Geometric Numerical Integration

(Ernst Hairer, TU München, winter 2009/10)

Development of numerical ordinary differential equations

- **Nonstiff differential equations** (since about 1850), see [4, 2, 1]
  Adams (1855), multistep methods, problem of Bashforth (1883)
  Runge (1895) and Kutta (1901), one-step methods.
- **Stiff differential equations** (since about 1950), see [5, 2, 1]
  Dahlquist (1963), A-stability of multistep methods
  Gear (1971), backward differentiation code.
- **Geometric numerical integration** (since 1986), see [3, 7, 6]
  structure-preserving integration of differential equations,
  Hamiltonian, reversible, divergence-free, Poisson systems.

Provisional contents of the lectures

- Hamiltonian systems
  - symplectic transformations, theorem of Poincaré
  - generating functions
- Symplectic numerical integrators
  - Störmer–Verlet method
  - symplectic Runge–Kutta methods
  - composition and splitting methods
- Backward error analysis
  - long-time energy conservation
  - perturbed integrable Hamiltonian systems
- Hamiltonian systems on manifolds
  - constrained mechanical systems (DAE's)
  - numerical integrator RATTLE
- Differential equations with highly oscillatory solutions
  - Fermi–Pasta–Ulam type problems
  - modulated Fourier expansion

1 Hamiltonian system (double well potential)

Consider a differential equation

$$\ddot{q} = -\nabla U(q)$$

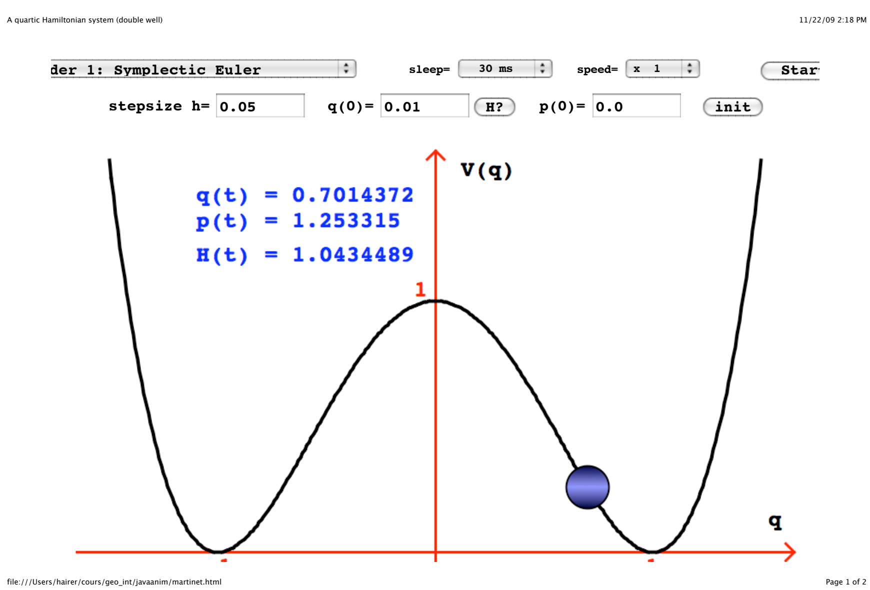
which can also be written as

$$\begin{aligned} \dot{q} &= p \\ \dot{p} &= -\nabla U(q) \end{aligned} \qquad \text{or} \qquad \begin{aligned} \dot{q} &= \nabla_p H(p,q) \\ \dot{p} &= -\nabla_q H(p,q) \end{aligned} \qquad \text{with} \quad H(p,q) = \frac{1}{2}\, p^{\mathsf{T}} p + U(q).$$

We have energy conservation along exact solutions:

$$H\big(p(t), q(t)\big) = Const$$

Numerical experiment with $U(q) = (q^2 - 1)^2$, taken from http://sma.epfl.ch/∼vilmart/



Explicit Euler

$$\begin{aligned} q_{n+1} &= q_n + h\, p_n \\ p_{n+1} &= p_n - h\, \nabla U(q_n) \end{aligned}$$

Symplectic Euler

$$\begin{aligned} q_{n+1} &= q_n + h\, p_n \\ p_{n+1} &= p_n - h\, \nabla U(q_{n+1}) \end{aligned} \qquad \text{or} \qquad \begin{aligned} q_{n+1} &= q_n + h\, p_{n+1} \\ p_{n+1} &= p_n - h\, \nabla U(q_n) \end{aligned}$$

