) = 0$, $p_2(0) = 2$, $q_1(0) = 0.4$, and $q_2(0) = 0$ so that the fundamental period of the motion is $T = 2\pi$ (see [1, 31]). We present simulation results for approximately 100 periods in the interval $[0, 630]$.

Geodesic Flow on Ellipsoid

Our last example considers the geodesic flow on the ellipsoid with three major axes of different lengths (a, b, c), which models the motion of a unit-mass point on the surface of the ellipsoid without any external forces. The corresponding Hamiltonian is

$$H(p_1, p_2; q_1, q_2) = \frac{g_{22}p_1^2 - 2g_{12}p_1p_2 + g_{11}p_2^2}{2|G|}, \tag{4.1}$$

where

$$\begin{aligned} g_{11} &= \cos^2 q_1 \left(a^2\cos^2 q_2 + b^2 \sin^2 q_2\right) + c^2 \sin^2 q_1, \\ g_{12} &= \frac{1}{4}(b^2 - a^2)\sin 2q_1 \sin 2q_2, \\ g_{22} &= \sin^2 q_1 (a^2 \sin^2 q_2 + b^2 \cos^2 q_2), \end{aligned}$$

and G is a symmetric matrix $\begin{pmatrix} g_{11} & g_{12} \\ g_{12} & g_{22} \end{pmatrix}$ with determinant $|G| = g_{11}g_{22} - g_{12}^2$. It is shown in ([55]) that in addition to the Hamiltonian, the quantity

$$A(p_1, p_2, q_1, q_2) = g_{11} + \frac{g_{22}}{\sin^2 q_1} - \frac{p_1^2}{13.5} - \frac{p_2^2}{13.5 \sin^2 q_1} \tag{4.2}$$

also represents an invariant. In the simulation, we set $a = 9.5$, $b = 5.5$, $c = 2.5$, and choose the initial values $p_1(0) = 8.846945$, $q_1(0) = \pi/2$, $p_2(0) = 5.436522$, and $q_2(0) = 0$.

4.2. **Symplectic Methods with Different Orders.** Traditionally, symplectic methods have been limited to lower orders due to reasons discussed in previous sections. Here, we compare the performance of the KDC accelerated GRK methods with different number of Gaussian nodes $s = 2, 4, 6, 8, 10$, which correspond to orders $4, 8, 12, 16, 20$, respectively. Our numerical code is written in matlab.

For each s in our numerical experiments, we compare the accuracy(for different stepsize) as a function of the CPU time (which is approximately equivalent to the total amount of operations). For the harmonic oscillator problem, as the analytical solution is known, we plot the real error in Figure 1. Similar results can be derived for the Kepler motion problem as shown in Figure 2. However, as the analytical solution is not readily available for this problem, we measure the error after each period where the exact solution should be $p_1 = 0, q_1 = 0.4, p_2 = 2, q_2 = 0$, the same as the initial condition. Finally for the geodesic flow on the Ellipsoid problem, neither the analytical solution nor the exact period is known. As the invariants $H(p_1, p_2, q_1, q_2)$ and $A(p_1, p_2, q_1, q_2)$ are not quadratic, which can not be exactly preserved by the GRK methods, therefore we measure the errors in these invariants as reasonable indicators for the solution error. These indicators have been verified by our numerical convergence analysis. The results are presented in Figure 3-4.

