Notes on a Symplectic Classical Trajectory Integrator

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Based on Brewer, Hulme, & Manolopoulos JCP 106 (1997) 4832 Appendix

- allows us to calculate both the action and the monodromy matrix

$$S = \int_0^t dt' \, T(\vec{p}) - V(\vec{q}) \qquad (i)$$

$$M = \begin{pmatrix} M_{pp} & M_{pq} \\ M_{qp} & M_{qq} \end{pmatrix} = \begin{pmatrix} \frac{\partial \vec{P}}{\partial \vec{p}} & \frac{\partial \vec{P}}{\partial \vec{q}} \\ \frac{\partial \vec{Q}}{\partial \vec{p}} & \frac{\partial \vec{Q}}{\partial \vec{q}} \end{pmatrix} \qquad (ii)$$

where $(p,q) = (p_0, q_0)$

$(P,Q) = (p_t, q_t)$

From Newton:

$$\dot{p} = -\frac{\partial V}{\partial q} \; ; \quad \dot{q} = \frac{\partial T}{\partial p} \qquad (iii)$$

from (i):

$$\dot{S} = T(p) - V(q) \qquad (iv)$$

from (ii) & (iii):

$$\cancel{\dot{M}_{pp} = \frac{\partial}{\partial t}\frac{\partial P}{\partial p} = \frac{\partial}{\partial p}\frac{\partial P}{\partial t} =}$$

$$\dot{M}_{pp} = -\frac{\partial^2 V}{\partial q^2} M_{qp} = -\frac{\partial^2 V}{\partial q^2}\frac{\partial Q}{\partial p} \qquad \dot{M}_{qp} = -\frac{\partial^2 V}{\partial q^2} M_{qq}$$

$$\dot{M}_{qp} = \frac{\partial^2 T}{\partial p^2} M_{pp} \qquad \dot{M}_{qq} = \frac{\partial^2 T}{\partial p^2} M_{pq}$$

prove these

Ideally, we want an integration strategy which preserves the symplectic property of the monodromy matrix:

$${}^tM J M = J \qquad \text{w/ } J = \begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix}$$

we do this by integrating according to the following scheme

$$p_k = p_{k-1} - b_k \frac{\partial V(q_{k-1})}{\partial q_{k-1}} \quad ; \quad q_k = q_{k-1} + a_k \frac{\partial T(p_k)}{\partial p_k}$$

$$S_k = S_{k-1} + a_k T(p_k) - b_k V(q_{k-1})$$

$$(M_{pp})_k = (M_{pp})_{k-1} - b_k \frac{\partial^2 V(q_{k-1})}{\partial q_{k-1}^2} (M_{qp})_{k-1} \, ; \quad (M_{pq})_k = (M_{pq})_{k-1} - b_k \frac{\partial^2 V(q_{k-1})}{\partial q_{k-1}^2} (M_{qq})_{k-1}$$

$$(M_{qp})_k = (M_{qp})_{k-1} + a_k \frac{\partial^2 T(p_k)}{\partial p_k^2} (M_{pp})_k \quad ; \quad (M_{qq})_k = (M_{qq})_{k-1} + a_k \frac{\partial^2 T(p_k)}{\partial p_k^2} (M_{pq})_k$$

for $k = 1, \dots, m$

This scheme will preserve the symplectic property for any coefficients a_k, b_k, but accuracy of the algorithm depends on a good choice of coefficients.

A good set, due to Gray (& Manolopoulos, apparently) is:

k	a_k	b_k
1	$\frac{1}{2}\left(1-\sqrt{\frac{1}{3}}\right)\Delta t$	0
2	$\sqrt{\frac{1}{3}}\,\Delta t$	$\frac{1}{2}\left(\frac{1}{2}+\sqrt{\frac{1}{3}}\right)\Delta t$
3	$-\sqrt{\frac{1}{3}}\,\Delta t$	$\frac{1}{2}\Delta t$
4	$\frac{1}{2}\left(1+\sqrt{\frac{1}{3}}\right)\Delta t$	$\frac{1}{2}\left(\frac{1}{2}-\sqrt{\frac{1}{3}}\right)\Delta t$

Actually, these parameters are apparently due to Candy and Rozmus, J. ~~Comput.~~ Computational Phys. 92 230-256 (1991)

Coding up Manolopoulos's Symplectic Integrator

time_step

$k=1,\ldots,4$:

$$p_k = p_{k-1} + b_k \, dt \, \dot{p}_{k-1}$$

$$q_k = q_{k-1} + a_k \, dt \, \dot{q}_k$$

action_time_step

$k=1,\ldots,4$:

$$S_k = S_{k-1} + a_k T_k - b_k V_{k-1}$$

monodromy_time_step

$k=1,\ldots,4$

$$(M_{pp})_k = (M_{pp})_{k-1} - b_k \, \text{hessian}(\text{sys}_{k-1}) \, (M_{qp})_{k-1}$$

$$(M_{pq})_k = (M_{pq})_{k-1} - b_k \, \text{hessian}(\text{sys}_{k-1}) \, (M_{qq})_{k-1}$$

$$(M_{qp})_k = (M_{qp})_{k-1} + a_k \left(\frac{\partial^2 T}{\partial p^2}\right)_k (M_{pp})_k$$

$$(M_{qq})_k = (M_{qq})_{k-1} + a_k \left(\frac{\partial^2 T}{\partial p^2}\right)_k (M_{pq})_k$$

update M_{px} before updating q

update M_{qx} after updating p

note: need to change if $V(p,q)$ or $T(p,q)$

things to add to md.h

- pot→T
- pot→hessian
- pot→d2Tdp2

- sys→S
- sys→Mpp
- sys→Mpq
- sys→Mqp
- sys→Mqq