2 N-body problem (planetary motion)

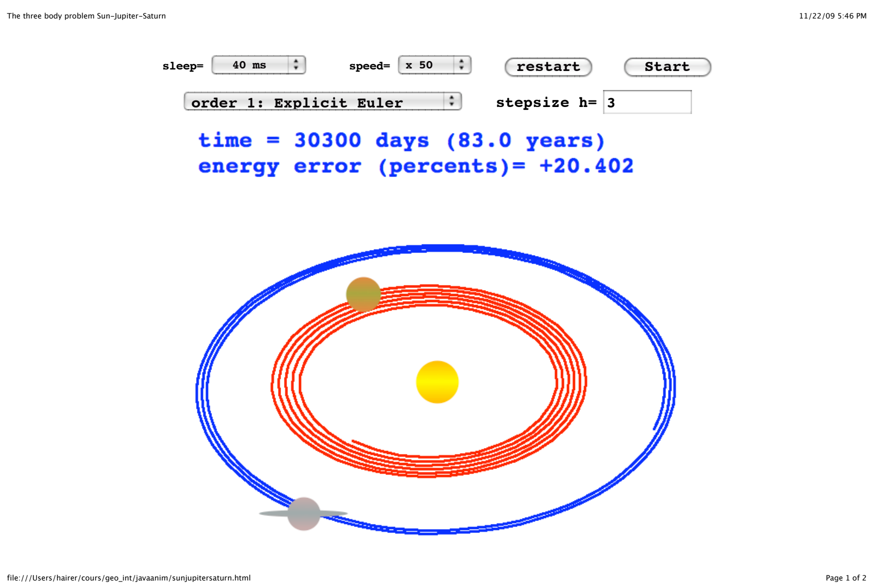
For $p_i, q_i \in \mathbb{R}^3$ we consider the Hamiltonian (kinetic plus potential energy)

$$H(p,q) \;=\; \frac{1}{2}\sum_{i=1}^{N} \frac{1}{m_i}\, p_i^{\mathsf{T}} p_i \;+ \sum_{1\le i<j\le N} U_{ij}\big(\|q_i - q_j\|\big)$$

with the gravitational potential

$$U_{ij}(r) = -G\,\frac{m_i\, m_j}{r}$$

Illustration: sun – jupiter – saturn (http://sma.epfl.ch/~vilmart/)



Conserved quantities (first integrals):

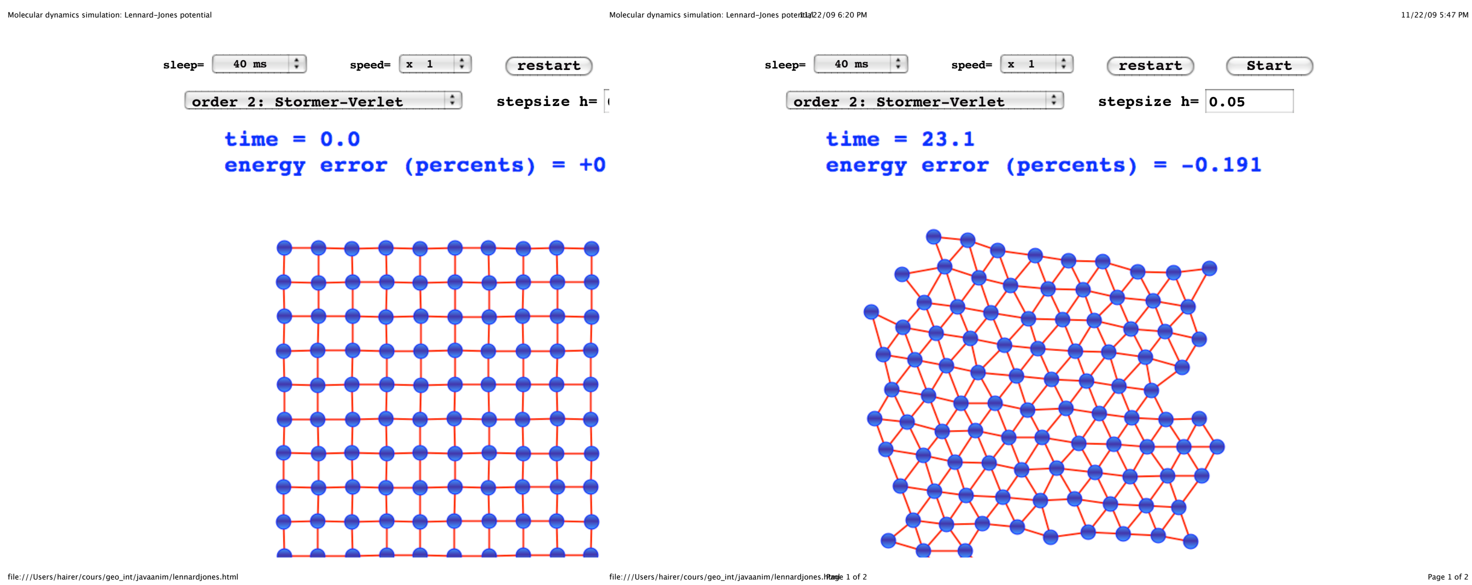
- Hamiltonian (total energy) $H(p,q)$
- linear momentum $P(p,q) = \sum_{i=1}^{N} p_i$
- angular momentum $L(p,q) = \sum_{i=1}^{N} q_i \times p_i$

