nevh: Numerical Evolution from the Hamiltonian

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1 Introduction

This package computes the trajectories of mechanical systems given their hamiltonian function and initial state alone.

The partial derivatives of the hamiltonian in order to the q's and p's are estimated numerically and their values used to set up and solve the time ODE.

2 Hamilton's Equations

The physical state of a system with N_f degreees of freedom is completely specified given the values of $2N_f$ variables q_i (coordinates) and p_i (momentums) $i = 1,\ldots,N_f$. Its time evolution is determined by the Hamilton's Equations,

$$\dot{q}_i = \frac{\partial H}{\partial p_i} \qquad\qquad \dot{p}_i = -\frac{\partial H}{\partial q_i}, \tag{1}$$

where $H = H(t,q,p)$ is the hamiltonian of the system which, in many situations, is simply the toal mechanical energy of the system, $H = T + U$. Once the partial derivatives in the rhs of Hamilton's equations are known, they define a system of $2N_f$ first order simultaneous ordinary differential equations (ODE) in time for the q's and the p's. The solution of this system is the trajectory (in phase space) followed by the system in its evolution.

In most cases, the above mentioned system of ODEs must be solved numerically, and a large number of computer packages, for all significant computer languages have been developed to do that. Here, we take this numerical approach a step further, and compute the partial derivatives of the hamiltonian also numerically. With this approach, the evolution of the system can be obtained from the hamiltonian alone, saving the need for the derivation of the right hand sides of the Hamilton's equations.

3 Hamilton's Equations in Numerical Form

Hamilton's Equations can be set in a more compact (and more suitable for numerical resolution using standard routines or in the current approach) form,

$$\dot{\psi} = f(t,\psi), \tag{2}$$

where $\psi = (\psi_1, \psi_2, \ldots, \psi_{2N_f}) = (q_i, p_i)$, $i = 1, \ldots N_f$ and

$$f(t,\psi) = \begin{pmatrix} \mathbb{0} & \mathbb{1} \\ -\mathbb{1} & \mathbb{0} \end{pmatrix} \nabla_\psi H(t,\psi). \tag{3}$$

Here, $\mathbb{0}$ and $\mathbb{1}$ represent the $N_f \times N_f$ zero matrix and identity matrix, respectively, and

$$\nabla_\psi H = \left(\frac{\partial H}{\partial \psi_1}, \frac{\partial H}{\partial \psi_2}, \ldots, \frac{\partial H}{\partial \psi_{2N_f}} \right).$$