Investigation on numeric methods solving heteroclinic trajectories in Hamilton systems

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Heteroclinic Trajectory

Here we restrict the topic to Hamiltonian systems, i.e. looking for a solution $(q(t), p(t)), -\infty \leq t \leq +\infty$ such that

$$\begin{cases} \dot{q} & = \dfrac{\partial H}{\partial p} \\ \dot{p} & = -\dfrac{\partial H}{\partial q} \end{cases}, \tag{1}$$

while the boundary conditon is

$$\nabla H(q(-\infty), p(-\infty)) = \nabla H(q(+\infty), p(+\infty)) = 0.$$

Gradient System - Special example

A simple system is proposed as

$$H_1 = \frac{1}{2}p^2 + p\left(q - q^3\right). \tag{2}$$

The analytical solution to Eqn 2 is

$$\begin{cases} q\left(t\right) &= -\frac{1}{\sqrt{1+\exp(2t)}} \\ p\left(t\right) &= 2\left(q\left(t\right)^3 - q\left(t\right)\right) \end{cases}.$$

Gradient System - Generalized

System described by Eqn 2 can be easily extended to higher dimensions, such as

$$H_2 = \frac{1}{2}\sum_{i=1}^{2} p_i^2 + \sum_{i=1}^{2} p_i \left(q_i - q_i^3\right) + \left[\left(q_2^2 - 1\right) q_1^2 - L\left(q_1^2 - 1\right) q_2^2\right]^2, \tag{3}$$

of which the solution is

$$(q_1, q_2, p_1, p_2) = \left(q_2\sqrt{\frac{L}{1+(L-1)\,q_2^2}}, \frac{1}{\sqrt{1+\exp(2t)}}, 2\left(q_1^3 - q_1\right), 2\left(q_2^3 - q_2\right)\right).$$

Cluster example

The system is a gradient one (see [Dellago et al., 1998]), proposed as

$$H = \frac{1}{2} p^T \cdot p + \nabla V^T \cdot p, \tag{4}$$

where

$$V = \sum_{i<j} v\left(r_{ij}\right), v\left(r\right) \triangleq 4\left(r^{-12} - r^{-6}\right).$$

Arclength parameterization

Suppose the solution can be arclength-parameterized, i.e.

$$S \triangleq \int_{-\infty}^{+\infty} \sqrt{\left(\frac{d}{dt} q\right)^2 + \left(\frac{d}{dt} p\right)^2} dt < \infty.$$

Thus a arclength mapping $s(t)$ can be defined as

$$s(t) \triangleq \frac{1}{S} \int_{-\infty}^{t} \sqrt{\left(\frac{d}{dt_1} q\right)^2 + \left(\frac{d}{dt_1} p\right)^2} dt_1. \tag{5}$$

We define $\widehat{q}$ and $\widehat{p}$ accordingly:

$$\widehat{q}(s) \triangleq q\left(t^{-1}(s)\right)$$
$$\widehat{p}(s) \triangleq p\left(t^{-1}(s)\right)$$

Local linearization

Introduce $\delta\widehat{q}(s) = \widehat{q}(s) - \widehat{q}(0), \delta\widehat{p}(s) = \widehat{p}(s) - \widehat{p}(0)$ and use Taylor expansion

$$\frac{d}{ds}\widehat{q}(s) = \left[H_{pq}\left(\widehat{q}(0), \widehat{p}(0)\right) \cdot \delta_0\widehat{q}(s) + H_{pp}\left(\widehat{q}(0), \widehat{p}(0)\right) \cdot \delta_0\widehat{p}(s) + \boldsymbol{O}\left(s^2\right)\right] \cdot \frac{dt}{ds} \tag{6}$$

$$\frac{d}{ds}\widehat{p}(s) = -\left[H_{qq}\left(\widehat{q}(0), \widehat{p}(0)\right) \cdot \delta_0\widehat{q}(s) + H_{qp}\left(\widehat{q}(0), \widehat{p}(0)\right) \cdot \delta_0\widehat{p}(s) + \boldsymbol{O}\left(s^2\right)\right] \cdot \frac{dt}{ds} \tag{7}$$

by using the fact that $\nabla H\left(\widehat{q}(0), \widehat{p}(0)\right) = 0$.