3 N-body problem (molecular dynamics)

N-body problem as before, but with Lennard–Jones potential

$$U_{ij}(r) = 4\,\varepsilon_{ij}\Big(\Big(\frac{\sigma_{ij}}{r}\Big)^{12} - \Big(\frac{\sigma_{ij}}{r}\Big)^{6}\Big)$$

Numerical simulation with initial configuration (left picture) and solution after sufficiently long time (right picture), see http://sma.epfl.ch/∼vilmart/



4 Idea of backward error analysis

For a differential equation $\dot y = f(y)$ consider a numerical solution obtained by a one-step method $y_{n+1} = \Phi_h(y_n)$.

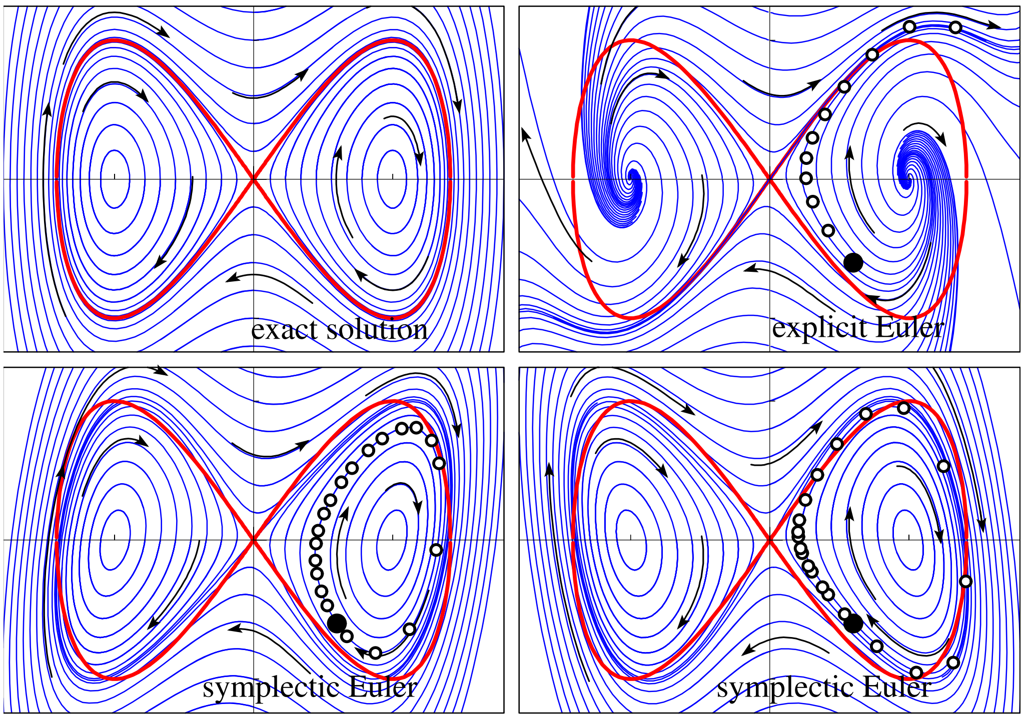
Find a **modified differential equation** $\dot y = f_h(y)$ of the form

$$\dot y = f(y) + hf_2(y) + h^2 f_3(y) + \ldots ,$$

such that its solution $\widetilde y(t)$ satisfies (formally) $y_n = \widetilde y(nh)$.

Numerical experiment with double well potential.