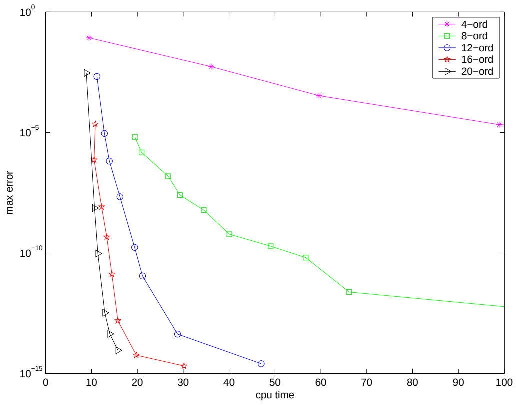

FIGURE 1. Harmonic Oscillator

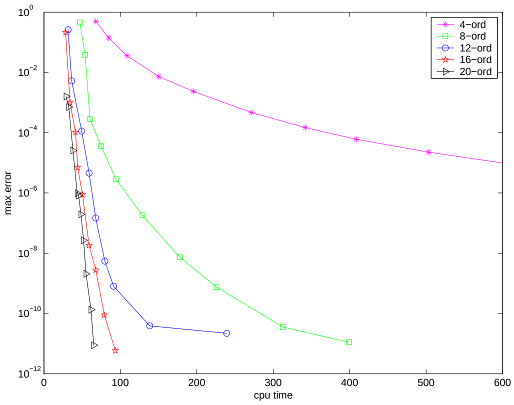

FIGURE 2. Kepler Motion

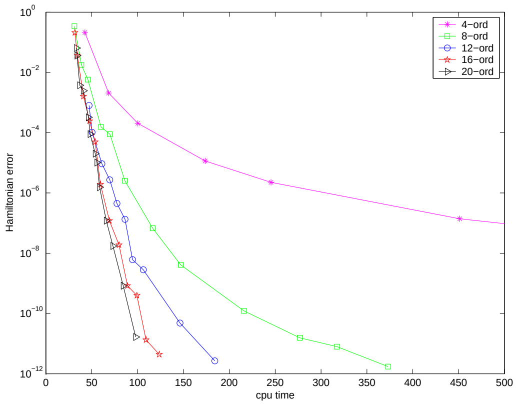

FIGURE 3. Geodesic Flows($H(p_1, p_2, q_1, q_2)$)

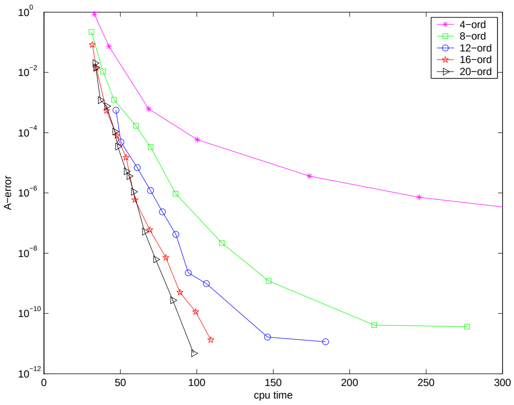

FIGURE 4. Geodesic Flows($A(p_1, p_2, q_1, q_2)$)

From the numerical experiments, we can see that higher order methods are more efficient than lower order ones, especially when very high accuracy is required. In fact, for the same stepsize, the error decays exponentially as the node number s increases. Therefore, for the same accuracy requirement, higher order methods take much larger time-step than lower order ones. This is extremely important for long-time simulations.

4.3. **Symplectic and Non-symplectic Methods.** Instead of Gaussian nodes, other quadrature points can be used in the collocation discretizations. The Radau IA method based on Legendre polynomial uses the left end point of the interval, the Radau IIA method uses the right end point, and the Lobatto nodes use both end points. Also, the Chebyshev polynomial based quadratures can be introduced and the resulting algorithms can be effectively accelerated by the fast Fourier transforms (FFTs). However, these methods are not symplectic. In this section, we compare the Radau IIA based initial value problem solvers with the GRK methods for the Hamiltonian systems. It is shown in [31, 32] that the Radau IIA collocation formulation is of order $2s-1$ when s nodes are used. Therefore for s=$2, 4, 6, 8, 10$, the corresponding orders of the nonsymplectic Radau IIA methods are $3, 7, 11, 15, 19$, respectively. In Figure 5-8, we compare the GRK methods with the nonsymplectic ones using the same number of nodes.