Local linearization

It implies that $\lim_{s\to 0}$ **normal** $\left(\delta_0 \widehat{q}\left(s\right), \delta_0 \widehat{p}\left(s\right)\right) = (u, v)$ is the eigen vector of the following eigen problem:

$$\lambda_0 \begin{bmatrix} u \\ v \end{bmatrix} = L_H\left(\widehat{q}\left(0\right), \widehat{p}\left(0\right)\right) \begin{bmatrix} u \\ v \end{bmatrix}, \tag{8}$$

$$L_H \triangleq \begin{bmatrix} \partial_{pq} & \partial_{pp} \\ -\partial_{qq} & -\partial_{qp} \end{bmatrix} H. \tag{9}$$

For λ_0, the eigenvalue should be the most positive since it dominates the limit.

Algorithm

S is not known beforehand. To address this, we can approxiamte that by

1. Choose a proper starting direction (u, v), which is a eigen vector. Assign $x_0 = (u, v) \cdot \Delta h + (q(-\infty), p(-\infty))$.
2. Based on $x_n = (\widetilde{q}(\widetilde{s}_n), \widetilde{p}(\widetilde{s}_n)), \widetilde{s}_n = n\Delta h$, calculate the update direction using an ODE integrator.
3. Determine if x_{n+1} is close to $(q(+\infty), p(+\infty))$ enough. If not, continue to Step 2.

Choice of the Initial Direction

- If $L_H\left(\widehat{q}(0), \widehat{p}(0)\right)$ has only one most positive eigenvalue λ_+, the direction is the corresponding eigen vector.
- If not, we can have a grid search in the space $\operatorname{Ker}\left(\lambda_+ I - L_H\left(\widehat{q}(0), \widehat{p}(0)\right)\right)$ by its coordinate form.

ODE Integrator

- Forward Euler
- Symplectic schemes
  - Mid-point Euler with estimation-correction
  - Implicit Runge-Kutta

Numerical Experiments

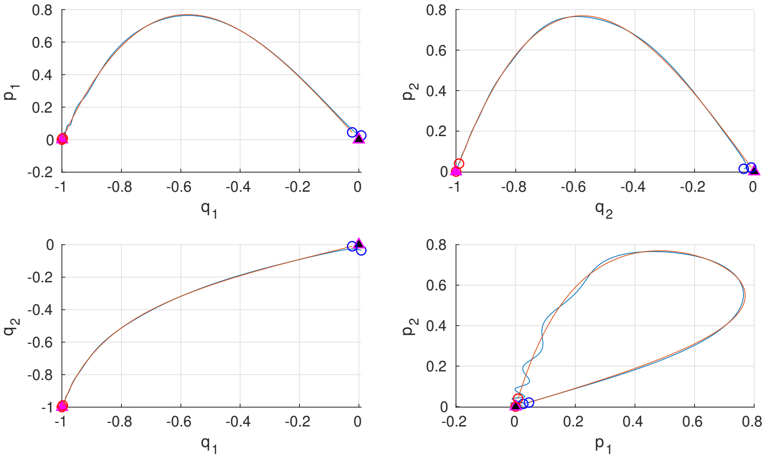

Figure: Solution obtained numerically(blue line) and analytically(red line). Notice that the solution starts to be unstable when reaching $s \to 1$(red circle).

Numerical Experiments

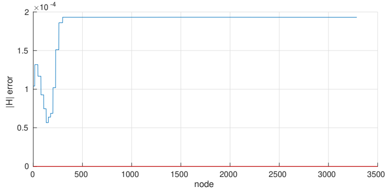

Figure: Estimating the error by measuring $|H|$.

Problems

- In general not quite as stable as the previous example.
- Illposedness near the steady points.

An observation

If the system is merely more than a gradient system, i.e.

$$H = \frac{1}{2}p^T p + b(q)^T p + l(q), b = \nabla V,$$

which leads to

$$\begin{cases} \dot{q} & = \dfrac{\partial H}{\partial p} = p + b \\ \dot{p} & = -\dfrac{\partial H}{\partial q} = -\left((\nabla b)^T p + \nabla l \right) \end{cases}, \tag{10}$$

we can explicitly solve p by the first line in Eqn 10 and take that into the second line, giving

$$\left(\nabla b - \nabla b^T \right) \dot{q} = \ddot{q} - \nabla b^T \cdot b + \nabla l.$$

In gradient systems

The vector gradient

$$\nabla b = \Delta V$$

will be symmetric,which leads to a second-order ODE

$$0 = \ddot{q} - \nabla b^T \cdot b + \nabla I. \tag{11}$$

ODE to PDE

Non-moving travelling wave solution to the following PDE:

$$\partial_t q = \partial_x^2 q - \nabla b^T \cdot b + \nabla I. \tag{12}$$

This can be interpreted as a "heat equation" with a reaction term $-\nabla b^T \cdot b + \nabla I$.