The following pictures show the exact solution (in phase space (q,p)) and solutions of the modified equation for various numerical integrators.



explicit in p, implicit in q explicit in q, implicit in p

Modified differential equation for explicit Euler:

$$\begin{pmatrix}\dot q\\ \dot p\end{pmatrix} = \begin{pmatrix}p\\ -U'(q)\end{pmatrix} + \frac{h}{2}\begin{pmatrix}U'(q)\\ U''(q)p\end{pmatrix} + \frac{h^2}{4}\begin{pmatrix}-2\,U''(q)p\\ 2\,U'U'' - U'''p^2\end{pmatrix} + \dots$$

Modified differential equation for symplectic Euler (expl. in q, impl. in p):

$$\begin{pmatrix}\dot q\\ \dot p\end{pmatrix} = \begin{pmatrix}p\\ -U'(q)\end{pmatrix} + \frac{h}{2}\begin{pmatrix}-U'(q)\\ U''(q)p\end{pmatrix} + \frac{h^2}{12}\begin{pmatrix}2\,U''(q)p\\ -2\,U'U'' - U'''p^2\end{pmatrix} + \dots$$

this modified equation is Hamiltonian with

$$\widetilde{H}(p,q) = \frac{1}{2}\,p^2 + U(q) - \frac{h}{2}\,U'(q)p + \frac{h^2}{12}\Big(U'(q)^2 + U''(q)p^2\Big) + \dots$$

5 Constrained mechanical system

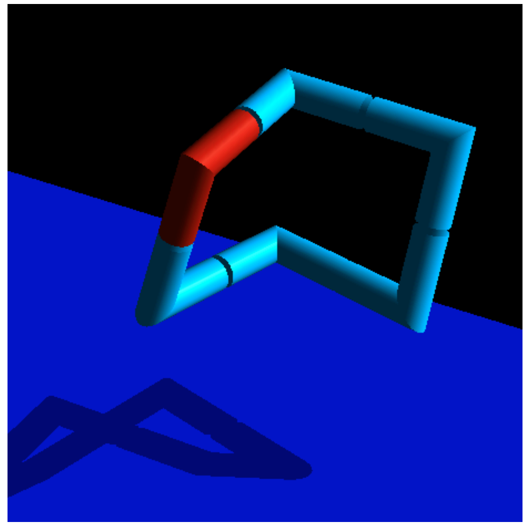
Position of corners

$q_i \in \mathbb{R}^3,\ i = 0, \ldots, 5$

$(6 \times 3 = 18$ variables)

Constraints

- motion of one piece (red) is prescribed, i.e., $q_0,\ q_1,\ q_2$ are fixed (9 conditions),
- distances between neighbor corners is unity (4 conditions),
- orthogonality between neighbor edges $(q_{n-1} - q_n) \perp (q_{n+1} - q_n)$ (5 conditions).



Graphics: J.-P. Eckmann & M. Hairer

Dynamics (red piece is fixed, corners have equal mass one, massless edges)

$$H(p,q) = \frac{1}{2} \sum_{i=3}^{5} p_i^{\mathsf{T}} p_i + \sum_{i=3}^{5} q_{iz},$$

where q_{iz} is the vertical component of q_i.

We obtain a differential-algebraic equation (DAE)

$$\begin{aligned} \dot{q}_i &= \nabla_{p_i} H(p,q) \\ \dot{p}_i &= -\nabla_{q_i} H(p,q) - G^{\mathsf{T}}(q)\lambda \\ 0 &= g(q) \end{aligned}$$

