Long-time-step methods for oscillatory Hamiltonian systems

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Talk based on:


Cambridge, INI, 21 March 2007
Oscillations and long time steps

\[ = \mathcal{O}(\varepsilon) \]
Outline

Highly oscillatory Hamiltonian systems
  Nearly constant high frequencies
  Time-dependent high frequencies
  State-dependent high frequencies

Building blocks of long-time-step methods
  Averaging
  Splitting
  Linearising
  Co-rotating

Trigonometric integrators for problems with constant frequencies
  see talks by D. Cohen, E. Hairer, C.L. next week

Adiabatic integrators for problems with varying frequencies
  Time-dependent frequencies
  Motion under a strong constraining force
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Canonical Hamiltonian equations of motion

\[
\begin{align*}
\dot{p} &= -\nabla_q H(p, q) \\
\dot{q} &= \nabla_p H(p, q)
\end{align*}
\]

\((p, q \in \mathbb{R}^d)\)
Systems with nearly constant high frequencies

\[ H(p, q) = \frac{1}{2} p^T M^{-1} p + \frac{1}{2} q^T A q + U(q) \]

A positive semi-definite constant stiffness matrix of large norm
\( M \) positive definite constant mass matrix
\( U \) smooth potential with moderately bounded derivatives

\[ A = \frac{1}{\varepsilon^2} \begin{pmatrix} 0 & 0 \\ 0 & I \end{pmatrix} \]


Systems with nearly constant high frequencies, ctd.

\[ H(p, q) = \frac{1}{2} p_0^T M_0(q)^{-1} p_0 + \frac{1}{2} p_1^T M_1^{-1} p_1 + \frac{1}{2} p^T R(q)p + \frac{1}{2\epsilon^2} q_1^T A_1 q_1 + U(q) \]

\[ R(q_0, 0) = 0 \]

water molecule
Time-dependent high frequencies

harmonic oscillator with time-dependent frequency

\[ H(p, q, t) = \frac{1}{2} p^2 + \frac{\omega(t)^2}{2\varepsilon^2} q^2 \]

quasi-period \( \sim \varepsilon \), but frequencies change on slower time scale \( \sim 1 \)

action \( I(t) = H(p(t), q(t), t)/\omega(t) \) is an adiabatic invariant

\[ H(p, q, t) = \frac{1}{2} p^T M(t)^{-1} p + \frac{1}{2\varepsilon^2} q^T A(t) q + U(q, t), \]

adiabatic invariants associated with each of the high frequencies as long as the frequencies remain separated

where eigenvalues almost cross: rapid non-adiabatic transitions
Adiabatic quantum dynamics

\[ i\varepsilon \dot{\psi} = H(t)\psi \]

finite-state Schrödinger equation with hermitian matrix \( H(t) \)
time-dependent Hamiltonian function \( \psi^* H(t) \psi \)

adiabatic invariants \( I_j = |\psi_j|^2 \) as long as the eigenvalues remain separated
State-dependent high frequencies

\[ H(p, q) = \frac{1}{2} p^T M(q)^{-1} p + \frac{1}{\varepsilon^2} V(q) + U(q) \]

constraining potential \( V(q) \) in appropriate coordinates:

\[ V(q) = \frac{1}{2} q_1^T A_1(q_0) q_1 \quad \text{for} \quad q = (q_0, q_1), \quad A_1 \text{ s.p.d.} \]

multiple spring pendulum
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Building blocks of long-time-step methods

handful of construction principles, to be discussed in the following
additionally preserve symmetry!
symplecticity? often too much to ask for
basic principle:

avoid isolated evaluations of oscillatory functions
rely on averaged quantities
\[ \ddot{q} = f(q), \quad f(q) = f^{[\text{slow}]}(q) + f^{[\text{fast}]}(q) \]