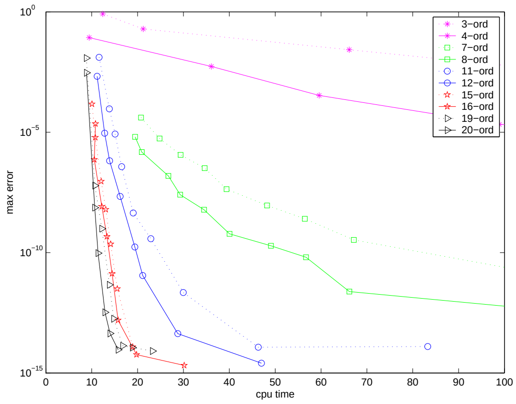

FIGURE 5. Harmonic Oscillator

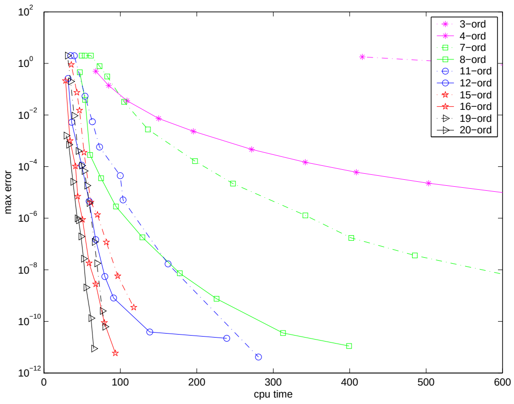

FIGURE 6. Kepler Motion

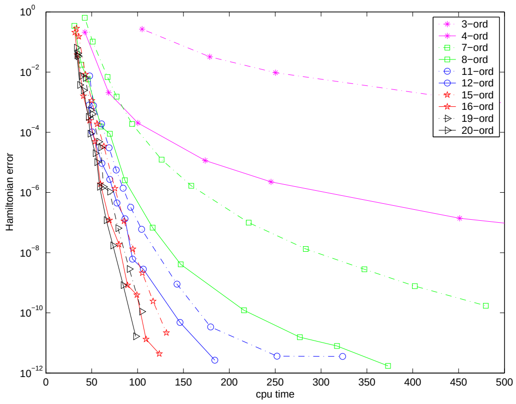

FIGURE 7. Geodesic Flows($H(p_1, p_2, q_1, q_2)$)

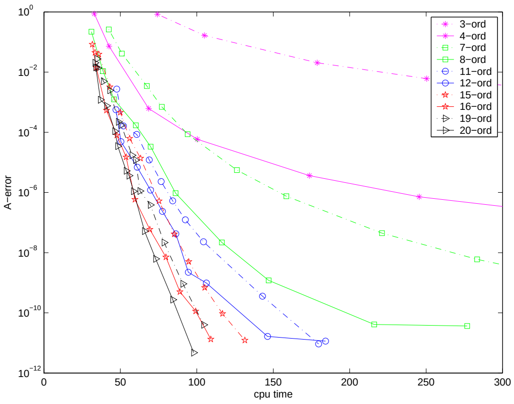

FIGURE 8. Geodesic Flows($A(p_1, p_2, q_1, q_2)$)

From the numerical experiments, it can be seen that for both symplectic and nonsymplectic techniques, higher order methods are more efficient than lower order ones for the same accuracy requirement. In addition, when using the same number of quadrature nodes, the GRK methods outperform the Radau IIA ones. This is not surprising as the GRK collocation formulation achieves optimal order of accuracy for a given s. However, we want to mention that for stiff systems and differential algebraic equations, the Radau IIA methods may outperform the GRK methods, as the GRK formulation may suffer severe order reduction and hence have lower B-convergence orders. The readers are referred to [32] for B-convergence and order reductions for different collocation formulations.

4.4. **Preserving the Invariants.** One advantage of the symplectic methods is their ability to better preserve the invariants of the Hamiltonian systems. In this section, we compare the accuracy of the symplectic and nonsymplectic methods in both the invariants and the solution itself. We want to mention that for many Hamiltonian systems, as the analytical solution is not readily available, one possible measure of the numerical error is to check how these invariants change as a function of time. However, such strategy may not work well for symplectic methods, especially when the invariants are preserved exactly by the numerical discretizations, as in the harmonic oscillator(Hamiltonian) and Kepler motion (angular momentum) problems. We also want to mention that when different sources of errors are considered, in particular, the error in solving the collocation formulations, the GRK methods can not preserve the invariants exactly. In the following, we show how the invariants change as a function of time for different methods and different systems.

We first consider the Harmonic Oscillator problem, in which the Hamiltonian function is a quadratic invariant and should be preserved exactly by the GRK methods when neglecting numerical errors in solving the collocation formulation. In Figure 4.4, we consider the order 8 GRK method and order 7 nonsymplectic Radau IIA method, both with stepsize $1/16$. It can be seen that for the nonsymplectic method, both the solution error and invariant error (Herror) grow as functions of time, while for the symplectic method, the error in the invariant grows extremely slowly as a function of time (it is not a constant due to the accuracy in solving the corresponding collocation formulations), and the solution error grows at about the same rate as the nonsymplectic method. In Figure 4.4, we consider the 20_{th} order GRK method and 19_{th} order Radau IIa method with stepsize 2. For these higher order schemes, as the solution is well resolved, it can be seen that the nonsymplectic method preserves the invariant to approximately the same accuracy level as the symplectic one, and the optimal symplectic method only marginally outperforms the nonsymplectic Radau IIa method.

