Cheap Implicit Symplectic Integrators*

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July 28, 1997

Abstract

The high frequency modes of Hamiltonian systems tend to have small amplitudes. Hence for moderately accurate integration of such problems, by say, the leapfrog method, the time step tends to be limited by stability restrictions rather than accuracy restrictions. Conventional implicit symplectic methods like implicit midpoint have less severe stability restrictions but the cost of solving large nonlinear systems with dense Jacobian matrices is probably too high to make them worthwhile. To bring down the cost of implicit methods, we have designed (i) mixed implicit-explicit and (ii) linearly implicit methods that retain the property of being symplectic.

Keywords: linearly implicit method, stiff oscillatory, symplectic integrator, Hamiltonian systems, implicit midpoint.

AMS(MOS) Subject Classifications: 65L20

CR Subject Classifications: G.1.3

1 Introduction

Physical phenomena like molecular dynamics, structural dynamics [4], and wave propagation are often modeled by Hamiltonian systems having multiple time scales. Because the energy

*This work was supported in part by DOE/NSF grant DE-FG02-91-ER25099/DMS-9304268, by NIH Grant P41RR05969, and by NSF/ARPA Grant BIR-9318159. The work of M. Z. was completed while at the University of Illinois. The work of R. S. was performed partly while visiting the Courant Institute.

tends to be equally partitioned among the different modes, the high frequency modes tend to have small amplitudes. In practical problems for which only moderate accuracy is needed, this amplitude can be less than the error tolerance, so it is not necessary to resolve this motion. (We could call such problems "stiff" or "stiff oscillatory.") We would hope then that the step size is limited only by the accuracy requirements of the low frequency part of the motion. Generally, this is not true though for explicit methods such as the leapfrog method, that have a short interval of stability on the imaginary axis. Conventional implicit methods like the implicit mid-point scheme have, of course, less severe stability restrictions if any at all, but the cost of solving large nonlinear systems with dense Jacobian matrices is probably too high to make them worthwhile.

To bring down the cost of implicit methods, we propose (i) mixed implicit-explicit and (ii) linearly implicit methods that retain the property of being symplectic. Linearly implicit methods need only to solve a linear system of equations—no matter whether the system we integrate is linear or nonlinear. Motivation for this work is its application to molecular dynamics [2, 7] although the ideas may be more suitable for other applications like structural dynamics and wave propagation, which are not so nonlinear as molecular dynamics. Numerical results are given at the end of this paper.

2 Mixed implicit-explicit methods

We begin by describing a family of simple implicit methods of conventional type for the system

$$\dot{x} = v, \quad \dot{v} = F(x)$$

where $F(x) = -U_x(x)$ and $U(x)$ is potential energy [6]. At the beginning of a typical step we have available the collective positions X_n and the collective velocities V_n. We advance one step as follows:

$$\begin{aligned} X_{n+1/2} &= X_n + \frac{\Delta t}{2} V_n, \\ F_{n+1/2} &= F(X_{n+1/2} + \alpha \Delta t^2 F_{n+1/2}) \\ V_{n+1} &= V_n + \Delta t F_{n+1/2}, \\ X_{n+1} &= X_{n+1/2} + \frac{\Delta t}{2} V_{n+1}, \end{aligned}$$

where α is the parameter for the family of methods. The case $\alpha = 0$ is the computationally inexpensive leapfrog/Verlet method, but a nonzero choice for α requires solving a system of nonlinear equations. That is, we use a force $F_{\Delta t}(X)$ which is defined implicitly by

$$F_{\Delta t} = F(X + \alpha \Delta t^2 F_{\Delta t}).$$

The value $F_{n+1/2}$ obtained in this way can be viewed as a modification of the force vector which attempts to compensate for the finite size of Δt. What is needed for symplecticness is merely that the Jacobian matrix of $F_{\Delta t}(X)$ be symmetric, which it is. The value $\alpha = \frac{1}{4}$, which yields essentially the implicit midpoint scheme, is special in that it guarantees that the total energy is exactly conserved for linear problems. (Also $\frac{1}{4}$ is the smallest value of α

that guarantees unconditional stability for any linear problem.) The choice $\alpha = \frac{1}{12}$ yields an effectively fourth-order method equivalent to the Störmer-Cowell method (also attributed to Numerov). Choices $\alpha = \frac{1}{3}$ or $\frac{1}{2}$ improve the stability for nonlinear problems [3].

