AMH Computational Methods in Applied Mathematics

Project 1B: Sympletic Integrator

Due date: Monday 5PM, 23 April 2012

Description

Hamiltonians of the form

\[ H = T(p_1, \ldots, p_N) + V(q_1, \ldots, q_N) \]

can be analysed using a split-step approach and alternating between the exact solutions of

\[ \dot{q}_i = \frac{\partial T}{\partial p_i} \quad i = 1, \ldots, N \]

and

\[ \dot{p}_i = -\frac{\partial V}{\partial q_i} \quad i = 1, \ldots, N. \]

The Fermi-Past-Ulam lattice models are a family of Hamiltonians that describe vibrating strings using a system of N interacting particles. The forces between neighbouring particles can be either linear or nonlinear. The FPU Hamiltonian can be written in the form

\[ H = \sum_{i=1}^{N} \left[ \frac{1}{2} p_i^2 + \frac{1}{2} (q_{i+1} - q_i)^2 + \frac{\alpha}{3} (q_{i+1} - q_i)^3 + \frac{\beta}{4} (q_{i+1} - q_i)^4 \right]. \]

For this project you may assume periodic boundary conditions \( q_{N+1} = q_1 \) and \( p_{N+1} = p_1 \) which correspond to a closed loop or string. When \( \alpha = \beta = 0 \) the system describes particles that interact via linear spring forces between nearest neighbour particles. Nonlinear springs are represented by adding cubic or quartic terms to the potential. Only weak nonlinearities with \( \alpha, \beta \ll 1 \) need be considered. Other related models are the Toda lattice

\[ H = \sum_{i=1}^{N} \left[ \frac{1}{2} p_i^2 + e^{q_{i+1} - q_i} \right] \]

and the diatomic Toda lattice

\[ H = \sum_{i=1}^{N} \left[ \frac{1}{2m_i} p_i^2 + e^{q_{i+1} - q_i} \right] \]

where the odd and even particles have slightly different masses \( m_{2i} = 1 + \epsilon \) and \( m_{2i+1} = 1 - \epsilon \).
Tasks

1. In no more than 2 or 3 pages, give a brief discussion of the Fermi-Pasta-Ulam problem and why the numerical results were unexpected (at the time). Also discuss the importance of the Toda lattice and its conservation laws.

2. Implement a symplectic integrator using a second-order split-step approach that can deal with any Hamiltonian of the form given above. It is recommended that you use a common main program but a separate function file for each potential/force.

3. Consider strings with $N = 32$ or $N = 64$ particles. Use an initial condition that corresponds to one of the linear modes of the string (eg. the fundamental mode is a half-period sine-wave). Verify that your numerical program reproduces the expected harmonic vibrational modes of a string when $\alpha = \beta = 0$.

4. Let $x_i = q_{i+1} - q_i$. Denote the Fourier transforms of $x_i$ and $p_i$ by $X_k$ and $P_k$ respectively. The energy in each vibrational mode $k$ is defined by

$$E_k = \frac{1}{2}|P_k|^2 + \frac{1}{2}|X_k|^2.$$ 

Verify that the energy in each vibrational mode is conserved if $\alpha = \beta = 0$.

5. Explore what happens when either $\alpha \neq 0$ or $\beta \neq 0$. Try initial conditions correspond to fundamental and other low order vibrational modes of the string. You should be able to reproduce the FPU result that the energy gradually moves into the other modes, but instead of reaching an equipartition between the modes, after a while almost all of the energy returns to the initial mode.

6. The Toda lattice is completely integrable and thus has $N$ independent conserved quantities. How closely are these quantities conserved by your program? Check the energy, total momentum and at least one of the other conservation laws.

7. Finally, explore and discuss what happens to the above observations for the unequal mass diatomic Toda lattice. Try very small differences in masses first (such as 1 or 2%).