Highly Oscillatory Problems

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- **Real solution:** The substitute for highly oscillatory problems with (nearly) constant frequencies is modulated Fourier expansions.

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Introduction

To be more specific consider the problem:

$$\ddot{q} = -\nabla V(q) \tag{0.1}$$

Note that the mass matrix is contained the function V. The standard way to integrate this problem is applying Störmer Verlet, which computes the new position as:

$$q_{n+1} - 2q_n + q_{n-1} = h^2 f_n, \quad f = -\nabla V(q_n) \tag{0.2}$$

Velocity approximations are given as:

$$\dot{q} = \frac{q_{n+1} - q_{n-1}}{2h} \tag{0.3}$$

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which leads to the one step formulation:

$$\dot{q}_{n+1/2} = \dot{q}_n \frac{1}{2} h f_n \tag{0.4}$$

$$q_{n+1} = q_n + h\dot{q}_{n+1/2} \tag{0.5}$$

$$q_{n+1} = \dot{q}_{n+1/2} \frac{1}{2} h f_{n+1} \tag{0.6}$$

recall that this methods is symmetric of second order. For bounded error propagation in linearised equations, the step-size must be restricted to:

$$h\omega < 2 \tag{0.7}$$

where ω is the largest eigenfrequency, i.e. square root of an eigenvalue, of the Hessian matrix $\nabla^2 V(q)$ along the solution

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However good energy conservation requires and even stronger demand, in MD a value of:

$$h\omega \approx \frac{1}{2} \tag{0.8}$$

for the harmonic oscillator ($V = \frac{1}{2}kq^2$) we have:

$$h\sqrt{k} \approx \frac{1}{2}. \tag{0.9}$$

The potential is often a sum of potentials which acts on different time scales such that:

$$V(q) = W(q) + U(q), \quad \|\nabla^2 W\| >> \|\nabla^2 U\| \tag{0.10}$$

solutions are now highly oscillatory on time scales $\tau \sim 1/\|\nabla^2 U\|^{1/2}$

Gautchi's and Deufhard's Trigonometric Methods

The first method to allow the use long time steps in oscillatory problems concerning quadratic potential $W(q) = \frac{1}{2}\omega^2 q^T q$ with $\omega >> 1$ for which the equations take the form:

$$\ddot{q} = -\omega^2 q + g(q) \tag{1.1}$$

Then Gautchi (1961) proposed to use:

$$q_{n+1} - 2q_n + q_{n-1} = h^2 sinc^2\left(\frac{1}{2}h\omega\right)\ddot{q}_n \tag{1.2}$$

and

$$\dot{q}_{n+1} - \dot{q}_{n-1} = 2hsinc(h\omega)\ddot{q}_n \tag{1.3}$$

with $sinc(x) = \frac{sin(x)}{x}$ and $\ddot{q}_n = -\omega^2 q_n + g_n$ with $g_n = g(q_n)$. This method gives the exact solution if $g = Constant$

Gautchi's and Deufhard's Trigonometric Methods

Further Deufhard (1979) suggested to use:

$$q_{n+1} - 2cos(h\omega)q_n + q_{n-1} = h^2 sinc(h\omega)q_n \tag{1.4}$$

with velocity updates:

$$2hsinc(hw)\dot{q}_n = q_{n+1} - q_{n-1}. \tag{1.5}$$

Both methods reduces to the Störmer Verlet for $\omega = 0$ and extends in a straightforward way to systems:

$$\ddot{q} = -Aq + g(q) \tag{1.6}$$

The Impulse Method

Another interpretation of the Störmer Verlet method is that it it approximates the exact solution φ_h^H of the Hamiltonian $H = T + V$ by:

$$\varphi_{h/2}^V \circ \varphi_h^T \circ \varphi_{h/2}^V \tag{1.7}$$

in this situation we have $V = W + U$ which gives us a new possibility to split the system $H = (W + T) + U$, which then yields

$$\varphi_{h/2}^U \circ \varphi_h^{T+W} \circ \varphi_{h/2}^U \tag{1.8}$$

This method has been proposed in several contexts and have a couple of names: Verlet-I scheme, r-RESPA and the Impulse method. I will go with the Impulse method as, the idea is:

1. Kick: set $p_n^+ = p_n - \frac{1}{2} h \nabla U(q_n)$
2. Oscillate: solve $\ddot{q} = -\nabla W(q)$ with initial values (q_n, p_n^+) over a time-step h to obtain (q_{n+1}, p_{n+1}^-).
3. Kick: set $p_{n+1} = p_{n+1}^- \frac{1}{2} h \nabla U(q_{n+1})$

The Impulse Method

- The second step must in general be computed approximately. If this method is symmetric and symplectic, so will the entire method be. Further typically you will use multiple steps, here as well. The natural choice is of course the Störmer Verlet method.
- Notice that this method reduces to the Deufhard's method for exact solution in step 2, and quadratic W.
- Though this method allows larger steps than the Störmer Verlet method (alone) in molecular dynamics, this method is not free of problems, which has been described in papers by Decki and Skeel (1993), and García-Archilla et al. (1999)
- So in these cases one typically uses the Mollified Impulse Method.

The Mollified Impulse Method, García-Archilla et al. (1999)

Difficulties with the impulse method can be intuitively seen to come from two sources:

- The slow force has only an effect at the end of an time-step
- The slow force is evaluated, somewhat arbitrarily, at isolated points of the oscillatory solution

To solve this García-Archilla et al. (1999) suggested to evaluate the slow force a an averaged value $\bar{q}_n = a(q_n)$. They replace the potential by $\bar{U}(q) = U(a(q))$, hence the mollified force:

$$-\nabla \bar{U}(q) = -a'(q)^T \nabla U(a(q)) \tag{1.9}$$

which is still symmetric and symplectic if care is taken.