This way of viewing the method suggests modifications that can significantly reduce the cost. The idea is to seek finite-Δt forces $F_{\Delta t}(X)$ which are cheap to compute and have a symmetric Jacobian matrix but retain a degree of implicitness.

One idea is to write

$$F = F^1 + F^2 + \cdots + F^m$$

where the splitting of collective force vectors is induced by a splitting of the potential energy function. Then define

$$F_{\Delta t} = F^1_{\Delta t} + F^2_{\Delta t} + \cdots + F^m_{\Delta t}$$

where

$$F^k_{\Delta t} = F^k(X + \alpha_k \Delta t^2 F^k_{\Delta t}).$$

For example, one can handle the "fast" forces as a single term in the splitting, with say $\alpha = \frac{1}{4}$, and the "slow" forces explicitly. This idea of mixing implicit and explicit differencing is used effectively in partial differential equations, such as reaction–diffusion equations. This splitting is, in principle, straightforward for molecular dynamics if the fast forces are chosen to include only bonded forces. However, nonbonded forces due to nearby atoms can be strong, if only temporarily, and full benefit of implicitness requires that these forces be treated implicitly. One way to do this is by a splitting of the nonbonded interaction into a slow long-range part and a fast short-range part. The short-range part is chosen to vanish beyond a certain cutoff and it is treated implicitly. For an example of such a splitting see [5].

3 Linearly implicit methods

To solve the equations of an implicit method requires several iterations, which can be costly even if only some forces F^1 are handled implicitly. If we do only one Newton iteration for forces F^1, the method would be much cheaper but we would sacrifice symplecticness. It would be desirable to have a symplectic linearly implicit method which reduces to some given implicit method for linear forces. Such a method is obtained by defining $F^1_{\Delta t}$ as the negative gradient of

$$U^1 - \frac{1}{2}\alpha_1 \Delta t^2 (U^1_x)^{\mathrm{T}} (I + \alpha_1 \Delta t^2 U^1_{xx})^{-1} U^1_x. \tag{1}$$

Omitting the index 1, we have

$$\begin{aligned} F_{\Delta t} &= -\left(U - \frac{1}{2}\alpha \Delta t^2 (U_x)^{\mathrm{T}} (I + \alpha \Delta t^2 U_{xx})^{-1} U_x\right)_x \\ &= -(I + \alpha \Delta t^2 U_{xx})^{-1} U_x - \frac{1}{2}\alpha^2 \Delta t^4 (U_x)^{\mathrm{T}} (I + \alpha \Delta t^2 U_{xx})^{-1} U_{xxx} (I + \alpha \Delta t^2 U_{xx})^{-1} U_x \end{aligned}$$

where there is a double summation implicit in the U_{xxx} term. This consists of one Newton iteration of the original implicit method plus a "correction term" involving the third derivative of U^1. In practice one might first compute $G = (I + \alpha \Delta t^2 U_{xx})^{-1} U_x$ and then

$$F^i_{\Delta t} = -G^i - \frac{1}{2}\alpha^2 \Delta t^4 G^{\mathrm{T}} \left(\frac{\partial}{\partial x^i} U_{xx}\right) G.$$

For molecular dynamics the third derivative correction term is small for the mildly nonlinear bonded forces but could be large for the highly nonlinear van der Waals forces. If the third derivative term is omitted from the force, the method is is still time reversible even though it is not symplectic, so in practice it may work as well.

Linearly implicit symplectic methods of a different kind can be derived using generating functions of the second kind [1, section 2.3], but the formulas proposed in [1] do not have extended intervals of stability.

4 Numerical experiments

We compare the following methods with $\alpha = \frac{1}{4}$ without any partitioning of the forces ($m = 1$):

1. the fully implicit method,
2. the symplectic linearly implicit method, and
3. the reversible nonsymplectic linearly implicit method, with the third derivative term omitted.

Our test problem is a nonlinear system with the Hamiltonian

$$H = \frac{1}{2}(v_1^2 + v_2^2) + \frac{1}{2\varepsilon^2}((x_1^2 + x_2^2)^{1/2} - 1)^2 + x_2 + 1 + \frac{1}{2}\varepsilon^2 \tag{2}$$

This models a two-dimensional stiff pendulum of unit length connected to a unit mass in a gravitional field of unit acceleration. The Hessian has a constant eigenvalue ε^{-2} associated with an eigenvector in the radial direction and a variable eigenvalue $\varepsilon^{-2}(1 - r^{-1})$ associated with an eigenvector in the angular direction. If this variable eigenvalue is much smaller in magnitude than the constant eigenvalue, the problem is stiff.

