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Numerical solution of highly oscillatory ordinary differential equations

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1. Introduction

One of the most difficult problems in the numerical solution of ordinary differential equations (ODEs) and in differential-algebraic equations (DAEs) is the development of methods for dealing with highly oscillatory systems. These types of systems arise, for example, in vehicle simulation when modelling the suspension system or tyres, in models for contact and impact, in flexible body simulation from vibrations in the structural model, in molecular dynamics, in orbital mechanics, and in circuit simulation. Standard numerical methods can require a huge number of time-steps to track the oscillations, and even with small stepsizes they can alter the dynamics, unless the method is chosen very carefully.

What is a highly oscillatory system, and what constitutes a solution of such a system? As we will see, this question is somewhat application-dependent, to the extent that it does not seem possible to give a precise mathematical definition which would include most of the problems that scientists, engineers and numerical analysts have described as highly oscillatory. *Webster's Ninth New Collegiate Dictionary* (1985) includes the following definitions for *oscillate*: 'to swing backward and forward like a pendulum; to move or travel back and forth between two points; to vary above and below a mean value.' Here we are mainly interested in systems whose solutions may be oscillatory in the sense that there is a *fast* solution which varies regularly about a *slow* solution. The problem will be referred to as *highly oscillatory* if the timescale of the fast solution is much shorter than the interval of integration.

We will begin with a simple example of an oscillating problem from multibody dynamics. In *Cartesian coordinates*, a simple stiff spring pendulum model with unit mass, length, and gravity, can be expressed as

$$0 = x' - u, \tag{1.1a}$$

$$0 = y' - v, \tag{1.1b}$$

$$0 = u' + x\lambda, \tag{1.1c}$$

$$0 = v' + y\lambda - 1, \tag{1.1d}$$

$$\epsilon^2\lambda = \frac{\sqrt{x^2+y^2}-1}{\sqrt{x^2+y^2}}, \tag{1.1e}$$

where $1/\epsilon^2 \gg 1$ is the spring constant. Preloading the spring by using $\epsilon = \sqrt{10^{-3}}$, the initial position $(x_0, y_0) = (0.9, 0.1)$, and the zero initial velocity $(u_0, v_0) = (0, 0)$, the results of the states (x, y, u, v) in the 0 to 10[s] simulation are shown in Fig. 1.

The solution to this problem consists of a low-amplitude, high-frequency oscillation superimposed on a slow solution. It is not immediately clear that a slow solution appears in the above problem. In fact, we can only identify

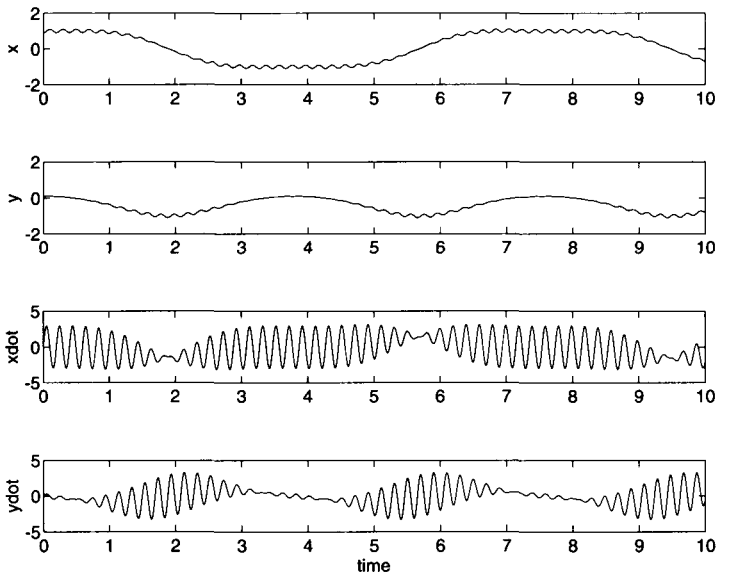

Fig. 1. Stiff spring pendulum in Cartesian coordinates

the slow solution of (1.1) using a proper nonlinear coordinate transformation $(x, y) = (r\cos(\theta), r\sin(\theta))$. In *polar coordinates* (r, θ), we obtain the equations of motion of (1.1):

$$0 = r' - z, \tag{1.2a}$$

$$0 = \theta' - \omega, \tag{1.2b}$$

$$0 = z' + r\omega^2 + \frac{1}{\epsilon^2}(r-1) - \sin\theta, \tag{1.2c}$$

$$0 = \omega' - \frac{1}{r}(2z\omega - \cos\theta), \tag{1.2d}$$

where (z, ω) is the velocity. In the 0 to 10[s] second simulation, using the same initial conditions, we obtain the solution in Fig. 2. It is clear that the length r represents the fast motion and the angle θ the slow motion.

One of the questions one must answer in selecting an appropriate mathematical or numerical method is: 'What do we mean by a solution?' For example, one might be interested only in finding the slow solution. On the other hand, in some situations it may be important to recover more information about the high-frequency oscillation, such as its amplitude, its energy or its envelope. The most detailed information about the high-frequency oscillation also includes its phase; this information is usually very difficult to recover, particularly over intervals which are long in comparison to the period of the oscillation. Efficiency is often an important consideration; one might be willing to give up on tracking some of the detailed information of

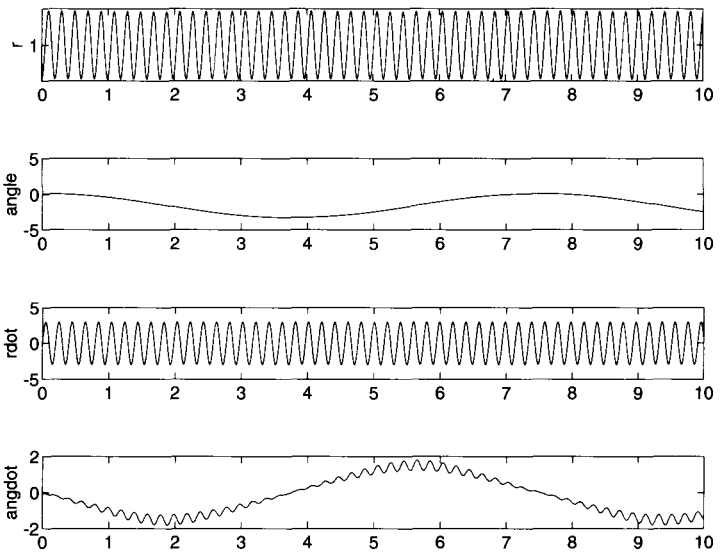

Fig. 2. Stiff spring pendulum in polar coordinates

the high-frequency oscillation in order to take much larger stepsizes. This is the case in real-time simulation of mechanical systems. For other problems, maintaining physical and mathematical properties in the numerical solution can be critical, particularly over long-time intervals. For example, in molecular dynamics it may be important to maintain invariants like the energy or the symplectic structure of the problem (Arnold 1989). What is meant by a solution is determined not only by the physical properties of the system and its mathematical structure, but also by how the information from the simulation is to be used.

The form and structure of the oscillating problem is highly application-dependent. Some problems are posed as a first-order ODE system, others as a second-order ODE system. Other problems include constraints, and hence are formulated as a DAE system. Often these ODE and DAE systems have a special mathematical structure. Some applications yield problems which are linear or nearly linear, while other applications require the solution of highly nonlinear oscillating systems. Some problems may have a single high frequency and be nearly periodic, whereas other problems may have multiple high-frequency components. Some oscillating problems, for example in ocean dynamics (Garrett and Munk 1979, Gjaja and Holm 1996), corrosion modelling (Tidblad and Graedel 1996), atmospheric modelling (Kopell 1985), nonlinear optics (Agrawal 1989), *ab initio* molecular dynamics (Tuckerman and Parrinello 1994) yield partial differential equation (PDE) systems; these problems are beyond the scope of the present paper although

many of the same considerations and types of methods apply for the time integration.

This paper will deal mainly with *numerical methods* for oscillating systems. There is an extensive literature in applied mathematics (Bogoliubov and Mitropolski 1961, Minorsky 1974, Fenichel 1979, Kevorkian and Cole 1981) including the method of averaging, the method of multiple scales, and the stroboscopic method, on approximating the solution to oscillating problems. Some of these techniques are related to the numerical methods described here. Methods from applied mathematics can sometimes be combined advantageously with numerical methods (Kirchgraber 1982) for the solution of oscillating problems. Most of the mathematical techniques require a nearly linear structure of the problem. For some applications, the equations naturally occur in this structure or can be easily reformulated; for others, casting the problem in this form is difficult or impossible. There is also a tradition of physically motivated mathematical or numerical methods that reformulate the system prior to numerical solution, using approximations that the scientist or engineer deems to be valid. These methods can be quite powerful when used carefully. The LIN method (see Subsection 4.4) for molecular dynamics, and modal analysis methods (see Subsection 3.4) for structural analysis are examples of these kinds of methods.

A wide variety of numerical methods has been developed for highly oscillatory problems. The best method to use is strongly dependent on the application. Small-amplitude oscillations in linear or nearly linear systems can often be damped via highly stable implicit numerical methods. We will see that it is also feasible to damp the oscillation in certain structured, highly nonlinear oscillating problems from mechanical systems. Even with numerical methods based simply on damping the oscillation, there can be unforeseen difficulties due to the nonlinear oscillation, for example in automatic stepsize control and in obtaining convergence of the Newton iteration of implicit numerical methods. In other applications, damping the oscillation can destroy important properties of the solution. For these problems, much attention has been focused on preserving important physical and mathematical properties like the energy or the symplectic structure of the system. Many of the numerical methods that can do this require relatively small stepsizes. Efficiency is also an important consideration, making these problems quite challenging. Still other problems yield systems with a single high-frequency oscillation. Methods based on envelope following can yield the smooth solution in this case.

It is important to recognize that, in general, one should not expect to be able to numerically solve nonlinear highly oscillatory problems using stepsizes which are large relative to the timescale of the fast solution. Standard numerical ODE methods make use only of local information about the problem, obtained from evaluating the right-hand side of the differential

equation. The methods which for some applications are able to take large stepsizes are able to do this by implicitly or explicitly making use of global information about the problem and/or its mathematical structure. For example, it is feasible to damp the oscillation for certain mechanical systems only because of a very specific mathematical structure. The LIN method of molecular dynamics makes use of both the mathematics and the physics of the problem. Envelope-following methods make use of the fact that for some problems it is known *a priori* that the fast solution has a single high-frequency component.

Unlike most stiff problems, which can be solved by strongly damped implicit numerical methods, effective solution of nonlinear highly oscillatory problems generally requires exploitation of the problem structure and a careful examination of the objectives and intended use of the computation. Therefore we have based the organization of this paper on classes of application problems. Section 2 covers linear problems and basic concepts that are fundamental to understanding numerical methods for highly oscillatory problems. Section 3 deals with highly oscillatory rigid and flexible mechanical systems, describing the nonlinear structure of these systems and implications for numerical methods, when and how the oscillation can be safely and efficiently damped, modal analysis techniques from structural analysis, and the problems and considerations in extending these techniques to flexible multibody systems. Section 4 briefly describes problems and numerical methods for molecular dynamics. Section 5 describes problems from circuit analysis and orbital mechanics for which envelope-following techniques are applicable, and describes those numerical methods.

2. Basic concepts and methods for linear oscillatory systems

Numerical methods used to treat oscillatory problems differ, depending on the formulation of the problem, the knowledge of certain characteristics of the solution, and the objectives of the computation (Gear 1984). However, certain concepts are common to most classes of methods. Since it is not possible to give a uniform presentation of these concepts, as an illustration we will consider the class of *partitioned Runge–Kutta* (PRK) methods which includes standard Runge–Kutta (RK) methods and other schemes of interest, such as the Verlet algorithm (4.2). For other classes of methods, the definitions are analogous.

To investigate the stability properties of numerical methods applied to oscillatory systems, the scalar *harmonic oscillator* equation

$$y'' = -\omega^2 y, \qquad (\omega > 0) \tag{2.1}$$

is chosen as a standard test equation. This is the analogue of Dahlquist's test equation $y' = \lambda y$ for first-order ODEs, although the situation is not

totally parallel to problems with large negative eigenvalues of the Jacobian matrix. The solutions to (2.1) are given by the family of *sine curves* $y(t) = A\sin(\omega t + \phi)$, where the expression $\omega t + \phi$ is called the *phase*. The real parameters $A \geq 0$, ω, and ϕ are called, respectively, the *amplitude*, the *pulse*, and the *phase-lag*. The *period* of the solution is $T := 2\pi/\omega$ and its *frequency* is $f := 1/T = \omega/2\pi$. The parameters A and ϕ are determined from the initial conditions. Sine curves are archetypal oscillatory functions and they form the basis of Fourier analysis.