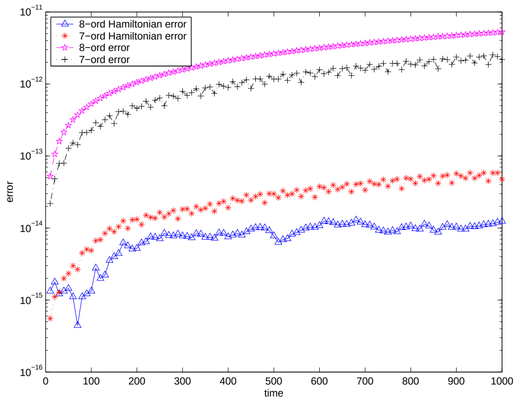

FIGURE 9. Lower-order Harmonic Oscillator

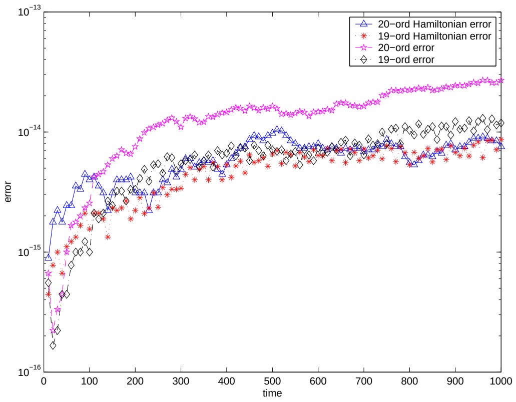

FIGURE 10. Higher-order Harmonic Oscillator

For the Kepler Motion problem, both the Hamiltonian H and angular momentum L are invariants. As the latter is quadratic, hence it is preserved by the GRK discretizations. Similar to the Harmonic Oscillator problem, the errors in the invariants and the solution are presented in Figure 4.4-4.4 for the two invariants. In the simulation, we use the stepsize $\pi/150$ for the lower order methods, and $\pi/8$ for higher order ones. Our numerical results show that the GRK methods give more accurate results in both the invariants and the solution, which is not surprising as the GRK methods are optimal in order and preserve the geometric structures of the original Hamiltonian system.

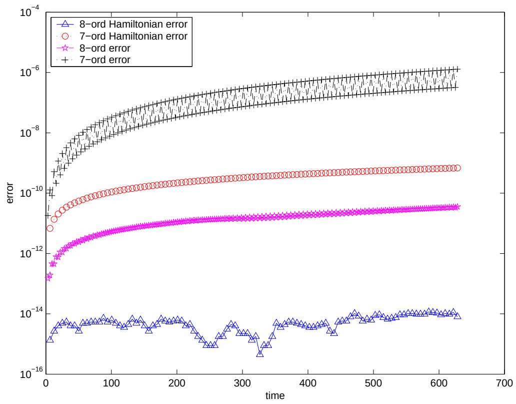

FIGURE 11. Lower-order Kepler(Hamiltonian)

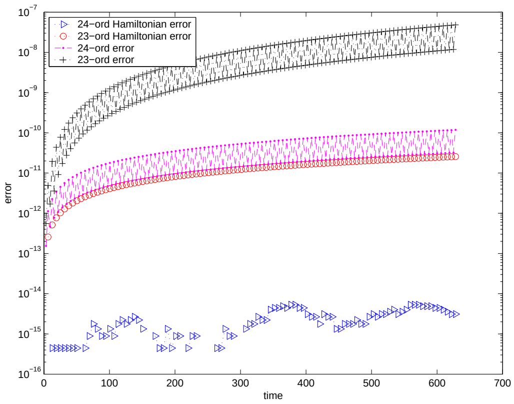

FIGURE 12. Higher-order Kepler(Hamiltonian)

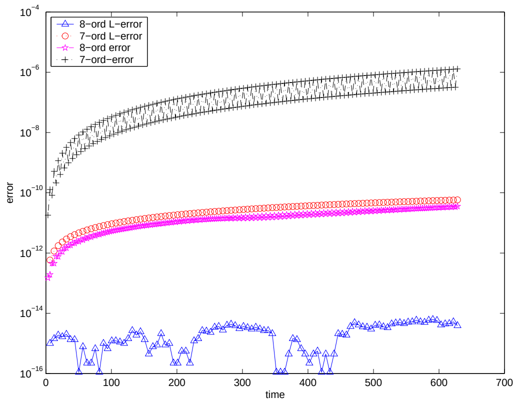

FIGURE 13. Lower order Kepler(angular momentum)