We choose initial conditions

$$x_1 = 0, \quad x_2 = -1 - \frac{1}{2}\varepsilon^2, \quad v_1 = 1, \quad v_2 = 1.$$

Hence the system begins near its equilibrium position with $\frac{1}{8}\varepsilon^2$ potential energy and with unit kinetic energy equally partitioned between radial and angular components. The constancy of the energy can be used to prove that the variable eigenvalue $\varepsilon^{-2}(1 - r^{-1})$ must lie in the range $-\sqrt{2}\varepsilon^{-1} - 1$ to $\sqrt{2}\varepsilon^{-1} - 1$ neglecting terms of order ε^2. To resolve the motion in the angular direction accurately, it is necessary to choose a time step Δt which is small compared to $\sqrt{\varepsilon}$. However, the use of the (explicit) leapfrog method requires that $\Delta t < 2\varepsilon$, because of stiffness in the radial direction.

For our experiments we choose $\varepsilon = 0.002$. As our time step we choose $\Delta t = 0.01$, which is greater than the maximum stable time step $2\varepsilon = 0.004$ for which the leapfrog method is stable. We compute energy and position error as a function of time on the time interval $[0, 60]$—about 10 periods of the pendulum. To get the position error, we also compute a (nearly) exact solution using $\alpha = \frac{1}{12}$ and $\Delta t = \frac{1}{5}\varepsilon$. Plotted in Figs. 1–3 are energy vs. time and position error vs. time for the fully and linearly implicit methods. We note that

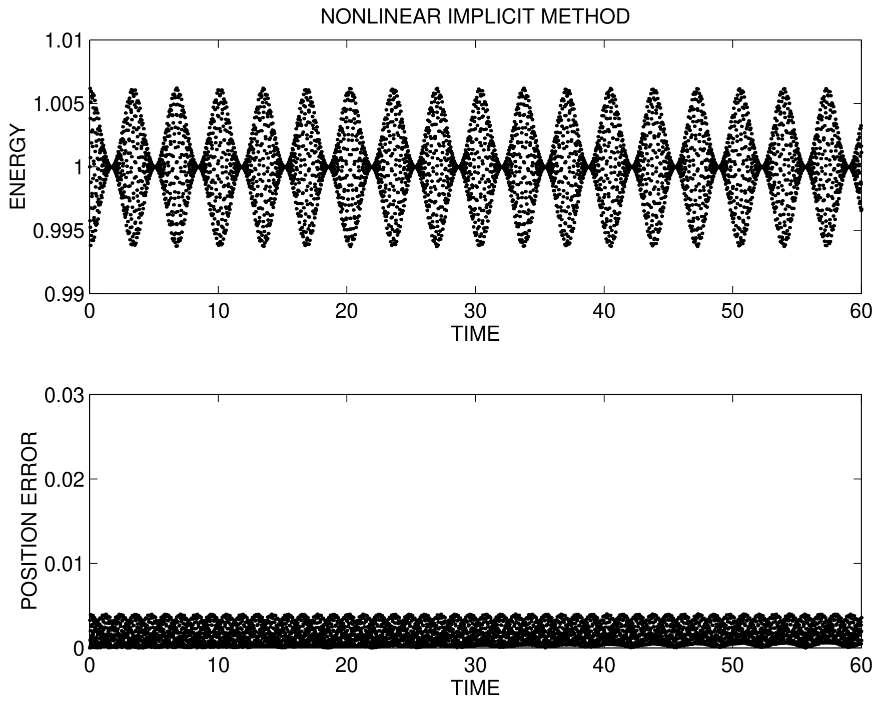

Figure 1: Energy and position error as a function of time for the fully implicit method.