To apply PRK methods, we must first rewrite (2.1) as a first-order system by introducing a new variable $z := y'$, yielding

$$y' = z, \qquad z' = -\omega^2 y. \tag{2.2}$$

This is one of the simplest systems for which the eigenvalues $(\pm i\omega)$ of the Jacobian matrix of the system are purely imaginary. This is also a linear Hamiltonian system with Hamiltonian $H(y,z) = (\omega^2 y^2 + z^2)/2$. PRK methods take advantage of the intrinsic partitioning of the equations by making use of the conjunction of two sets of RK coefficients. One step of an *s-stage PRK method* applied to partitioned systems of the form

$$y' = f(t,y,z), \qquad z' = g(t,y,z),$$

with initial values (y_0, z_0) at t_0 and stepsize h, is defined by

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

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

where $t_i := t_0 + c_i h$. The coefficients (b_i, a_{ij}, c_i) and $(b_i, \widehat{a}_{ij}, c_i)$ are the coefficients of two RK methods based on the same quadrature formula (b_i, c_i). Applying the PRK method to (2.2) we get

$$\begin{pmatrix} y_1 \\ z_1 \end{pmatrix} = D_\omega M(\mu) D_\omega^{-1} \begin{pmatrix} y_0 \\ z_0 \end{pmatrix},$$

where $\mu := h\omega$, $D_\omega := \mathrm{diag}(1, \omega)$, and $M(\mu)$ is the 2×2 *stability matrix* of the PRK method. This matrix is given by

$$M(\mu) = I_2 + \mu \begin{pmatrix} O & b^T \\ b^T & O \end{pmatrix} \begin{pmatrix} I_s & -\mu A \\ \mu\widehat{A} & I_s \end{pmatrix}^{-1} \begin{pmatrix} \mathbb{1}_s & O \\ O & \mathbb{1}_s \end{pmatrix}, \tag{2.3}$$

where we have used $\mathbb{1}_s$ to denote the s-dimensional vector $(1, \ldots, 1)^T$, I_n for the identity matrix in $\mathbb{R}^{n\times n}$, $\{A, \widehat{A}\}$ for the matrices of the RK coefficients, and b for the vector of the RK weights. Other expressions for the stability matrix can be derived with the help of Van Der Houwen and Sommeijer

(1989, Lemma 2.1). The exact solution to (2.2) at $t_0 + h$ can be expressed by

$$\begin{pmatrix} y(t_0+h) \\ z(t_0+h) \end{pmatrix} = D_\omega \Theta(\mu) D_\omega^{-1} \begin{pmatrix} y_0 \\ z_0 \end{pmatrix}, \quad \Theta(\mu) = \begin{pmatrix} \cos(\mu) & \sin(\mu) \\ -\sin(\mu) & \cos(\mu) \end{pmatrix}.$$

The eigenvalues of the rotation matrix $\Theta(\mu)$ are of modulus one. This motivates the following definition.

Definition 2.1 For a PRK method, an interval I with $\{0\} \subset I \subset \mathbb{R}$ is an *interval of periodicity* if for all $\mu \in I$ the eigenvalues $\lambda_i(\mu)$ $(i = 1, 2)$ of the stability matrix $M(\mu)$ (2.3) satisfy $|\lambda_i(\mu)| = 1$ $(i = 1, 2)$ and, if $\lambda_1(\mu) = \lambda_2(\mu)$, then this eigenvalue must possess two distinct eigenvectors. A method is said to be *P-stable* if $\mathbb{R}$ is an interval of periodicity.

If the interval of periodicity is not reduced to $\{0\}$, the method is usually called *nondissipative*. These concepts are due to Lambert and Watson (1976) and were originally introduced for linear multistep methods applied to $y'' = g(t, y)$. They proved that nondissipative linear multistep methods must be symmetric. They also stated that P-stable linear multistep methods cannot have order greater than two. A proof of this result in a more general setting was given by Hairer (1979). This is a result similar to the famous Dahlquist's second barrier (Dahlquist 1963). To overcome this order barrier, several hybrid multistep methods have been derived (Cash 1981, Chawla and Rao 1985, Hairer 1979), for instance, a P-stable modification to the fourth-order Numerov method (Hairer 1979). For standard RK methods ($A = \widehat{A}$) the eigenvalues of the stability matrix are simply given by $\lambda_1(\mu) = R(\mathrm{i}\mu)$ and $\lambda_2(\mu) = R(-\mathrm{i}\mu) = \overline{\lambda_1(\mu)}$, where $R(z) = 1 + zb^T(I_s - zA)^{-1}\mathbb{1}_s$ is the usual stability function of the RK method. Hence, we have the following well-known result.

Theorem 2.1 Symmetric RK methods are P-stable.

For example, the implicit midpoint rule is P-stable. However, a similar theorem does not hold for PRK methods. For example, we can consider the coefficients of the two-stage Lobatto IIIA–IIIB method (Jay 1996)

$$A = \begin{pmatrix} 0 & 0 \\ 1/2 & 1/2 \end{pmatrix}, \qquad \widehat{A} = \begin{pmatrix} 1/2 & 0 \\ 1/2 & 0 \end{pmatrix}, \qquad b^T = \begin{pmatrix} 1/2 & 1/2 \end{pmatrix}.$$

This symmetric and symplectic method is equivalent to the famous leapfrog/Störmer/Encke/Verlet method (4.2) used for second-order ODEs. Necessary conditions on the coefficients of the stability matrix $M(\mu)$ to satisfy the conditions of Definition 2.1 are given by

$$\det(M(\mu)) = 1, \qquad |\operatorname{tr}(M(\mu))| \leq 2. \tag{2.4}$$

The stability matrix of the two-stage Lobatto IIIA–IIIB method is

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

It satisfies $\det(M(\mu)) = 1$, but only $|\operatorname{tr}(M(\mu))| = |2 - \mu^2|$. Thus, according to (2.4) this method is not P-stable; its interval of periodicity (and of absolute stability, see below) is $(-2, 2)$. As pointed out in Lambert and Watson (1976), the relevance of the property of P-stability seems restricted to situations exhibiting *periodic stiffness*, that is, where the oscillatory solution is of negligible amplitude. The reason is that the stepsize of a method is not only limited by stability requirements but is also dictated by accuracy requirements. A stepsize of the same magnitude as the period of oscillation with highest frequency is required even for P-stable methods to follow this oscillation in order to preserve the accuracy of the method, unless its amplitude is sufficiently small.

The weaker property of nondissipativity is of primary interest in celestial mechanics for orbital computation, where it is desired that the numerically computed orbits do not spiral inwards or outwards. In this context, a related notion is the property of *orbital stability* of Cooper (1987), that is, the preservation of quadratic invariants by the numerical method. The construction of nondissipative explicit Runge–Kutta–Nyström (RKN) methods of order two to five with a minimal number of function evaluations per step and possessing relatively large intervals of periodicity is given in Chawla and Sharma (1981*a*) and (1981*b*). In Portillo and Sanz-Serna (1995), it is shown with an example that, for Hamiltonian systems, nondissipative methods do not in general share the advantageous error propagation mechanism possessed by symplectic methods (Sanz-Serna and Calvo 1994). In this framework, an explicit symplectic method of effective order four with three function evaluations per step and with a maximal interval of periodicity is presented in López-Marcos, Sanz-Serna and Skeel (1995*b*).

In certain applications, it can be desirable to leave the fast oscillation modes unresolved. For example, in many structural dynamics applications (see Subsection 3.5), high-frequency oscillations are spurious and should be damped out. Hence, we can consider a less stringent notion of stability.

Definition 2.2 Replacing the condition $|\lambda_i(\mu)| = 1$ by $|\lambda_i(\mu)| \leq 1$ in Definition 2.1 we define the notions of an *interval of absolute stability* and of *I-stability*.

For standard RK methods we recover the usual definition of *I-stability* (Hairer and Wanner 1996). *L-stable* RK methods, *i.e.*, RK methods satisfying $R(\infty) = 0$ and $|R(z)| \leq 1$ when $\operatorname{Re}(z) \leq 0$, such as the implicit Euler method, may be appropriate to damp out highly oscillatory components (corresponding to large μ) since they are I-stable and satisfy $\lim_{\mu\to\infty} |\lambda_i(\mu)|$

$= 0$ $(i = 1, 2)$. When the eigenvalues of the stability matrix (2.3) are conjugate, we can write

$$\lambda_1(\mu) = \overline{\lambda_2(\mu)} = \rho(\mu)e^{i\theta(\mu)},$$

where $\rho(\mu)$ and $\theta(\mu)$ are real-valued functions. Notice that the exact solution of (2.2) in $\mathbb{C}$ is reproduced if $\rho(\mu) \equiv 1$ and $\theta(\mu) \equiv \mu$. Following Brusa and Nigro (1980), we can define the functions $a(\mu)$ and $b(\mu)$ by the relations $\rho(\mu) = e^{-\mu a(\mu)}$ and $\theta(\mu) = \mu b(\mu)$. The function $a(\mu)$ is called the *factor of numerical (or algorithmic) damping.* Owren and Simonsen (1995) have constructed families of L-stable *singly diagonally implicit Runge–Kutta* (SDIRK) methods with controllable numerical damping. The expression $|b(\mu) - 1|$ is called the *frequency distortion.* In the *phase-lag expansion* of the *relative period error* $b(\mu) - 1 = b_r(\mu)\mu^r + \mathcal{O}(\mu^{r+1})$ with $b_r(\mu) \not\equiv 0$, the exponent r is called the *dispersion order.* In Van Der Houwen and Sommeijer (1987) and (1989), several nondissipative RKN methods and diagonally implicit RK (DIRK) methods with high order of dispersion are derived. On certain test problems with oscillatory solutions, they show that the accuracy of the method is mostly determined by its dispersion rather than by its usual local truncation error. Other related error measures are often used in the literature to compare the merits of different methods, such as the *(relative) amplitude (or amplification) error* for $1 - \rho(\mu)$ and the *phase (or period) error (or dispersion or phase-lag)* for $\mu - \theta(\mu)$.

In addition to the natural free modes of oscillation of a system, modelled by the harmonic oscillator equation (2.2), the presence of forcing terms of oscillation may be considered. A simple inhomogeneous test equation in $\mathbb{C}$ is given by

$$y'' = -\omega^2 y + \delta e^{i\omega_f t}, \qquad (\omega \neq \omega_f, \omega > 0, \omega_f > 0),$$

where $\omega_f/2\pi$ represents the frequency of the forcing term. The exact solution is

$$y(t) = Ae^{i(\omega t + \phi)} + \frac{\delta}{\omega^2 - \omega_f^2} e^{i\omega_f t}.$$

It may be of interest to know how well a numerical method approximates the second term of the solution, corresponding to the forcing term. Nevertheless, it must be emphasized that the *inhomogeneous phase error* introduced by the forcing term remains constant, whereas the *homogeneous phase error* due to the free oscillation accumulates with time and is therefore the main source of errors (Van Der Houwen and Sommeijer 1987). Methods with no inhomogeneous phase error are said to have *in-phase forced oscillations* (Gladwell and Thomas 1983).

