Kharagpur Lectures

Numerical Accuracy, Error Control and Applications

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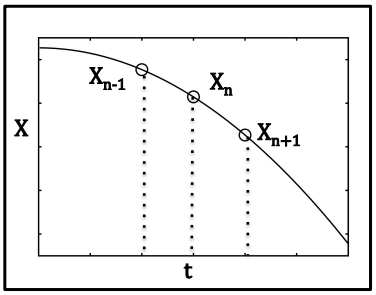
Outline

1. Integration Methods and Accuracy
   Accuracy checks with the harmonic oscillator or a benchmark problems
   Symplectic Integrators for Hamiltonian Systems
   Runge-Kutta Integrators for NonHamiltonian Systems
2. Cell Model evaluation of integration techniques
3. Predictor-Corrector Methods
   Milne method
   Gear predictor-Corrector
4. Stiff Differential Equations :
   The Nosé Oscillator
   Adaptive Integration
5. Addendum
   Periodic orbits for the Nosé and Nosé-Hoover oscillator
   Regular and Chaotic Orbits for the springy pendulum

1. Integration Methods and Accuracy

Numerical Approximations with Taylor's Series at t_n



Carl Störmer

$$x(t_{n+1}) = x(t_n) + \Delta t\frac{dx}{dt} + \frac{(\Delta t^2)}{2!}\frac{d^2x}{dt^2} + \frac{(\Delta t^3)}{3!}\frac{d^3x}{dt^3} + O(\Delta t^4)$$

$$x(t_{n-1}) = x(t_n) - \Delta t\frac{dx}{dt} + \frac{(\Delta t^2)}{2!}\frac{d^2x}{dt^2} - \frac{(\Delta t^3)}{3!}\frac{d^3x}{dt^3} + O(\Delta t^4)$$

$$x(t_{n+1}) - 2x(t_n) + x(t_{n-1}) = \Delta t^2 F(x_n) + O(\Delta t^4)$$

Second-Order Symplectic Integration Algorithms

Harmonic oscillator : $\dot{q} = p$; $\dot{p} = -q$; $(q,p)_0 = (1,0)$

Solve one second order equation or two first order equations :

$\frac{d^2x}{dt^2} = F(x)$ $\qquad$ $\frac{dx}{dt} = \mathrm{v}$; $\frac{d\mathrm{v}}{dt} = F(x)$.

Störmer-Verlet .

$$x_{n+1} = 2x_n - x_{n-1} + dt^2\, F(x_n)$$

Leapfrog ; 3 stages .

$$x_n = x_{n-1} + \mathrm{v}_{n-(1/2)}\, dt\,;$$

$$a_n = F(x_n)\ ;$$

$$\mathrm{v}_{n+(1/2)} = \mathrm{v}_{n-(1/2)} + a_n dt\,.$$

The Stormer-Verlet difference equation can be solved analytically :

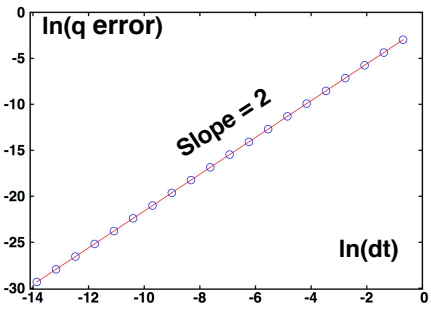
$$q_0 = e^{i\omega 0}\ ;\ q_{+1} = e^{i\omega dt}\ ;\ q_{-1} = e^{i\omega(-dt)}\ ;$$

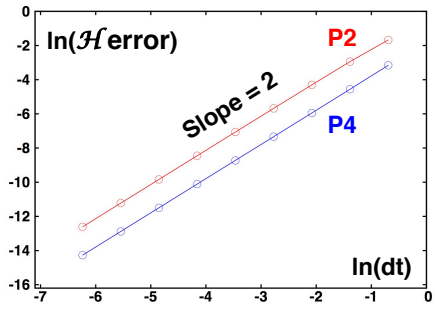
$$\omega = (1/dt)\ cos^{-1}(1 - dt^2/2\,)$$

Then $q\ error = max\left(\sqrt{(cos(time) - cos\,(\omega j dt))^2}\ \right)$

Wm. G. Hoover and Carol G. Hoover, "Comparison of Very Smooth Cell-Model Trajectories", ariXiv:1504.00620 .

Stormer-Verlet Coordinate and Energy Errors





The momentum must be approximated from the values of the coordinates. The two curves shown for the energy error are for second- and fourth-order centered approximations for the momentum :

$$\text{P2}: \quad p_i = \frac{(q_{i+1} - q_{i-1})}{2dt} - \left(\frac{dt^2}{6}\right) q'''$$

$$\text{P4}: \quad p_i = \frac{2(q_{i+1} + q_{i-1})}{3dt} - \frac{(q_{i+2} + q_{i-2})}{12dt} + \left(\frac{dt^4}{30}\right) q'''''$$

Notice that the energy remains second order. However, the calculated data shows that the energy error is about five times smaller for the higher order momentum .