Störmer–Verlet method uses a pointwise evaluation of \( f \):

\[ q_{n+1} - 2q_n + q_{n-1} = h^2 f(q_n) \]

whereas the exact solution has a weighted average:

\[ q(t + h) - 2q(t) + q(t - h) = h^2 \int_{-1}^{1} (1 - |\theta|) f(q(t + \theta h)) \, d\theta \]
Averaged-force method

\[ q(t + h) - 2q(t) + q(t - h) = h^2 \int_{-1}^{1} (1 - |\theta|) f(q(t + \theta h)) \, d\theta \]

freeze the slow part and approximate

\[ f(q(t_n + \theta h)) \approx f^{[\text{slow}]}(q_n) + f^{[\text{fast}]}(u(\theta h)) \]

where \( u(\tau) \) solves

\[ \ddot{u} = f^{[\text{slow}]}(q_n) + f^{[\text{fast}]}(u) \]

insert

\[ h^2 \int_{-1}^{1} (1 - |\theta|) \left( f^{[\text{slow}]}(q_n) + f^{[\text{fast}]}(u(\theta h)) \right) \, d\theta = u(h) - 2u(0) + u(-h) \]
Averaged-force method

\[ \ddot{u} = f^{[\text{slow}]}(q_n) + f^{[\text{fast}]}(u) \quad \text{with } N \text{ microsteps over } [-h, h] \]

\[
q_{n+1} - 2q_n + q_{n-1} = u^N(h) - 2u^N(0) + u^N(-h)
\]

\[
\dot{q}_{n+1} - \dot{q}_{n-1} = \dot{u}^N(h) - \dot{u}^N(-h) .
\]

Hochbruck & L. 1999 and Sect. VIII.4 in HLW

different symmetric averaging schemes:

Leimkuhler & Reich 2001, E 2003, Engquist & Tsai 2005
Splitting

for \( H(p, q) = [T(p) + V^{[\text{fast}]}(q)] + V^{[\text{slow}]}(q) \) approximate the flow by

\[
\varphi^H_h \approx \varphi_{h/2} \circ \varphi_h \circ T + V^{[\text{fast}]} \circ \varphi_{h/2}.
\]

Impulse method:

1. kick: set \( p_n^+ = p_n - \frac{1}{2} h \nabla V^{[\text{slow}]}(q_n) \)
2. oscillate: solve \( \ddot{q} = -\nabla V^{[\text{fast}]}(q) \) with initial values \((q_n, p_n^+)\)
   over a time step \( h \) to obtain \((q_{n+1}, p_{n+1}^-)\)
3. kick: set \( p_{n+1} = p_{n+1}^- - \frac{1}{2} h \nabla V^{[\text{slow}]}(q_{n+1}) \).

Grubmüller, Heller, Windemuth & Schulten 1991
Tuckerman, Berne & Martyna 1992
Garcia-Archilla, Sanz-Serna & Skeel 1999:
mollified impulse method, uses \( V^{[\text{slow}]}(\text{average}(q)) \)
Linearising: variation-of-constants formula

\[ \ddot{q} = -Aq + g(q) \]

\[ A = \Omega^2 \text{ symmetric positive semi-definite, of large norm} \]

\[
\begin{pmatrix}
\Omega q(t) \\
\dot{q}(t)
\end{pmatrix}
= \begin{pmatrix}
\cos t\Omega & \sin t\Omega \\
-\sin t\Omega & \cos t\Omega
\end{pmatrix}
\begin{pmatrix}
\Omega q_0 \\
\dot{q}_0
\end{pmatrix}
\]

\[
+ \int_0^t \begin{pmatrix}
\sin(t - s)\Omega \\
\cos(t - s)\Omega
\end{pmatrix}
\begin{pmatrix}
g(q(s))
\end{pmatrix}
\, ds .
\]

discretize the integral \( \rightarrow \text{trigonometric integrators} \)

earliest references: Hersch 1958 and Gautschi 1961
Transformation to corotating variables

needed when frequencies and eigenspaces depend on time or state
illustrate the procedure for Schrödinger-type equations

\[ i\varepsilon \dot{\psi} = H(t)\psi, \quad H(t) \text{ hermitian} \]

transform \( \eta(t) = T_{\varepsilon}(t)\psi(t) \) for \( |t - t_0| \leq h \):

\[ \dot{\eta}(t) = S_{\varepsilon}(t)\eta(t) \quad \text{with} \quad S_{\varepsilon} = \dot{T}_{\varepsilon} T_{\varepsilon}^{-1} - \frac{i}{\varepsilon} T_{\varepsilon} HT_{\varepsilon}^{-1}. \]

simple first idea: freeze \( H(t) \approx H_\ast = H(t_0 + h/2) \), transform

\[ T_{\varepsilon}(t) = \exp \left( \frac{it}{\varepsilon} H_\ast \right) \quad \rightarrow \quad S_{\varepsilon}(t) = \mathcal{O}(h/\varepsilon) \]

step sizes restricted by \( h = \mathcal{O}(\varepsilon) \) in general!