The Mollified Impulse Method, García-Archilla et al. (1999)

We now have to choose the averaging function $a(q)$. Here we have numerous possibilities, but we have to note that it may **only** depend on the position. What one does is to solve the auxiliary problem:

$$\ddot{x} = -\nabla W(x), \quad x(0) = q, \dot{x}(0) = 0 \tag{1.10}$$

together with the variational equation (using the same method and the same step size)

$$\ddot{X} = -\nabla^2 W(x(t)), \quad X(0) = I, \dot{X}(0) = 0 \tag{1.11}$$

and computes the time average over an interval of length ch for some $c > 0$

$$a(q) = \frac{1}{ch} \int_0^{ch} x(t)dt \tag{1.12}$$

$$a'(q) = \frac{1}{ch} \int_0^{ch} X(t)dt \tag{1.13}$$

The Mollified Impulse Method, García-Archilla et al. (1999)

García-Archilla et al. (1999) found that the choice $c = 1$ gives the best result. Further they also found that weighted averages does now yield any improvements.
Izaguirre, Reich and Skeel (1999) propose to take $a(q)$ as a projection of q to the manifold where $\nabla W(q) = 0$. for situations where all non-zero eigenvalues of the Hessian of $W(q)$ are much larger than those of the Hessian of $U(q)$, this choice is motivated by the fact that solutions oscillates around this manifold.

Gautchi's Methods Revisited, Hochbruck and Lubich (1999)

Recall that the ordinary method reads:

$$q_{n+1} - 2q_n + q_{n-1} = h^2 sinc^2\left(\frac{1}{2}h\omega\right)\ddot{q}_n \tag{1.14}$$

$$\dot{q}_{n+1} - \dot{q}_{n-1} = 2hsinc(h\omega)\ddot{q}_n \tag{1.15}$$

where $\ddot{q} = -\omega^2 q_n + g_n$ with $g_n = g(q_n)$. We now change the argument of g such that:

$$g_n = g(\phi(h\Omega)q_n), \quad \Omega = A^{1/2}. \tag{1.16}$$

Functions, ϕ, with $\phi(0) = 1$ that vanish at integral multiples of π give a huge improvement over the original method. Further the specific choice

$$\phi(x) = sinc\left(x(1 + \frac{1}{3}sin^2\frac{1}{2}x)\right) \tag{1.17}$$

was in particular good.

Two-Force Methods, Hairer and Lubich (2000)

Hairer and Lubich compared the analytical solution to the numerical solution in the Fermi-Pasta-Ulam model using modulated Fourier series. This lead them to suggest the following method:

$$q_{n+1} - 2cos(h\Omega)q_n + q_{n-1} = h^2 sinc(h\Omega)g(q_n) + h^2 d_n \quad (1.18)$$

where $d_n = sinc^2(h\Omega)g(q_n) - sinc(h\Omega)g(sinc(h\Omega)q_n)$.
This method gives the correct slow energy exchange between stiff components in the model problem. It also has better energy preserving properties than the Deufhard and Impulse method.

General formulation

All the previous methods were written in their two-step form, and has the same general form:

$$x_{n+1} - 2cos(h\Omega)x_n + x_{n-1} = h^2 \Psi g(\Phi x_n) \tag{1.19}$$

where $\Psi = \psi(h\Omega)$ and $\Phi = \phi(h\Omega)$. ψ and ϕ are called filter functions and are for all methods even and fulfil $\phi(0) = \psi(0) = 0$, additionally they are given as:

ID:	$\psi(x) =$	$\phi(x) =$	Method:
(A)	$sinc^2(\frac{1}{2}x)$	1	Gautschi
(B)	$sinc(x)$	1	Deuflhard
(C)	$sinc(x)\phi(x)$	$sinc(x)$	Mollified Impulse
(D)	$sinc^2(\frac{1}{2}x)$	Eqn (1.17)	Gautschi rev.
(E)	$sinc^2(x)$	1	Two Force

(1.20)

One step formulation

Including a velocity approximation we can rewrite the above two step formulation into one step formulations:

$$
\begin{aligned}
x_{n+1} &= \cos(h\Omega x_n) + \Omega^{-1}\sin(h\Omega \dot{x}_n) + \frac{1}{2}h^2\Psi g_n \\
\dot{x}_{n+1} &= -\Omega\sin(h\Omega x_n) + \cos(h\Omega \dot{x}_n) + \frac{1}{2}h\left(\Psi_0 g_n + \Psi_1 g_{n+1}\right)
\end{aligned}
$$

where $\Psi_0 = \psi_0(h\Omega)$, $\Psi_1 = \psi_1(h\Omega)$ and $g_n = g(\Phi x_n)$ with even function ψ_0 and ψ_1 satisfying $\psi_0(0) = \psi_1(0) = 1$.

Theorem (Symplecticity and symmetricity)

If and only if the functions ψ_1 and ψ_0 satisfies that $\psi(x) = sinc(x)\psi_1(x)$ and $\psi_0(x) = cos(x)\psi_1(x)$ then the method is symmetric.
If and only if the $\psi(x) = sinc(x)\phi(x)$ then the method is symplectic.