Fourth-Order Symplectic Algorithm (Candy and Rozmus)

The fourth-order symplectic algorithms solve first order differential equations. The number of stages in a timestep is four .

$$\dot{q} = p \; ; \; \dot{p} = F$$
$$Specify \; q_0 \; and \; p_0 \; ;$$

$$q_i = q_{i-1} + a_i \, p_{i-1} dt \; ; \quad p_i = p_{i-1} + b_i F_i dt \; ; \quad for \; i = 1, 4$$

$$a_1 = a_4 = \left(2 + 2^{1/3} + 2^{-1/3}\right)/6 \; ; \; b_1 = b_3 = \left(2 - 2^{1/3}\right)^{-1}$$
$$a_2 = a_3 = \left(1 - 2^{1/3} - 2^{-1/3}\right)/6 \; ; \; b_2 = \left(1 - 2^{2/3}\right)^{-1} .$$

Programming steps :

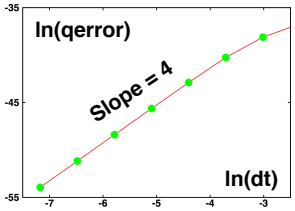
```
Q = Q + a1*P*dt
P = P + b1*F*dt
Q = Q + a2*P*dt
P = P + b2*F*dt
Q = Q + a2*P*dt
P = P + b1*F*dt
Q = Q + a1*P*dt
```

Stephen K. Gray, Donald W. Noid and Bobby G. Sumpter, "Symplectic integrators for large scale molecular dynamics: A comparison of several explicit methods", J. Chem. Phys., Vol. 101, (September 1994).

Fourth-Order Symplectic Monte-Carlo Algorithm

An algorithm with five force evaluations per timestep was developed by Monte-Carlo sampling adjusting the coefficients subject to the constraints of time reversibility and normalization so that the Monte-Carlo trajectory optimization occurs in a four-dimensional space. This method was successful in modeling many-body dynamics. There are 5 force evaluations per step. The programming steps for the oscillator are given below.

```
q = q + 0.005904d00*p*dt
p = p + 0.171669d00*(-q)*dt
q = q + 0.515669d00*p*dt
p = p - 0.516595d00*(-q)*dt
q = q - 0.021573d00*p*dt
p = p + 1.689852d00*(-q)*dt
q = q - 0.021573d00*p*dt
p = p - 0.516595d00*(-q)*dt
q = q + 0.515669d00*p*dt
p = p + 0.171669d00*(-q)*dt
q = q + 0.005904d00*p*dt
```



Notice that for each variable the coefficients add up to 1.0 .

William G. Hoover, Oyeon Kum, and Nancy E. Owens, "Accurate symplectic integrators via random sampling", J. Chem. Phys., Vol. 103, No. 4, (22 July 1995).

Runge-Kutta Methods

Fourth-Order Runge-Kutta Method

1. **Four steps calculate approximate derivatives :**
   - **Calculate new values of v and F using updated values of x and p (right-hand-side evaluation)**
   - **Update x and v for dt/2 or dt .**
2. **Calculate updated values of x and v over the full time step using a weighted average of the derivatives computed in the previous four-step calculation .**

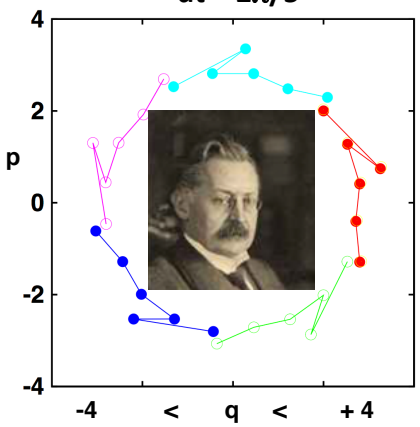
Fifth-Order Runge-Kutta Method

1. **Six update steps to calculate approximate derivatives . Some update steps use weighted derivatives .**
2. **Final step uses a weighted average of six approximate derivatives .**

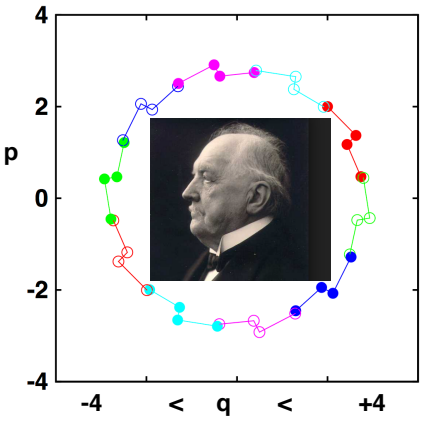
Derivative points for Runge-Kutta integrators