Several different methods have been proposed for problems whose solutions are known to be periodic and such that the period can be estimated

a priori. In Section 5 we will treat in detail the envelope-following techniques. Another category of methods which can be interpreted as *exponentially fitted* methods (Liniger and Willoughby 1970) is based on the exact integration of the trigonometric polynomials $\cos(\ell\omega t), \sin(\ell\omega t)$ $(\ell = 1, \ldots, r)$ with ω fixed. Such methods depend on a parameter $\widetilde{\omega}$ approximating ω. They are exact when $\widetilde{\omega} = \omega$, but they may be sensitive to an inaccurate estimate of ω. Gautschi (1961) was the first to develop a basic theory for linear multistep methods with modified coefficients depending on $\widetilde{\mu} := \widetilde{\omega}h$. In the limit as $\widetilde{\mu} \to 0$, those methods reduce to the classical Adams and Störmer methods. As an example, the modified two-step explicit Störmer method of classical order $p = 2$ and of trigonometric order $r = 1$ applied to $y'' = g(t, y)$ is given by

$$y_{n+1} - 2y_n + y_{n-1} = h^2 \left(\frac{2\sin(\widetilde{\mu}/2)}{\widetilde{\mu}} \right)^2 g(t_n, y_n).$$

Methods of Nyström and Milne–Simpson type, less sensitive to inaccuracy in estimating ω, can be found in Neta and Ford (1984). Using different techniques from mixed interpolation (De Meyer, Vanthournout and Vanden Berghe 1990), Vanthournout, Vanden Berghe and De Meyer (1990) have constructed methods of Adams, Nyström, and Milne–Simpson type with an elegant derivation of their local truncation error. More general, and requiring more parameters, is the exact integration of products of ordinary polynomials and trigonometric functions with multiple frequencies given in Stiefel and Bettis (1969) and Bettis (1970), where methods of Störmer type are constructed. This was motivated from applications in celestial mechanics to take into account secular effects of orbit motion. Still in the same framework, the *minimax* methods of multistep type proposed by Van Der Houwen and Sommeijer (1984) attempt to minimize the local truncation error over a given interval of frequencies $[\omega_{\min}, \omega_{\max}]$. Such methods are less sensitive to inaccurate prediction of the frequencies. However, as for all methods mentioned in this paragraph, the presence of perturbations superimposed on the oscillations generally decreases dramatically the performance of these methods. Using an approach based on the 'principle of coherence' of Hersch (1958), numerical methods of multistep type for nearly linear ODEs are proposed in Denk (1993) and (1994), but they require the exact computation of the matrix exponential.

For certain problems with slow and fast components, *multirate methods* may be applied to reduce the total computational effort. A first method is used with one *macrostep* H to integrate the slow components and a second method is applied N times with a *microstep* h ($H = Nh$ to ensure synchronization) to integrate the fast components. The main difficulty with multirate methods is the assumption, before performing a macrostep, that the splitting between slow and fast components is known. In a counterintuitive but

justified 'slowest first strategy' (Gear and Wells 1984), the slow components are integrated first using extrapolated values for the fast components and then the fast components are integrated using interpolated values for the slow components. Multirate Rosenbrock–Wanner (MROW) methods are analysed in detail in Günther and Rentrop (1993*a*) and (1993*b*). They have constructed a four-stage A-stable method of order three with a second-order embedded formula for error estimation. Their partitioning strategy is based on the stepsizes predicted for each component. In highly integrated electrical circuits applications, where most of the elements at any given time are inactive, they also make use of some information about the neighbourhood of the active elements to improve the performance of the partitioning strategy. A multirate extrapolation method based on the explicit Euler method has been developed by Engstler and Lubich (1995). An inexpensive partitioning strategy is implemented, which consists of stopping to build the extrapolation tableau for the components recognized as sufficiently accurate. Closely related to multirate methods are *multiple time-stepping* (MTS) methods. The right-hand side of the ODE is split as a sum of fast and slowly varying functions which are evaluated at different rates (see Subsection 4.5).

In the next sections we will deal with different classes of problems exhibiting oscillatory behaviour. For each class of problems we will discuss the structure of the equations, the objectives of the numerical simulation, the computational challenges, and some numerical methods that may be appropriate.

3. Mechanical systems

3.1. Multibody systems

The governing equations of motion of a mechanical system of stiff or highly oscillatory force devices may be written as a system of DAEs (Brenan, Campbell and Petzold 1995)

$$M(q)q'' + G^T(q)\lambda - (f^s(q', q, t) + f^n(q', q, t)) = 0, \quad (3.1a)$$

$$g(q) = 0, \quad (3.1b)$$

where $q = (q_1, \ldots, q_n)^T$ are the generalized coordinates, $q' = dq/dt$ the generalized velocities, $q'' = d^2q/dt^2$ the generalized accelerations, $\lambda = (\lambda_1, \ldots, \lambda_m)^T$ the Lagrange multipliers, M is the mass-inertia matrix, $g = (g_1, \ldots, g_m)^T$ the holonomic constraints, and $G = \partial g/\partial q$. The *stiff* or *oscillatory force* is $f^s = \sum_i^{n_f} f_i^s$, and f^n includes all the field forces and the external forces which are nonstiff compared to the stiff components, that is,

$$\left\| \frac{\partial f^s}{\partial (q, q')} \right\| \gg \left\| \frac{\partial f^n}{\partial (q, q')} \right\|.$$

The stiff force components in (3.1a) can often be written in the form

$$f_i^s = -B_i(q)\left(K_i\eta_i(q) + C_i\frac{d\eta_i}{dt}\right), \tag{3.2}$$

where η_i is smooth, $i \in \{1,\ldots,n_f\}$, $B_i = (\partial\eta_i/\partial q)^T$, and K_i, C_i are the associated stiffness and damping matrices. For some generalized coordinate sets, the functions η_i may be linear, or even the identity. When the components of the coefficient matrices K_i and C_i are large, these force components may cause rapid decay or high frequency oscillation in the solution of (3.1). It is well known that the characteristics of the fast or slow solution are determined not only by the modelling aspects, for example the coefficients of the stiffness and damping matrices, but also by the initial conditions and events that may excite stiff components in the system during the simulation.

To demonstrate some of the potential difficulties caused by highly oscillatory forces in mechanical systems, we consider two common oscillatory forces: a spring force (which is exemplified by the stiff spring pendulum of Section 1), and a 2D *bushing* force. The former is a very simple example of a type of system often seen in molecular dynamics (see Section 4), and the latter is a general form of modelling force devices in multibody mechanical systems.

Spring force

The stiff spring pendulum of Section 1 is an example of a point-mass connected to a stiff spring force. The equations of motion of the particle in Cartesian coordinates are given by (1.1), where the spring force is given by $(x\lambda, y\lambda)^T$. This problem is highly nonlinear, due to (1.1e). Since most of the mathematical methods for oscillatory problems assume a nearly linear form of the problem, and many numerical techniques are implicitly based on linearization, we will begin by examining the structure of the local linearized system. The eigenvalues of the *underlying ODE* of (1.1), that is, substituting (1.1e) into (1.1c, 1.1d), are illustrated for $\epsilon = \sqrt{10^{-3}}$ in Fig. 3. The dominant eigenvalues are $\pm\mathrm{i}/\epsilon$. As $\epsilon \to 0$, the dominant pair of eigenvalues approaches $\pm\infty$ along the imaginary axis. The other pair of eigenvalues oscillates on the complex plane, with amplitude and frequency approaching $\pm\infty$. The amplitude of the oscillations in the eigenvalues depends on the initial conditions for the problem. If the initial conditions are on the slow solution, then the amplitude is zero. In Fig. 3, we have chosen the initial conditions to be slightly off the slow solution, which is the situation for most numerical methods. From this we can see that methods based on linearization are likely to fail for this problem unless the stepsizes are very small or the linearization is performed exactly on the slow solution.

In Section 1, we showed that a slow solution for this problem could be identified by shifting to polar coordinates. One might guess that perhaps

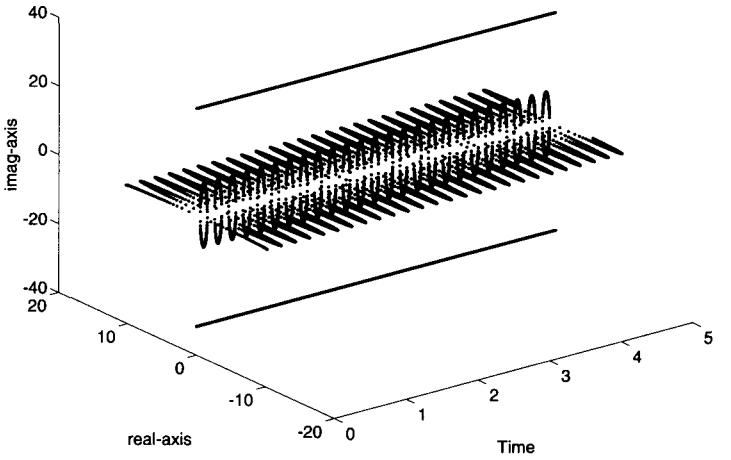

Fig. 3. Eigenvalues of stiff spring pendulum in Cartesian coordinates, $\epsilon = 10^{-1.5}$

the oscillation in the eigenvalues described above is due to the choice of the Cartesian coordinate system, which is unnatural for this problem. This is true, but only partly so. The eigenvalues along the solution trajectory in polar coordinates are shown in Fig. 4. The dominant eigenvalues are of the same magnitude as those in (1.1); see Fig. 3. This is because the coordinate transformation is linear with respect to the fast moving r. The oscillation of the other pair of eigenvalues along the real axis persists.

Bushing force

Nonlinear oscillations in general multibody systems are often generated by forces from components such as bushings. This type of component is used in modelling vehicle suspension systems. Unlike the spring, this element is usually an *anisotropic* force, that is, it has different spring coefficients along the principle axes of the bushing local coordinate frame. The bushing force between *body-i* and *body-j* may be defined using the relative displacement d_{ij}, its time derivative d'_{ij}, and the relative angle θ_{ij} and its time derivative θ'_{ij} of two body-fixed local coordinate frames at the bushing location on two bodies. Using the vectors s_i and s_j representing the bushing location in *body-i*'s and *body-j*'s centroid local coordinate systems, respectively, we have

$$d_{ij} = \begin{pmatrix} x_i \\ y_i \end{pmatrix} - \begin{pmatrix} x_j \\ y_j \end{pmatrix} + A_i s_i - A_j s_j,$$

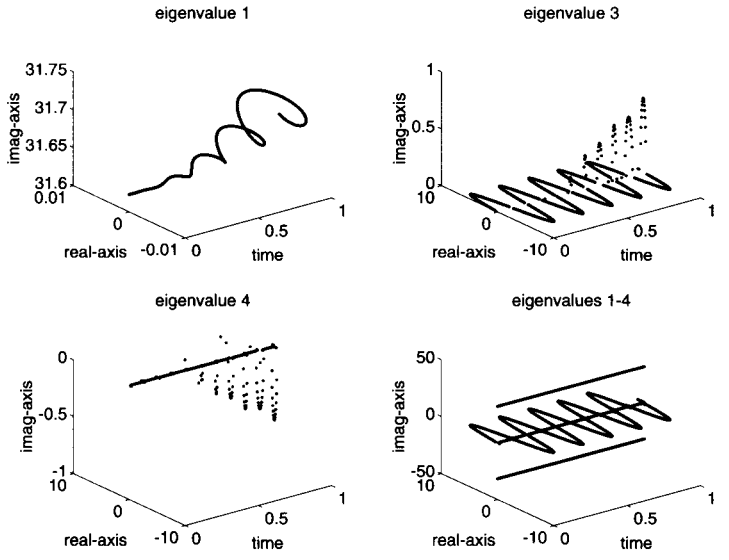

Fig. 4. Eigenvalues of stiff spring pendulum in polar coordinates, $\epsilon = 10^{-1.5}$

where the orientation transformation matrices A_k are

$$A_k = A(\theta_k) = \begin{pmatrix} \cos(\theta_k) & -\sin(\theta_k) \\ \sin(\theta_k) & \cos(\theta_k) \end{pmatrix},$$

and (x_k, y_k, θ_k) are coordinates at body-fixed frames. The bushing force f_b can then be written as

$$f_b = \begin{pmatrix} f_b^x \\ f_b^y \end{pmatrix} = A_i \begin{pmatrix} k^x & 0 \\ 0 & k^y \end{pmatrix} A_i^T d_{ij} + A_i \begin{pmatrix} c^x & 0 \\ 0 & c^y \end{pmatrix} A_i^T d'_{ij},$$

and the applied torque is

$$\tau_b = k^\theta \theta_{ij} + c^\theta \frac{d\theta_{ij}}{dt},$$

where k^x, k^y, and k^θ are the spring coefficients associated with the x, y, and θ coordinates, and c^x, c^y, and c^θ are the corresponding damping coefficients.

An example of a simple mechanical system incorporating this force may be obtained from this model using unit mass-inertia and gravity, and setting the bushing location on the body to $s = (-1/2, 0)$. A bushing element with no damping, attached at the global position of $(1/2, 0)$, yields

$$0 = x'' - k^x \left(\frac{1}{2} - x + \frac{\cos(\theta)}{2} \right), \tag{3.3a}$$

$$0 = y'' + k^y \left(y - \frac{\sin(\theta)}{2} \right) + 1, \tag{3.3b}$$

$$0 = \theta'' + k^\theta \theta - \frac{\sin(\theta)}{2} k^x \left(\frac{1}{2} - x + \frac{\cos(\theta)}{2} \right) - \frac{\cos(\theta)}{2} k^y \left(y - \frac{\sin(\theta)}{2} \right). \quad (3.3c)$$

It can be seen from (3.3) that the local eigenstructure of the system may change rapidly, depending on the size of the stiffness coefficients. Using the initial values $(x, y, \theta) = (1.1, 0.1, 0.0)$ with $(k^x, k^y, k^\theta) = (10^4, 10^4, 10^3)$, the solution of (3.3) exhibits high-frequency oscillations in all variables, as shown in Fig. 5. Solving the eigenvalue problem of (3.3) at each time-step yields three pairs of eigenvalues as illustrated in Fig. 6.