Accuracy Comparison

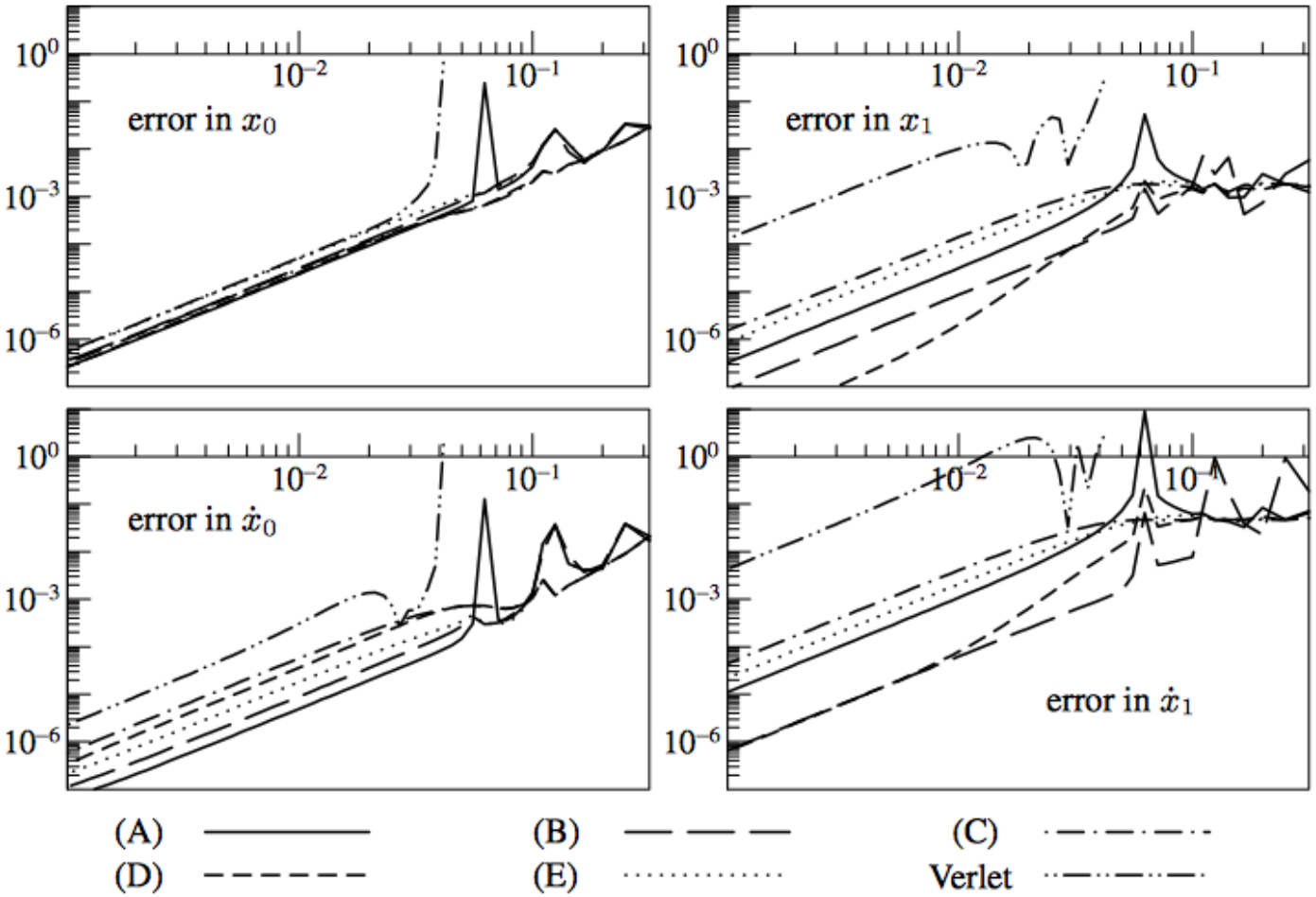

Fig. 2.2. Global error at $t = 1$ for the different components and for the five methods (A) - (E) and the Störmer–Verlet method as a function of the step size h

