

HIGHLY OSCILLATORY SYSTEMS AND PERIODIC-STABILITY

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Abstract. We are concerned with the numerical solution of highly oscillatory systems such as Hamiltonian and mechanical systems containing strong potentials forcing the motion to be close to a smooth manifold. We are interested in methods taking stepsizes much larger than the shortest period of oscillation. As a simple model problem we consider the system of the harmonic oscillator. For this system methods preserving the amplitudes of the oscillations for arbitrary high frequencies and arbitrary stepsize lengths are called periodic (P)-stable. Symmetric Runge-Kutta methods are shown to be P-stable. We also demonstrate that the Lobatto IIIA-III B partitioned Runge-Kutta methods are not P-stable. The (Rattle)-Verlet algorithm is therefore not P-stable. For nonlinear highly oscillatory Hamiltonian and mechanical systems P-stability is not sufficient. The convergence of the method is mostly dictated by its behaviour when applied to a nearby holonomically constrained system. We emphasize the fact that the (Rattle)-Verlet algorithm, the midpoint rule, and the trapezoidal rule fail for large stepsizes even if the amplitudes of the oscillations are neglectable (smooth motion). To overcome all these difficulties we propose the use of P-stable schemes with sufficiently high order, like the s -stage ($s \geq 4$) Gauss methods or the s -stage ($s \geq 3$) Lobatto IIIA methods. We also propose some modifications in the simplified Newton iterations. For the starting values of these iterations and for the simplified Jacobian used in the simplified Newton iterations we make use of projected values on a nearby slow manifold. Some numerical experiments with the stiff spring pendulum equations are given.

Key words. differential-algebraic equations, Hamiltonian systems, highly oscillatory systems, holonomic constraints, index three, mechanical systems, Newton iterations, partitioned Runge-Kutta methods, periodic-stability, slow and smooth manifolds, strong potential, symmetric methods

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1. Introduction. *Highly oscillatory systems* are differential systems $y' = f(y)$ where the Jacobian matrix $\partial f / \partial y$ possesses large eigenvalues on or near the imaginary axis of the complex plane. These eigenvalues are the cause of oscillations with high frequencies. Examples of such systems are given by Hamiltonian and mechanical systems containing strong potentials of the form

$$\frac{1}{\varepsilon^2} V(q) \text{ with } 0 < \varepsilon \ll 1$$

where q are the generalized coordinates. Under some technical assumptions it can be shown that such potentials force the motion to be close to a smooth manifold [22]. In this paper we assume that the amplitudes of the oscillations are sufficiently small to ensure existence and uniqueness of the numerical solution (see section 4).

Any numerical method preserving accurately the phase of the oscillations must generally take stepsizes smaller than the shortest period of oscillation in order to track the exact trajectory of the solution. In this article we are interested in methods able to take stepsizes much larger than the shortest period of oscillation. Obviously such

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methods will generally lose the phase information. Nevertheless, in many practical applications the phase of the oscillations is not relevant and may be neglected, e.g., in molecular dynamics simulation [1]. A first approach consists of replacing a strong potential by a holonomic constraint. This may be satisfactory in certain specific situations, e.g., for bond stretchings in molecular dynamics, but generally this approach fails due to the introduction of artificial rigidity in the system, e.g., for bond-angle bendings in molecular dynamics. A second approach is to damp the oscillations by the use of super-stable methods like the k -step BDF methods ($1 \leq k \leq 6$) [2] or any L-stable Runge-Kutta methods, like the s -stage Radau IIA schemes [15]. This approach also obviously fails to reflect the correct motion of the system because of the artificial numerical damping introduced by the method, which is reflected by a decrease of the energy level of the system. In this article we are interested in methods taking large stepsizes and preserving satisfactorily the amplitudes of the oscillations, i.e., allowing flexibility without artificial damping or blowing up of the oscillations.

In section 2 as a simple model problem we consider the equation of the harmonic oscillator $\ddot{y} = -\lambda^2 y$. For this system methods preserving the amplitudes of the oscillations for arbitrary large values of λ and arbitrary stepsize lengths are called *periodic (P)-stable*. Methods which are not P-stable are not well-suited for solving highly oscillatory systems with large stepsizes. That is one of the main motivations to look at P-stable methods. Symmetric Runge-Kutta methods are shown to be P-stable. We also demonstrate that the combination of the s -stage Lobatto IIIA and Lobatto IIIB methods as partitioned Runge-Kutta methods is not P-stable. This may seem surprising since these methods have proved to be very efficient when solving holonomically constrained systems [16, 19] and the Lobatto IIIA and Lobatto IIIB methods are both symmetric Runge-Kutta methods. For separable Hamiltonians the (Rattle)-Verlet algorithm is equivalent to the 2-stage Lobatto IIIA-IIIB scheme, it is therefore not P-stable.

For nonlinear highly oscillatory Hamiltonian and mechanical systems P-stability is not sufficient. This is the subject of section 3. The convergence of the method is mostly dictated by its behaviour when applied to a nearby holonomically constrained system, which is a differential-algebraic system of index three. That is the reason why the midpoint rule and the trapezoidal rule, although both P-stable, usually fail when applied with large stepsizes to highly oscillatory systems, because they do not converge when applied to such index three problems. We emphasize the fact that the (Rattle)-Verlet algorithm, the midpoint rule, and the trapezoidal rule fail even if the amplitudes of the oscillations are neglectable (smooth motion). To overcome all these difficulties we propose the use of P-stable schemes with sufficiently high order, like the s -stage ($s \geq 4$) Gauss methods or the s -stage ($s \geq 3$) Lobatto IIIA methods.

In section 4 we propose some modifications in the simplified Newton iterations, which are needed for convergence with large stepsizes. For the starting values of these iterations we make use of projected values on a nearby slow manifold.

Finally, in section 5 some numerical experiments with the stiff spring pendulum equations are given.

2. Periodic-stability analysis. As a simple model problem of a highly oscillatory system we consider the equation of the *harmonic oscillator* $\ddot{y} = -\lambda^2 y$ where by definition $\lambda > 0$. Introducing a new variable for the velocity $z := \dot{y}$, this equation can be rewritten as a first-order linear differential system

$$(1) \quad \begin{pmatrix} \dot{y} \\ \dot{z} \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -\lambda^2 & 0 \end{pmatrix} \begin{pmatrix} y \\ z \end{pmatrix}.$$

This is a Hamiltonian system with Hamiltonian $H(y, z) = (\lambda^2 y^2 + z^2) / 2$. This is one of the simplest systems where the eigenvalues of the Jacobian matrix ($\pm i\lambda$) are purely imaginary. Considering the linear canonical transformation

$$(2) \quad \begin{pmatrix} q \\ p \end{pmatrix} = \begin{pmatrix} \sqrt{\lambda} & 0 \\ 0 & 1/\sqrt{\lambda} \end{pmatrix} \begin{pmatrix} y \\ z \end{pmatrix},$$

in these new variables the system (1) reads

$$(3) \quad \begin{pmatrix} \dot{q} \\ \dot{p} \end{pmatrix} = \begin{pmatrix} 0 & \lambda \\ -\lambda & 0 \end{pmatrix} \begin{pmatrix} q \\ p \end{pmatrix}$$

which is obviously again Hamiltonian with Hamiltonian $H(q, p) = \lambda (q^2 + p^2) / 2$.

We are mainly interested in partitioned Runge-Kutta methods. For partitioned systems of the form

$$(4) \quad y' = f(y, z), \quad z' = g(y, z)$$

these methods make use of the conjunction of two Runge-Kutta (RK) methods.

DEFINITION 2.1. One step of an s -stage partitioned Runge-Kutta (PRK) method applied to the partitioned system (4), with initial values (y_0, z_0) and stepsize h reads

$$y_1 = y_0 + h \sum_{i=1}^s b_i f(Y_i, Z_i), \quad z_1 = z_0 + h \sum_{i=1}^s \hat{b}_i g(Y_i, Z_i),$$

$$Y_i = y_0 + h \sum_{j=1}^s a_{ij} f(Y_j, Z_j), \quad Z_i = z_0 + h \sum_{j=1}^s \hat{a}_{ij} g(Y_j, Z_j).$$

The coefficients (b_i, a_{ij}) and $(\hat{b}_i, \hat{a}_{ij})$ are the coefficients of two Runge-Kutta methods generally based on the same quadrature formula, i.e., $b_i = \hat{b}_i$.