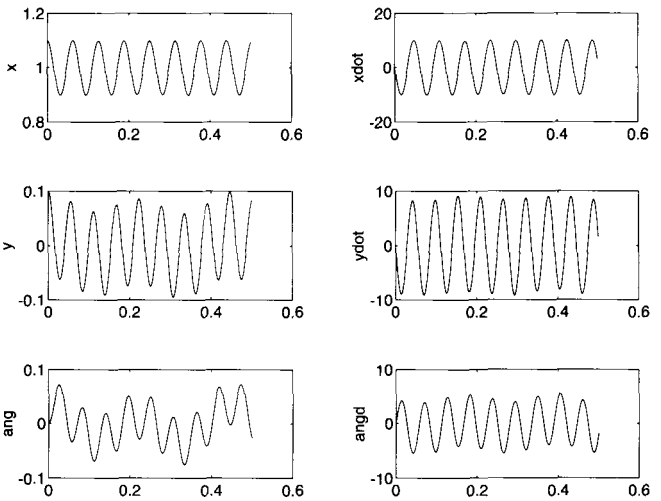

Fig. 5. Bushing problem in Cartesian coordinates

Structure of limiting DAE

Another source of difficulties for the numerical solution arises from the structure of stiff multibody systems. These systems are *singular singular perturbation problems* (O'Malley 1991). In the limit as the fast timescale tends to infinity, the system becomes a *high-index DAE*. For example, as $\epsilon \to 0$ in the stiff spring pendulum problem (1.1) or (1.2), the equations become those of a rigid pendulum. This index-3 DAE has a *Hessenberg structure*. Numerical solution of high-index DAE systems of Hessenberg structure has been extensively studied (Brenan et al. 1995, Hairer, Lubich and Roche 1989, Hairer and Wanner 1996). There are well-known difficulties with numerical accuracy, matrix conditioning, error control, and stepsize selection. Roughly speaking, the higher the index of a DAE, the more difficulties for its numerical solution. Hence, it is not surprising that there would be difficulties for the numerical solution of highly oscillatory mechanical systems.

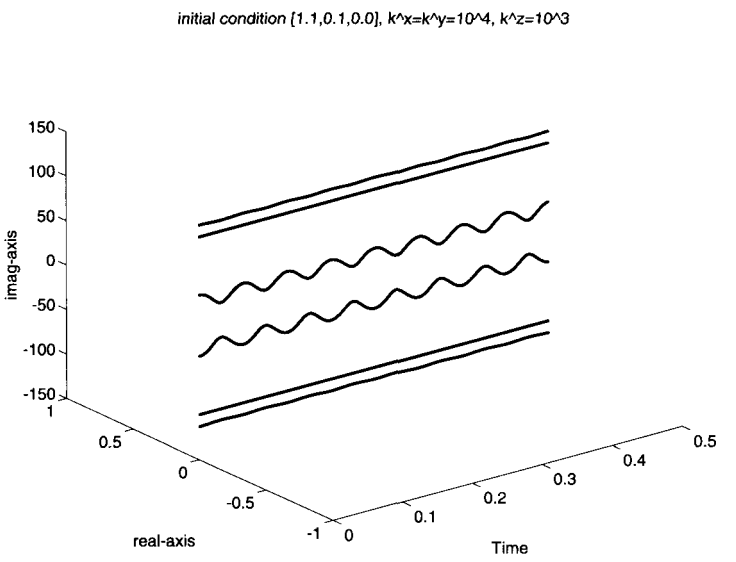

Fig. 6. Eigenvalues of bushing problem

3.2. Finding the slow solution

Given the situation of a rapidly changing local eigenstructure, perhaps the simplest strategy for numerical solution is to consider damping the oscillation, when it is of sufficiently small amplitude, via highly stable implicit numerical methods. First, we want to emphasize that damping the oscillation for general nonlinear systems is not safe and can easily lead to an erroneous solution! However, the system may have a very special structure such that this approach is appropriate.

Lubich (1993) has shown that the numerical solution of stiff spring mechanical systems of a strong potential energy (for instance, a stiff spring force such as in (1.1)) by a class of implicit Runge–Kutta methods with stepsize independent of the parameter ϵ, converges to the slowly varying part of the solution. These results have been extended to a class of multistep Runge–Kutta methods (Schneider 1995). Unfortunately, it is not clear that these results may apply directly to all the types of oscillatory components in multibody systems. As indicated in Lubich (1993), the representation of stiff or oscillatory components in an appropriate coordinate system is not always possible, that is, the constraints associated with the stiff or oscillatory potential force can be difficult to obtain in general. Nevertheless, for (3.1), an approximation of the dynamics of such local coordinates can be obtained for oscillatory force components of the form (3.2).

The amount of damping in a highly stable implicit method is controlled by the stepsize; for the types of methods that one would consider using

for this purpose, the damping increases with the stepsize. One might hope that the automatic stepsize selection mechanisms used in variable-stepsize ODE/DAE codes would increase the stepsize whenever the magnitude of the oscillation is small compared with the local error tolerances. This works well, but only if the usual error control strategy is changed to one that is appropriate for the limiting high-index DAE.

There are also difficulties with Newton convergence for implicit numerical methods applied to highly oscillatory nonlinear mechanical systems (Lubich 1993, Yen and Petzold 1997). The Newton iteration at each time-step does not converge for large (relative to the period of the high-frequency oscillation) stepsizes. The problem is due to the linearization on which Newton's method is based. With the eigenstructure of the local Jacobian matrix changing so rapidly, Newton's method does not yield good directions to the slow solution unless the initial guess (prediction) is extremely accurate; such an accurate initial guess can only be attained by using very small stepsizes. Some variables can be predicted more accurately than others. Variables that play the role of Lagrange multipliers in (3.1) are not predicted well by polynomial extrapolation, which is used in many ODE/DAE codes. This is not surprising: these variables depend directly on the second derivatives of the highly oscillatory position variables.

Yen and Petzold (1997) have recently proposed a *coordinate-split* formulation of the equations of motion which eliminates difficulties due to obtaining an accurate predictor for the Lagrange multiplier variables, because these variables are no longer present in the computation. These methods are particularly effective for oscillatory multibody systems with components such as the stiff bushing. The coordinate-split formulation is described as follows. Direct numerical integration of the index-3 DAE (3.1) suffers from the well-known difficulties inherent in the solution of high-index DAEs. One way to lower the index involves introducing derivatives of the constraint $g(q)$, along with additional Lagrange multipliers μ. This yields the *stabilized index-2* or *GGL* formulation of the constrained equations of motion (Gear, Gupta and Leimkuhler 1985)

$$\begin{aligned} q' - v + G^T(q)\mu &= 0, && \text{(3.4a)} \\ M(q)v' + G^T(q)\lambda - f(v,q,t) &= 0, && \text{(3.4b)} \\ G(q)v &= 0, && \text{(3.4c)} \\ g(q) &= 0, && \text{(3.4d)} \end{aligned}$$

where $v = q'$ and $f = f^s + f^n$, which has been used widely in simulation. The Lagrange multiplier variables λ and μ fulfil the role of projecting the solution onto the *position* (3.4d) and the *velocity* (3.4c) constraints, respectively. Many of the numerical methods for multibody systems solve the system (3.4) directly. It is also possible to eliminate the Lagrange multipliers and

reduce the size of the system to the number of degrees of freedom. One way to accomplish this begins with the stabilized index-2 system (3.4). Suppose that $G(p)$ is full-rank on the constraint manifold $\mathcal{M} = \{q \in \mathbb{R}^n : g(q) = 0\}$. Then one can find an annihilation matrix $P(q) \in \mathbb{R}^{(n-m)\times n}$ such that $P(q)G^T(q) = 0$, for all $q \in \mathcal{M}$. Premultiplying (3.4a) and (3.4b) by $P(q)$ yields an index-1 DAE

$$\begin{aligned} P(q)\,(q' - v) &= 0, && \text{(3.5a)} \\ P(q)\,(M(q)v' - f(v,q,t)) &= 0, && \text{(3.5b)} \\ G(q)v &= 0, && \text{(3.5c)} \\ g(q) &= 0. && \text{(3.5d)} \end{aligned}$$

An important practical consequence of (3.5) is that (μ, λ) have been eliminated from the DAE, via multiplication of (3.4a, 3.4b) by the nonlinear $P(q)$. Thus, the error test and the Newton iteration convergence test in a numerical implementation of (3.5) no longer need to include the problematic Lagrange multipliers (μ, λ).

The coordinate-split method gives an inexpensive way to find $P(q)$ via a splitting of the Cartesian basis (Yen and Petzold 1996). Discretizing the coordinate-split formulation by an implicit method like BDF or an implicit Runge–Kutta method, it seems at first glance that the local Jacobian matrix might be difficult to compute, because it involves derivatives of $P(q)$. However, this is easily overcome by using the formulæ for the derivative of a projector given by Golub and Pereyra (1973) and the resulting method lends itself to efficient implementation.

The performance of damped numerical methods for highly oscillatory mechanical systems is improved by using the coordinate-split formulation. However, for problems with very high-frequency oscillations, there are still difficulties for Newton convergence. To obtain rates of convergence which are independent of the frequency of the oscillation, Yen and Petzold (1997) have introduced a modification to the Newton iteration, that is, the *modified coordinate-split (CM)-iteration.* The basic idea of the CM-iteration is that there are terms in the Jacobian which involve derivatives of the projection onto the constraint manifold. These terms are large and complicated to compute, but small on the slow solution. For example, applying a (low-order) BDF formula to (3.5) yields the nonlinear system

$$\begin{aligned} P(q_n)h(\rho_h q_n - v_n) &= 0, && \text{(3.6a)} \\ P(q_n)h(M(q_n)\rho_h v_n - f(v_n, q_n, t_n)) &= 0, && \text{(3.6b)} \\ G(q_n)v_n &= 0, && \text{(3.6c)} \\ g(q_n) &= 0, && \text{(3.6d)} \end{aligned}$$

where ρ_h is the discretization operator, and h is the stepsize of the time

discretization. Given an initial prediction $(q_n^{(0)}, v_n^{(0)})$, applying Newton-type methods to (3.6) requires the solution of a linear system

$$J(q_n, v_n)(\Delta q_n, \Delta v_n) = -r(q_n, v_n)$$

such that Δq_n and Δv_n are the increments of q_n and v_n,

$$J(q_n, v_n) = \begin{pmatrix} P(q_n)[(\frac{dG^T(q_n)}{dq_n})s_1 + h\frac{\partial \rho_h q_n}{\partial q_n}] & -hP(q_n) \\ P(q_n)[(\frac{dG^T(q_n)}{dq_n})s_2 + \frac{dr_2(q_n,v_n)}{dq_n}] & P(q_n)\frac{\partial r_2(q_n,v_n)}{\partial v_n} \\ \frac{\partial (G(q_n)v_n)}{\partial q_n} & G(q_n) \\ G(q_n) & 0 \end{pmatrix},$$

and

$$r(q_n, v_n) = (P(q_n)r_1(q_n, v_n), P(q_n)r_2(q_n, v_n), G(q_n)v_n, g(q_n)),$$

where $s_1 = -(GY)^{-T}Y^T r_1$, $s_2 = -(GY)^{-T}Y^T r_2$, $r_1 = h(\rho_h q_n - v_n)$, and $r_2 = h(M(q_n)\rho_h v_n - f(v_n, q_n, t_n))$. The terms which cause the Newton convergence problem are those involving s_1 and s_2. Away from the slow solution, small perturbations in the positions can result in large changes in these terms, leading to convergence difficulties for the Newton iteration. The CM-iteration sets these terms to zero, yielding a reliable direction towards the slow solution for the Newton-type iteration. Convergence results for the CM-iteration are given in Yen and Petzold (1997). For nonoscillatory mechanical systems, the convergence behaviour of the CM-modification is similar to that of standard Newton.