Accuracy Comparison

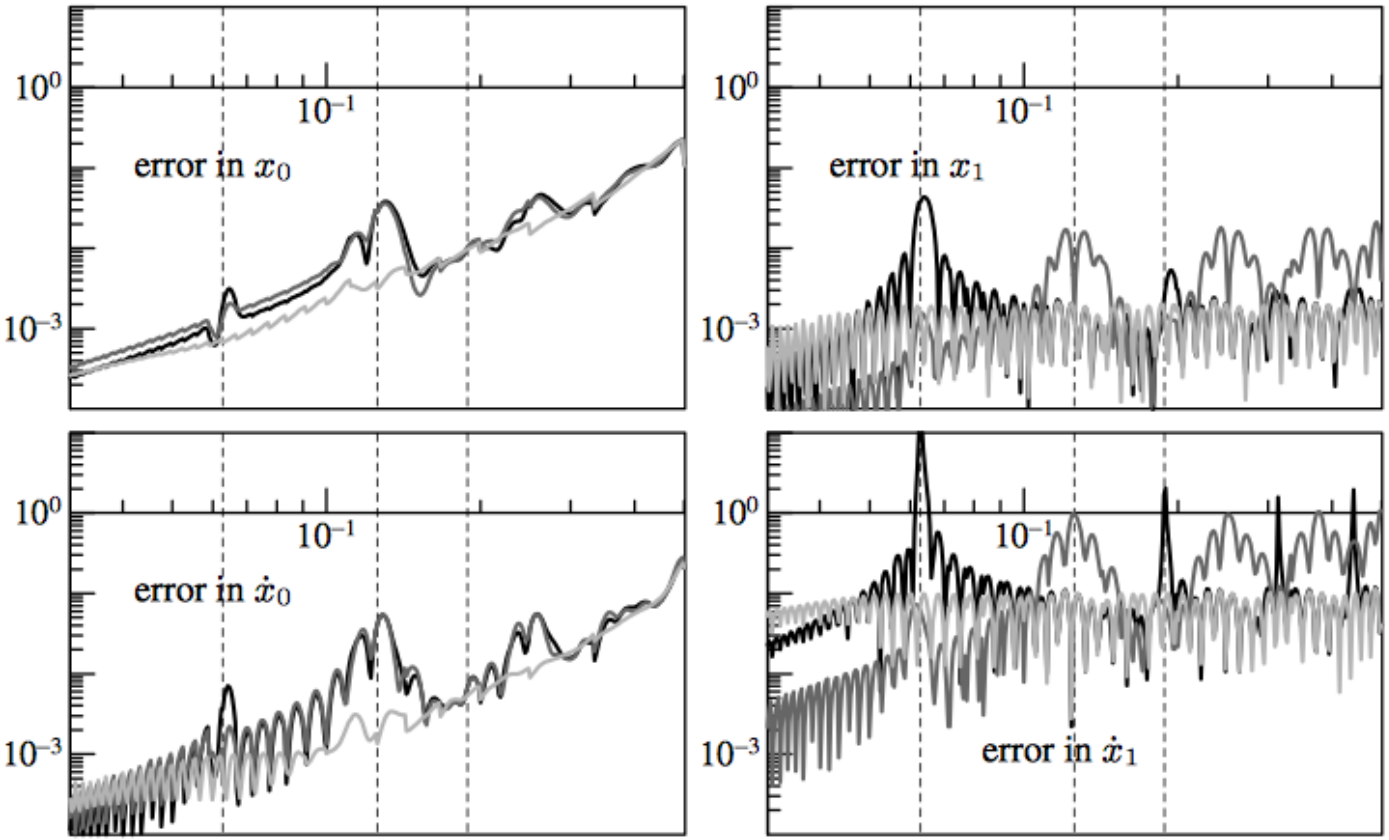

Fig. 2.3. Global error at the first grid point after $t = 1$ for the different components as a function of the step size h. The error for method (A) is drawn in black, for method (B) in dark grey, and for method (C) in light grey. The vertical lines indicate step sizes for which $h\omega$ equals π, 2π, or 3π

Energy Exchange between Stiff Components

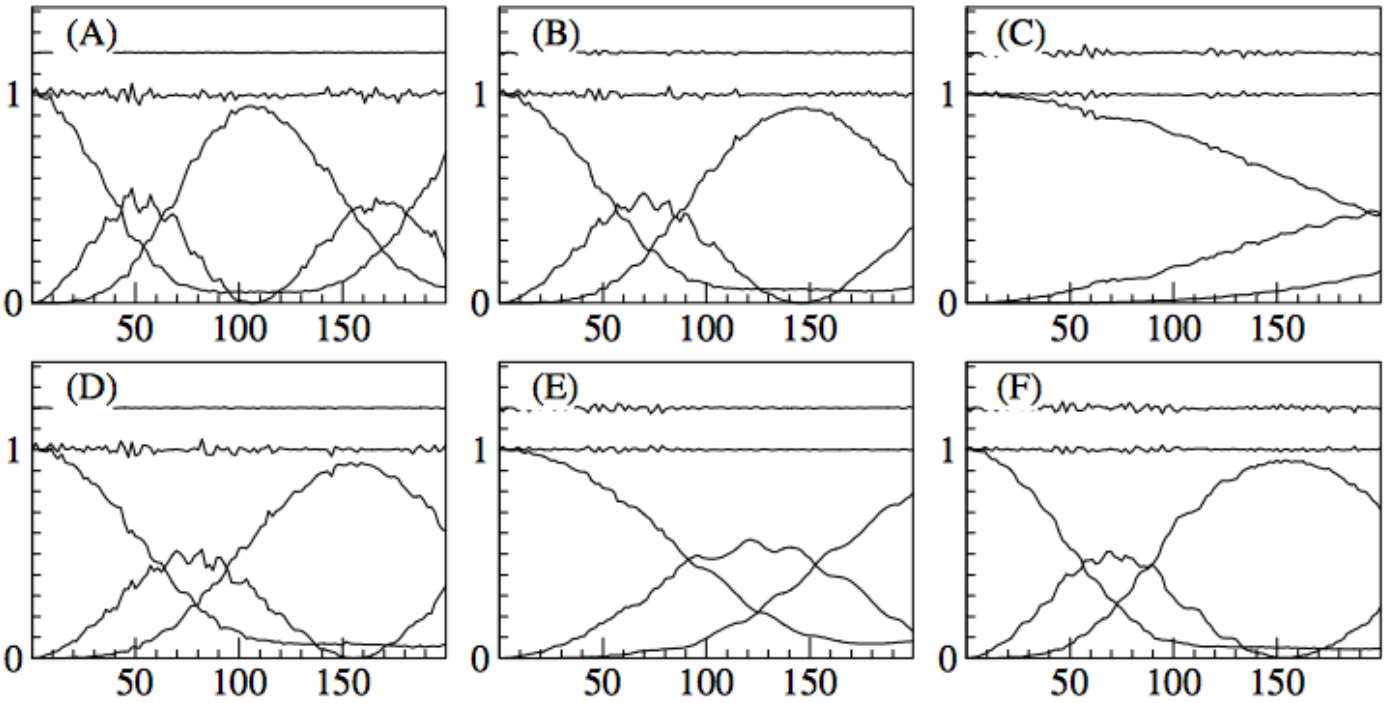

Fig. 2.4. Energy exchange between stiff springs for methods (A)-(F) ($h = 0.03$, $\omega = 50$)

