ETH Zurich
Department of Mechanical and Process Engineering
Statistical Mechanics of Elasticity
Exercise 1 - Summer 2007

Institute for Mechanical Systems
Center of Mechanics
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Useful Definitions

Hamilton's Equations

The Hamiltonian H as a function of coordinates $\mathbf{q}_i$ and momenta $p_i = m_i \dot{q}_i$ of a system is most generally defined as the Legendre transform of its Lagrangian L,

$$H(\mathbf{p}, \mathbf{q}) = \sum_k \dot{q}_k p_k - L(\mathbf{q}, \dot{\mathbf{q}}). \tag{1}$$

For the systems we will consider, the Hamiltonian is equal to their total energy and can be written as

$$H(\mathbf{p}, \mathbf{q}) = K(\mathbf{p}) + V(\mathbf{q}), \tag{2}$$

where $K(\mathbf{p}) = \sum_i p_i^2 / 2m_i$ and $V(\mathbf{q})$ are the system's kinetic and potential energy, respectively. This property does not hold necessarily in case of e.g. moving geometrical constraints or time-dependent potentials. Once the Hamiltonian is known, the equations of motion can be obtained using

$$\dot{q}_i = \frac{\partial H}{\partial p_i}, \qquad \dot{p}_i = -\frac{\partial H}{\partial q_i}. \tag{3}$$

Explicit time integration schemes for the equations of motion

Consider the equation of motion of a single particle with mass m one degree of freedom x and a (time-dependent) force acting on it:

$$m\ddot{x}(t) = F(t). \tag{4}$$

Given the state of the system at time t (and possibly $t - \Delta t$), we now look for ways to obtain $x^{n+1} = x(t + \Delta t)$ and $v^{n+1} = v(t + \Delta t)$ where $v = \dot{x}$.

Forward Euler

For the given problem with a linear spring, the Forward Euler scheme is unconditionally unstable.

Variant of Newmark

Following directly from the Taylor series, an approximation of (4) is:

$$\begin{aligned} x^{n+1} &= x^n + \Delta t \cdot v^n + \frac{\Delta t^2}{2} \frac{F^n}{m}, \\ v^{n+1} &= v^n + \Delta t \frac{F^n}{m}. \end{aligned} \tag{5}$$

This coincides with an (unusual) Newmark's scheme for $\beta = 0$ and $\gamma = 0$.

Classical Verlet

A second-order approximation of (4) is:

$$\begin{aligned} x^{n+1} &= 2x^n - x^{n-1} + \Delta t^2 \frac{F^n}{m}, \\ v^n &= \frac{x^{n+1} - x^{n-1}}{2\Delta t}, \end{aligned} \tag{6}$$

where the velocity is not needed for the integration and is (inconveniently) only obtained at the previous step.

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Velocity Verlet

A variation of the classical Verlet algorithm that allows an accurate update of the velocity is given by:

$$\begin{aligned} x^{n+1} &= x^n + \Delta t \cdot v^n + \frac{\Delta t^2}{2}\frac{F^n}{m}, \\ v^{n+1} &= v^n + \frac{\Delta t}{2}\left(\frac{F^n}{m} + \frac{F^{n+1}}{m}\right). \end{aligned} \tag{7}$$

Problem 1

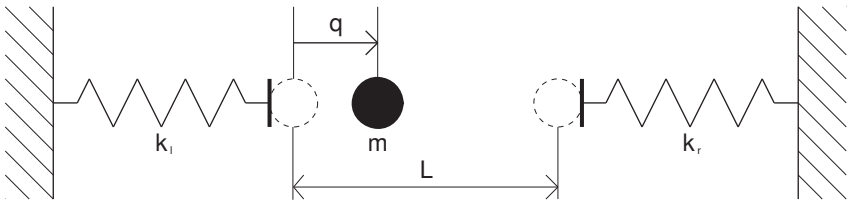

Figure 1: A particle confined between two massless springs (show in undeformed state).