For the stability analysis of PRK methods, instead of considering directly the system (1) we will consider the more convenient system (3). This is justified since the application of a PRK method commutes with the transformation (2). The exact solution of the system (3) is given by

$$(5) \quad \begin{pmatrix} q(t) \\ p(t) \end{pmatrix} = \begin{pmatrix} \cos(\mu) & -\sin(\mu) \\ \sin(\mu) & \cos(\mu) \end{pmatrix} \begin{pmatrix} q_0 \\ p_0 \end{pmatrix}$$

where $\mu = h\lambda$ and $h = t - t_0$. From now on we use the notation I_s for the identity matrix in \mathbb{R}^s , $\mathbf{1}_s$ is the s -dimensional vector $(1, \dots, 1)^T$, A and \hat{A} are the matrices of the RK coefficients, and b and \hat{b} are the vectors of the RK weights. The application of a PRK method to (3) yields the linear system

$$(6) \quad \begin{pmatrix} I_s & -\mu A \\ \mu \hat{A} & I_s \end{pmatrix} \begin{pmatrix} Q \\ P \end{pmatrix} = \begin{pmatrix} \mathbf{1}_s q_0 \\ \mathbf{1}_s p_0 \end{pmatrix},$$

$$\begin{pmatrix} q_1 \\ p_1 \end{pmatrix} = \begin{pmatrix} q_0 \\ p_0 \end{pmatrix} + \mu \begin{pmatrix} O & \hat{b}^T \\ -\hat{b}^T & O \end{pmatrix} \begin{pmatrix} Q \\ P \end{pmatrix}.$$

Hence we get

$$(7) \quad \begin{pmatrix} q_1 \\ p_1 \end{pmatrix} = M(\mu) \begin{pmatrix} q_0 \\ p_0 \end{pmatrix}$$

where the 2×2 stability matrix $M(\mu)$ is given by

$$(8) \quad M(\mu) = I_2 + \mu \begin{pmatrix} O & \hat{b}^T \\ -\hat{b}^T & O \end{pmatrix} \begin{pmatrix} I_2 & -\mu A \\ \mu \hat{A} & I_2 \end{pmatrix}^{-1} \begin{pmatrix} \mathbb{1}_2 & O \\ O & \mathbb{1}_2 \end{pmatrix}.$$

Now we look at PRK methods which preserve in a certain sense the amplitudes of the oscillations of the true solution (5) for all μ . Such methods are called *periodic-stable*. We give a precise definition of this concept which relates the norm of the eigenvalues of the stability matrix $M(\mu)$ to those of the matrix in (5). Our definition is slightly more precise than the usual ones.

DEFINITION 2.2. For a PRK method, an interval $I \subset \mathbb{R}$ is an interval of periodicity if for all $\mu \in I$ the eigenvalues of the stability matrix $M(\mu)$, denoted by $\lambda_i(\mu) \in \mathbb{C}$ ($i = 1, 2$), satisfy $|\lambda_i(\mu)| = 1$ ($i = 1, 2$) and $\lambda_1(\mu) = \lambda_2(\mu) = \pm 1$ only for a discrete set of μ -values in I . A PRK method is said to be periodic (P)-stable if \mathbb{R} is an interval of periodicity.

It is easily seen that the conditions on the eigenvalues of the stability matrix $M(\mu)$ are equivalent to the conditions

$$(9) \quad \det(M(\mu)) = 1, \quad |\operatorname{tr}(M(\mu))| \leq 2,$$

and $|\operatorname{tr}(M(\mu))| = 2$ only for a discrete set of μ -values.

The concept of P-stability has been considered in the literature for general multistage-multistep methods, including Runge-Kutta methods, Nyström methods, multistep methods, and some hybrid methods. The first result (without proof) about P-stability is due to Lambert & Watson [20] which states that P-stable multistep methods can not have order greater than two. A proof of this result in a more general setting is given by Hairer in [12]. This is a result similar to the famous Dahlquist's second barrier [8] and more generally to the Daniel & Moore conjecture [9] (proved in [30] with the beautiful order stars theory). The construction of explicit Nyström methods possessing relatively large intervals of periodicity can be found in [6, 7]. To overcome the order-barrier of multistep methods, hybrid P-stable methods with constant stepsizes have been derived in [3, 5, 12].

For pure Runge-Kutta methods ($A = \hat{A}$, $b = \hat{b}$) we have the following result.

THEOREM 2.3. *Symmetric Runge-Kutta methods are P-stable.*

Proof. We consider the unitary transformation in \mathbb{C}^2 given by

$$(10) \quad \begin{pmatrix} u \\ v \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix} \begin{pmatrix} q \\ p \end{pmatrix}.$$

In these new variables the system (3) reads

$$\begin{pmatrix} \dot{u} \\ \dot{v} \end{pmatrix} = \begin{pmatrix} i\lambda & 0 \\ 0 & -i\lambda \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix}.$$

The application of a RK method commutes with the transformation (10). We trivially have $u_1 = R(i\lambda)u_0$ and $v_1 = R(-i\lambda)v_0$ where R is the usual stability function of the RK method (see [15, Formula IV.3.2]). It only remains to show that $|R(i\lambda)| = 1$ for all $\lambda \in \mathbb{R}$ (this also implies I-stability, see [15, Formula IV.3.6]). Since the coefficients of the rational polynomial $R(z)$ are real, this result comes directly from $R(-z) = R(z)^{-1}$ by symmetry of the method [15, Ex. IV.3.1]. \square

Examples of P-stable Runge-Kutta methods are thus given by the Gauss methods, the Lobatto IIIA methods, and the Lobatto IIIB methods (see [15, Chapter IV.5] and

[4]). It is amazing to observe further that the combination of Lobatto IIIA and Lobatto IIIB as PRK methods leads to non P-stable schemes, although their combination is still symmetric!

For general PRK methods the situation is slightly more intricate to analyze. A more detailed representation of the stability matrix (8) can be given.

THEOREM 2.4. *The stability matrix $M(\mu)$ (8) of a PRK method is given by*

$$(11) \quad M(\mu) = \begin{pmatrix} 2 - \frac{\det(I_s + \mu^2 AA + \mu^2 \mathbb{1}_s b^T \hat{A})}{\det(I_s + \mu^2 AA)} & -\mu + \mu \frac{\det(I_s + \mu^2 \hat{A}A + \mathbb{1}_s b^T)}{\det(I_s + \mu^2 AA)} \\ \mu - \mu \frac{\det(I_s + \mu^2 A\hat{A} + \mathbb{1}_s \hat{b}^T)}{\det(I_s + \mu^2 AA)} & 2 - \frac{\det(I_s + \mu^2 \hat{A}A + \mu^2 \mathbb{1}_s \hat{b}^T A)}{\det(I_s + \mu^2 AA)} \end{pmatrix}$$

In the proof we will make use of the following lemma.

LEMMA 2.5 ([29]). *Let N be a nonsingular $n \times n$ matrix and v and w n -dimensional vectors. Then*

$$v^T N^{-1} w = \frac{\det(N + wv^T)}{\det(N)} - 1. \quad \square$$

Proof of Theorem 2.4. The inverse matrix in (8) can be expressed by

$$(12) \quad \begin{pmatrix} I_s & -\mu A \\ \mu \hat{A} & I_s \end{pmatrix}^{-1} = \begin{pmatrix} (I_s + \mu^2 A\hat{A})^{-1} & \mu A (I_s + \mu^2 \hat{A}A)^{-1} \\ -\mu \hat{A} (I_s + \mu^2 A\hat{A})^{-1} & (I_s + \mu^2 \hat{A}A)^{-1} \end{pmatrix}$$

leading to

$$(13) \quad M(\mu) = \begin{pmatrix} 1 - \mu^2 b^T \hat{A} (I_s + \mu^2 A\hat{A})^{-1} \mathbb{1}_s & \mu b^T (I_s + \mu^2 \hat{A}A)^{-1} \mathbb{1}_s \\ -\mu \hat{b}^T (I_s + \mu^2 A\hat{A})^{-1} \mathbb{1}_s & 1 - \mu^2 \hat{b}^T A (I_s + \mu^2 \hat{A}A)^{-1} \mathbb{1}_s \end{pmatrix}$$