For nonlinear mechanical systems with small-amplitude, high-frequency oscillations, the CS formulation combined with a highly stable implicit method to damp the oscillations and the CM-modification to the Newton iteration can be highly effective. A two-body pendulum problem in 2D Cartesian coordinates, with a bushing force, as given in Subsection 3.1, which is the source of the high-frequency oscillation, is described in Yen and Petzold (1997). In experiments at very high frequencies using the BDF code DASSL (Brenan et al. 1995) with the method order restricted to two, the CS formulation is solved twice as efficiently as the GGL formulation (3.4). The CM modification to the Newton iteration further improves the efficiency by a factor of more than a hundred. At lower frequencies, of course, the comparison is less dramatic.

An alternative to numerical methods that use damping to find the slow solution is to approximate the slow solution directly. Reich (1995) has extended the *principle of slow manifold*, which has been widely used in the approximation of multiple timescale systems (Fenichel 1979, Kopell 1985), to the DAEs of multibody systems with highly oscillatory force terms. Algebraic constraints corresponding to the slow motion were introduced with

a relaxation parameter to preserve the slow solution, while adding flexibility to it in the slow manifold approach.

3.3. Flexible multibody mechanical systems

The numerical solution of flexible multibody systems is required for nonlinear dynamic analysis of articulated structures. The need for modelling deformable bodies has been kindled by the dynamic simulation of physically large and massive mechanisms, such as aeroplanes, industrial robots and automobiles. These are structures in which kinematic connections permit large relative motion between components that undergo small elastic deformation. A source of difficulty in the solution of flexible multibody equations of motion is the coupling between the elastodynamic equations and the gross motion. The methods for analysing flexible mechanisms can generally be divided into two categories:

(i) methods that focus on the structure, while using the gross multibody motion as a source of dynamic loading
(ii) methods that incorporate flexibility effects into the multibody dynamic analysis.

Simulation of flexible multibody systems has been an active research topic for the last two decades. Many of the methods for flexible multibody systems have been implemented in multibody dynamic analysis codes (Haug 1989, Nikravesh 1988, Pereira and Ambrósio 1993). For such systems, an important feature of the solution is the nonlinear oscillations induced by the elastodynamics equations. Moreover, since the governing equations of flexible multibody systems are often modelled using algebraic constraints, the numerical solution of DAEs is required. As discussed in the two previous subsections, the numerical solution of the resulting highly oscillatory DAEs presents many challenging problems.

Modelling of flexibility effects in multibody systems can significantly alter the dimension and solutions of the governing equations of motion. It is well documented that adding flexible components to rigid body models can drastically increase the computational complexity. For instance, a typical rigid-body model of a ground vehicle, such as a passenger car, may consist of several rigid bodies of 10–100 coordinates. Replacing the chassis of the car with its flexible model can increase the number of coordinates to millions. Compounding the difficulty of an increased dimension are the high-frequency oscillations that arise from the modal stiffness and damping coefficients. They represent both the physical and geometrical approximations of the elastic, plastic, and viscoelastic effects of the flexible bodies, and their eigenvalues are usually of magnitudes greater than those of the gross motion. It has been shown for some flexible multibody systems that

the coupling of unresolved high frequencies to the rigid motion may result in a nonlinear instability. In Simo, Tarnow and Doblare (1993), the numerical simulation of a flexible rod illustrates the nonlinear instability in Hamiltonian systems. For nonconservative flexible mechanisms, such problems can be found in the approximation of the deformation of elastic bodies in constrained multibody systems (Yoo and Haug 1986, Yen, Petzold and Raha 1996). Special care must be taken to maintain the stability of the oscillatory components in the solution. In the following, we give an overview of the numerical techniques used for handling oscillations in flexible multibody systems. We begin with a summary of computational methods used in structural dynamics.

3.4. Modal analysis of structures

Applying spatial discretization to the elastomechanical PDE, the dynamic equations of the response of a discrete structural model are given by

$$M^e u'' + C^e u' + K^e u = f(t), \tag{3.7}$$

where u is the nodal displacement, $f(t)$ is the load, and M^e, C^e, and K^e are constant mass, damping, and stiffness matrices of the node coordinates, respectively. Numerical methods have been developed based on spectral decomposition of this linear ODE system. Rewriting (3.7) as a first-order ODE, we obtain

$$\begin{pmatrix} 0 & M^e \\ M^e & C^e \end{pmatrix} \frac{\mathrm{d}}{\mathrm{d}t} \begin{pmatrix} u' \\ u \end{pmatrix} + \begin{pmatrix} -M^e & 0 \\ 0 & K^e \end{pmatrix} \begin{pmatrix} u' \\ u \end{pmatrix} = \begin{pmatrix} 0 \\ f(t) \end{pmatrix}. \tag{3.8}$$

Denoting $z = (u', u)^T$, the solution of (3.8) can be written explicitly,

$$z = e^{-tA} z_0 + F(t), \tag{3.9}$$

where z_0 and $F(t)$ are two vectors that depend on the initial values and loading function, and

$$A = \begin{pmatrix} 0 & M^e \\ M^e & C^e \end{pmatrix}^{-1} \begin{pmatrix} -M^e & 0 \\ 0 & K^e \end{pmatrix}.$$

Using (3.9), numerical solution techniques for (3.7) can be unified in the framework of approximating the exponential of the matrix A times a vector.

A straightforward approach for dealing with the high frequencies in (3.7) is to truncate the higher *eigenmodes*, which were obtained from the *generalized eigenvalue problem* of the matrix $K^e - \omega^2 M^e$ (Bathé and Wilson 1976, Craig and Bampton 1968). For most structures the eigenvectors, or *normal modes* ϕ_i, span the nodal coordinate space, and form the coordinate transformation, for instance the *modal matrix*, from the nodal coordinates u to the modal

coordinates η,

$$u = \sum_{i=1}^{N} \phi_i \eta_i = \Phi \eta. \tag{3.10}$$

Note that the nodal and modal coordinates in (3.10) are those corresponding to the undamped system of (3.7).

To approximate the harmonic frequencies of (3.7) with fewer modes, one can apply the *Rayleigh–Ritz method* to the undamped system, employing the *Rayleigh quotient* and *Ritz vectors* (Bathé and Wilson 1976). In contrast to the *mode-superposition method*, which requires all the natural frequencies (eigenvalues) and modes (eigenvectors) to satisfy

$$(K^e - \omega_i^2 M^e)\phi_i = 0, \quad for\ i = 1, 2, \ldots, N,$$

the Rayleigh–Ritz method allows the use of a few *shape vectors* (Ritz vectors) to approximate the solution of (3.7). For some classes of problems, the Rayleigh–Ritz method is more efficient than eigenvector mode superposition methods for computing the dynamic response of (3.7). Efficient numerical procedures have been developed for determining a set of lowest orthonormalized Ritz vectors (Chen and Taylor 1989, Wilson, Yuan and Dickens 1982). For flexible multibody simulation, the oscillatory solution can be eliminated by removing the high modes, provided that the reduced structural model is consistent. More precisely, the deformations at the locations of kinematic joint and force attachment nodes must be taken into account for some proper mode shapes, for instance *constraint* or *attachment* modes (Craig 1981).

For damped systems, the aforementioned methods assume proportional damping or, more generally, modal damping of (3.7) (*i.e.*, that the damping matrix satisfies $\phi_i^T C^e \phi_j = 0, i \neq j$) for lack of a more realistic representation in many of the structural models. This approach may be too simplistic to be effective in some applications. A general approach to the numerical solution of (3.7) solves the generalized *unsymmetric eigenvalue problem* (Lanczos 1950), where the equations of dynamic equilibrium are first transformed into a first-order system (3.8) (Nour-Omid and Clough 1984). The development of numerical solution techniques for this problem has been one of the most active research topics in iterative solution of linear systems (Freund, Golub and Nachtigal 1992). Some efficient numerical methods developed in recent years are based on *Krylov subspace* approximations to (3.9) (Friesner, Tuckerman, Dornblaser and Russo 1989, Gallopoulos and Saad 1992). Such Krylov subspace approximations have been used in structural dynamics (Nour-Omid and Clough 1984) and chemical physics (Park and Light 1986). A recent study (Hochbruck, Lubich and Selhofer 1995) indicated that a class of *exponential integrators* has favourable properties in the numerical integration of large oscillatory systems. What remains to be seen is

an effective application of these exponential integrators for simulating large *flexible* mechanisms.

Another approach to incorporating flexible components in multibody dynamics is to use *nonlinear beam theory*, which applies finite element approximation to the forces resulting from body deformation (Hughes 1987, Simo and Vu-Quoc 1986, Cardona and Géradin 1993). An appropriate nonlinear beam formalism requires in many cases incorporating geometric nonlinear effects such as *geometric stiffening*, which contribute inertia forces to the global motion. The approximation of the inertia force due to geometric nonlinearity usually depends on the nodal position and velocity, for instance, the damping and stiffness matrices of (3.7) become nonconstant. In some cases, these nonlinear forces introduce additional oscillations, which can hinder efficient numerical solution of flexible multibody systems (Simeon 1996).

3.5. Numerical integration methods

Time integration algorithms for solving structural dynamics problems have been developed since the late 1950s (Newmark 1959). General requirements and the foundations of these methods have been well documented (Bathé and Wilson 1976, Chung and Hulbert 1993, Hilber, Hughes and Taylor 1977, Hoff and Pahl 1988, Wood, Bossak and Zienkiewicz 1980). Although their main application area is to linear structural dynamics, these methods can be directly applied to initial value problems of nonlinear second-order ODEs

$$q'' = f(q', q, t). \tag{3.11}$$

Accuracy and stability analysis hold for the numerical methods, provided the discretized nonlinear equations have been solved accurately, that is, within a small enough tolerance. For example, the HHT-α method (Hilber et al. 1977) for (3.11) is given by

$$a_{n+1} = (1+\alpha)f_{n+1} - \alpha f_n, \tag{3.12a}$$

$$q_{n+1} = q_n + hv_n + h^2((\frac{1}{2} - \beta)a_n + \beta a_{n+1}), \tag{3.12b}$$

$$v_{n+1} = v_n + h((1-\gamma)a_n + \gamma a_{n+1}), \tag{3.12c}$$

where h is the stepsize, $\alpha \in [-1/3, 0]$, $\beta = (1-\alpha)^2/4$, and $\gamma = 1/2 - \alpha$. It is well known that the HHT-α family is second-order accurate and A-stable. Numerical damping is maximum for $\alpha = -0.3$, and zero for $\alpha = 0$. Controllable numerical damping and unconditional stability are needed to deal with the high-frequency modes which often result from standard finite element spatial discretization. For nonlinear oscillations, these properties are also required in the solution of flexible multibody systems. Rather than using *ad hoc* mode-selection processes, this approach is desirable because

the elimination of higher frequencies is controlled by selection of the method parameters.

Recent work has dealt with extending these types of methods to treat flexible multibody systems (Cardona and Géradin 1989, Yen et al. 1996). The basic form of constrained multibody equations of motion is given by (3.1), which is a DAE of index-3. Due to the problems of numerical instability in solving index-3 DAEs, most of the solution techniques for (3.1) have been developed using differentiation of the constraints (3.1b). Assuming that M is invertible, direct application of (3.12) to the *underlying ODE* of (3.1) (Führer and Leimkuhler 1991), for instance,

$$q'' = \phi(q', q, t) = M^{-1}(q)(f(q', q, t) - G^T(q)\lambda), \tag{3.13}$$

where

$$\lambda = (GM^{-1}G^T)^{-1}\left(GM^{-1}f + \frac{\partial Gq'}{\partial q}q'\right),$$

can be carried out. However, the numerical solution will not generally preserve the constraint (3.1b) and its derivative. To enforce the constraints, the numerical solution should be projected onto the constraint manifold. Applying the method of Lagrange multipliers to combine the projection with the solution of (3.13), which has been discretized using (3.12), leads to the *DAE α-method* (Yen et al. 1996)

$$\begin{aligned}
M_{n+1}(q_{n+1} - \hat{q}_n) - \hat{\beta}h^2 f_{n+1} + G_{n+1}^T \nu_{n+1} &= 0, && \text{(3.14a)}\\
M_{n+1}(v_{n+1} - \hat{v}_n) - \hat{\gamma}h f_{n+1} + G_{n+1}^T \mu_{n+1} &= 0, && \text{(3.14b)}\\
G_{n+1}v_{n+1} &= 0, && \text{(3.14c)}\\
g(q_{n+1}) &= 0, && \text{(3.14d)}
\end{aligned}$$

where $\hat{\beta} = \beta(1+\alpha)$, $\hat{\gamma} = \gamma(1+\alpha)$,

$$\begin{aligned}
\hat{q}_n &= q_n + hv_n + h^2\left(\left(\frac{1}{2} - \beta\right)a_n - \beta\alpha\phi_n\right),\\
\hat{v}_n &= v_n + h\left((1-\gamma)a_n - \gamma\alpha\phi_n\right),
\end{aligned}$$

$\phi_n = M_n^{-1}(f_n - G_n^T\lambda_n)$, $a_0 = \phi_0$ and $a_n = (1+\alpha)\phi_n + \alpha\phi_{n-1}$ for $n \geq 1$. The *algebraic* variables ν_{n+1} and μ_{n+1} in (3.14) comprise $h^2\hat{\beta}\lambda_{n+1}$ and the corresponding *correction* terms, which project the position and velocity variables onto the constraint manifold. A convergence analysis of (3.14) was given by Yen et al. (1996).