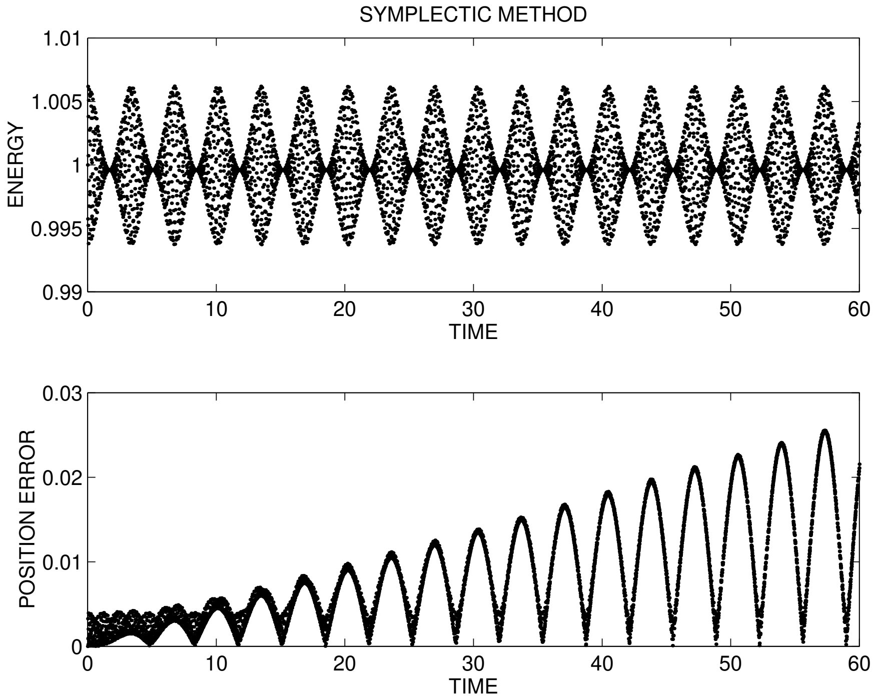

Figure 2: Energy and position error as a function of time for the symplectic linearly implicit method.

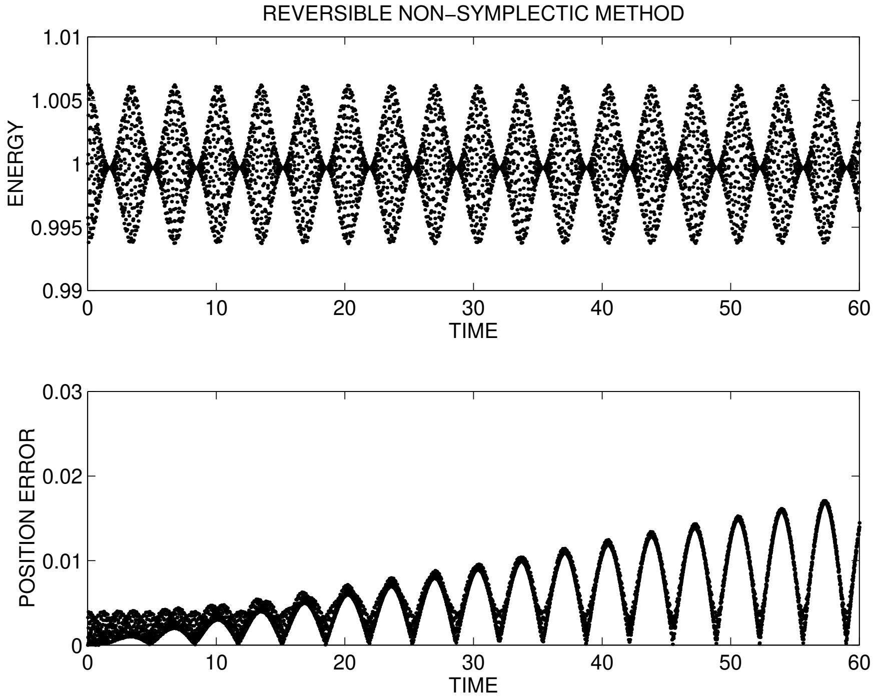

Figure 3: Energy and position error as a function of time for the reversible but nonsymplectic linearly implicit method.

energy is conserved equally well for all three methods but that position error is markedly larger for the linearly implicit methods with the symplectic variant doing a little worse than the merely reversible one. The fully implicit method is much more costly, however, with an average of 9.3 iterations per time step to achieve machine precision accuracy in the solution of the implicit equations.

These experiments indicate the potential of linearly implicit methods to outperform both explicit and nonlinearly implicit methods on Hamiltonian systems.

Acknowledgment

We are grateful to Roger Steffen for programming assistance.

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