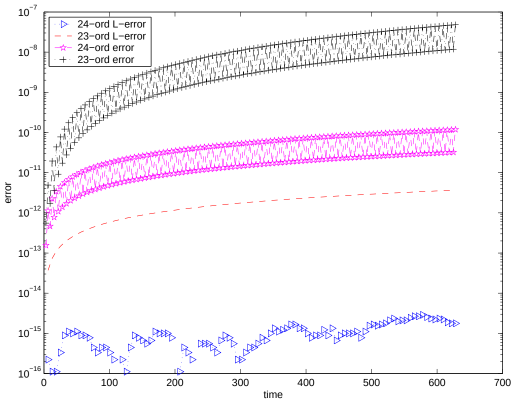

FIGURE 14. Higher order Kepler(angular momentum)

Finally for the geodesic flow on ellipsoid problem, Figure 15 shows how the errors in the Hamiltonian function H and the other invariant A evolve as functions of time for lower-order symplectic (order 8) and nonsymplectic (order 7) methods using stepsizes $1/60$. Similarly in Figure 16, results are presented for higher-order symplectic (order 24) and nonsymplectic (order 23) methods with stepsize $1/5$.

Our numerical results show that the symplectic methods significantly improve the accuracy of the invariants and stability of the numerical results when compared with lower order nonsymplectic ones. Also, higher order methods are more efficient than lower order ones, especially when higher accuracy is required in long-time simulations. However when the order increases, the advantages of the symplectic methods become less significant.

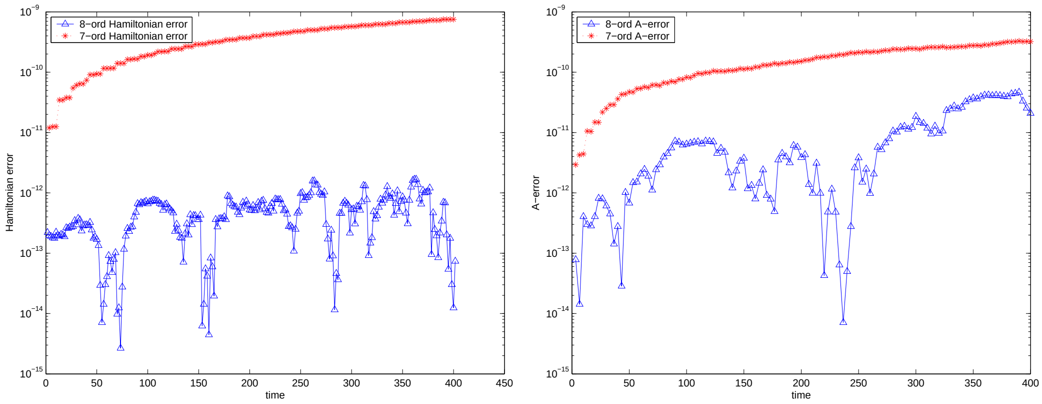

Figure 15. Low-order Geodesic flow(Hamiltonian and A)

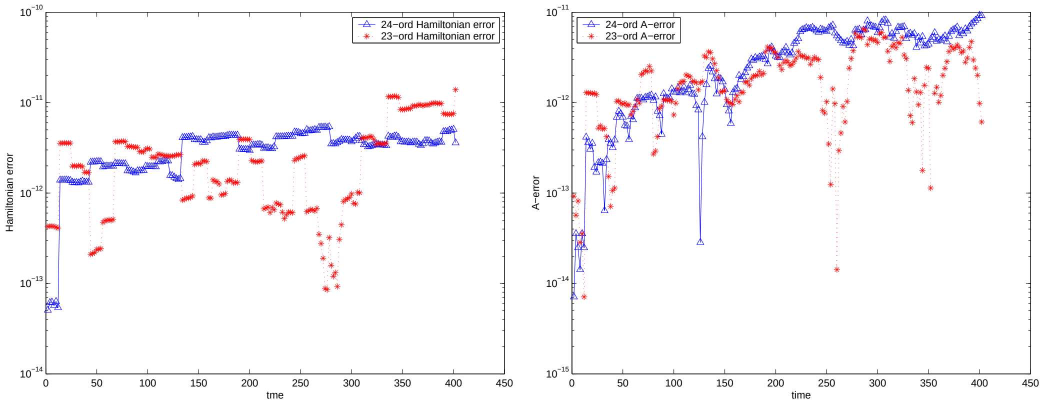

Figure 16. High-order Geodesic flow(Hamiltonian and A)

5. Concluding Remarks

In this paper, we present an efficient arbitrary order numerical technique for solving Hamiltonian systems, in which existing Gaussian Runge-Kutta collocation formulations are combined with the recently developed Krylov deferred correction methods. Many interesting features of the symplectic GRK schemes are confirmed and our preliminary numerical experiments show that the symplectic GRK methods are optimal in order, more stable numerically, and outperform other initial value problem solvers (including the nonsymplectic Radau IIA schemes) in preserving the geometric structures of the underlying system. Also, for the same accuracy requirements, higher order symplectic GRK methods are optimal in stepsize and more efficient than lower order versions, especially when very high accuracy is required.