A straightforward application of Lemma 2.5 to each component of the stability matrix gives the desired result. \square

For the numerical solution (q_1, p_1) (7) of the test problem (3) if the matrices of Runge-Kutta coefficients A, \hat{A} are invertible we get from (13) for $\mu \rightarrow \infty$

$$(14) \quad M(\infty) = \begin{pmatrix} R(\infty) & 0 \\ 0 & \hat{R}(\infty) \end{pmatrix}$$

where $R(\infty) = 1 - b^T A^{-1} \mathbb{1}_s$ and $\hat{R}(\infty) = 1 - \hat{b}^T \hat{A}^{-1} \mathbb{1}_s$. For the s -stage Gauss method we have $R(\infty) = \hat{R}(\infty) = (-1)^s$. This explains the highly oscillatory behaviour for the Gauss methods with an odd stage number s and the smooth behaviour for an even stage number s (see the numerical experiments in section 5). With respect to the preservation of oscillations, Gauss methods with an odd stage number s are therefore qualitatively superior. However, with respect to accuracy, they are comparable, the numerical solution remaining in a vicinity of the envelope of the oscillations in both cases. For the s -stage Lobatto IIIA method the matrix $M(\infty)$ is also of the form (14) with $R(\infty) = \hat{R}(\infty) = (-1)^{s-1}$. This also explains the highly oscillatory behaviour for Lobatto IIIA methods with an even stage number s and the smooth behaviour for an odd stage number s .

The coefficients of the 2-stage Lobatto IIIA-III B PRK method, which is equivalent to the famous (Rattle)-Verlet algorithm for separable Hamiltonians, are given by

$$A = \begin{pmatrix} 0 & 0 \\ 1/2 & 1/2 \end{pmatrix}, \quad \hat{A} = \begin{pmatrix} 1/2 & 0 \\ 1/2 & 0 \end{pmatrix}, \quad b^T = \hat{b}^T = (1/2 \quad 1/2).$$

The stability matrix of the (Rattle)-Verlet algorithm can be computed with the help of (11) and we obtain

$$(15) \quad M(\mu) = \begin{pmatrix} 1 - \mu^2/2 & \mu \\ -\mu + \mu^3/4 & 1 - \mu^2/2 \end{pmatrix}.$$

We have $\det(M(\mu)) = 1$, but only $|\operatorname{tr}(M(\mu))| = |2 - \mu^2|$. Thus according to (9) the (Rattle)-Verlet algorithm is not P-stable as its interval of periodicity is $[-2, 2]$. This may seem surprising since the 2-stage Lobatto IIIA method (the trapezoidal rule) is P-stable, as is also its symmetric and symplectic counterpart the 2-stage Lobatto III B method. Hence the (Rattle)-Verlet algorithm is not well-suited for stiff oscillatory systems. The time-scale of integration with such a method is clearly limited by this instability, since the stepsizes are restricted by the shortest period of oscillation, even if the amplitudes of the oscillations are neglectible (smooth motion, i.e., without the presence of oscillations). To overcome to this instability, modified formulations for some highly oscillatory differential systems have been proposed in [24, 25], allowing more flexibility than a constrained formulation. However, it is still not clear firstly if such modified formulations reproduce the correct behaviour of the system and secondly if the instability of the (Rattle)-Verlet scheme is really overcome, i.e., if large stepsizes are possible. We will see below that the whole family of s -stage Lobatto IIIA-III B PRK methods are not P-stable. Such methods have proved recently to be very successful when integrating Hamiltonian or conservative mechanical systems with holonomic constraints [16, 19]. These schemes preserve the symplectic and reversible characters of the flow, they preserve the manifold of constraints, they are superconvergent with order $2s - 2$, and they quasi-preserve the energy of the system. One defect is precisely that they are not P-stable, that is the main reason why they fail with large stepsizes when integrating, e.g., the stiff spring pendulum equations [14] even for the smooth motion.

THEOREM 2.6. *The s -stage Lobatto IIIA-III B PRK methods are not P-stable.*

Proof. By direct application of Lemma 2.5 to (8) we can express the stability matrix as

$$M(\mu) = \frac{1}{q(\mu)} \begin{pmatrix} p_{11}(\mu) & p_{12}(\mu) \\ p_{21}(\mu) & p_{22}(\mu) \end{pmatrix}$$

with

$$\begin{aligned} p_{11}(\mu) &= \det \begin{pmatrix} I_s & -\mu(A - \mathbb{I}_s b^T) \\ \mu \hat{A} & I_s \end{pmatrix}, \quad p_{12}(\mu) = \det \begin{pmatrix} I_s & -\mu A \\ \mu \hat{A} & I_s + \mu \mathbb{I}_s b^T \end{pmatrix} - 1, \\ p_{21}(\mu) &= \det \begin{pmatrix} I_s - \mu \mathbb{I}_s \hat{b}^T & -\mu A \\ \mu \hat{A} & I_s \end{pmatrix} - 1, \quad p_{22}(\mu) = \det \begin{pmatrix} I_s & -\mu A \\ \mu(\hat{A} - \mathbb{I}_s \hat{b}^T) & I_s \end{pmatrix}, \\ q(\mu) &= \det \begin{pmatrix} I_s & -\mu A \\ \mu \hat{A} & I_s \end{pmatrix}. \end{aligned}$$

To prove the theorem we will show that for the s -stage Lobatto IIIA-IIIIB PRK method the rational polynomial

$$\text{tr}(M(\mu)) = \frac{p_{11}(\mu) + p_{22}(\mu)}{q(\mu)}$$

is unbounded as $\mu \rightarrow \infty$. More precisely we will show that for these methods $\deg(p_{11}(\mu) + p_{22}(\mu)) = 2s - 2$ and $\deg(q(\mu)) \leq 2s - 4$.

We first show that $\deg(q(\mu)) \leq 2s - 4$. The Runge-Kutta matrices A and \hat{A} of the s -stage Lobatto IIIA and Lobatto IIIIB can be expressed respectively as

$$A = \begin{pmatrix} 0 & \cdots & 0 \\ & A_0 & \\ & & \ddots \\ & & & 0 \end{pmatrix} = \begin{pmatrix} 0 & \cdots & 0 \\ & \tilde{A}_0 & \\ a_{s,1} & \cdots & a_{s,s} \end{pmatrix},$$

$$\hat{A} = \begin{pmatrix} 0 \\ \hat{A}_0 \\ \vdots \\ 0 \end{pmatrix} = \begin{pmatrix} \hat{a}_{11} & 0 \\ \vdots & \tilde{\hat{A}}_0 \\ \hat{a}_{s,1} & 0 \end{pmatrix}$$

since the first row of A and the last column of \hat{A} are zero. Thus we have

$$\begin{pmatrix} I_s & -\mu A \\ \mu \hat{A} & I_s \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ & \ddots & & & -\mu \tilde{A}_0 \\ 0 & & 1 & -\mu a_{s,1} & \cdots & -\mu a_{s,s} \\ \mu \hat{a}_{11} & & 0 & 1 & & 0 \\ \vdots & \mu \tilde{\hat{A}}_0 & \vdots & & \ddots & \\ \mu \hat{a}_{s,1} & & 0 & 0 & & 1 \end{pmatrix}.$$

For the computation of the determinant of this matrix we can suppress its first row, its first column, its s -th row, and its s -th column. Hence we can express $q(\mu)$ as

$$q(\mu) = \det \begin{pmatrix} I_{s-2} & -\mu \tilde{A}_0 \\ \mu \tilde{\hat{A}}_0 & I_s \end{pmatrix}.$$

Since the matrix \tilde{A}_0 has $s - 2$ rows and the matrix $\tilde{\hat{A}}_0$ has $s - 2$ columns, we have $\deg(q(\mu)) \leq 2s - 4$.