Boundary Conditions

There are roughly two conditions to choose: Dirichlet and Neumann condition.

- Dirichlet condition: $q(-A,t) = q_{-\infty}, q(+A,t) = q_{+\infty}$.
- Neumann condition: $\partial_x q(-A,t) = \partial_x q(+A,t) = 0$.

Update Scheme

We included the following three schemes (donoting $f(q) \triangleq -\nabla b^T \cdot b + \nabla l$)

- Forward Euler (explicit scheme):

$$\frac{\Delta_{+\tau}}{\tau}(q(x,t)) = \frac{\delta_h^2}{h^2}(q(x,t)) + f(q(x,t)). \tag{13}$$

- Backward Euler (implicit scheme):

$$\frac{\Delta_{+\tau}}{\tau}(q(x,t)) = \frac{\delta_h^2}{h^2}(q(x,t+\tau)) + f(q(x,t+\tau)).$$

- Crank-Nicolson (implicit scheme)

Stop Criterion

- Use $\left|H\left(q\left(\xi\right),p\left(\xi\right)\right)\right|_{\infty}$ as an indication.
- To obtain H, we have to obtain $p\left(\xi\right)$ by

$$p\left(\xi\right)=\dot{q}\left(\xi\right)-b\left(q\left(\xi\right)\right). \tag{14}$$

Change in coordinate

- One feasible mapping is the arctan function:

$$\mathring{q}\left(y,t\right) \triangleq q\left(\tan\left(x\right),t\right).$$

- To tranform Eqn 14 into coordinate (y,t),

$$\frac{\partial^2}{\partial x^2}q = \left(\frac{\partial^2}{\partial y^2}\mathring{q}\right)\cdot\left(\frac{dy}{dx}\right)^2 - \left(\frac{\partial}{\partial y}\mathring{q}\right)\cdot\left(\frac{d^2x}{dy^2}\right)\cdot\left(\frac{dy}{dx}\right)^3 \tag{15}$$

$$= \left(\frac{\partial^2}{\partial y^2}\mathring{q}\right)\cos^4\left(y\right) - 2\left(\frac{\partial}{\partial y}\mathring{q}\right)\sin\left(y\right)\cos\left(y\right)^3.$$

Numerical Experiment 1 - which boundary condition

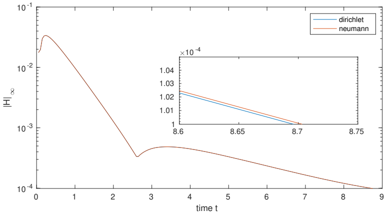

Figure: ∞-norm error in the hamiltonian. Inset: a close look at where the stop criterion is about to be statisfied. The x-domain is grid$(-6, 6, 1/16)$.

Numerical Experiment 1 - spacial resolution

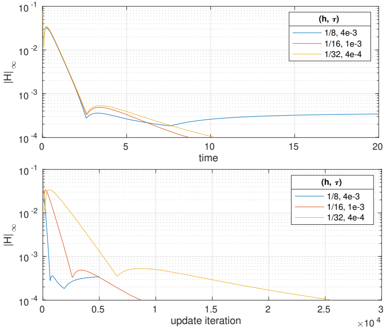

Figure: ∞-norm error in the hamiltonian when using different space discretization step.

Numerical Experiment 1 - implicit or explicit

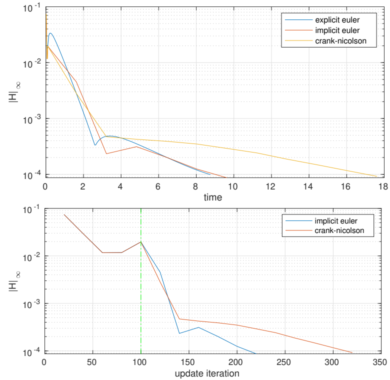

Figure: ∞-norm error in the hamiltonian when using different update schemes. Green dashed line indicates that we assume the solution is close enough so that implicit method can take on over explicit methods.