However, we notice that the differences between the symplectic GRK methods and the nonsymplectic Radau IIA schemes become less significant as the order increases. In fact, it was shown in [32] that the Radau IIA schemes are better choices for stiff ODEs and differential algebraic equation systems. Finally, we want to mention that to fully take advantage of these higher order symplectic methods for Hamiltonian systems, many numerical implementation details have to be taken care of. In particular, the selections of the optimal stepsize and order, and specialized Newton-Krylov methods. More importantly, the technique discussed in this paper can be generalized to Hamiltonian systems governed by partial differential equations. Results along these directions will be reported in the future.

References

1. V.I. Arnold, *Mathematical Methods of Classical Mechanics*, Springer-Verlag, New York, 1978, Second Edition, 1989.
2. U.M. Ascher, and L.R. Petzold, *Computer Methods for Ordinary Differential Equations and Differential-Algebraic Equations*, SIAM, Philadelphia, 1998.
3. W. Auzinger, H. Hofstatter, W. Kreuzer, and E. Weinmuller, *Modified defect correction algorithms for ODEs. Part I: General theory*, Numer. Algorithms, **36** (2004), 135-156.
4. R. Barrett, et al, *Templates for the Solution of Linear Systems: Building Blocks for Iterative Methods*, 2nd Edition, SIAM, Philadelphia, 1994.
5. K.E. Brenan, S.L. Campbell, and L.R. Petzold, *Numerical Solution of Initial-Value Problems in Differential-Algebraic Equations*, SIAM, Philadelphia, 1995.
6. J.C. Butcher, *Implicit Runge-Kutta Processes*, Math. Comput., **18** (1964), 50-64.
7. M.P. Calvo, and C. Palencia, *Avoiding the order reduction of Runge-Kutta methods for linear initial boundary value problems*, Math. Comput., **71**(2002), 1529-1543.
8. C. Canuto, M.Y. Hussaini, A. Quarteroni, and T.A. Zang, *Spectral Methods in Fluid Dynamics*, Springer-Verlag, 1988.
9. P.J. Channel, and J.C. Scovel, *Symplectic integration of Hamiltonian systems*, *Nonlinearity* **3**(2) (1990), 231-259.
10. K. Chen, A. Iserles, and P.G. Ciarlet (Editors), *Matrix Preconditioning Techniques and Applications*, Cambridge University Press, 2005.
11. K. Dekker, and J.G. Verwer, *Stability of Runge-Kutta methods for stiff nonlinear differential equations*, CWI Monographs. North-Holland, 1984.
12. S. Dutt, L. Greengard, and V. Rokhlin, *Spectral deferred correction methods for ordinary differential equations*, BIT, **40**(2) (2000), 241-266.
13. A. Dutt, M. Gu, and V. Rokhlin, *Fast Algorithms for Polynomial Interpolation, Integration, and Differentiation*, SIAM J. Nume. Anal., **33**(5) (1996), 1689-1711.
14. B. L. Ehle, *On Pad Approximation to the Exponential Function and A-stable Methods for the Numerical Solution of Initial Value Problems*, Research Report *CSRR* 2010, Dept. AACS, University of Waterloo(1969).
15. B.L. Ehle, *High order A-Stable methods for the numerical solution of systems of D.E.'S*, BIT **8** (1968),276-278.
16. K. Feng, *On Difference Schemes and Symplectic Geometry*, in *Proceedings of the 1984 Beijing Symposium on Differential Geometry and Differential Equations*, Edited by K. Feng, Beijing, Science Press, 1985, pp. 42–58.
17. K. Feng, *Difference Schemes for Hamiltonian Formalism and Symplectic Geometry*, J. Comput. Math., **4**(3) (1986), 279-289.
18. K. Feng, and M.Z. Qin, *Hamiltonian Algorithms for Hamitonian Systems and a Comparative Numerical Study*, Comput. Phys. Communi., **65** (1991), 173-187.
19. K. Feng & D.L. Wang, *Symplectic Difference Schemes for Hamiltonian Systems in General Symplectic Structure*, J. Computa. Math., **9**(1) (1991), 86-96.
20. K. Feng, H.M. Wu, M.Z. Qin, and D.L. Wang, *Construction of canonical difference schemes for Haniltonian formalism via generating functions*, J. Comput. Math., **7**(1) (1989), 71-96.
21. Q.D. Feng, Y.D. Jiao & Y.F. Tang, *Conjugate Symplecticity of 2nd-Order Linear Multi-Step Methods*, J. Computa. Appli. Math., **203**(1) (2007), 6-14.
22. E. Forest, and R.D. Ruth, *Fourth-Order Symplectic Integration*, Physica D, **43** (1990), 105-117.
23. Z. Ge and K. Feng, *On the approximation of linear Hamiltonian-systems*, J. Comput. Math., **6**(1) (1988), 88-97.
24. D. Gottlieb, and S.S. Orszag, *Numerical Analysis of Spectral Methods*, SIAM, Philadelphia, 1977.
25. L. Greengard, *Spectral Integration and Two-Point Boundary Value Problems*, SIAM J. Nume. Anal., **28** (1991), 1071-1080.
26. L.Greengard, V.Rokhlin, *A new version of the fast multipole method for the Laplace in three dimensions*, Acta Numerica, 1997, pp. 229–269.