The DAE α-methods are most effective when combined with the CS formulation and CM iteration described earlier. In the Lagrange multipliers formulation there may be convergence difficulties with the Newton iteration. Premultiplying (3.14a) and (3.14b) by the CS matrix $P(q)$ yields

$$P(q_{n+1})(M_{n+1}(q_{n+1} - \hat{q}_n) - \hat{\beta}h^2 f_{n+1}) = 0, \tag{3.15a}$$

$$P(q_{n+1})(M_{n+1}(v_{n+1} - \hat{v}_n) - \hat{\gamma} h f_{n+1}) = 0, \quad (3.15b)$$

$$G_{n+1} v_{n+1} = 0, \quad (3.15c)$$

$$g(q_{n+1}) = 0. \quad (3.15d)$$

Accuracy and stability of the α-methods for ODEs are preserved. More importantly, the high-index variables (ν_{n+1}, μ_{n+1}), which exhibit high-frequency oscillations of large amplitudes, are not present in (3.15). Compared to the Lagrangian form (3.14), much improved Newton convergence was observed in a number of flexible multibody simulations (Yen et al. 1996). When applying strong numerical damping to the higher modes, the CM iteration illustrated even better convergence in these examples.

4. Classical molecular dynamics

Classical molecular dynamics (MD) has become an important tool in the study of (bio)molecules, such as nucleic acids, polymers, and proteins (Allen and Tildesley 1987, Board Jr., Kalé, Schulten, Skeel and Schlick 1994, Gerschel 1995). In classical MD, quantum effects are neglected and the motion of the atoms is often described by *Newton's equations*

$$q' = v, \qquad Mv' = -\nabla U(q), \quad (4.1)$$

where the vector q contains the Cartesian coordinates of the atoms, the vector v contains their velocities, M is the diagonal matrix of atomic masses, and $U(q)$ is a semi-empirical potential energy function. Defining the momenta $p := Mv$, these equations form a Hamiltonian system with Hamiltonian $H(q,p) := \frac{1}{2} p^T M^{-1} p + U(q)$. Therefore, the Hamiltonian (the energy) and the symplectic form $dq \wedge dp$ are invariant under the action of the flow (Arnold 1989). More sophisticated dynamics are also often considered in MD simulation. In Langevin dynamics (4.5), stochastic and friction forces are introduced to model additional aspects (see Subsection 4.4). In Nosé dynamics, temperature and pressure constraints are included to treat nonequilibrium situations (Nosé 1984, Hoover 1991).

The potential energy function $U(q)$ is generally given by a repeated sum over the atoms of pairwise potentials modelling interactions of diverse type (Gerschel 1995): electrostatic, dipolar, polar, dispersive, repulsive, etc. These interactions vary with the interatomic distance and have different ranges of influence: localized for the covalent bondings, short-range for the Van der Waals forces, and long-range for the electrostatic forces. They also differ in their strength and timescale, making the dynamics of (bio)molecules very complex, even chaotic. The equations of MD are highly nonlinear and extremely sensitive to perturbations. A perturbation grows roughly by a factor of 10 every picosecond ($= 10^{-12}$[s]). Therefore, due to various sources of approximation and error in MD simulation, it is not reasonable from the

viewpoint of forward error analysis to ask for an accurate representation of the molecular configuration after several picoseconds. The framework of MD is actually statistical mechanics. To emphasize this point, let us mention that the initial velocities of the atoms of a (bio)molecule are usually chosen randomly to follow a Boltzmann–Maxwell distribution. What is actually desired in MD is to generate a statistically acceptable motion or to obtain a good sampling of phase space over sufficiently long periods of time to provide spatial and temporal information; it is not usually necessary to follow an exact trajectory. Monte Carlo simulation, by generating random configurations, is another technique used in the study of molecular systems based on their statistical properties, but this falls outside the scope of this article. For large (bio)molecules, MD simulation is usually preferred.

Conformational changes of a (bio)molecule arise on a continuum from 1[ps] to 10^2[s]. In MD simulation the main difficulty in the integration of the equations is the presence of a spectrum of very high-frequency oscillations of Brownian character. The fastest vibrations are the bond stretchings and the bond-angle bendings which are orders of magnitude stronger than the other interactions. For example a C–H stretch has an oscillation around an equilibrium position of approximate frequency $0.9 \cdot 10^{14}$[Hz] (Streitwieser Jr. and Heathcock 1985). This imposes a severe limit on the stepsize used by standard integration schemes in order to resolve these high-frequency oscillations; for example, a stepsize around 1[fs] ($= 10^{-15}$[s]) is necessary for the widely used Verlet algorithm (4.2). Computing the forces for a large system at each step is computationally expensive. Therefore, with today's computer technology this stepsize constraint limits the horizon of integration to the order of a nanosecond ($= 10^{-9}$[s]), several orders of magnitude less than the biological timescale for which phenomena like protein folding ($\approx 10^{-1}$[s]) take place. Decreasing the ratio of force evaluation per step is therefore a major goal to speed up the integration.

There are three ways of handling the high-frequency components in MD: resolve them, model their effects, or suppress them. Methods combining these different approaches are of course possible. The desire is that the dynamics should be correctly reproduced from the point of view of statistical mechanics. A recent detailed survey on MD integration methods is Schlick, Barth and Mandziuk (1997); other references are Skeel, Biesiadecki and Okunbor (1993) and Leimkuhler, Reich and Skeel (1995). In this section we will briefly present different approaches, stressing some of their strengths and weaknesses.

4.1. The Verlet algorithm

The most commonly used method in MD is the *Verlet algorithm* (Verlet 1967). Using the momenta $p = Mv$, this explicit second-order method

applied to (4.1) can be expressed as follows:

$$\begin{aligned} p_{n+1/2} &= p_n - \frac{h}{2}\nabla U(q_n), \\ q_{n+1} &= q_n + hM^{-1}p_{n+1/2}, \\ p_{n+1} &= p_{n+1/2} - \frac{h}{2}\nabla U(q_{n+1}). \end{aligned} \tag{4.2}$$

Given the inaccuracy of the governing force field, such a low-order integration method is adequate in MD. Besides being relatively easy to program, this method possesses several attractive features. It preserves two important geometric properties of the flow: symplecticness and reversibility under the involution $p \mapsto -p$. For more details about symplectic discretization we refer the reader to Sanz-Serna (1992) and Sanz-Serna and Calvo (1994). The main interest in preserving the symplectic structure of the flow lies in the following result of mixed backward–forward error analysis: for constant stepsizes the numerical solution of a symplectic method can be interpreted over long-time intervals as being exponentially close to the exact solution of a perturbed Hamiltonian system (Hairer 1994, Hairer and Lubich 1997, Reich 1996*a*). This long-time stability property is the main distinction of the Verlet algorithm, compared to nonsymplectic methods used in MD for short-time integration, such as the Beeman algorithm (Beeman 1976). When applied to the harmonic oscillator (2.2), the Verlet algorithm also possesses the largest relative interval of periodicity among explicit RKN methods (Chawla 1985). However, its use with variable stepsizes destroys not only the aforementioned backward–forward error result but also the existence of an interval of periodicity (Skeel 1993). Nevertheless, a strategy has been discovered recently by Hairer (1996) and Reich (1996*a*) combining variable stepsizes with symplectic integration: the symplectic method is simply applied with constant stepsizes to a modified Hamiltonian function $s(q,p)\,(H(q,p) - H(q_0,p_0))$ where the scaling function $s(q,p)$ corresponds to a time-reparametrization of the original Hamiltonian system.

Since the Verlet method is explicit, the stepsize is usually limited to approximately 1[fs], to resolve the high-frequency vibrations. As for other symplectic integrators, resonance phenomena at certain stepsizes have also been observed (Mandziuk and Schlick 1995). At those given stepsizes, large fluctuations of energy or even instability may occur due to repeated sampling of a component at certain points.

4.2. Implicit symplectic methods

To overcome the stability barrier of the explicit Verlet algorithm while preserving its favourable long-time stability property, it is tempting to consider the application of implicit symplectic methods, for instance the implicit mid-

point (IM) rule. Applied to (4.1), one step of IM is given by the solution of a nonlinear system

$$\begin{aligned} q_{n+1} &= q_n + \frac{h}{2}(v_n + v_{n+1}), \\ v_{n+1} &= v_n - hM^{-1}\nabla U\left(\frac{q_n + q_{n+1}}{2}\right). \end{aligned}$$

Having to solve a nonlinear system is the major drawback of implicit methods. Here, the solution can also be seen as a minimum of an optimization problem, for instance, for IM q_{n+1} is a minimum of a 'dynamics function'

$$\Phi(q) := \frac{1}{2}(q - q_n - hv_n)^T M(q - q_n - hv_n) + h^2 U\left(\frac{q + q_n}{2}\right). \tag{4.3}$$

Therefore, optimization techniques can be applied (Schlick and Fogelson 1992).

The IM method is known to be P-stable. However, in the limit of large stepsizes, the high-frequency oscillations are misrepresented by being aliased to one lower frequency. Moreover, as for the Verlet algorithm, instability at certain stepsizes may occur due to numerical resonance. Recently, Ascher and Reich (1997) have shown that, for implicit symmetric schemes applied to highly oscillatory Hamiltonian systems, unless the stepsize is restricted to the order of the square root of the period of the high-frequency oscillation, then even the errors in slowly varying quantities, like energy, can grow undesirably. This error growth is due to the fact that, at large stepsizes, the numerical method fails to accurately represent the time-dependent transformation that decouples the system into a slowly varying and highly oscillatory part (for example, the transformation from Cartesian to polar coordinates in the stiff spring pendulum). In Skeel, Zhang and Schlick (1997), a general one-parameter family of symplectic integrators has been studied in detail, including the explicit Verlet method and several implicit methods: IM, the trapezoidal rule, the Numerov method, and the scheme LIM2 of Zhang and Schlick (1995). Although the interval of periodicity of implicit symplectic methods is larger than that of the Verlet algorithm, implicit methods do not seem competitive in MD. Even when solving the nonlinear equations in parallel by functional iterations, the two-stage implicit Gauss RK method has been found on a standard test problem involving long-range forces to be less efficient than the Verlet algorithm (López-Marcos, Sanz-Serna and Díaz 1995*a*). Implicit symplectic methods are not recommended for resolving high-frequency oscillations efficiently, because of their large overhead for only a modest increase in the allowable stepsize.