Near Conservation of Total Energy

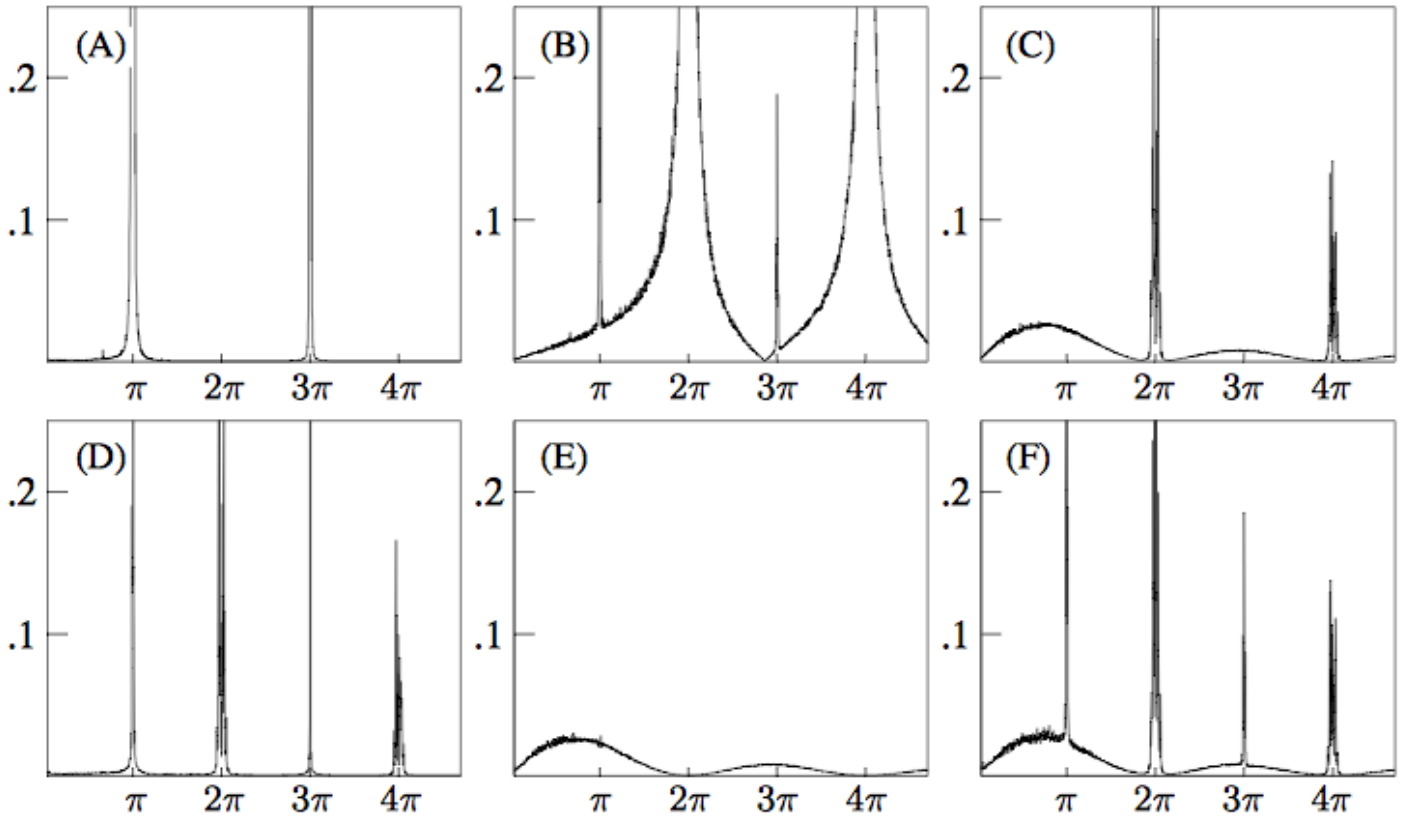

Fig. 2.5. Maximum error of the total energy on the interval $[0, 1000]$ for methods (A) - (F) as a function of $h\omega$ (step size $h = 0.02$)

Modulated Fourier Expansions of Exact Solutions

We first expand the exact solution, to later be able to compare with the expansion of the numerical solution.

Theorem (Modulated Fourier Expansion, Hairer and Lubich 2000a)

Consider a solution $x(t)$ of $\ddot{x} + \Omega^2 x = g(x)$ and satisfies that $\frac{1}{2}\|\dot{x}(0)\|^2 + \frac{1}{2}\|\Omega x(0)\|^2 \leq E$ and stays in a compact set K for $t \in [0, T]$.
Then, the solution admits an expansion:

$$x(t) = y(t) + \sum_{0<|k|<N} e^{ik\omega t} z^k(t) + R_N(t) \qquad (1.21)$$

for arbitrary $N \geq 2$ and $\dot{R}_N(t) = \mathcal{O}(\omega^{-N-1})$ for $t \in [0, T]$

Theorem (Continued)

For real valued function $y = (y_0, y_1)$ and complex valued functions $z^k = (z_0^k, z_1^k)$ together with all their derivatives are bounded by:

$$\begin{array}{lll} y_0 = \mathcal{O}(1) & z_0^1 = \mathcal{O}(\omega^{-3}) & z^k = \mathcal{O}(\omega^{-k-2}) \\ y_1 = \mathcal{O}(\omega^{-2}) & z_1^1 = \mathcal{O}(\omega^{-1}) & \end{array} \tag{1.22}$$

for $k = 2, \ldots, N-1$. Moreover, $z^{-k} = \overline{z^k}$ for all k. These functions are unique up to terms of size $\mathcal{O}(\omega^{-N-2})$. Constants symbolized by Big-O notation are independent of ω and t.