Given is a rigid mass m whose position is described by the coordinate q. It is bouncing back and forth one-dimensionally between two massless springs of stiffnesses $k_l = 2$ and $k_r = 3$. Between the impacts with the springs the free path of the mass has length $L = 1$ as shown in Figure 1.

a) Derive the Hamiltonian $H(p, q)$ of the system.

b) Use Hamilton's equations to obtain the equations of motion from $H(p, q)$.

c) Sketch $q(t)$ for $0 \leq t \leq T$, where T is one period of the system if its total energy is E.

d) Derive and sketch the trajectory of the given system in phase space if its total energy is E.

Homework 1

Consider the system treated already in **Problem 1** . Download the compressed Matlab-files *hw1.zip* that are an incomplete (one-dimensional) *molecular dynamics* code meant to compute and plot the time evolution of the given system in two-dimensional phase space (see example given in Weiner, p. 82).

a) Place two replicas of the system at $q = 0$ and $p = 1.25$ (just set $q_{min} = q_{max} = 0$, $p_{min} = p_{max} = 1.25$, $n_q = 2$ and $n_p = 1$). Use the described *Variant of Newmark* for the integration of the trajectory of one of the two particles and calculate the other's motion using *Velocity-Verlet* for $nstep = 10,000$ steps up to a time of $T = 100$. Store the total energy of both particles at each timestep. Plot the evolution of the energies and the final positions of both particles at $t = T$.

b) Now populate the phase space with a 20×20 equidistant grid of replicas lying between $q_{min} = 0$ and $q_{max} = 0.5$ on the coordinate axis and between $p_{min} = 1$ and $p_{max} = 1.5$ on the momentum axis. Use *Velocity-Verlet* to

calculate the evolution of the replicas for $T = 15$ using $nstep = 1000$ steps. The initial configuration is shown in Figure 2 (right). Plot the final configuration. The volume of the chosen ensemble should be preserved in phase space (Liouville's theorem).

c) Now populate the space with $n = 500$ equidistant replicas lying at $q = 0$ on the coordinate axis and between $p_{min} = 1$ and $p_{max} = 1.5$ on the momentum axis and let them evolve for $T = 1000$ using $nstep = 100,000$ (You might want to let this run overnight). If your computational ressources (or your time) don't allow this, reduce n, T and $nstep$ accordingly. The initial configuration is shown in Figure 2 (left). Plot the final configuration. The whole (accessible) phase space should be uniformly covered with replicas of the system (property of mixing, guarantees ergodicity).

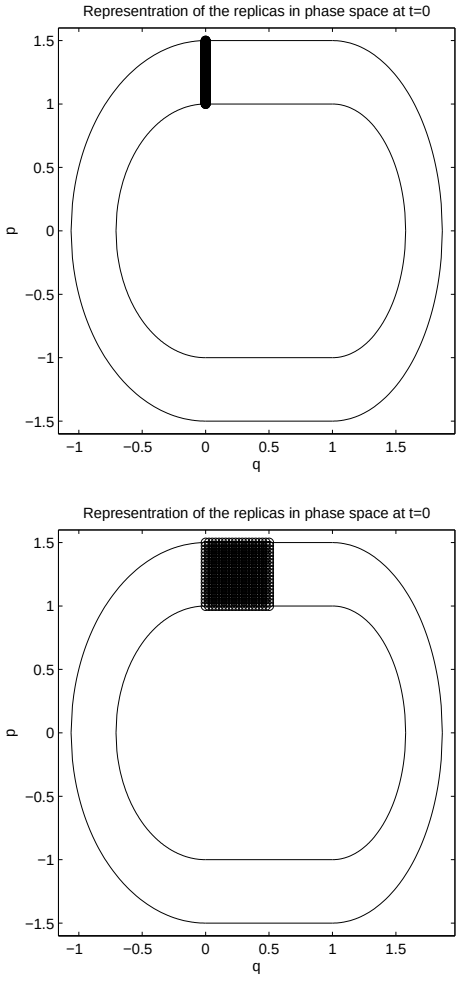

Figure 2: Initial setups for b) (left) and c) (right).

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