27. Guillou &J.L.Soulé, *La résolution numérique des problèmes différentiels aux conditions initiales par des méthodes de collocation*, Rev.Francaise Informat.Recherche Opŕationnelle 3, Ser.R-3,17-44,[II.1],1969.
28. E. Hairer, and M. Hairer,*”GniCodes - Matlab programs for geometric numerical integration”*, Frontiers in Numerical Analysis (Durham 2002), Springer, Berlin, 2003.
29. E. Hairer & P. Leone, *Order Barriers for Symplectic Multi-Value Methods*, in: *Numerical Analysis 1997, Proceedings of the 17th Dundee Biennial Conference, June 24-27, 1997* (Edited by D.F. Griffiths, D.J. Higham and G.A. Watson), Pitman Research Notes in Mathematics Series Vol. 380, 1998, pp. 133-149.
30. E. Hairer, Ch. Lubich, and M. Roche, *The Numerical Solution of Differential-Algebraic Systems by Runge-Kutta Methods*, Springer-Verlag, 1989.
31. E. Hairer, Ch. Lubich, and G. Wanner, *Geometric Numerical Integration*, Springer, 2002.
32. E. Hairer, and G. Wanner, *Solving Ordinary Differential Equations II*, Springer, 1996.
33. J.F. Huang, J. Jia, and M. Minion, *Accelerating the Convergence of Spectral Deferred Correction Methods*, J. Comput. Phys., **214**(2) (2006), 633-656.
34. J.F. Huang, J. Jia & M. Minion, *Arbitrary Order Krylov Deferred Correction Methods for Differential Algebraic Equations*, J. Comput. Phys., **221**(2) (2007), 739-760.
35. Hisashi Ishida, Yoshinori Nagai, and Akinori Kidera, *Symplectic integrator for molecular dynamics of a protein in water*, Chemical Physics Letters, **282**(2) (1998), 115-120.
36. C.T. Kelly, *Iterative Methods for Linear and Nonlinear Equations*, SIAM, 1995.
37. C.T. Kelly, *Solving Nonlinear Equations with Newton's Method*, SIAM, 2003.
38. D.A. Knoll, and D.E. Keyes, *Jacobian-free Newton-Krylov methods: a survey of approaches and applications*, J. Comput. Phys., **193** (2004), 357-397.
39. M.P. Laburta, *Construction of starting algorithms for the RK-Gauss methods*, J. Comput Appl. Math., **90**(2) (1998), 239-261.
40. F.M. Lasagni, *Canonical Runge-Kutta Methods*, ZAMP, **39**(6) (1988), 952-953.
41. A.T. Layton, and M.L. Minion, *Conservative multi-implicit spectral deferred correction methods for reacting gas dynamics*, J. Comput. Phys., **194**(2) (2004), 697C714.
42. V. Pereyra, *Iterated Deferred Correction for Nonlinear Boundary Value Problems*, Numer. Math., **11** (1968), 111-125.
43. L.R. Petzold, *A Description of DASSL: A Differential-Algebraic System Solver*, SAND82-8637, Sandia National Lab, 1982.
44. Joel R. Phillips and J. K. White, *A precorrected-FFT method for electrostatic analysis of complicated 3D structures*, IEEE Transactions on Computer-Aided Design of Integrated Circuits and Systems, 1997, pp. 1059–1072.
45. Y. Saad, and M.H. Schultz, *GMRES: a generalized minimal residual algorithm for solving non-symmetric linear systems*, SIAM J. Sci. Stat. Comp., **7** (1986), 856–869.
46. J.M. Sanz-Serna, *Runge-Kutta schemes for Hamiltonian systems*, BIT, **28** (1998), 877-883.
47. J.M. Sanz-Serna and M.P. Calvo, *Numerical Hamiltonian Problems*, Chapman & Hall, London, (1994).
48. J.C. Scovel, *Symplectic numerical integration of Hamiltonian systems*, The Geometry of Hamiltonian Systems, MSRI Series, Vol. 22, (Edited by T.Ratiu), Springer-Verlag, New York, 1991, pp. 463-496.
49. Z.J. Shang, *KAM theorem of symplectic algorithms for Hamiltonian systems*, Numer. Math., **83** (1999), 477-496.
50. Z.J. Shang, *Resonant and Diophantine step sizes in computing invariant tori of Hamiltonian systems*, Nonlinearity, **13** (2000), 299-308.
51. J. Strain, *Fast Stable Deferred Correction Methods for Two-Point Boundary Value Problems*, Preprint.
52. Y.B. Suris, *On the preservation of the symplectic structure for numerical integration of Hamiltonian systems*, Numerical Solution of Differential Equations, (Edited by S.S. Filippov), USSR Academy of Sciences, Moscow, 1988, pp. 148-160.
53. M. Suzuki, *Fractal Decomposition of Exponential Operators with Applications to Many-Body Theories and Monte Carlo Simulations*, Phys. Lett. A, **146**(6) (1990), 319-323.
54. Y.F. Tang, *The Symplecticity of Multi-Step Methods*, Computers Math. Applic., **25**(3) (1993), 83-90.
55. Y.F. Tang, *Geodesic Flows on Compact Surfaces—As an Application of Hamiltonian Formalism*, Computers Math. Applic., **26**(1) (1993), 21-33.
56. Y.F. Tang, J.W. Cao, X.T. Liu & Y.C. Sun, *Symplectic methods for the Ablowitz-Ladik discrete nonlinear Schrödinger equation*, J. Phys. A: Math. Theor., **40** (2007), 2425-2437.
57. L.N. Trefethen, and M.R. Trummer, *An instability phenomenon in spectral methods*, SIAM J. Numer. Anal., **24** (1987).
58. G. Wanner, *A short proof on nonlinear A-stability*, BIT, **16**(2) (1976), 226-227.