Harmonic Oscillator $\dot{q} = +p$ $\dot{p} = -q$

5th order Runge-Kutta
dt = 2π/5



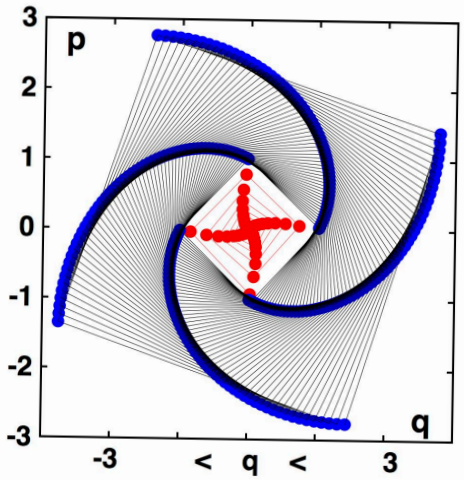
4th order Runge-Kutta
dt = 2π/10



Storage Layout for the Runge-Kutta Algorithms
5 particles

YY Array Position and Momenta	YYP Array Derivatives
x1 = yy(1)	yyp(1) = p1
x2 = yy(2)	yyp(2) = p2
x3 = yy(3)	yyp(3) = p3
x4 = yy(4)	yyp(4) = p4
x5 = yy(5)	yyp(5) = p5
p1 = yy(6)	yyp(6) = f1
p2 = yy(7)	yyp(7) = f2
p3 = yy(8)	yyp(8) = f3
p4 = yy(9)	yyp(9) = f4
p5 = yy(10)	yyp(10) = f5

A Comparison of RK4 and RK5 for the Oscillator with a Large Timestep



dt = 2π/4 ; 250 steps
Initial condition : q,p = (1.0,0.0)
60 periods

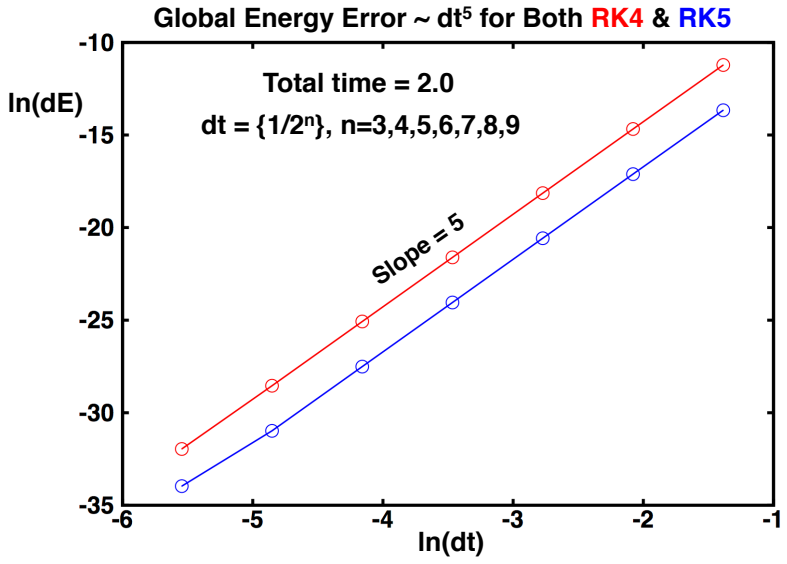
Results for a large timestep :

The Fourth-Order Runge-Kutta solution decays.

The Fifth-Order Runge-Kutte solutions grows.

Similarly the energy drifts upward for the RK5 and decays for RK4.

Energy Errors for RK4 and RK5 for the Harmonic Oscillator



2. Cell Model evaluation of integration techniques

Integration Accuracy for a Chaotic System

- **A Cell Model**
  A Chaotic Trajectory generated with a very smooth, soft potential

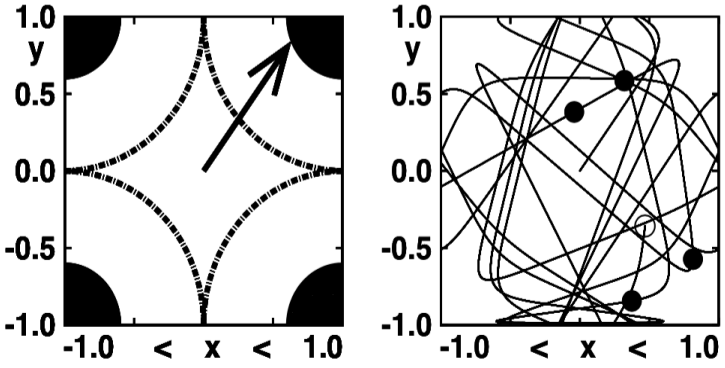
- **6 Integration Methods**
  Symplectic :
  - 2nd Order LeapFrog
  - 4th Order Candy-Rozmus
  - 4th Order Method with Coefficients determined by Monte-Carlo
  - 6th Order Yoshida Method

  Runge-Kutta Methods :
  - 4th Order Runge-Kutta
  - 5th Order Runge-Kutta

- Results compared with an accurate 8th order Telroy-Schlier-Sieter symplectic method.

A Very Smooth Cell-Model Trajectory

t = (10, 20, 30, 40, 50)



$$\Phi = \sum \left[1 - (r - r_i)^2\right]^4 \text{ for } \left| r - r_i \right| < 1 \ .$$

Periodic boundary conditions ; RK5 quadruple precision ; chaotic Hamiltonian .

Wm. G. Hoover and Carol G. Hoover, "Comparison of Very Smooth Cell-Model Trajectories", ariXiv:1504.00620 .

Evaluation Criteria for the Cell Model Calculations

1. Trajectory Accuracy
We find the time for which the coordinates are accurate to 0.01 when compared with the Schlier-Seiter-Telroy 8th order integration.

2. Reversibility
The time for which a trajectory can be reversed to within 0.01 of the origin.

3. Energy Accuracy
Energy conservation is a diagnostic. The difference between the initial energy and the energy at the final time is the energy error.