4.3. Constrained dynamics and the Rattle algorithm

As mentioned previously, the highest frequencies in MD are due to the bond stretchings and to the bond-angle bendings. The potential due to these bonds can be expressed as follows,

$$U_{\text{bond}}(q) = \frac{1}{2} g^T(q) K g(q), \tag{4.4}$$

where K is a diagonal matrix of large force constants and the vector $g(q)$ contains the stretches $r(q) - \overline{r}$ and the angle bends $\phi(q) - \overline{\phi}$, where $\overline{r}$ and $\overline{\phi}$ are equilibrium values. The potential $U(q)$ can thus be decomposed as $U(q) = V(q) + U_{\text{bond}}(q)$. Introducing the new variable $\lambda := Kg(q)$, we can rewrite the corresponding Hamilton's equations as follows:

$$q' = M^{-1}p, \qquad p' = -\nabla V(q) - G^T(q)\lambda, \qquad K^{-1}\lambda = g(q),$$

where $G(q) := g_q(q)$. If the elements of K are all of the same size and are very large compared to $\|V_{qq}\|$, the last equation can be replaced by holonomic constraints

$$0 = g(q).$$

Mathematical conditions under which this approach is legitimate have been analysed in detail by Bornemann and Schütte (1995*b*). Constraining the bond interactions has the effect of suppressing the presence of the high-frequency oscillations associated with them, hence of allowing an increase in the stepsize at the cost of some added complexity per integration step. We have obtained a system of DAEs of index 3 where λ plays the role of a Lagrange multiplier (Brenan et al. 1995, Hairer and Wanner 1996, Jay 1996). Differentiating the constraint equations twice, we get two additional constraints:

$$\begin{aligned} 0 &= G(q)M^{-1}p, \\ 0 &= G_q(q)\left(M^{-1}p, M^{-1}p\right) - G(q)M^{-1}\left(\nabla V(q) + G^T(q)\lambda\right). \end{aligned}$$

To integrate the above DAE system numerically, a generalization of the Verlet algorithm is given by the *Rattle algorithm* (Andersen 1983)

$$\begin{aligned} p_{n+1/2} &= p_n - \frac{h}{2}\left(\nabla V(q_n) + G^T(q_n)\Lambda_n\right), \\ q_{n+1} &= q_n + hM^{-1}p_{n+1/2}, \\ 0 &= g(q_{n+1}), \\ p_{n+1} &= p_{n+1/2} - \frac{h}{2}\left(\nabla V(q_{n+1}) + G^T(q_{n+1})\lambda_{n+1}\right), \\ 0 &= G(q_{n+1})M^{-1}p_{n+1}. \end{aligned}$$

The computation of the projected value p_{n+1} can actually be avoided by using the relation

$$p_{n+1/2} = p_{n-1/2} - h\left(\nabla V(q_n) + G^T(q_n)\Lambda_n^*\right)$$

which is the basis of the *Shake algorithm* (Ryckaert, Ciccotti and Berendsen 1977). The method is semi-explicit in the sense that it requires only one evaluation of $\nabla V(q)$ per step. The above equations form a nonlinear system for the Lagrange multiplier Λ_n^* which can be solved iteratively. The Shake iterations consist of a combination of Newton and Gauss–Seidel iterations. An overrelaxation procedure that may improve the performance of the Shake iterations by up to a factor two has been advocated in Barth, Kuczera, Leimkuhler and Skeel (1995).

From a physical point of view, constraining a bond corresponds to freezing the interaction. The dynamics of the constrained system is called the *slow dynamics* (Reich 1994). Whereas this approach seems appropriate for bond stretchings, it is inappropriate for bond-angle bendings since the original dynamics is altered (Van Gunsteren and Karplus 1982). The justification in MD for a constrained dynamics borrows arguments from mathematics and statistical mechanics. From a mathematical point of view, one is interested in a running average of the solution

$$\begin{pmatrix} q_\alpha(t) \\ p_\alpha(t) \end{pmatrix} = \frac{1}{\alpha}\int_{-\infty}^{+\infty} \rho\left(\frac{t-s}{\alpha}\right) \cdot \begin{pmatrix} q(t) \\ p(t) \end{pmatrix} \mathrm{d}s$$

for $0 < \alpha \ll 1$ with an appropriate weight function ρ, for example,

$$\rho(x) = \begin{cases} 1 & \text{if } -1/2 \le x \le 1/2, \\ 0 & \text{otherwise.} \end{cases}$$

The goal is to find the dynamics of $(q_{\sqrt{\varepsilon}}(t), p_{\sqrt{\varepsilon}}(t))$ for $\varepsilon \approx \sqrt{\|V_{qq}\| \cdot \|K\|^{-1}}$ called the *smoothed dynamics* (Reich 1995, Schütte 1995) and which generally differs from the slow dynamics. By introduction of an additional soft potential $W(q)$ aimed at correcting the dynamics of the constrained system, the smoothed dynamics can be reestablished. The establishing of the correcting potential has been the subject of recent controversy (Bornemann and Schütte 1995*b*, Bornemann and Schütte 1995*a*, Reich 1996*b*). A standard correction is given by the *Fixman potential* (Fixman 1974)

$$W_F(q) = \frac{k_B T}{2} \log\left(\det\left(G(q)M^{-1}G^T(q)\right)\right),$$

where k_B is the Boltzmann constant and T is the temperature. The computation of the Fixman potential is rather expensive in practice, but it can be simplified by approximating the matrix $G(q)M^{-1}G^T(q)$ by block-diagonal parts (Reich 1997). To improve the correction it has also been proposed to

replace the *hard* constraints $0 = g(q)$ by *soft* constraints (Reich 1995)

$$0 = \tilde{g}(q) = g(q) + K^{-1}\left(G(q)M^{-1}G^T(q)\right)^{-1} G(q)M^{-1}\nabla V(q),$$

restoring some flexibility in the dynamics (Reich 1997). The controversy about the correctness of the Fixman potential seems to be due to the intrusion of physical arguments in its derivation. The principle of *equipartition of energy* of statistical mechanics (Diu, Guthmann, Lederer and Roulet 1989) used to derive the Fixman potential (Fixman 1974, Reich 1995, Reich 1997) is the likely source of the controversy, because of the hypothesis of ergodicity postulated in statistical mechanics.

4.4. Normal-mode techniques in Langevin dynamics

To take into account the effects of a heat bath, of the constant energy transfer between the slow and fast degrees of freedom due to molecular collisions, and of various simplifications in the model, a more realistic dynamics in MD is reflected by the *Langevin dynamics*. The Langevin equations are given by

$$q' = v, \qquad Mv' = -\nabla U(q) - \gamma M v + \zeta(t), \tag{4.5}$$

where γ is a collision frequency (friction) parameter and $\zeta(t)$ is a random force chosen to counterbalance the frictional damping to establish temperature equilibrium. One of the main motivations for the *Langevin/implicit-Euler/normal-mode* (LIN) method of Zhang and Schlick (1993) is to mitigate the undesirable severe high-frequency damping of the implicit Euler method, which may alter the dynamics, while maintaining its ability to take large stepsizes (Peskin and Schlick 1989). In LIN the solution is decomposed into *fast* and *slow* components, that is, $q = q_f + q_s$. A linear approximation to the Langevin equations is used for the fast components

$$q_f' = v_f, \qquad Mv_f' = -\nabla U(q_r) - \overline{H}(q_r)(q_f - q_r) - \gamma M v_f + \zeta(t), \tag{4.6}$$

where q_r is a reference point and $\overline{H}(q_r)$ is a sparse (usually block-diagonal) approximation to $U_{qq}(q_r)$. These equations are solved over a relatively large stepsize, for instance, by using standard *normal-mode techniques*: by diagonalizing the matrix $M^{-1/2}\overline{H}(q_r)M^{-1/2}$, the system (4.6) is rewritten as a set of decoupled equations

$$\tilde{q}' = \tilde{v}, \qquad \tilde{v}' = -D\tilde{q} - \gamma\tilde{v} + \theta(t),$$

where $\tilde{q} = TM^{1/2}(q_f - q_r)$, $\tilde{v} = TM^{1/2}v_f$, $D = TM^{-1/2}\overline{H}(q_r)M^{-1/2}T^{-1}$ is diagonal, and $\theta(t) = TM^{-1/2}(\zeta(t) - \nabla U(q_r))$; these equations can then be solved analytically (Zhang and Schlick 1994). Nevertheless, it has been observed recently in Barth, Mandziuk and Schlick (1997) and Schlick et al. (1997) that the direct numerical integration of (4.6) can in fact be much faster than computing the normal modes, for instance, by application of

the second-order Lobatto IIIA–IIIB PRK method with small inner stepsizes. The above procedure, consisting of computing the fast components, turns out to be a very competitive method in itself, and constitutes the *Langevin/normal* (LN) method. In LIN there is an additional correction step for the slowly varying anharmonic part of the solution

$$q_s' = v_s, \qquad Mv_s' = -\nabla U(q_f + q_s) + \nabla U(q_r) + \overline{H}(q_r)(q_f - q_r) - \gamma M v_s.$$

This system is integrated by the implicit Euler method with one large stepsize h or, equivalently, by minimizing a dynamics function similar to (4.3).

4.5. Multiple time-stepping methods in MD

Since the forces in MD can be decomposed as a sum of *hard* short-range interactions and *soft* long-range interactions on a different time-scale, it is natural to consider the application of *multiple time-stepping* (MTS) methods. The idea is to reduce the overall computational work by evaluating the soft forces less often than the hard forces (Streett, Tildesley and Saville 1978). In (4.1) the potential $U(q)$ is decomposed into hard and soft parts

$$U(q) = U^{\text{hard}}(q) + U^{\text{soft}}(q).$$

The bonded interactions (4.4) enter into the hard part. Moreover, an artificial partitioning of a long-range interaction into one hard and one soft part has been proposed in Skeel and Biesiadecki (1994), for example, an electrostatic interaction $V(r) = C/r$ can be decomposed as

$$V^{\text{soft}}(r) = \begin{cases} C(3r_{\text{cut}}^2 - r^2)/2r_{\text{cut}}^3 & \text{if } r < r_{\text{cut}}, \\ C/r & \text{if } r \geq r_{\text{cut}}, \end{cases}$$

and $V^{\text{hard}}(r) = V(r) - V^{\text{soft}}(r)$ where r_{cut} is a cut-off distance. MTS methods do not generally preserve the symplectic and reversible character of the flow of (4.1). However, the *Verlet-I* algorithm (Grubmüller, Heller, Windemuth and Schulten 1991, Biesiadecki and Skeel 1993) or, equivalently, the *r-RESPA* method (Tuckerman, Berne and Martyna 1992), is an MTS method retaining these properties. One macrostep H of this method can be seen as a composition method: the Verlet algorithm is first applied with stepsize $H/2$ to

$$q' = 0, \qquad Mv' = -\nabla U^{\text{soft}}(q); \tag{4.7}$$

then it is applied N times with a microstep $h = H/N$ to

$$q' = v, \qquad Mv' = -\nabla U^{\text{hard}}(q);$$

finally it is again applied with stepsize $H/2$ to (4.7). Basically, the soft forces are evaluated every macrostep H while the hard forces are evaluated every microstep $h = H/N$. It must be mentioned that resonance and other

problems have been reported (Grubmüller et al. 1991, Biesiadecki and Skeel 1993).

5. Circuit simulation

5.1. Introduction

There are a number of applications where the solution has the property that the fast solution is composed of an oscillation with a single high frequency. In this section we will explore some problems from circuit simulation, and a class of methods based on envelope-following ideas, which exploit this property. These methods are often able to take stepsizes that are much larger than the period of the oscillation. The problem of transient simulation in this case is very closely related to the problem of finding a periodic steady state; we will also discuss how similar ideas have been employed in numerical methods for this problem.

Circuit simulation programs like SPICE (Nagel 1975) often need to employ hundreds of thousands of time-steps to simulate the transient behaviour of clocked analog circuits like switching power converters and phase-locked loops. This is because in circuit simulation the stepsizes must be chosen (for accuracy) to be much smaller than a clock period, but the time interval of interest to a designer can be thousands of clock periods. Circuit designers are typically not interested in the details of the node voltage behaviour in every clock cycle, but instead are interested in the *envelope* of that behaviour. With that in mind, the *quasi-envelope* is defined to be a continuous function derived by the following process. Starting at the initial value or at some other point on the solution, define a discrete sequence of points by sampling the state of the system after every clock period T (see Fig. 7). The quasi-envelope is derived by interpolating that sequence to form a smooth curve. We note that the quasi-envelope is different from the more standard notion of envelope because the quasi-envelope is not unique but instead depends on the initial time used to generate the sequence.

Envelope-following methods are based on the idea that if the sequence of points formed by sampling the state at the beginning of each cycle changes slowly as a function of the cycle number, then the quasi-envelope will vary relatively slowly and we will be able to approximate it using stepsizes which are large relative to the length of a cycle.