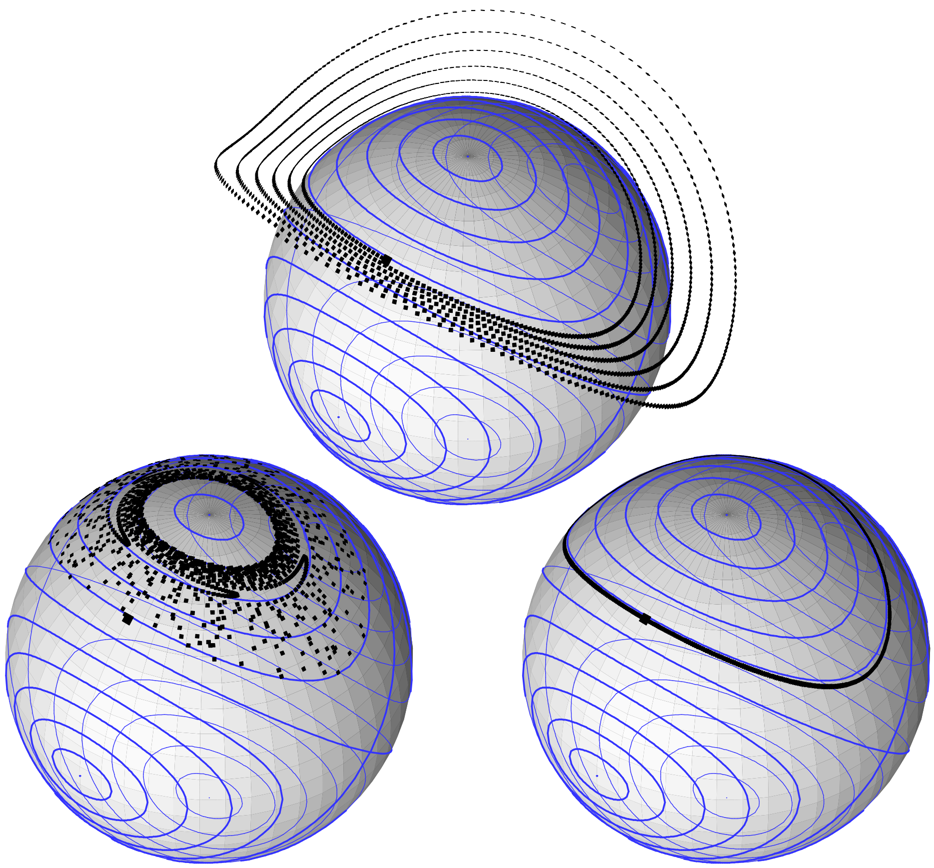
Here, q is the vector composed by $q_3,\ q_4,\ q_5$, $p = \dot{q}$ is the velocity, $g(q) = 0$ represents the 9 constraints for q, and $G(q) = g'(q)$ (matrix of dimension 9×9).

6 Euler's equations of motion for a free rigid body

The angular momentum vector $y = (y_1, y_2, y_3)^\mathsf{T}$ satisfies

$$\begin{aligned} \dot y_1 &= (I_3^{-1} - I_2^{-1})\, y_3\, y_2 \\ \dot y_2 &= (I_1^{-1} - I_3^{-1})\, y_1\, y_3 \\ \dot y_3 &= (I_2^{-1} - I_3^{-1})\, y_2\, y_1 \end{aligned} \qquad \text{or} \qquad \begin{pmatrix} \dot y_1 \\ \dot y_2 \\ \dot y_3 \end{pmatrix} = \begin{pmatrix} 0 & -y_3 & y_2 \\ y_3 & 0 & -y_1 \\ -y_2 & y_1 & 0 \end{pmatrix} \begin{pmatrix} y_1/I_1 \\ y_2/I_2 \\ y_3/I_3 \end{pmatrix}$$

Hamiltonian: $H(y) = \dfrac{1}{2}\Big(\dfrac{y_1^2}{I_1} + \dfrac{y_2^2}{I_2} + \dfrac{y_3^2}{I_3}\Big)$, Casimir: $C(y) = \dfrac{1}{2}\Big(y_1^2 + y_2^2 + y_3^2\Big)$



1st picture: integration with explicit Euler
2nd picture: trapezoidal rule with projection onto the sphere
3rd picture: implicit midpoint rule

References

[1] J. C. BUTCHER, *Numerical Methods for Ordinary Differential Equations*, John Wiley & Sons Ltd., Chichester, 2nd ed., 2008.

[2] P. DEUFLHARD AND F. BORNEMANN, *Numerische Mathematik 2*, de Gruyter Lehrbuch. [de Gruyter Textbook], Walter de Gruyter & Co., Berlin, revised ed., 2008. Gewöhnliche Differentialgleichungen. [Ordinary differential equations].

[3] E. HAIRER, C. LUBICH, AND G. WANNER, *Geometric Numerical Integration. Structure-Preserving Algorithms for Ordinary Differential Equations*, Springer Series in Computational Mathematics 31, Springer-Verlag, Berlin, 2nd ed., 2006.

[4] E. HAIRER, S. P. NØRSETT, AND G. WANNER, *Solving Ordinary Differential Equations I. Nonstiff Problems*, Springer Series in Computational Mathematics 8, Springer, Berlin, 2nd ed., 1993.

[5] E. HAIRER AND G. WANNER, *Solving Ordinary Differential Equations II. Stiff and Differential-Algebraic Problems*, Springer Series in Computational Mathematics 14, Springer-Verlag, Berlin, 2nd ed., 1996.

[6] B. LEIMKUHLER AND S. REICH, *Simulating Hamiltonian Dynamics*, Cambridge Monographs on Applied and Computational Mathematics 14, Cambridge University Press, Cambridge, 2004.

[7] J. M. SANZ-SERNA AND M. P. CALVO, *Numerical Hamiltonian problems*, vol. 7 of Applied Mathematics and Mathematical Computation, Chapman & Hall, London, 1994.