4. What else do we need to consider?

A Comparison of Integration Methods for the Cell Model

	Method	Order	Accurate Trajectory Time	Energy Accuracy	Reversal Time	Force Evaluations
	Leapfrog	2nd	18	10^{-7}	47	1
Symplectic	Candy Rozmus	4th	34	10^{-15}	42	3
Symplectic	Monte Carlo	4th	31	10^{-13}	43	5
Symplectic	Yoshida	6th	36	10^{-15}	42	7
	Runge-Kutta	4th	35	10^{-13}	42	4
	Runge-Kutta	5th	34	10^{-15}	42	6

Accurate trajectory time occurs for coordinate errors less than 0.01 compared to 8th order Telroy-Schlier-Sieter symplectic method. Coefficients are extended precision . Here dt = 0.001, a typical MD timestep

Conclusions
Comparison of 6 Integration Methods

- Energy conservation and reversibility do not guarantee an accurate trajectory. Leapfrog integration is an example.
- Leapfrog integration has a longer reversibility time than any of the other more accurate integration methods. For chaotic systems it is nearly as useful as the higher order, more accurate integrators because of the Lyapunov instability for the cell model.
- The Lyapunov instability is a physical instability rather than a numerical inaccuracy that occurs in chaotic systems. The Lyapunov exponent measures the exponential separation rate between two trajectories initially separated by a "small" perturbation (~ 10^{-6}). The largest Lyapunov exponent for the cell model is 0.7 . Consider an initial error of 10^{-16} . For a run to a time of 50 the separation will increase to 10^{15} :

$$e^{\lambda t} = e^{0.7x50} = e^{35} \cong 10^{15} .$$

- Trajectory accuracy is the most important criterion to use when calculating detailed atomistic mechanisms such as energy barrier crossings. Leapfrog integration (or the Monte-Carlo method) is a good choice for equilibrium problems at constant energy.

3. Predictor – Corrector Methods

- Used for stiff equations
- Often stiff equations arise for problems with two time scales in the solution
- Two steps :
- The Predictor step is explicit
- The Corrector step is implicit
- Predictor-Corrector schemes are not self-starting
  Fourth and fifth order Runge-Kutta algorithms are self-starting !
  Combining the two Runge-Kutta algorithms results in an excellent adaptive integrator for the Nosé oscillator
- Second Order Störmer-Verlet is self starting
- Stability is important **
- Stable time steps are usually larger for implicit than for explicit algorithms
- Molecular dynamics : Nosé's thermostated oscillator
- Continuum mechanics : Viscoplasticity and other nonlinear effects
- Other examples include chemical reactions with two time scales, and circuit analysis
- Milne's two methods can be analyzed with the Harmonic Oscillator . The first uses the two first order equations of motion and the second uses the second order equation of motion

** For more details on implicit methods see the following :

http://qucs.sourceforge.net/tech/node25.html
http://qucs.sourceforge.net/tech/node24.html

Milne's Predictor-Corrector Methods for the Oscillator

Method 1 : Two first order differential equations – Error term is 5th order .

Predictor Step : Explicit

$$q_{n+1} = q_{n-3} + (4dt/3)(2\dot{q}_n - \dot{q}_{n-1} + 2\dot{q}_{n-2}) + (28/90)dt^5 \ \dddot{\dddot{q}}$$

$$p_{n+1} = p_{n-3} + (4dt/3)(2\dot{p}_n - \dot{p}_{n-1} + 2\dot{p}_{n-2}) + (28/90)dt^5 \ \dddot{\dddot{q}} \ ; \ (\dot{p} = -q)$$

Corrector Step : Implicit

$$q_{n+1} = q_{n-1} + (h/3)(\underline{\dot{q}_{n+1}} + 4\dot{q}_n + \dot{q}_{n-1}) - (1/90)dt^5 \ \dddot{\dddot{q}}$$

$$p_{n+1} = p_{n-1} + (h/3)(\underline{\dot{p}_{n+1}} + 4\dot{p}_n + \dot{p}_{n-1}) - (1/90)dt^5 \ \dddot{\dddot{p}} \ ; \ (\dot{p} = -q)$$

Method 2 : One second order differential equation – Error term is 6th order .

Predictor Step : Explicit

$$q_{n+1} = q_n + q_{n-2} - q_{n-3} + (dt^2/4)(5\ddot{q}_n + 2\ddot{q}_{n-1} + 5\ddot{q}_{n-2}) + (17/240)dt^6 \ \ddddot{\ddddot{q}}$$

Corrector Step : Implicit

$$q_{n+1} = 2q_n - q_{n-1} + (dt^2/12)(\underline{\ddot{q}_{n+1}} + 10\ddot{q}_n + \ddot{q}_{n-1}) - (1/240)dt^6 \ \ddddot{\ddddot{q}}$$

Predictor-Corrector Algorithms are not Self-Starting

If the analytical form of the solution is known, it can used to evaluate nearby points to start up the algorithm .

Taylor's series can always be used to generate the extra points needed to start the algorithm . This can also be done numerically .

Evaluate the function and its derivative each at two nearby points. This is the finite difference technique .

Accuracy can be evaluated using analytical solutions for the numerical approximation and comparing the error when the time step in reduced in a systematic way .