Envelope-following methods are closely related to the *stroboscopic method* proposed in 1951 by Minorsky (1974) for the study of differential equations. Numerical methods using the envelope-following idea were first introduced by astronomers in 1957 for calculating the orbits of artificial satellites (Mace and Thomas 1960, Taratynova 1960) and were called *multirevolution methods.* Unlike circuit designers, who are interested in the envelope of the oscillations but not in the details, the astronomers were concerned with com-

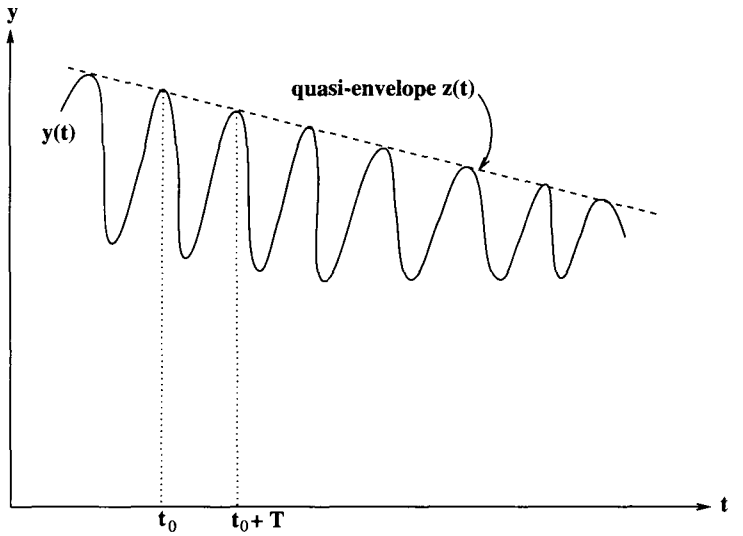

Fig. 7. ODE solution and quasi-envelope

puting future orbits accurately. The multirevolution methods developed in Mace and Thomas (1960), Taratynova (1960) and Graff and Bettis (1975) were generalizations of explicit multistep and Runge–Kutta methods for ODEs to approximately solve the difference equation which generates the sequence of points defining the quasi-envelope. Thus they would always take stepsizes which are multiples of the period of the oscillation. Rather than using an arbitrary starting point to define the quasi-envelope, as above, they used a physical reference point (for example, node, apogee, or perigee). Petzold (1981) extended these methods to more general systems by defining the smooth quasi-envelope as above (independent of any physical reference points), by providing a separate algorithm for finding the period of the oscillation in the fast solution, and by showing how to handle the case of a slowing changing period of the oscillation. Convergence results for envelope-following numerical methods were also given in Petzold (1981). Gear and Gallivan (Gallivan 1980, Gallivan 1983, Gear 1984) explored the design of general ODE codes which incorporate multirevolution techniques and attempt to detect the onset of oscillations. Kirchgraber (1982, 1983) proposed a novel class of methods which synthesize ideas from the method of averaging with envelope-following techniques. White et al. (White and Leeb 1991, Kundert, White and Sangiovanni-Vincentelli 1988*b*, Kundert, White and Sangiovanni-Vincentelli 1988*a*, Telichevesky, Kundert and White 1995, Telichevesky, Kundert and White 1996) applied envelope-following methods to circuit simulation, developing implicit methods which are quite efficient for this application and for finding the periodic steady state.

5.2. Envelope-following methods

Given the initial value problem

$$y' = f(y,t), \quad y(0) = y_0, \quad 0 \le t \le L, \tag{5.1}$$

where $y(t)$ is periodic or nearly periodic with period T, the quasi-envelope $z(t)$ is defined more precisely by

$$z(t+T) = z(t) + Tg(z(t),t), \quad 0 \le t \le L - T, \tag{5.2}$$

where

$$g(z,t) = \frac{1}{T}\big(\tilde{y}(t+T,t) - \tilde{y}(t,t)\big)$$

and

$$\frac{d}{ds}\tilde{y}(t+s,t) = f(\tilde{y}(t+s,t), t+s), \quad \tilde{y}(t,t) = z.$$

It is easy to see that if $z(0) = y(0)$ then $z(KT) = y(KT)$, $0 \le KT \le L$, so that z agrees with y at multiples of the period. Since y is nearly periodic, the values of z at points $\{KT\}$, K an integer, should change slowly. Solving (5.2) exactly amounts to solving the differential equation (5.1) over the entire interval $[0, L]$, because $g(z,t)$ is determined by integrating the differential equation over one period of the oscillation. The basis of envelope-following methods is to compute an approximation to z, that is, to solve the difference equation (5.2) approximately with stepsizes H much larger than T. For some applications, like circuit simulation, it is possible to define a smooth z over the entire interval $[0, L]$. For other applications like orbit calculations, it is best to consider z as a discrete function and to take stepsizes in the approximation method which are multiples of T. We note that the solution to the differential equation can be recovered at any time from the (discrete) quasi-envelope, by solving the original ODE with initial condition on the quasi-envelope for no more than one cycle.

Envelope-following methods that are generalizations of linear multistep methods or Runge–Kutta methods have been derived (Gallivan 1983, Graff and Bettis 1975, Petzold 1981, Taratynova 1960). For example, the 'trapezoidal' envelope-following method is given by

$$z_{n+1} = z_n + \left(\frac{H-T}{2}\right) g(z_{n+1}, t_{n+1}) + \left(\frac{H+T}{2}\right) g(z_n, t_n).$$

We note that the coefficients of these methods reduce to those of standard ODE methods as $T \to 0$, and that the methods are 'exact' (up to errors in solving the original ODE numerically over each individual cycle) when $T = H$. For efficiency, the objective is to be able to take $H \gg T$.

In some applications, the period (cycle length) of the oscillation might also be slowly varying. This is handled in envelope-following methods by

means of a change of independent variable t so that in the new variable $\hat{t}$ the period τ of the oscillation is a constant, that is,

$$t(\hat{t}+\tau) - t(\hat{t}) = T(t(\hat{t})), \quad t(0) = 0.$$

Defining $\hat{y}(\hat{t}) := y(t(\hat{t}))$ and $\hat{z}(\hat{t}) := z(t(\hat{t}))$, the difference equations that define the quasi-envelope in the case of a slowly varying period of the oscillation are given by

$$\begin{aligned} \hat{z}(\hat{t}+\tau) &= \hat{z}(\hat{t}) + \tau \hat{g}(\hat{z}(\hat{t}), \hat{t}). \quad \hat{z}(0) = z(0), \\ t(\hat{t}+\tau) &= t(\hat{t}) + \tau \left(\frac{T(t(\hat{t}))}{\tau} \right), \quad t(0) = 0, \end{aligned}$$

where

$$\hat{g}(\hat{z}, \hat{t}) := \left(\frac{T(t(\hat{t}))}{\tau} \right) g(\hat{z}, t(\hat{t})).$$

The accuracy and stability of these formulæ have been analysed by Petzold (1981).

5.3. Finding the period

In some applications, such as circuit simulation, the period of the oscillation is known *a priori*. In other applications, and in finding a periodic steady state, finding the period of the high-frequency oscillation is an important part of the method.

Several algorithms have been proposed for finding the period. Noting that if y were periodic, $\|y(t) - y(t+T)\| = 0$, Petzold (1981) proposed finding the period T by miminizing $\|y(t) - y(t+T)\|$ over one approximate period. More precisely, T_{m+1} is defined as the value of T^* that satisfies

$$\min_{0<\epsilon\leq T^*\leq I} \int_0^{T_m} (y(t) - y(t+T^*))^2 \, \mathrm{d}t.$$

In practice, in order to better model problems whose solutions are given by a fast oscillation superimposed on a slowly varying solution, the period is found by solving

$$\min_{0<\epsilon\leq T^*\leq I} \int_0^{T_m} (y - p_{m+1} - (y(t+T_{m+1}) - p_{m+1}(t+T_{m+1})))^2 \, \mathrm{d}t,$$

where p_{m+1} is a polynomial which approximates the slow solution that is found at each iteration for T_{m+1} via another minimization. It is shown in Petzold (1978) that this algorithm converges, given a sufficiently smooth initial guess. A similar approach has been used in finding the periodic steady state, as we will discuss below.

The above method of comparing the solution over two periods to find the period of the oscillation is quite general; however, it suffers from the drawback that it is somewhat inefficient. In particular, each time the period needs to be found, the original problem must be solved over two cycles, whereas the envelope-following formulæ require the solution over only one cycle. For problems with a slowly varying period (where the period needs to be recomputed often) this is a relatively large expense. To remedy this problem, another algorithm was proposed by Gallivan and Gear (Gallivan 1980, Gallivan 1983, Gear 1984). This algorithm is based on the idea of defining the period by identifying certain points on the solution at which a simple characterization is repeated, such as zero crossing. Astronomers did this for the multirevolution methods by identifying points of physical interest, such as node, apogee or perigee. For a general problem, the solution itself may have no zero crossing, and there may be difficulty in choosing any value which is crossed periodically. However, the derivative will have periodic sign changes, so the method examines the zero crossings of $c^T y'$, where c is a vector of constant weights. Since there may be more than one zero crossing in a single period, $\|y'(t_1) - y'(t_2)\|$ is also examined, where t_1 and t_2 are the times of zero crossings. If the norm is small, the possibility of a period is considered. For some problems, the solution may not start out oscillatory. This type of algorithm can be used to detect the onset of oscillations, by monitoring the sequence of periods T which are computed. In the event that highly oscillatory behaviour is detected, the software can switch to envelope-following methods.

5.4. Stiffness and implicit methods

As we have noted, the objectives of circuit designers for simulation differ from those of astronomers because circuit designers are not usually interested in the fine details of the oscillation. There are also significant differences in the properties of the ODE systems which influence the choice of numerical methods. In particular, circuit simulation problems are usually quite stiff. Thus they require the use of implicit versions of the envelope-following methods.

White et al. (White and Leeb 1991, Kundert et al. 1988*b*, Kundert et al. 1988*a*, Telichevesky et al. 1995, Telichevesky et al. 1996) have developed efficient implicit algorithms based on the envelope-following idea, and applied them to circuit simulation. The simplest implicit envelope-following method is based on the implicit Euler method and is given by

$$z_{n+1} = z_n + Hg(z_{n+1}, t_{n+1}). \tag{5.3}$$

Solving the nonlinear system (5.3) for z_{n+1}, which is accomplished in stiff ODE codes by a modified Newton iteration, requires an approximate Jac-

obian matrix $\partial g/\partial z$. Gallivan (1983) has considered the implementation of implicit envelope-following methods and suggests computing the Jacobian by finite difference approximation. This can work well for small problems, but for large systems it is prohibitively expensive because each evaluation of g requires solving the original problem over one cycle.

A more efficient and accurate approach (White and Leeb 1991) is to view this computation as finding the sensitivities of g with respect to perturbations in z. The sensitivity problem is solved concurrently with the original system over one cycle. This can be implemented very efficiently by noting that the Jacobian matrix at every time-step for the sensitivities with respect to each parameter is the same as the Jacobian matrix of the original system. Hence this matrix, if it is dense, can be formed and decomposed once, then used in the Newton iteration for each sensitivity. Differencing in this way is also more accurate than directly differencing the numerical solution over each cycle, because the original system and the sensitivity equations use the same sequence of stepsizes and orders (Hairer, Nørsett and Wanner 1993). White and Leeb (1991) have further noted that if the implicit Euler envelope-following method is used unmodified, the stepsize H will be constrained by the component of y with the fastest-changing envelope. This can be unnecessarily conservative; components of y which have rapidly changing envelopes in stiff problems are likely to be 'nearly algebraic' functions of other, more slowly changing components, over the timescale of one period. These nearly algebraic components of y are computed in White and Leeb (1991) directly from the other components via a DC (steady-state) analysis, and hence are not computed by the envelope-following method. A component y_i of y is considered *quasi-algebraic* if the ith column of the sensitivity matrix is nearly zero.

For large-scale systems, approximating the Jacobian matrix directly is too expensive, because there are so many sensitivities to be computed. Telichevesky et al. (1996) have applied preconditioned iterative methods to solve the linear system at each Newton iteration. These Krylov subspace methods have the property that the Jacobian is never needed directly. Instead, the iterative method needs the product of the Jacobian matrix times a given vector. This can be approximated by a directional difference (a sensitivity in the direction of the given vector). Further efficiency is attained by exploiting the structure of the system in a 'recycled' version of the Krylov algorithm. Telichevesky et al. (1996) found that this method can be as much as forty times faster than direct factorization, for large circuits.

Finally, we note that the solution of stiff oscillatory systems by implicit envelope-following methods has much in common with finding the periodic steady state. That problem can be described as finding y and T such that

$$y(T) - y(0) = 0,$$

which can also be written as

$$g(z(0), T) = 0.$$

Aprille Jr. and Trick (1972) proposed a Newton-type algorithm for solving the steady-state problem in circuit analysis. Telichevesky et al. (1995) have efficiently performed steady-state analysis for large-scale circuits making use of the Krylov subspace approach described above. Lust, Roose, Spence and Champneys (1997) have proposed an algorithm for computing periodic steady states of general ODE systems which combines the recursive projection method of Shroff and Keller (1993), which separates the slow from the fast components, with a Krylov method.

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