To show that $\deg(p_{11}(\mu) + p_{22}(\mu)) = 2s - 2$ we will make use of the W -transformation. For details about the W -transformation we refer the reader to [15, Section IV.5] and [4, 10]. Here the aim is to express $p_{11}(\mu)$ and $p_{22}(\mu)$ in terms of the transformed matrices $X := W^T B A W$ and $\tilde{X} := W^T \tilde{B} \hat{A} W$ where $B = \text{diag}(b_1, \dots, b_s)$, the coefficients of the matrix W are given by $w_{ij} = P_{j-1}(c_i)$ with $P_{j-1}(x)$ the $(j-1)$ -th shifted Legendre polynomial, and the c_i are the nodes of the Lobatto quadrature. The matrices X, \tilde{X} for the Lobatto IIIA and Lobatto IIIIB coefficients are given respectively by [10]

$$X = \begin{pmatrix} X_0 & \vdots \\ & 0 \end{pmatrix} = \begin{pmatrix} 1/2 & -\zeta_1 & & 0 & 0 \\ \zeta_1 & 0 & \ddots & & 0 \\ & \ddots & \ddots & -\zeta_{s-2} & \vdots \\ & & \zeta_{s-2} & 0 & 0 \\ 0 & & & \zeta_{s-1} u & 0 \end{pmatrix},$$

$$\hat{X} = \begin{pmatrix} 0 & \hat{X}_0 & 0 \end{pmatrix} = \begin{pmatrix} 1/2 & -\zeta_1 & & & 0 \\ \zeta_1 & 0 & \ddots & & \\ & \ddots & \ddots & -\zeta_{s-2} & \\ 0 & & \zeta_{s-2} & 0 & -\zeta_{s-1}u \\ 0 & 0 & \dots & 0 & 0 \end{pmatrix}$$

where $\zeta_k = \frac{1}{2\sqrt{4k^2-1}}$ and $u = \sum_i^s b_i P_{s-1}^2(c_i)$. It is important to notice that these two matrices satisfy the relation $X = -\hat{X}^T + e_1 e_1^T$ where e_1 is the s -dimensional vector $(1, 0, \dots, 0)^T$. The matrix $W^T B W$ is diagonal and is equal to $D_s = \text{diag}(1, \dots, 1, u)$, hence $\det(W^T B W) = \det(D_s) = u$. Using also the relations $W e_1 = \mathbb{1}_s$, and $W^T B \mathbb{1}_s = e_1$ we can express $p_{11}(\mu)$ and $p_{22}(\mu)$ as

$$\begin{aligned} p_{11}(\mu) &= \det \left(\begin{pmatrix} O & (W^T B)^{-1} \\ (W^T B)^{-1} & O \end{pmatrix} \begin{pmatrix} O & W^T B \\ W^T B & O \end{pmatrix} \times \right. \\ &\quad \left. \begin{pmatrix} I_s & -\mu(A - \mathbb{1}_s b^T) \\ \mu \hat{A} & I_s \end{pmatrix} \begin{pmatrix} O & W \\ W & O \end{pmatrix} \begin{pmatrix} O & W^{-1} \\ W^{-1} & O \end{pmatrix} \right) \\ &= \det(D_s)^{-2} \cdot \det \begin{pmatrix} D_s & \mu \hat{X} \\ \mu \hat{X}^T & D_s \end{pmatrix}, \\ p_{22}(\mu) &= \det \left(\begin{pmatrix} O & (W^T B)^{-1} \\ (W^T B)^{-1} & O \end{pmatrix} \begin{pmatrix} O & W^T B \\ W^T B & O \end{pmatrix} \times \right. \\ &\quad \left. \begin{pmatrix} I_s & -\mu A \\ \mu(\hat{A} - \mathbb{1}_s b^T) & I_s \end{pmatrix} \begin{pmatrix} O & W \\ W & O \end{pmatrix} \begin{pmatrix} O & W^{-1} \\ W^{-1} & O \end{pmatrix} \right) \\ &= \det(D_s)^{-2} \cdot \det \begin{pmatrix} D_s & -\mu X^T \\ -\mu X & D_s \end{pmatrix}. \end{aligned}$$

Since the last row of the matrices \hat{X} and X^T and the last column of the matrices X and \hat{X}^T vanish, we can suppress the s -th columns and the s -th rows in the computation of $p_{11}(\mu)$ and $p_{22}(\mu)$ and multiply the results by u leading to

$$\begin{aligned} p_{11}(\mu) &= \frac{1}{u} \det \begin{pmatrix} I_{s-1} & \mu \hat{X}_0 \\ \mu \hat{X}_0^T & D_s \end{pmatrix} = \det \begin{pmatrix} I_{s-1} & \mu \hat{X}_0 \\ \mu D_s^{-1} \hat{X}_0^T & I_s \end{pmatrix}, \\ p_{22}(\mu) &= \frac{1}{u} \det \begin{pmatrix} I_{s-1} & -\mu X_0^T \\ -\mu X_0 & D_s \end{pmatrix} = \det \begin{pmatrix} I_{s-1} & -\mu X_0^T \\ -\mu D_s^{-1} X_0 & I_s \end{pmatrix}. \end{aligned}$$

The leading terms of these polynomials of degree $2s-2$ are given by

$$\begin{aligned} p_{11}(\mu) &= (-1)^{s-1} \det(\hat{X}_0 D_s^{-1} \hat{X}_0^T) \mu^{2s-2} + \dots, \\ p_{22}(\mu) &= (-1)^{s-1} \det(X_0^T D_s^{-1} X_0) \mu^{2s-2} + \dots. \end{aligned}$$

For the Lobatto quadratures we have $b_i > 0$ [15, Theorem IV.12.7], implying that $u > 0$. Thus we can express D_s^{-1} as $D_s^{-1/2} D_s^{-1/2}$. The matrices $D_s^{-1/2} X_0$ and $D_s^{-1/2} \hat{X}_0^T$ are of full rank $s-1$. Thus the matrices $\hat{X}_0 D_s^{-1} \hat{X}_0^T$ and $X_0^T D_s^{-1} X_0$ are strictly positive definite, hence their determinant is strictly positive. Therefore the leading terms (of degree $2s-2$) of $p_{11}(\mu)$ and $p_{22}(\mu)$ do not vanish and are of the same sign. Thus we finally conclude $\deg(p_{11}(\mu) + p_{22}(\mu)) = 2s-2$. \square

To remedy the non periodic-stability of the Lobatto IIIA-III B PRK methods for highly oscillatory systems, we propose instead the use of the s -stage P-stable Lobatto IIIA schemes with $s \geq 3$ to treat the terms responsible of the oscillations [18] (see also the next section).

3. Nonlinear highly oscillatory systems. For nonlinear highly oscillatory Hamiltonian and mechanical systems P-stability is not sufficient. The convergence of the method is mostly dictated by its behaviour when applied to a nearby holonomically constrained system. A rigorous analysis for the smooth motion of stiff oscillatory mechanical systems and for a certain subclass of Runge-Kutta methods is given by Lubich in [22]. In the article [22] the considered equations are

$$(16) \quad \begin{aligned} \dot{q} &= v, \\ M(q)\dot{v} &= f(q, v) - \frac{1}{\epsilon^2} V_q^T(q) \end{aligned}$$

with $0 < \epsilon \ll 1$. It is assumed that:

- H1. $M(q)$ is symmetric and positive definite.
- H2. $V(q)$ attains a (local) minimum on a d -dimensional manifold V .
- H3. In a neighbourhood of V , $V(q)$ is strongly convex along directions non-tangential to V .

It is shown that for the smooth motion the convergence of the considered Runge-Kutta methods is dictated by their behaviour when applied (direct approach) to a nearby holonomically constrained system

$$(17) \quad \begin{aligned} \dot{\tilde{q}} &= \tilde{v}, \\ M(\tilde{q})\dot{\tilde{v}} &= f(\tilde{q}, \tilde{v}) - G^T(\tilde{q})\tilde{\lambda}, \\ 0 &= g(\tilde{q}) \end{aligned}$$

with $0 = g(\tilde{q})$ if and only if $\tilde{q} \in V$, $G^T(\tilde{q}) := g_{\tilde{q}}^T(\tilde{q})$, and

$$\begin{pmatrix} M(\tilde{q}) & G^T(\tilde{q}) \\ G(\tilde{q}) & 0 \end{pmatrix} \text{ invertible.}$$

This system (17) is a differential-algebraic system of index three.