Student problem

Any of the algorithms can be evaluated with the oscillator .

Is the stability behavior different when using previous points versus future points in Taylor series ?

Numerically Evaluate the Order of the Global Error for Milne's Methods Using the Harmonic Oscillator

Coordinate Error q(2π) = True Solution - Numerical Solution

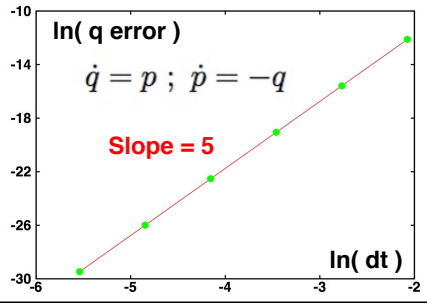
Plot : ln(Error) as a function of ln(dt) for several values of dt .
The slope of a straight line gives the power of dt in the error term .

$$\text{Initial condition} \; : \; q = cos(t) \; ; \; p = -sin(t) \; ; \; F = -q \; .$$

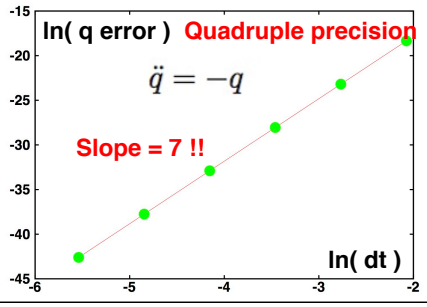
$$dt = \frac{2\pi}{50} \; , \; \frac{2\pi}{100} \; \cdots \; \frac{2\pi}{1600}$$

Starting values calculated from the analytical solution .

Method 1 : First Order-Equations



Method 2 : Second-Order Equation



Gear Predictor-Corrector Method

$$r^p_{t+dt} = r_t + dt(v_t) + \frac{dt^2}{2}a_t + \frac{dt^3}{6}b_t + \cdots$$

$$v^p_{t+dt} = v_t + dt(a_t) + \frac{dt^2}{2}b_t + \cdots$$

$$a^p_{t+dt} = a_t + dt(b_t) + \cdots$$

$$b^p_{t+dt} = b_t$$

Predictor Step

$$\begin{pmatrix} r \\ v \\ a \\ b \end{pmatrix}^p_{t+dt} = \begin{pmatrix} 1 & dt & \frac{dt^2}{2} & \frac{dt^3}{6} \\ 0 & 1 & dt & \frac{dt^2}{2} \\ 0 & 0 & 1 & dt \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} r \\ v \\ a \\ b \end{pmatrix}_t \; ; \qquad r^p_{t+dt} \rightarrow a^c_{t+dt} \; ;$$

$$\Delta a_0 = (a^c_{t+dt} - a^p_{t+dt})dt^2/2$$

Corrector Step

$$\begin{pmatrix} r \\ v \\ a \\ b \end{pmatrix}^{c,0}_{t+dt} = \begin{pmatrix} r \\ v \\ a \\ b \end{pmatrix}^p_{t+dt} + (c_0 + c_1 + c_2 + c_3)\Delta a_0 \begin{pmatrix} 1 \\ 1/dt \\ 2/dt^2 \\ 6/dt^3 \end{pmatrix} ; \quad (c_1, c_2, c_3, c_4) = \left(\frac{1}{6}, \frac{5}{6}, 1, \frac{1}{3}\right)$$

Student Problem

Consult Gear's book for a fourth order gear algorithm with an iteration scheme for the corrector step.

Gear, G. W., *Numerical Initial Value Problems in Ordinary Differential Equations*, Prentice-Hall, Englewood Cliffs, N. J. (1971).

Gear Algorithm with a single iteration of the Corrector Step

```
c Gear algorithm for the harmonic oscillator

      ro  =  1.0d00  ! initial condition
      vo  =  0.0d00
      ao  = -1.0d00
      bo  =  0.0d00
      dt  =  (1/2)**n  ! Pick dt for n = 1,9

      rp = 0.0d00    ! Predictor values
      vp = 0.0d00
      ap = 0.0d00
      bp = 0.0d00

      rc = 0.0d00    ! Corrector values
      vc = 0.0d00
      ac = 0.0d00
      bc = 0.0d00

      time = 0.0d00
      Ham  = 0.5d00*(ro**2 + vo**2)
      Ham0 = Ham
      write(6,*)"energy ",time,Ham

      c0 = 1.0d00/6.0d00
      c1 = 5.0d00/6.0d00
      c2 = 1.0d00
      c3 = 1.0d00/3.0d00
```

```
      do it = 1,itmax
c predictor
      rp =  ro + dt*vo + 0.5d00*(dt**2)*ao +
     &          (1.0d00/6.0d00)*(dt**3)*bo
      vp =  vo + dt*ao + 0.5d00*(dt**2)*bo
      ap =  ao + dt*bo
      bp =  bo
      ac = -rp
      dela = (ac - ap)
      DA   = 0.5d00*dela*dt*dt
c corrector
      rc = rp + c0*DA
      vc = vp + c1*DA/dt
      ac = ap + 2.0d00*c2*DA/(dt**2)
      bc = bp + 6.0d00*c3*DA/(dt**3)
      time = it*dt
      Ham  = 0.5d00*(rc**2 + vc**2)
      write(6,*)time,rc,vc,ac,bc,Ham
      ro = rc   ! reset the variables
      vo = vc
      ao = ac
      bo = bc
      end do
```