Lawson 1967 and studied for oscillatory problems by
Corotating: adiabatic transformation

with diagonalized $H(t) = U(t) \Lambda(t) U(t)^*$, set

$$
\eta(t) = \exp\left(\frac{i}{\varepsilon} \Phi(t)\right) U(t)^* \psi(t) \quad \text{with} \quad \Phi(t) = \int_0^t \Lambda(s) \, ds,
$$

Born & Fock 1928
Corotating: ODE in adiabatic variables

with \( W(t) = \dot{U}(t)^* U(t) \) obtain

\[
\dot{\eta}(t) = \exp\left( -\frac{i}{\varepsilon} \Phi(t) \right) W(t) \exp\left( \frac{i}{\varepsilon} \Phi(t) \right) \eta(t)
\]

simple method: freeze slow \( \eta(t) \) and \( W(t) \), linear approximation to phases \( \Phi(t) \), then integrate exactly over the time step

\[ \Rightarrow \text{adiabatic integrator:} \]

\[
\eta_{n+1} = \eta_n + hB(t_{n+1}/2) \frac{1}{2}(\eta_n + \eta_{n+1}) \quad \text{with}
\]

\[
b_{jk} = \text{sinc}\left( \frac{h}{2\varepsilon} (\lambda_j - \lambda_k) \right) \exp\left( -\frac{i}{\varepsilon} (\phi_j - \phi_k) \right) w_{jk}
\]

+ more accurate methods  
\[ \text{Jahnke & L. 2003, Jahnke 2004} \]

need adaptive step sizes near avoided crossings of eigenvalues
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Mechanical systems with time-dep. frequencies

\[ H(p, q, t) = \frac{1}{2} p^T M(t)^{-1} p + \frac{1}{2\varepsilon^2} q^T A(t) q \]

approximately separate the fast and slow time scales by time-dependent canonical linear coordinate transformations done numerically by standard numerical linear algebra routines

end up with adiabatic variables, use adiabatic integrator

Chapter XIV in HLW
Canonical linear coordinate transformations

- Cholesky decomposition of $M(t) \rightarrow$ new mass matrix $= I$
- Eigendecomposition

$$A(t) = Q(t) \begin{pmatrix} 0 & 0 \\ 0 & \Omega(t)^2 \end{pmatrix} Q(t)^T,$$

$\Omega(t) = \text{diag}(\omega_j(t))$

splits positions $q = (q_0, q_1)$ and momenta $p = (p_0, p_1)$ into slow and fast variables

- rescale fast positions and momenta by $\varepsilon^{-1/2}$ and $\varepsilon^{1/2}$, resp.
- remove term $\varepsilon^{-1/2} q^T K(t) p$ by another canonical transform
Hamiltonian in the new coordinates

\[ H(p, q, t) = \frac{1}{2} p_0^T p_0 + \frac{1}{2\varepsilon} p_1^T \Omega(t)p_1 + \frac{1}{2\varepsilon} q_1^T \Omega(t)q_1 \]

\[ + q^T L(t)p + \frac{1}{2} q^T S(t)q \]

Equations of motion: with functions bounded uniformly in \( \varepsilon \),

\[ \dot{p}_0 = f_0(p, q, t) \]
\[ \dot{q}_0 = p_0 + g_0(q, t) \]

\[ \begin{pmatrix} \dot{p}_1 \\ \dot{q}_1 \end{pmatrix} = \frac{1}{\varepsilon} \begin{pmatrix} 0 & -\Omega(t) \\ \Omega(t) & 0 \end{pmatrix} \begin{pmatrix} p_1 \\ q_1 \end{pmatrix} \begin{pmatrix} f_1(p, q, t) \\ g_1(q, t) \end{pmatrix} \]

oscillatory part: \( 1/\varepsilon \times \) skew-symmetric matrix
Transform to adiabatic variables

diagonalize and consider the diagonal phase matrix $\Phi$:

$$
\begin{pmatrix}
0 & -\Omega(t) \\
\Omega(t) & 0
\end{pmatrix} = \Gamma i \Lambda(t) \Gamma^*, \quad \Gamma = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i \\ -i & i \end{pmatrix}
$$

$$
\Lambda(t) = \begin{pmatrix}
\Omega(t) & 0 \\
0 & -\Omega(t)
\end{pmatrix}, \quad \Phi(t) = \int_{t_0}^{t} \Lambda(s) \, ds
$$

adiabatic variables

$$
\eta = \varepsilon^{-1/2} \exp \left( -\frac{i}{\varepsilon} \Phi(t) \right) \Gamma^* \begin{pmatrix} p_1 \\ q_1 \end{pmatrix}
$$
Equations of motion in adiabatic variables

\[ \dot{p}_0 = -L_{00} p_0 - S_{00} q_0 - \varepsilon S_{01} Q_1 \eta \]
\[ \dot{q}_0 = p_0 + L_{00}^T q_0 + \varepsilon L_{10}^T Q_1 \eta \]

for the slow variables, and

\[ \dot{\eta} = \exp\left(-\frac{i}{\varepsilon} \Phi\right) W \exp\left(\frac{i}{\varepsilon} \Phi\right) \eta - P_1^* (L_{10} p_0 + S_{10} q_0) \]

for the adiabatic variables, where

\[ W = \Gamma^* \begin{pmatrix} -L_{11} & -\varepsilon S_{11} \\ 0 & L_{11}^T \end{pmatrix} \Gamma, \quad \begin{pmatrix} P_1 \\ Q_1 \end{pmatrix} = \Gamma \exp\left(\frac{i}{\varepsilon} \Phi\right). \]

Slow and fast degrees of freedom are only weakly coupled.
for separated frequencies $\omega_j(t)$, the functions $I_j = |\eta_j|^2$ are adiabatic invariants:

$$I_j(t) - I_j(0) = O(\varepsilon) \quad \text{for} \quad t = O(1)$$

$I_j$ is the action (energy divided by frequency)

$$I_j(t) = \frac{1}{\omega_j(t)} \left( \frac{1}{2} p_j(t)^2 + \frac{\omega_j(t)^2}{2\varepsilon^2} q_j(t)^2 \right).$$
1. Propagate the slow variables \((p_0, q_0)\) with a half-step of the symplectic Euler method: for the oscillatory function \(Q_1(t)\), replace the evaluation at \(t_{n+1/2}\) by the average

\[
Q_1^{-} \approx \frac{2}{h} \int_{t_n}^{t_{n+1/2}} Q_1(t) \, dt
\]

with linear phase approximation and analytic integration.

2. Propagate the adiabatic variable \(\eta\) with a full step of an adiabatic integrator.

3. Propagate the slow variables \((p_0, q_0)\) with a half-step of the adjoint symplectic Euler, with an appropriate average of \(Q_1\).

Approximation properties for \(t = O(1)\) in the original variables: 
\(O(h^2)\) in positions and \(O(h)\) in momenta uniformly in \(\varepsilon\) for \(h \leq \sqrt{\varepsilon}\)
Example

\[ A(t) = \left( \begin{array}{cc} t + 3 & \delta \\ \delta & 2t + 3 \end{array} \right)^2, \quad M(t) = I, \quad \varepsilon = 0.01 \]

Frequencies \( \omega_j \) (upper) and \( \| \dot{Q} \| \) (lower) for \( \delta = 1, 0.1, 0.01 \).
Adiabatic variables $\eta_j$ as functions of time.
Example: symmetric adaptive stepsize selection

Non-adiabatic transition: step sizes as function of $t$

Step size vs. time for $\delta = 2^0, 2^{-2}, 2^{-4}, 2^{-6}$
Motion under a strong constraining force

\[ H(p, q) = \frac{1}{2} p^T M(q)^{-1} p + \frac{1}{2\varepsilon^2} q_1^T A(q_0) q_1 \]

Methods and techniques for the time-dependent case can be extended to problems with state-dependent high frequencies again: series of canonical transformations to transform numerically to a system with nearly-separated slow and fast components difficulties with nearly crossing frequencies (Takens chaos)

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Lorenz 2006 Thesis, Chapter XIV in HLW
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