Since the midpoint rule and the trapezoidal rule do not converge when applied to such index three systems (17) for the direct approach [13], they usually fail when applied with large stepsizes to highly oscillatory systems, although both methods are P-stable [11, 26, 27]. We emphasize the fact that the (Rattle)-Verlet algorithm, the midpoint rule, and the trapezoidal rule fail even if the amplitudes of the oscillations are neglectible (smooth motion). To overcome all these difficulties when solving highly oscillatory Hamiltonian and mechanical systems, we propose the use of P-stable schemes which are convergent when applied (direct approach) to index three systems of the form (17). Examples of such methods are given by the s -stage ($s \geq 4$) Gauss methods and the s -stage ($s \geq 3$) Lobatto IIIA methods. Although they suffer from some order reduction, a common phenomenon when stiffness is encountered, this order reduction is not drastic. Such phenomenon can also be observed for any other numerical method like the Radau IIA RK schemes [22] and also for other types of stiffness, e.g., in the theory of B-convergence [15, Sections IV.15, V.8 & V.9]. For the Gauss methods we have the following convergence result.

THEOREM 3.1 ([13]). Consider the index three problem (17) with consistent initial values $(\tilde{q}_0, \tilde{v}_0, \tilde{\lambda}_0)$. Then the global error for the s -stage ($s \geq 4$) Gauss methods (direct approach) satisfies

$$\tilde{q}(t_n) - \tilde{q}_n = O(h^s), \quad \tilde{v}(t_n) - \tilde{v}_n = O(h^{s-2}), \quad \tilde{\lambda}(t_n) - \tilde{\lambda}_n = O(h^{s-4})$$

where $h = \max_i h_i$ and $nh \leq \text{Const.}$ For constant stepsizes $h_i = h$ and $s \geq 3$ odd, the convergence rate is one order higher for all three components. \square

For the Lobatto IIIA methods, since the first row of their Runge-Kutta matrix is zero, the first internal stage value for $\tilde{\lambda}$, denoted by $\tilde{\Lambda}_1$, must be carefully determined to be consistent with the definition of the direct approach. Since these methods are stiffly accurate, i.e., $a_{si} = b_i$ for $i = 1, \dots, s$, it is easily seen that at the n th-step we have $\tilde{\Lambda}_{1n} = \tilde{\Lambda}_{s,n-1}$ the last stage for $\tilde{\lambda}$ of the previous step. For the initial step we must take $\tilde{\Lambda}_1 = \tilde{\lambda}_0$ a consistent initial value for (17). For this application of Lobatto IIIA methods (direct approach) we have the following convergence result.

THEOREM 3.2. Consider the index three problem (17) with consistent initial values $(\tilde{q}_0, \tilde{v}_0, \tilde{\lambda}_0)$. Then the global error for the s -stage ($s \geq 3$) Lobatto IIIA methods (direct approach) satisfies

$$\tilde{q}(t_n) - \tilde{q}_n = O(h^{2s-4}), \quad \tilde{v}(t_n) - \tilde{v}_n = O(h^{s-1}), \quad \tilde{\lambda}(t_n) - \tilde{\lambda}_n = O(h^{s-3})$$

where $h = \max_i h_i$ and $nh \leq \text{Const.}$

A proof of this theorem in a more general situation will be given in [17].

In the paper of Lubich [22] Runge-Kutta methods satisfying $|R(i\omega)| < 1 \forall \omega \in \mathbb{R}$ and $|R(\infty)| < 1$ were considered where $R(z)$ is the stability function of the method. Symmetric Runge-Kutta methods are known to satisfy $|R(i\omega)| = 1 \forall \omega \in \mathbb{R}$ and $|R(\infty)| = 1$. A first reason why such methods were not included in [22] was because the main interest was in methods able to damp the oscillations with high frequency. A second reason was because convergence results for index three problems were only known for methods satisfying $|R(\infty)| < 1$ at this time [14, Theorem 6.4]. Since then convergence results for Gauss methods have been given in [13] (see Theorem 3.1). For Lobatto IIIA methods such results will be established in [17] (see Theorem 3.2). For stiff oscillatory mechanical systems, with the help of these two convergence results, following the lines of [22], we arrive at the following result.

THEOREM 3.3. Let us consider a stiff oscillatory mechanical system (16) satisfying the assumptions H1-H3. Let us suppose that the exact solution $(q^e(t), v^e(t))$ of (16) with initial values (q_0^e, v_0^e) is smooth. Let us consider the application of the s -stage Gauss methods and of the s -stage Lobatto IIIA methods to this system. Then for $0 < \epsilon \leq h \leq h_0$, with h_0 sufficiently small but independent of ϵ , there exists a unique numerical solution of the stiff oscillatory mechanical system (16), whose error satisfies for the s -stage ($s \geq 4$) Gauss methods

$$q_n^e - q^e(t_n) = O(h^s + \epsilon^2 h^{s-2}), \quad v_n^e - v^e(t_n) = O(h^{s-2} + \epsilon^2 h^{s-4}),$$

and for the s -stage ($s \geq 3$) Lobatto IIIA methods

$$q_n^e - q^e(t_n) = O(h^{2s-4} + \epsilon^2 h^{s-1}), \quad v_n^e - v^e(t_n) = O(h^{s-1} + \epsilon^2 h^{s-3}),$$

uniformly for $h = \max_i h_i$ and $nh \leq \text{Const.}$ For the Gauss methods applied with constant stepsizes $h_i = h$ and $s \geq 3$ odd, the convergence rate is one order higher in h .

As mentioned in [13] the stage order s of Gauss methods and Lobatto IIIA methods has to be sufficiently high to ensure convergence. The midpoint rule and the trapezoidal rule do not converge. This has been numerically observed in [11, 26, 27].

For the solution of oscillatory systems, any numerical scheme obviously introduces phase errors up to its order of accuracy. A phase error analysis of Runge-Kutta methods can be found in [29], where forcing oscillating forces have also been considered. It has even been proved in [28] that symmetric Runge-Kutta methods introduce no phase lag for the forcing oscillating forces. This is however not especially relevant since this is generally not the main source of phase errors.

It is also worth mentioning that when using stepsizes much larger than the shortest period of oscillation the actual high frequencies of the system are all aliased to a lower 'numerical frequency' and are therefore not sampled correctly in a certain sense. This is however not a drawback due entirely to the numerical approximation, but inherently a sampling problem. Even if the exact values were known at the given large time steps then the actual high frequencies of the system could not be recovered from these values according to Shannon's criteria in sampling theory.

4. Simplified Newton iterations. Up to this point we have assumed implicitly that the nonlinear systems arising in the definition 2.1 of (P)RK methods are solved exactly. In practice they are solved iteratively by the use of simplified Newton iterations. Standard simplified Newton iterations may fail for highly oscillatory systems, unless the stepsizes are chosen sufficiently small so that the system is no longer stiff, making implicit methods less efficient than explicit methods [21]. We therefore propose some modifications in the simplified Newton iterations. For the starting values of the internal stages of an implicit (P)RK method we make use of a nearby *slow manifold*

$$(18) \quad M = \{(\bar{q}, \bar{v}) \in \mathbb{R}^n \times \mathbb{R}^n \mid 0 = g(\bar{q}), 0 = G(\bar{q})\bar{v}\}$$

coming from (17). We stress the point that we do not make use of the dynamics of a slow solution, but only of one of its geometric invariants, the slow manifold M . The dynamics on the slow manifold can differ significantly over mid and long-time intervals to that on the *smooth manifold* of (16), i.e., on the manifold of smooth motion. The projection on the slow manifold is purely geometric and does not require further analysis of the differential system as needed for the smooth manifold. These two manifolds are in a $O(\varepsilon^2)$ -neighbourhood and the corresponding values of $\frac{1}{\varepsilon^2}V_q$ differ only by an order $O(\varepsilon^2)$ [22, Theorem 2.2]. If $\frac{1}{\varepsilon^2}V(q)$ is of the form $\frac{1}{2\varepsilon^2}g(q)^T K g(q)$ with K a strictly positive definite symmetric matrix then the constraint function g in (17) can be chosen as g in $\frac{1}{2\varepsilon^2}g(q)^T K g(q)$. In molecular dynamics such potentials represent for covalent bond stretchings and bond-angle bendings [23]. For such potentials we can use Hairer's reformulation [14, p. 120] of the system (16)

$$(19a) \quad \dot{q} = v,$$

$$(19b) \quad M(q)\dot{v} = f(q, v) - G^T(q)\lambda,$$

$$(19c) \quad 0 = Kg(q) - \varepsilon^2\lambda.$$

For more general strong potentials we advocate the use of the modifications proposed in [22, Section 8].