Gear Corrector Coefficients for First and Second Order Equations

Table E.1 *Gear corrector coefficients for a first-order equation*

Values	c_0	c_1	c_2	c_3	c_4	c_5
3	5/12	1	1/2			
4	3/8	1	3/4	1/6		
5	251/720	1	11/12	1/3	1/24	
6	95/288	1	25/24	35/72	5/48	1/120

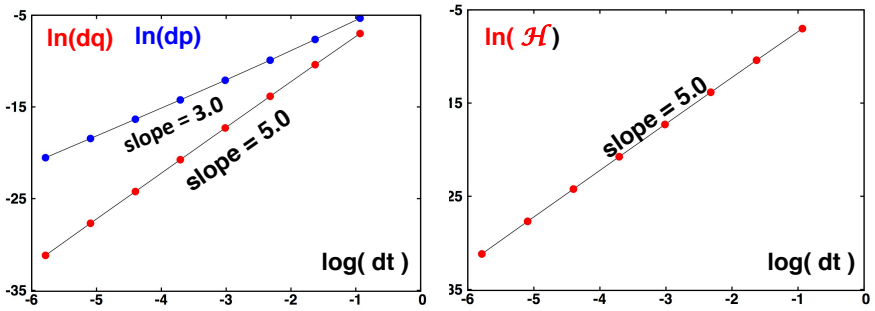
Table E.2 *Gear corrector coefficients for a second-order equation*

Values	c_0	c_1	c_2	c_3	c_4	c_5
3	0	1	1			
4	1/6	5/6	1	1/3		
5	19/120	3/4	1	1/2	1/12	
6	3/20	251/360	1	11/18	1/6	1/60

Gear integration for the Harmonic Oscillator
Energy, Coordinate, and Momentum Error in one period

Initial condition (q, p, a, b, $\mathcal{H}$) = (1, 0, -1, 0, .5)

dt = π / 2^n for n = 4, . . ., 11



Gear's method. Extra material for *Introduction to Chemical Engineering Computing*, 2nd ed., Bruce A. Finlayson, Wiley (2012).

If the numerical problem has some components that change quickly, but you have to integrate for a long time, the problem is called stiff (see p. 360 and Perry and Green, p. 3-50, 2008). Implicit methods are then needed. The best ones are based upon the work by Gear (1971). For the problem

$$\frac{dy}{dt} = f(t,y), \quad y(0) = y_0$$

http://www.chemecomp.com/Gear.pdf ;
https://people.maths.ox.ac.uk/suli/nsodes.pdf

where y and f can be vectors, the methods of different order are:

$$(1): \; y^{n+1} = y^n + \Delta t \, f(y^{n+1})$$

$$(2): \; y^{n+1} = \frac{4}{3}y^n - \frac{1}{3}y^{n-1} + \frac{2}{3}\Delta t \, f(y^{n+1})$$

$$(3): \; y^{n+1} = \frac{18}{11}y^n - \frac{9}{11}y^{n-1} + \frac{2}{11}y^{n-2} + \frac{6}{11}\Delta t \, f(y^{n+1})$$

$$(4): \; y^{n+1} = \frac{48}{25}y^n - \frac{36}{25}y^{n-1} + \frac{16}{25}y^{n-2} - \frac{3}{25}y^{n-3} + \frac{12}{25}\Delta t \, f(y^{n+1})$$

$$(5): \; y^{n+1} = \frac{300}{137}y^n - \frac{300}{137}y^{n-1} + \frac{200}{137}y^{n-2} - \frac{75}{137}y^{n-3} + \frac{12}{137}y^{n-4} + \frac{60}{137}\Delta t \, f(y^{n+1})$$

In Gear's method, the nonlinear equations are solved. If they cannot be solved, then the step size is reduced and you try again. Keep reducing the step size until the implicit equations can be solved. If the step size is extremely small, the computer program will stop. The order can be changed, too, and it is changed in the Gear algorithm to minimize the computational cost for a specified accuracy.

Reference

Gear, G. W., *Numerical Initial Value Problems in Ordinary Differential Equations*, Prentice-Hall, Englewood Cliffs, N. J. (1971).

Perry, R. H. and Green, D. W. (ed.), *Perry's Chemical Engineers' Handbook*, 8th ed., McGraw-Hill: New York, 2008.

4. Stiff Differential Equations

Purpose: To understand adaptive integration and to study techniques for analyzing results

1. **Hamiltonian mechanics with temperature**

   Nosé (1984) modified Hamiltonian mechanics to include temperature . We compare two versions of the modified mechanics : Nosé mechanics and Nosé-Hoover mechanics for the harmonic oscillator.