Modulated Fourier Expansions of Numerical Solutions

Theorem (Modulated Fourier Expansion, Hairer and Lubich 2000a)

Consider a numerical solution of the system $\ddot{x} + \Omega^2 x = g(x)$ *which satisfies* $\frac{1}{2}\|\dot{x}(0)\|^2 + \frac{1}{2}\|\Omega x(0)\|^2 \leq E$ *by the previously seen two step methods with step-size* h*, with starting approximations obtained from the one step formulation. Now assume that the following holds:*

- $h\omega \geq c_0 \geq 0$
- $|sin(\frac{1}{2}kh\omega)| \geq c\sqrt{h}$ *(Non-resonance condition)*
- $|\psi(h\omega)| \leq C_1 sinc^2(\frac{1}{2}h\omega)$
- $|\phi(h\omega)| \leq C_2|sinc(\frac{1}{2}h\omega)|$
- $|\psi(h\omega)\phi(h\omega)| \leq C_2|sinc(h\omega)|$

Theorem (Continued)

Then, the numerical solution admits an expansion

$$x_n = y_h + \sum_{0<|k|<N} e^{ik\omega t} z_h^k(t) + R_{h,N}(t) \tag{1.23}$$

uniformly for $t \in [0, T]$. *The remainder term is of the form*

$$R_{h,N} = t^2 h^N \Psi r(t), \quad r(t) = \mathcal{O}(\phi(h\omega)^N + h^m) \tag{1.24}$$

where $m \geq 0$ *can be chosen arbitrarily. The coefficient functions together with all their derivatives are bounded by:*

$$\begin{array}{ccc} y_{h,0} = \mathcal{O}(1) & z_{h,0}^1 = \mathcal{O}(\omega^{-2}) & z_{h,0}^k = \mathcal{O}(\omega^{-k}) \\ y_{h,1} = \mathcal{O}(\omega^{-2}) & z_{h,1}^1 = \mathcal{O}(\omega^{-1}) & z_{h,1}^k = \mathcal{O}(\omega^{-k}) \end{array} \tag{1.25}$$

for $k = 2, \ldots, N-1$

Theorem (Continued)

Moreover, $z_h^{-k} = \overline{z_h^k}$ for all k. As in the previous theorem, the constants symbolized with Big-O notation are independent of ω and h, but may depend on the rest.

Modulated Fourier Expansions of Velocity approximations

Theorem (Modulated Fourier Expansion, Hairer and Lubich 2000a)

Under the assumptions of the previous theorem, the velocity approximations $\dot{x}_n$ from the one step formulation has an expansion:

$$\dot{x}_n = v_n(t) + \sum_{0<|k|<N} e^{ik\omega t} w_h^k(t) + \mathcal{O}(t^2 h^{N-1}) \qquad (1.26)$$

uniformly in the time interval $t \in [0, T]$, where the real valued functions $v_h = (v_{h,0}, v_{h,1})$ and the complex valued functions $w_h^k = (w_{h,0}^k, w_{h,1}^k)$ together with their derivatives satisfy:

Theorem (Continued)

$$\begin{aligned} v_{h,0} &= \dot{y}_{h,0}\mathcal{O}(h^2) & w^1_{h,0} &= \mathcal{O}(\omega^{-1}) & w^k_{h,0} &= \mathcal{O}(\omega^{-k}) \\ w_{h,1} &= iwz^1_{h,1}\mathcal{O}(\omega^{-1}) & v^1_{h,1} &= \mathcal{O}(\omega^{-1}) & w^k_{h,1} &= \mathcal{O}(\omega^{-k}) \end{aligned} \tag{1.27}$$

for $k = 2, \ldots, N-1$. Moreover $w_h^{-k} = \overline{w_h^k}$. The constants symbolized by the Big-O notation are independent of ω and h, but may depend on the rest.

Long Time Near-Conservation

Applying the modulated Fourier series to the exact problem, yields a so called "almost Hamiltonian" which is the highly oscillatory counterpart to the Backward Error analysis' shadow Hamiltonian.

Theorem

Under all the previously defined conditions, the numerical solution of $\ddot{x} + \Omega^2 x = g(x)$ *which satisfies that* $\frac{1}{2}\|\dot{x}(0)\|^2 + \frac{1}{2}\|\Omega x(0)\|^2 \leq E$ *obtained by the one step methods satisfies:*

$$\begin{aligned} H(x_n, \dot{x}_n) &= H(x_0, \dot{x_0}) + \mathcal{O}(h), \quad t \in [0, h^{-N+1}] \\ I(x_n, \dot{x}_n) &= I(x_0, \dot{x_0}) + \mathcal{O}(h), \quad t \in [0, h^{-N+1}] \end{aligned}$$

where H *is the total energy and* I *is the oscillatory energy. The constants symbolized by the Big-O notation are independent of* n, h *and* ω.

The Sörmer-Verlet Method

Let us now consider the Sörmer-Verlet method again. We know that it does not preserve the energy very good as this would require to small step sizes, but due to this next theorem, we might be able to apply it anyway.
We first define the modified energies:

Definition (Modified Energy)

In the following we will call the following for the modified total energy:

$$H^*(x,\dot{x}) = H(x,\dot{x}) + \frac{1}{2}\gamma\|\dot{x}_1\|^2, \gamma = \frac{1}{1-\frac{1}{4}(h\omega)^2} - 1 \quad (1.28)$$

Like we will call the following for the modified oscillatory energy:

$$I^*(x,\dot{x}) = I(x,\dot{x}) + \frac{1}{2}\gamma\|\dot{x}_1\|^2, \gamma = \frac{1}{1-\frac{1}{4}(h\omega)^2} - 1 \quad (1.29)$$

The Sörmer-Verlet Method

Theorem (Hairer and Lubich 2000b)

Let the Sörmer-Verlet method be applied to the typical problem, with step-size h for which $0 < c_0 \leq h\omega \leq c_1 < 2$ and $|\sin(\frac{1}{2}kh\tilde{\omega})| \geq c\sqrt{h}$ for $k = 1, \ldots, N$ for some $N \geq 2$, $c > 0$ and $\tilde{\omega}$ fulfilling $\sin(\frac{1}{2}h\tilde{\omega}) = \frac{1}{2}h\omega$. Suppose further that the numerical solution values x_n stay in a region on which all derivatives of U are bounded. Then, the so called modified energies (total and oscillatory respectively) satisfies:

$$H^*(x_n, \dot{x}_n) = H(x_0, \dot{x}_0) + \mathcal{O}(h), \quad t \in [0, h^{-N+1}]$$
$$I^*(x_n, \dot{x}_n) = I(x_0, \dot{x}_0) + \mathcal{O}(h), \quad t \in [0, h^{-N+1}]$$