In the simplified Newton iterations, for the starting values of the internal stages of an implicit (P)RK method based on a unique quadrature formula (b_i, c_i) , our choice comes from the analysis of the harmonic oscillator (1). For h fixed and letting

$\mu \rightarrow \infty$, when the matrices of Runge-Kutta coefficients A, \hat{A} are invertible the internal stages of the PRK solution satisfy $Y_i = 0$ and $Z_i = -(1/h) \cdot e_i^T \hat{A} (A \hat{A})^{-1} \mathbb{1}_s \cdot y_0$, and $\Lambda_i = (1/h^2) \cdot e_i^T (A \hat{A})^{-1} \mathbb{1}_s \cdot y_0 + (1/h) \cdot e_i^T A (\hat{A} A)^{-1} \mathbb{1}_s \cdot z_0$ with $\lambda = y/\varepsilon^2$. This can be seen from (2), (6), and (12). As initial guesses for the system (19a)-(19c) we therefore propose to use (see also [14, p. 95]) for $i = 1, \dots, s$

$$\begin{aligned} Q_i^{(0)} &= \tilde{q}_0 + hc_i \tilde{v}_0, \\ V_i^{(0)} &= \tilde{v}_0 - \frac{1}{h} \cdot e_i^T \hat{A} (A \hat{A})^{-1} \mathbb{1}_s \cdot (q_0 - \tilde{q}_0), \\ \Lambda_i^{(0)} &= \frac{1}{h^2} \cdot e_i^T (A \hat{A})^{-1} \mathbb{1}_s \cdot (q_0 - \tilde{q}_0) + \frac{1}{h} \cdot e_i^T A (\hat{A} A)^{-1} \mathbb{1}_s \cdot (v_0 - \tilde{v}_0), \end{aligned}$$

where $(\tilde{q}_0, \tilde{v}_0) \in M$ are projected values of (q_0, v_0) [16, Subsection III.1.3] on the slow manifold M

$$\begin{aligned} 0 &= M(\tilde{q}_0)(\tilde{q}_0 - q_0) + G^T(\tilde{q}_0)\mu_0, \\ 0 &= g(\tilde{q}_0), \\ 0 &= M(\tilde{q}_0)(\tilde{v}_0 - v_0) + G^T(\tilde{q}_0)\nu_0, \\ 0 &= G(\tilde{q}_0)\tilde{v}_0. \end{aligned}$$

A value for $\tilde{\lambda}_0$ would be simply $\tilde{\lambda}_0 = (1/\varepsilon^2)Kg(\tilde{q}_0) = 0$. We also advocate the use of $(\tilde{q}_0, \tilde{v}_0)$ instead of (q_0, v_0) when evaluating the simplified Jacobian matrix. Moreover, the quantities $\|\tilde{q}_0 - q_0\|$ and $\|\tilde{v}_0 - v_0\|$ could be used as measures of the size of the oscillations. They could be used in the stepsize control mechanism. If these quantities are larger than the desired precision TOL then the stepsize should not be larger than one period of oscillation and should therefore be restricted by accuracy requirements. However, if one still wants to take large stepsizes, since the phase information of the oscillations is lost, arbitrarily large errors should be allowed in directions orthogonal to the smooth and slow solutions. Nevertheless, we conjecture that the projections of the numerical solution onto the smooth or slow manifolds will still converge to the corresponding projections of the exact solution onto these manifolds.

For Lobatto IIIA methods the Runge-Kutta matrix $A = \hat{A}$ is not invertible. For the harmonic oscillator (1), for h fixed and by letting $\mu \rightarrow \infty$, the internal stages satisfy $Y_1 = y_0$, $Z_1 = z_0$, $\Lambda_1 = \lambda_0 = y_0/\varepsilon^2$, and for $i = 2, \dots, s$ $Y_i = R_i(\infty)y_0$, $Z_i = R_i(\infty)z_0 - (1/h) \cdot e_{i-1}^T \tilde{A}^{-2}(\tilde{A}_1 + \tilde{A}\mathbb{1}_{s-1}) \cdot y_0$, $\Lambda_i = R_i(\infty)\lambda_0 + (1/h^2) \cdot e_{i-1}^T \tilde{A}^{-2} \mathbb{1}_{s-1} \cdot y_0 + (1/h) \cdot e_i^T \tilde{A}^{-2}(\tilde{A}_1 + \tilde{A}\mathbb{1}_{s-1}) \cdot z_0$ where $R_i(\infty) = -e_{i-1}^T \tilde{A}^{-1} \tilde{A}_1$, e_j^T is the j -th unit vector in R^{s-1} , and the Runge-Kutta matrix A of Lobatto IIIA coefficients is given by

$$A = \begin{pmatrix} 0 & 0 & \dots & 0 \\ \tilde{A}_1 & \tilde{A} & & \end{pmatrix}.$$

This can be seen by computing the inverse of the matrix in the left-hand side of (6)

$$\begin{pmatrix} I_s & -\mu A \\ \mu A & I_s \end{pmatrix}^{-1} = \begin{pmatrix} 1 & 0 & \dots & 0 & 0 & 0 & \dots & 0 \\ v_1(\mu) & N(\mu) & & -v_2(\mu) & P(\mu) & & & \\ 0 & 0 & \dots & 0 & 1 & 0 & \dots & 0 \\ v_2(\mu) & -P(\mu) & & v_1(\mu) & N(\mu) & & & \end{pmatrix}$$

where $v_1(\mu) = \mu \tilde{A} v_2(\mu)$, $v_2(\mu) = -\mu N(\mu) \tilde{A}_1$, $N(\mu) = (I_{s-1} + \mu^2 \tilde{A}^2)^{-1}$, $P(\mu) = \mu \tilde{A} N(\mu)$, by using (2), and by letting $\mu \rightarrow \infty$. For the Lobatto IIIA methods we thus

propose to use instead $Q_1 = q_0$, $V_1 = v_0$, $\Lambda_1 = \lambda_0 = (1/\epsilon^2)Kg(q_0)$, and for $i = 2, \dots, s$

$$Q_i^{(0)} = \tilde{q}_0 + R_i(\infty)(q_0 - \tilde{q}_0) + hc_i \tilde{v}_0,$$

$$V_i^{(0)} = \tilde{v}_0 + R_i(\infty)(v_0 - \tilde{v}_0) - \frac{1}{h} \cdot e_{i-1}^T \tilde{A}^{-2} (\tilde{A}_1 + \tilde{A} \mathbb{1}_{s-1}) \cdot (q_0 - \tilde{q}_0),$$

$$\Lambda_i^{(0)} = R_i(\infty)\lambda_0 + \frac{1}{h^2} \cdot e_{i-1}^T \tilde{A}^{-2} \mathbb{1}_{s-1} \cdot (q_0 - \tilde{q}_0) + \frac{1}{h} \cdot e_i^T \tilde{A}^{-2} (\tilde{A}_1 + \tilde{A} \mathbb{1}_{s-1}) \cdot (v_0 - \tilde{v}_0),$$

For large amplitudes in the oscillations the above approach will generally fail, i.e., the Newton iterations will not converge. Unlike stiff problems with very large negative eigenvalues [15, Theorem IV.14.2], existence and uniqueness of the numerical solution cannot be proved for highly oscillatory systems, unless the amplitudes of the oscillations are sufficiently small [22, Lemma 5.1].