2. **We discuss numerical stiffness, errors, and Lyapunov instability**

3. **We discuss fixed time step calculations (Fourth-Order Runge-Kutta) for the Nosé and Nosé-Hoover oscillators ; we find numerical instability .**

4. **We present an adaptive integration technique based on fourth-order Runge-Kutta .**

5. **We compare the adaptive method for the Nosé and Nosé-Hoover oscillators**

6. **Summary**

The Thermostated Harmonic Oscillator

The Nosé oscillator is the motion of a harmonic oscillator with a specified average temperature ! Nosé's idea (1984) was to replace isoenergetic mechanics with a temperature-based mechanics. To do this he developed a temperature dependent Hamiltonian consistent with Gibbs' canonical distribution. When this Hamiltonian is applied to the harmonic oscillator the resulting equations of motion are very stiff !

$$2\mathcal{H} = q^2 + p^2/s^2 + \mathrm{T}\ln\left(s^2\right) + \zeta^2 \equiv 0 \;\rightarrow$$

Nosé Oscillator Equations

$$\dot{q} = (p/s^2)\,;\; \dot{p} = -q\,;\; \dot{s} = \zeta \;;\; \dot{\zeta} = (p^2/s^3) - 1/s$$

$$for\ \kappa, T, k, m = 1\ .$$

Dettmann and Morris later modified the original Nosé Hamiltonian and showed that the following Nosé-Hoover equations (Hoover 1985) can be derived from it.

Nosé-Hoover Oscillator Equations

$$\dot{q} = p/s \;;\; \dot{p} = -sq \;;\; \dot{s} = s\zeta \;;\; \dot{\zeta} = p^2/s^2 - 1 \qquad \#\ 1$$

$$p/s \rightarrow p\,;\; \dot{q} = p\,;\; \dot{p} = -q - \zeta p\,;\; \dot{\zeta} = p^2 - 1\ . \qquad \#\ 2$$

Adaptive Integration for stiff differential equations : Compare the Nosé and Nosé-Hoover Oscillators

- We will compare the smooth Nosé-Hoover equations to the stiff Nosé oscillator equations with the same phase-space trajectories .
- Nosé-Hoover oscillator trajectories are both (Lyapunov stable) and chaotic (Lyapunov unstable) .
- A trajectory is considered "Lyapunov" unstable if the distance between the trajectory and nearby a neighbors' trajectory grows exponentially :

$$\delta \propto e^{+\lambda t} \; Lyapunov\ unstable\ \lambda\ for > 0$$

$$Lyapunov\ stable\ for\ \lambda \leq 0$$

- The trajectory considered in this Lecture is Lyapunov unstable (chaotic). However, Lyapunov instability occurs perpendicular to the trajectory whereas numerical errors give rise to phase-error fluctuations parallel to the trajectory.
- The unusual aspect of these two oscillators is that the two trajectories are exactly the same but the dynamical rates of progress along the common trajectory are different. This is referred to as "time scaling" in Nosé's original paper. We will show that this is the cause of the numerical stiffness !

Numerical Stiffness

- In mathamatics, a stiff equation is a differential equation for which the usual numerical methods for solving the equation are numerically unstable, unless the step size is taken to be extremely small .
- Adaptive methods can be used in some cases to overcome numerical instability. We will illustrate this with the Nosé oscillator example .
- Adaptive methods cannot be used for singular integrands such as the "event-driven" hard sphere collision models.
- Other examples of numerical stiffness arise in problems with two time scales as in circuit analysis. In these cases the stiffness is treated with predictor-corrector methods including implicit methods . Matrix solutions are required for the implicit methods.
  - Most molecular dynamics motion equations are solved with explicit techniques !

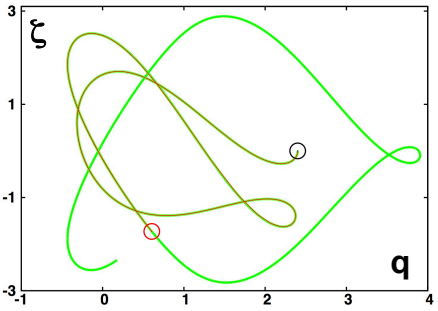
Fourth-Order Runge-Kutta Integration for the Nosé and Nosé-Hoover Oscillators

If the Hamiltonian is set to 0 and p = ζ = 0 initially then $0 < s \leq 1$, the Nosé and Nosé-Hoover oscillator phase-space trajectories are identical. We can use this fact to compare the integration results for the two oscllators.

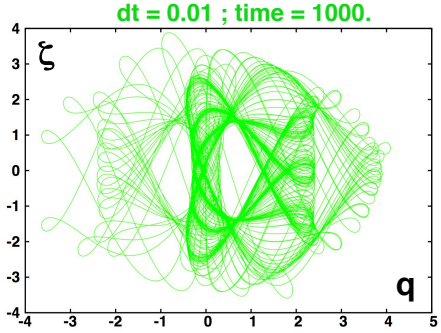
Initial condition : (q,p,s, ζ) = (2.4, 0, $e^{-2.88}$, 0) ; $\mathcal{H} = 0$.

Nosé
dt = 0.001
time = 5.

Nosé-Hoover
dt = 0.01
time = 25.