Numerical Experiment 1 - coordinate transform

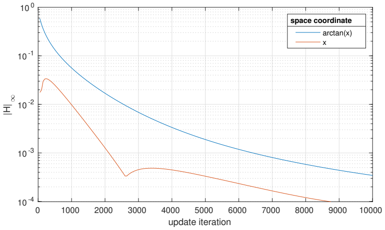

Figure: Comparison between two space coordinates choices. A change in space coordinate does require more calculation, but we can use less nodes and achieve faster speed (0.694s compared to 0.726s when there is no such change).

Numerical Experiment 1 - coordinate transform

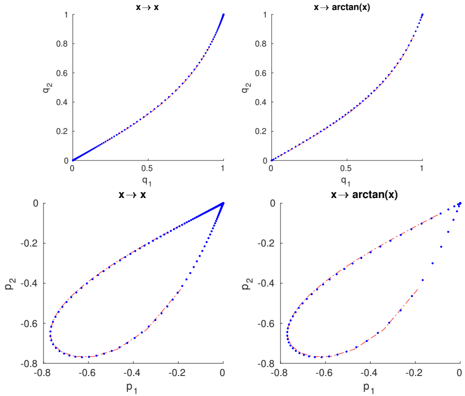

Figure: Comparison between solution obtained under different space coordinate settings. Red dashed line indicates the analytical solution. Nodes on the right side plots are much separated.

Numerical Experiment 1 - coordinate transform

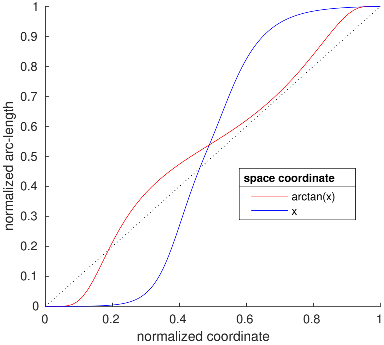

Figure: Relation between normalized space coordinate and normalized arc-length. Back dotted line indicates perfect arc-length parameterization.

Numerical Experiment 2

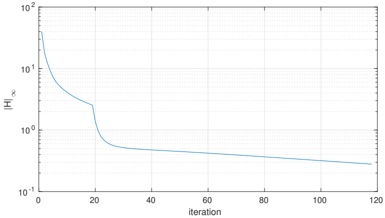

Figure: ∞-norm error in the hamiltonian. $(h,\tau) = \left(\frac{1}{8}, 10^{-5}\right)$, time update scheme: explicit Euler. Total time used for 2000 iterations: 75.80s.

Numerical Experiment 2 - Potential

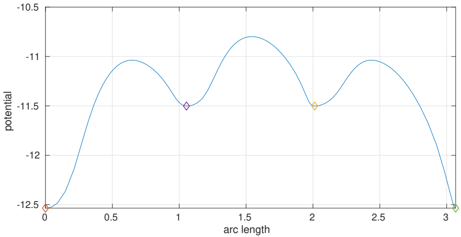

Figure: Potential changing along the arc length parameter. From left to right: A(red), B(purple), C(yellow), D(green).

Numerical Experiment 2 - Structures

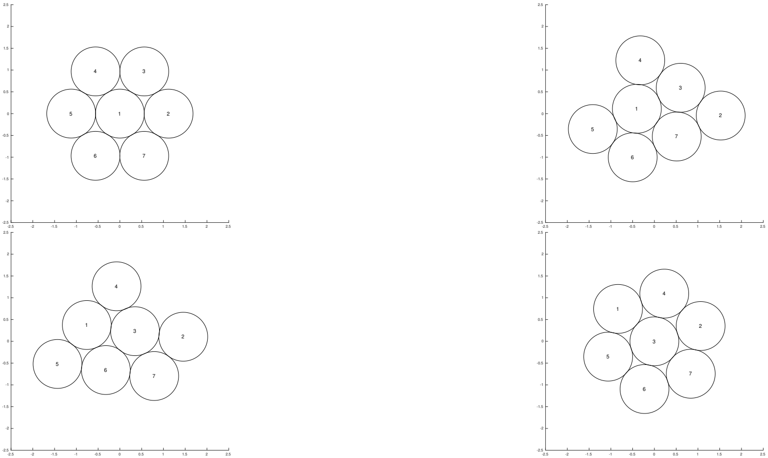

Figure: From left to right, top to bottom: configuration A(left-top), B(right-top), C(left-bottom), D(right-bottom).

References

Dellago, C., Bolhuis, P. G., and Chandler, D. (1998).
Efficient transition path sampling: Application to lennard-jones cluster rearrangements.
The Journal of Chemical Physics, 108(22):9236–9245.