5. Numerical experiments. A typical example of a stiff oscillatory mechanical system is given by the *stiff spring pendulum* [14, 22]. It consists of a point of mass m suspended by a massless spring with a large Hooke's constant $1/\epsilon^2$, $0 < \epsilon \ll 1$. Using Cartesian coordinates $q = (q_1, q_2)^T$, the kinetic energy T and the potential energy U of the system are given respectively by

$$T(\dot{q}) = \frac{m}{2} (\dot{q}_1^2 + \dot{q}_2^2), \quad U(q) = mgq_2 + \frac{1}{2\epsilon^2} \left(\sqrt{q_1^2 + q_2^2} - \ell \right)^2$$

where ℓ denotes the rest position of the spring and g the gravity. The Lagrange equations of motion can be written, using Hairer's reformulation (19c)

$$(21a) \quad \begin{pmatrix} \dot{q}_1 \\ \dot{q}_2 \end{pmatrix} = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix},$$

$$(21b) \quad m \begin{pmatrix} \dot{v}_1 \\ \dot{v}_2 \end{pmatrix} = \begin{pmatrix} -\frac{q_1}{\sqrt{q_1^2 + q_2^2}} \lambda \\ -mg - \frac{q_2}{\sqrt{q_1^2 + q_2^2}} \lambda \end{pmatrix},$$

$$(21c) \quad 0 = \sqrt{q_1^2 + q_2^2} - \ell - \epsilon^2 \lambda.$$

By using the generalized momenta $p = (p_1, p_2)^T = (mv_1, mv_2)^T$ these equations form also a Hamiltonian system with Hamiltonian $H = T + U$. For the limit case $\epsilon \rightarrow 0$, we obtain the pendulum equations with the holonomic constraint

$$0 = \sqrt{q_1^2 + q_2^2} - \ell$$

and λ has now the role of a Lagrange multiplier. Differentiating once this constraint leads to

$$0 = q_1 v_1 + q_2 v_2.$$

Another differentiation gives

$$\lambda = \frac{m}{\ell^2} (v_1^2 + v_2^2 - gq_2).$$

In the following numerical experiments the parameters have been taken as $m = 1$, $\ell = 1$, $g = 1$, and $\epsilon = 10^{-5}$. For those values the Jacobian of the system possesses

two eigenvalues with large imaginary part of size $\pm 1/\epsilon$ leading to highly oscillatory behaviour for small ϵ . Different numerical methods have been applied on the interval $[0, 20]$ with a constant stepsize $h = 10^{-2}$ which is 10^3 times greater than ϵ . For the initial values we have chosen $q_2(0) = 0$, $v_1(0) = v_2(0) = 0$, and different values for $q_1(0)$. A smooth solution is given by $q_1(0) = 1 - 3\epsilon^4 - 90\epsilon^8 + O(\epsilon^{10})$. A numerical approximation of the solution has been computed using the 5-stage Gauss method and is plotted in Fig. 1. The energy of the smooth solution is equal to $H = 4.5\epsilon^6 + O(\epsilon^8)$. The behaviour of the computed energy is mainly due to the errors at the end of the Newton process. For the slow solution $q_1(0) = 1$, i.e., the solution starting on the slow manifold (18), the obtained numerical results were identical since ϵ^4 was smaller than the machine precision.

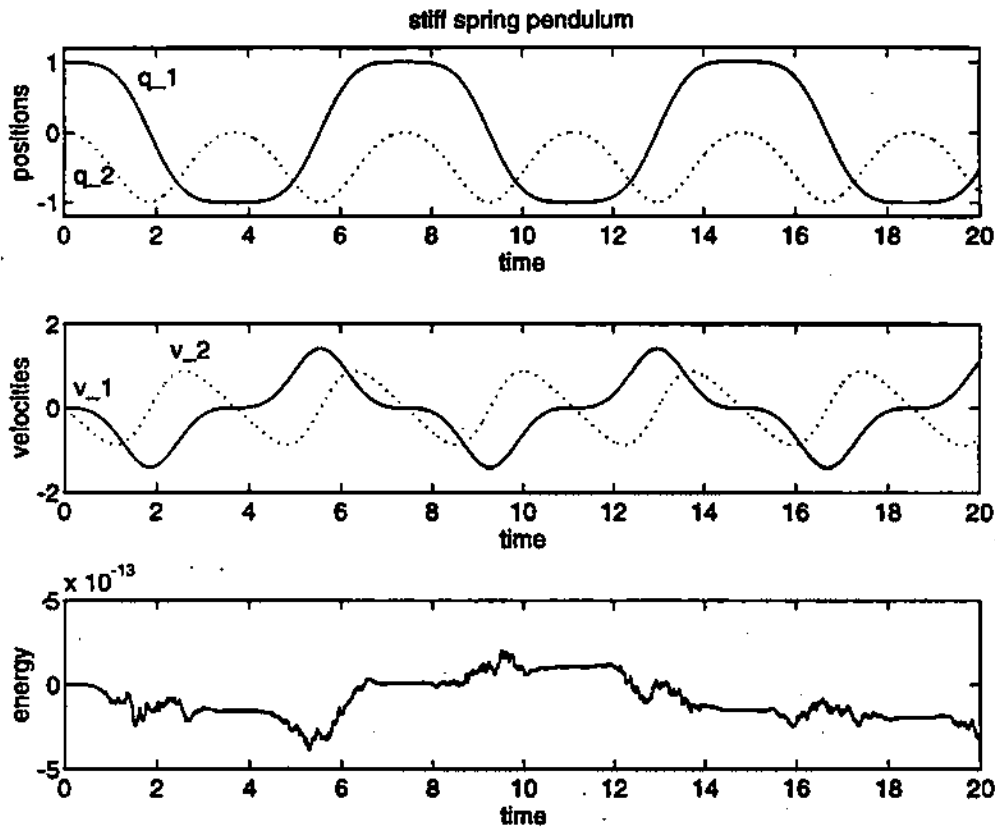


FIG. 1. Smooth solution with the 5-stage Gauss method, $h = 0.01$.

We have perturbed the smooth solution by adding a perturbation 10^{-5} to the previous value of $q_1(0)$, leading to the highly oscillatory solution drawn in Fig. 2. This perturbation has been chosen sufficiently small to ensure existence and uniqueness of the numerical solution (see [22, Lemma 5.1]). The 5-stage Gauss method mimics well the highly oscillatory behaviour in the velocities, the amplitudes of the oscillations in the positions being too small to be observed. The energy of the system oscillates around its exact value $H \approx 0.5$, this is a typical behaviour for a symplectic integrator.

In Fig. 3 these oscillations are not present when using the 4-stage Gauss method since this method satisfies $R(\infty) = 1$, whereas the 5-stage Gauss method satisfies

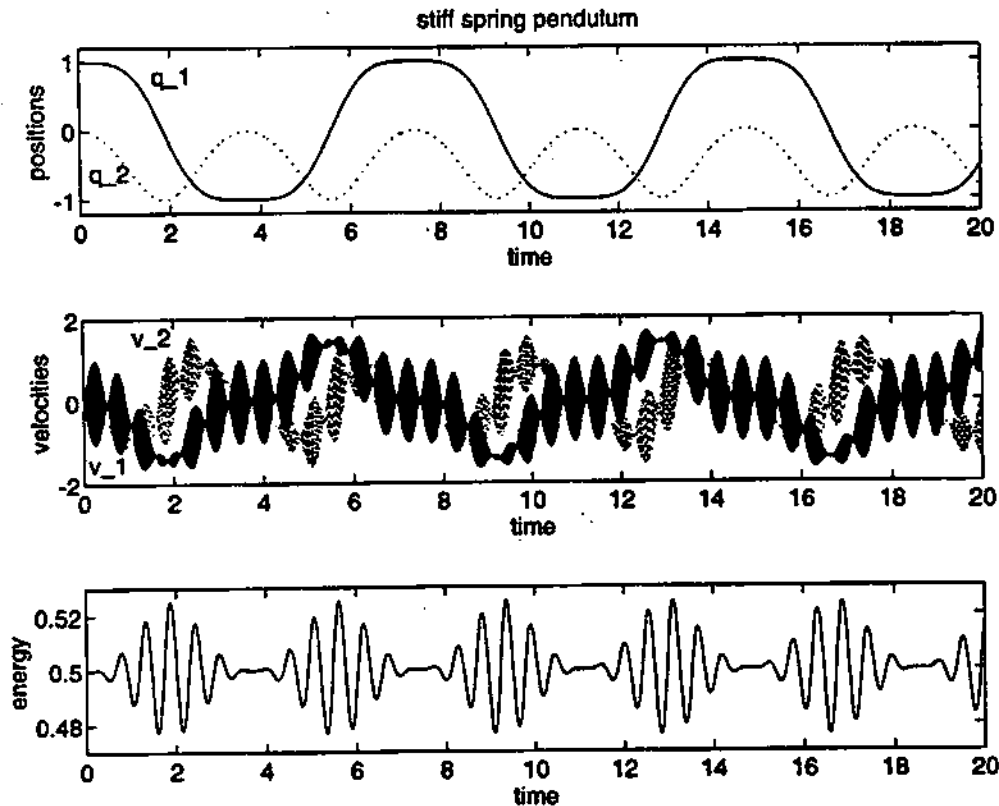


FIG. 2. Highly oscillatory solution with the 5-stage Gauss method, $h = 0.01$.