59. K.Wright, *Some relationships between implicit Runge-Kutta, collocation and Lanczos τ methods, and their stability properties*, BIT, **10** (1970), 217-227, [II.1].
60. Hans Van de Vyver, *A fourth-order symplectic exponentially fitted integrator*, Computer Phys. Commun., **174**(4) (2006), 255-262.
61. H. Yoshida, *Construction of Higher-Order Symplectic Integrators*, Phys. Lett. A, **150**(5-7) (1990), 262-268.
62. P.E. Zadunaisky, *A method for the estimation of errors propagated in the numerical solution of a system of ordinary differential equations: The Theory of Orbits in the Solar System and in Stellar Systems*, Proceedings of International Astronomical Union, Symposium, **25**, 1964.
63. P.E. Zadunaisky, *On the Estimation of Errors Propagated in the Numerical Integration of Ordinary Differential Equations*, Numer. Math., **27** (1976), 21-40.

LSEC, ICMSEC, Academy of Mathematics & Systems Science, Chinese Academy of Sciences, P.O. Box 2719, Beijing 100080, P.R. China
Current address: College of Science, Beijing Forestry University, Beijing 100083, P.R. China
E-mail address: `fqd@lsec.cc.ac.cn`

LSEC, ICMSEC, Academy of Mathematics & Systems Science, Chinese Academy of Sciences, P.O. Box 2719, Beijing 100080, P.R. China, And Graduate School of the Chinese Academy of Sciences, Beijing 100080, P.R. China
E-mail address: `nienm@lsec.cc.ac.cn`

Department of Mathematics, University of North Carolina at Chapel Hill, Phillips Hall, CB #3250, NC 27599, USA
E-mail address: `huang@amath.unc.edu`

Institute of Mathematics, Academy of Mathematics & Systems Science, Chinese Academy of Sciences, Beijing 100080, P.R. China
E-mail address: `zaijiu@amss.ac.cn`

LSEC, ICMSEC, Academy of Mathematics & Systems Science, Chinese Academy of Sciences, P.O. Box 2719, Beijing 100080, P.R. China
E-mail address: `tyf@lsec.cc.ac.cn`