The Sörmer-Verlet Method

So as we are dealing with an invariant, it must be constant over time. So it is obvious to see how the Störmer-Verlet method preserves the time averages of the energies:

Theorem

Under the conditions of the previous theorem, the time averages of the total and oscillatory energy along the numerical solution satisfies.

$$\overline{H}_n = \overline{H}_0 + \mathcal{O}(h), \quad t \in [0, h^{-N+1}] \tag{1.30}$$

$$\overline{I}_n = \overline{I}_0 + \mathcal{O}(h), \quad t \in [0, h^{-N+1}] \tag{1.31}$$

Systems with Several Constant Frequencies

Under the constraints:

- The energy of the initial values is bounded independently of ϵ
- The numerical solution values Φx_n stay inside a compact subset of a domain on which the potential U is smooth.
- We impose a lower bound on the step size $\frac{h}{\epsilon} \geq c_0 > 0$
- We assume the numerical non-resonance condition
- For the filter functions we assume

$$|\psi(\xi_j)| \leq C_1 sinc^2(\frac{1}{2}\xi_j) \quad (1.32)$$

$$|\phi(\xi_j)| \leq C_2 |sinc(\frac{1}{2}\xi_j)| \quad (1.33)$$

$$|\psi(\xi_j)| \leq C_3 |sinc(\xi_j)\phi(\xi_j)| \quad (1.34)$$

The previous theorems also holds for several frequencies.

Non-Constant Mass Matrix

Algorithm (Algorithm XIII.10.3)

1. *Apply a half step with the symplectic Euler method to the system with the Hamiltonian* $\frac{1}{2}p^T R(q)p$.
2. *Treat the oscillatory components of the variables* p *and* q *with any of the seen one step methods, and the slow components with the Störmer-Verlet scheme.*
3. *Apply a half step with the adjoint symplectic Euler method to the system with the Hamiltonian* $\frac{1}{2}p^T R(q)p$.

Non-Constant Mass Matrix

The algorithm applied to the a model for the water molecule ($\epsilon = 0.01$):

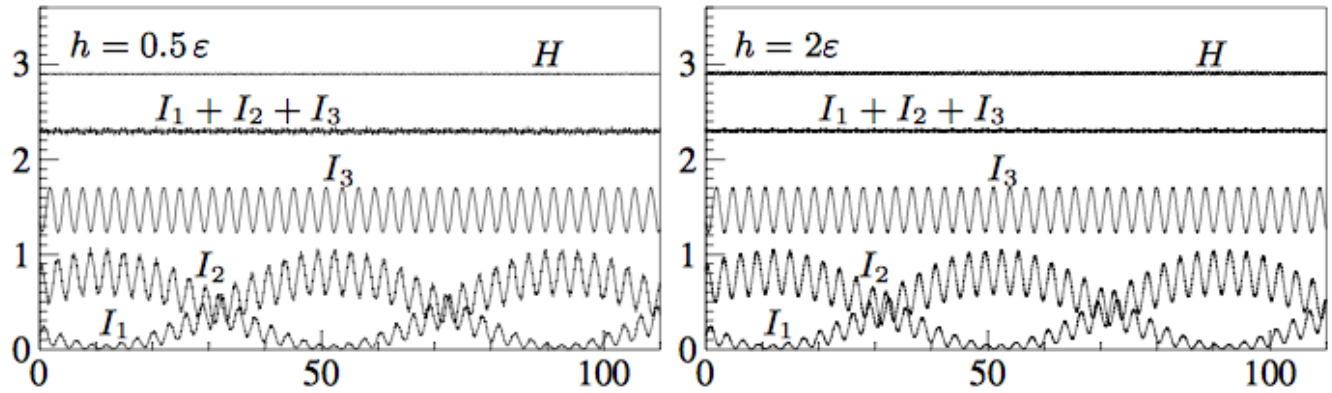

Fig. 10.2. Oscillatory energies and total energy for the method of Algorithm 10.2

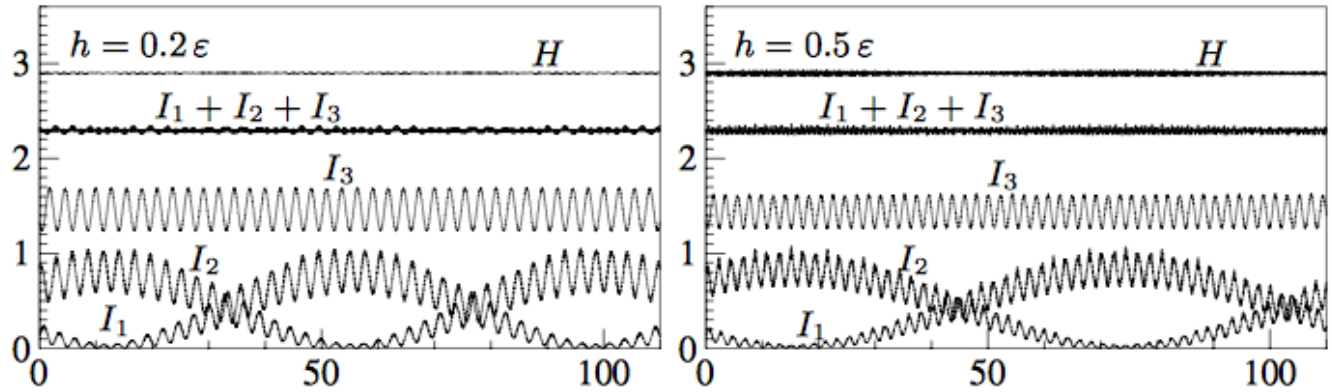

Fig. 10.3. Oscillatory energies and total energy for the Störmer–Verlet method

Varying High Frequencies

We now turn to consider oscillatory problems, where the frequencies are no longer constant, but depends on either time or the solution.
The general idea is to:

- Rewrite into so called adiabatic variables
- Solve using adiabatic solvers

A General Transform

Consider the equation:

$$\dot{y} = \frac{1}{\epsilon} Z(t) y(t) \tag{2.1}$$

where $Z(t)$ is a real or complex skew symmetric (/hermitian) matrix valued function, with time derivatives bounded independently of the small parameter ϵ.
Together with the transformation:

$$\nu(t) = T_\epsilon(t) y(t) \tag{2.2}$$

which takes the system into the form:

$$\dot{\nu} = S_\epsilon(t)\nu(t), \quad S_\epsilon = \dot{T}_\epsilon T_\epsilon^{-1} + \frac{1}{\epsilon} T_\epsilon Z T_\epsilon^{-1} \tag{2.3}$$

The Adiabatic Transformation

Before we choose the transformation we first diagonalize $Z(t)$:

$$Z(t) = U(t)i\Lambda(t)U(t) \tag{2.4}$$

where $\Lambda = diag(\lambda_j(t))$ and unitary matrix $U(t)$ of eigenvectors. We further let:

$$\Phi(t) = \int_0^t \Lambda(s)ds \tag{2.5}$$

We can now define the adiabatic transformation

The Adiabatic Transformation

Definition (Adiabatic Transformation)

Choose:

$$T_\epsilon(t) = exp\left(-\frac{i}{\epsilon}\Phi(t)\right) U(t)^* \tag{2.6}$$

Which yields the differential equation:

$$\dot{\nu}(t) = exp\left(-\frac{i}{\epsilon}\Phi(t)\right) W(t) exp\left(\frac{i}{\epsilon}\Phi(t)\right) \nu(t) \tag{2.7}$$

where $W(t) = \dot{U}(t)^* U(t)$.
We call this transformation "the adiabatic transformation".

Time Dependent Frequencies

Consider the mechanical system:

$$H(p,q,t) = \frac{1}{2}p^T M(t)^{-1} p + \frac{1}{2\epsilon^2} q^T A(t) q + U(q,t) \quad (2.8)$$

Such Hamiltonian describes oscillations in a mechanical system that at the same time exerts a driven motion on a slower time scale. We only consider cases where the total energy is bounded.

To solve such a system, one now follow this idea

1. Transform the mass matrix into the identity matrix
2. Diagonalize the stiffness matrix
3. Rescale the position and momenta
4. Tidy up
5. Rewrite into adiabatic variables using the transformation
6. (Optional) Let $\epsilon \to 0$. We call this the "slow limit"

Doing so we obtain equations for q_0, p_0 and η

Adiabatic Integrators

Algorithm (Simple)

Solving the equations in the slow limit in stead of the "correct" one yields an error bounded by $\mathcal{O}(\epsilon^2)$. Accepting this error we obtain and algorithm that simply reads:

1. *Solve the equations in the slow limit e.g. using the Störmer-Verlet.*
2. *Keep $\eta = \eta(0)$.*

then the total error is $\mathcal{O}(\epsilon)$

Adiabatic Integrators

Algorithm (Not nearly as simple)

An alternative is to solve the correct system, in that case we obtain

- *Solve the equations for q_0 and p_0 e.g. using the Störmer-Verlet.*
- *Solve the adiabatic equation η using an adiabatic solver.*

then the total error is $\mathcal{O}(\epsilon)$

Alternative Integrators

Note that there might very well exist cases where the decomposition is more expensive that doing many small steps with the methods used for constant frequencies. In that case one should apply those methods.

Solution Dependent Frequencies

Consider the mechanical system:

$$H(p,q,t) = \frac{1}{2}p^T M(q)^{-1} p + \frac{1}{\epsilon^2}V(q) + U(q) \qquad (2.9)$$

With strong potential $\epsilon^{-2}V(q)$ that for instance penalizes some directions of motion

To solve such a system, apply nearly the same idea as before

1. Transform the stiffness matrix into the identity matrix
2. Eliminate off-diagonal blocks in the mass matrix
3. Diagonalize the mass matrix of the fast variables
4. Rescale the position and momenta
5. Rewrite into adiabatic variables using the transformation
6. (Optional) Ignore the fast variables, this is again called the slow limit

Doing so we obtain equations for q_0, p_0 and η

Long time Integrator

Algorithm

- *Solve the equations in the slow limit*
- *Together with (Note that all variables are in the adiabatic coordinates):*

$$\dot{\eta} = exp\left(-\frac{i}{\epsilon}\Phi\right) Wexp\left(\frac{i}{\epsilon}\Phi\right) \qquad (2.10)$$

More integrators

For more adiabatic integrators applied to systems in quantum - classical molecular dynamics see:

- T. Jahnke, Numerische Verfahren für fast adiabatische Quantendynamik, Doctoral Thesis, Univ. Tübingen, 2003.
- T. Jahnke, Long-time-step integrators for almost-adiabatic quantum dynamics, SIAM J. Sci. Comput. 25 (2004a) 2145–2164.
- T. Jahnke, A long-time-step method for quantum-classical molecular dynamics, Report, 2004b.
- T. Jahnke and Ch. Lubich, Numerical integrators for quantum dynamics close to the adiabatic limit, Numer. Math. 94 (2003), 289–314.

Alternatively as in the previous case, if the decomposition is to expensive, it might be more efficient to apply a method for constant frequencies, but with lower step-sizes.