$R(\infty) = -1$. Qualitatively the behaviour of methods satisfying $R(\infty) = -1$ is therefore preferable to those satisfying $R(\infty) = 1$, although in terms of precision they are comparable. The behaviour of the computed energy is similar however. By increasing too much the perturbation in the smooth solution, the Newton iterations begin to fail. This can be simply explained by the fact that existence and uniqueness of the numerical solution fails to hold for large perturbations (see [22, Lemma 5.1]).

Finally we have applied the 3-stage Radau IIA method, an L -stable method, with the same previous initial values on the highly oscillatory solution. The intrinsic damping property of this numerical scheme suppresses the highly oscillatory behaviour of the solution, this can be observed in Fig. 4. For the first two steps the numerical energy decreases from 0.5 to $4.5 \cdot 10^{-6}$ and $-2.6 \cdot 10^{-10}$ respectively. Such behaviour has been analyzed in detail in a more general setting in [22].

6. Conclusion. In this article we have identified and analyzed numerical methods which are able to obtain satisfactorily solutions with large stepsizes to highly oscillatory systems such as Hamiltonian and mechanical systems. The amplitude of the high-frequency oscillation must be small to ensure existence and uniqueness of the numerical solution for nonlinear problems.

The methods that we propose are the s -stage ($s \geq 4$) Gauss methods or the s -stage ($s \geq 3$) Lobatto IIIA methods. These methods have the important property of P -stability, which requires the method to preserve the amplitude of high-frequency

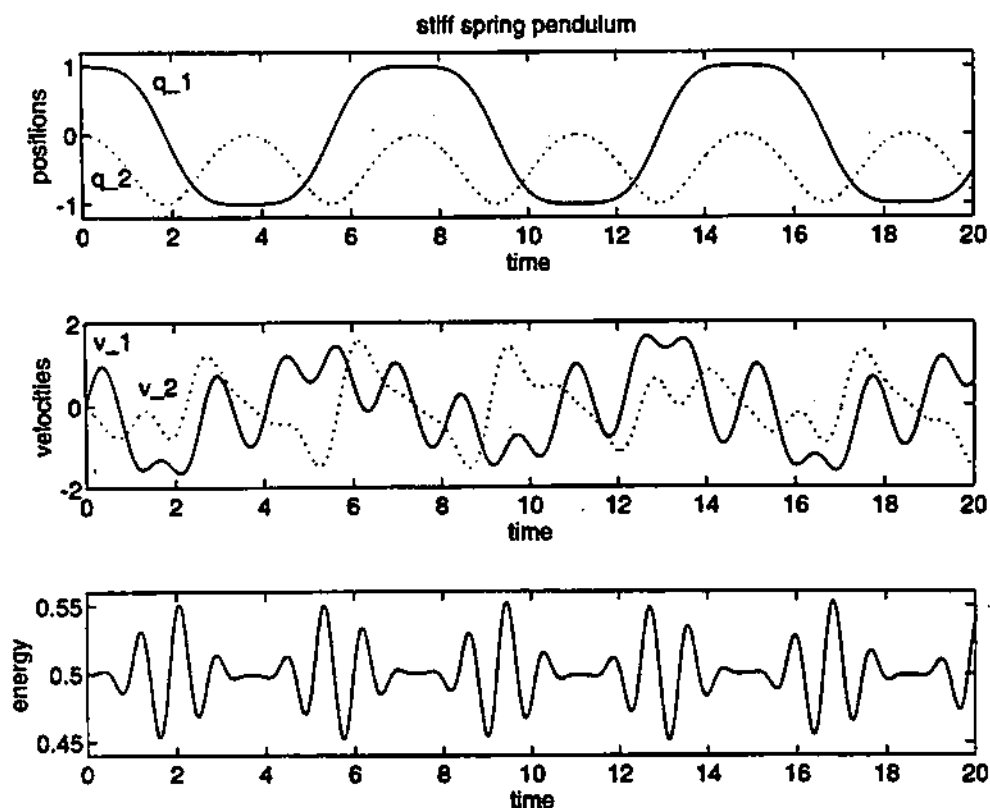


FIG. 3. Highly oscillatory solution with the 4-stage Gauss method, $h = 0.01$.

oscillations for linear systems, and of sufficiently high order that they are convergent for the Hessenberg index-3 DAE system which is the limit as $\epsilon \rightarrow 0$ of the considered oscillatory system. We show that for smooth solutions to the class of problems under consideration, these methods are convergent for stepsizes of size independent of the frequency of the oscillation. Some numerical experiments with the stiff spring pendulum equations are given.

The proposed methods are implicit. For such large stepsizes, convergence cannot be achieved without some modifications in the Newton iteration at each time step. In particular, we have reformulated the system as suggested by Hairer [13]. The starting values for the internal stages are obtained by using projection onto the slow manifold. The Jacobian matrix is also evaluated on the slow manifold. The projection is purely geometric and numerical, and does not require further analysis of the differential system.

We note that the Lobatto IIIA-III B partitioned Runge-Kutta methods, of which (Rattle)-Verlet is a member, that are widely in use for this type of oscillatory Hamiltonian system are not effective for stepsizes which are much larger than the smallest period of the oscillation. This is because they are not P-stable. Other widely-used methods, the trapezoidal and midpoint, are also not effective for large stepsizes and nonlinear oscillatory problems because their order is not high enough for the method to be convergent for the limiting index-3 DAE.

We wish to emphasize that the proposed methods are effective only for small-

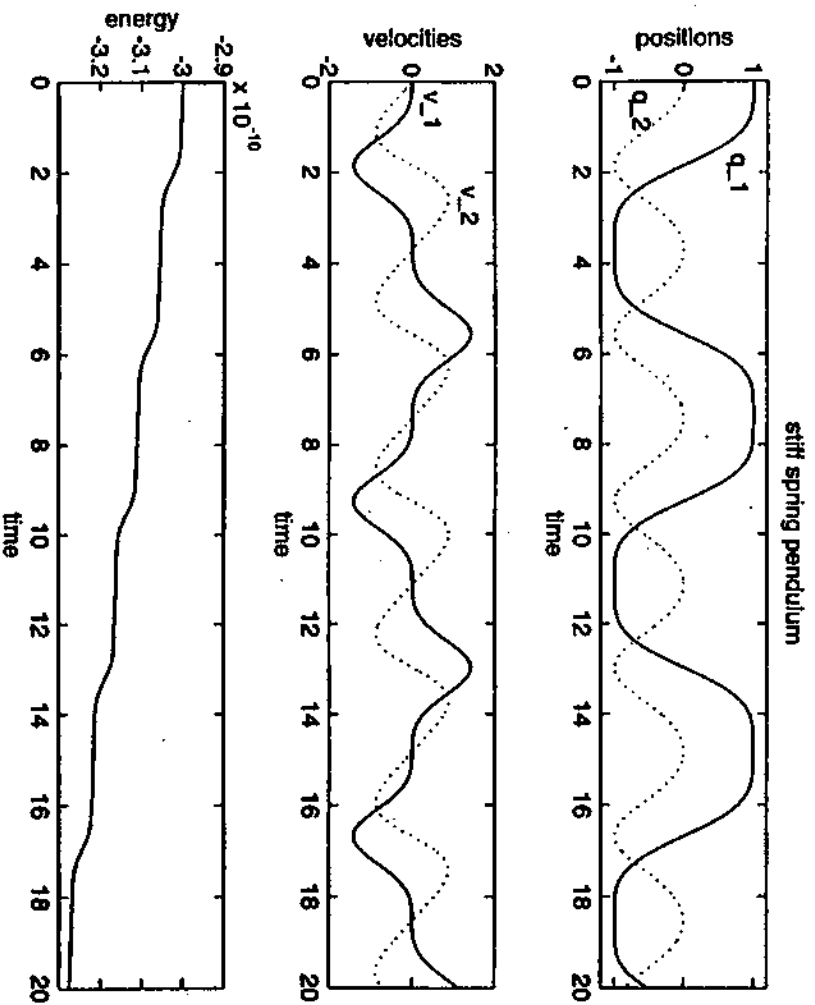


Fig. 4. Highly oscillatory solution with the 3-stage Runge-Kutta method, $h = 0.01$.

amplitude oscillations. A different approach is necessary if the amplitudes of the oscillation are large, which is the case in most molecular dynamics applications.

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