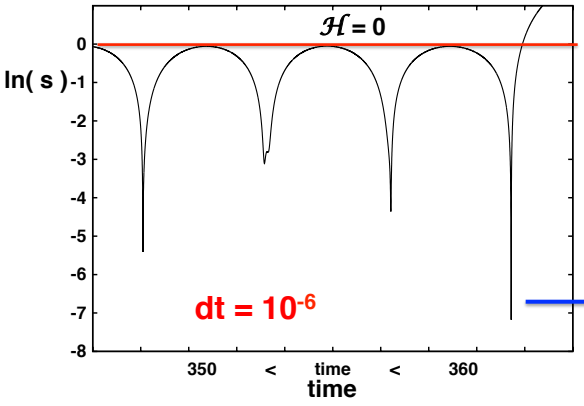
Nosé-Hoover Oscillator
dt = 0.01 ; time = 1000.



Identical phase-space trajectories. RK4 algorithm is unstable for Nosé oscillator using dt = 0.001, time ~ 5.0 . Nosé-Hoover oscillator is stable for dt = 0.01 .

What is a stable time step for the Nosé Oscillator ?

The Hamiltonian will be zero if $0 < s < 1$. For the Nosé Oscillator the variables scale as $1/(s^2)$. For small s the rates become large. What is the minimum value of s for which the algorithm will remain stable and at what time does this minimum occur?



Initial condition :
(q,p,s, ζ) = (2.4, 0, $e^{-2.88}$, 0)
$\mathcal{H} = 0$.

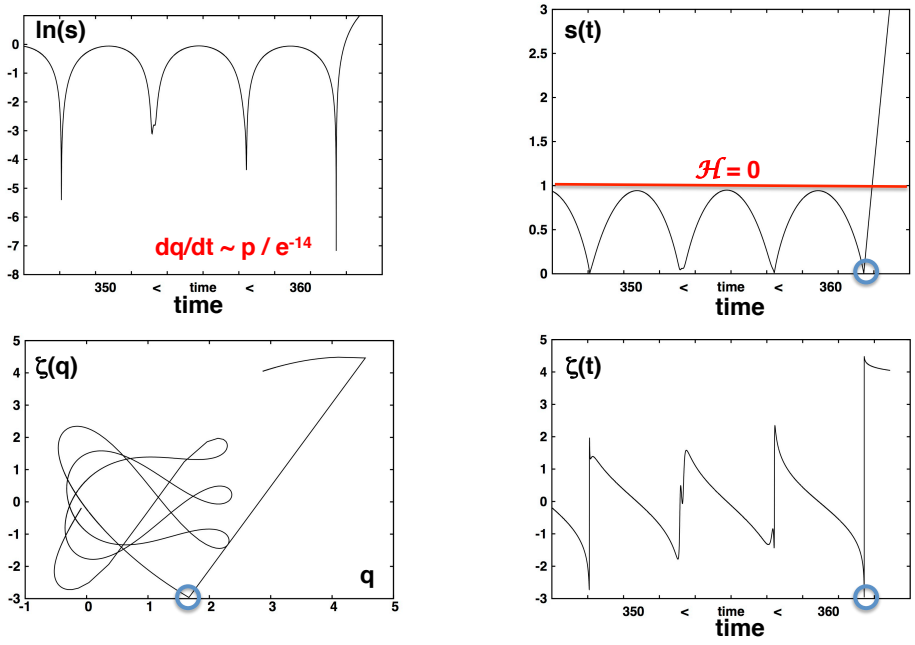
s is a time scaling variable

dq/dt ~ p / e^{-14}

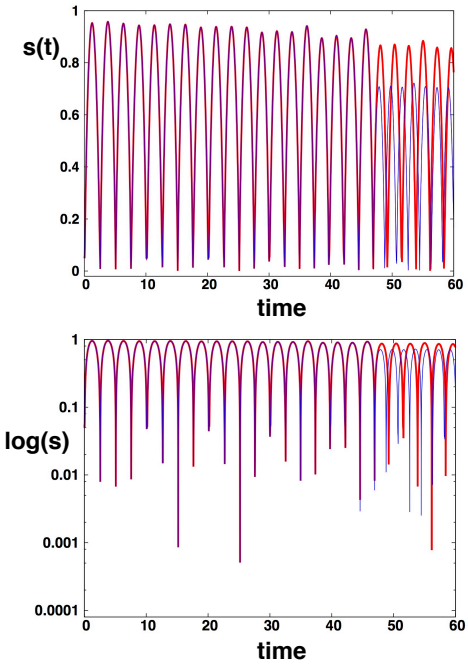
$\dot{q} = (p/s^2)\ ;\ \dot{p} = -q\ ;\ \dot{s} = \zeta\ ;\ \dot{\zeta} = (p^2/s^3) - 1/s$ Nosé

$\dot{q} = p/s\ ;\ \dot{p} = -sq\ ;\ \dot{s} = s\zeta\ ;\ \dot{\zeta} = p^2/s^2 - 1$ Nosé-Hoover

Nosé Oscillator Trajectories for dt = 10^{-6}



How well does the algorithm perform for dt = 0.0001 ?



Double Precision

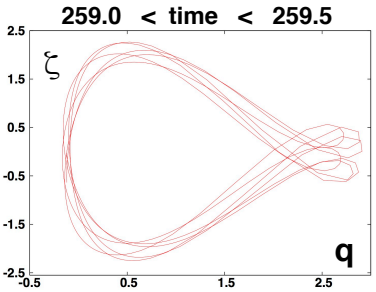
Quadruple Precision

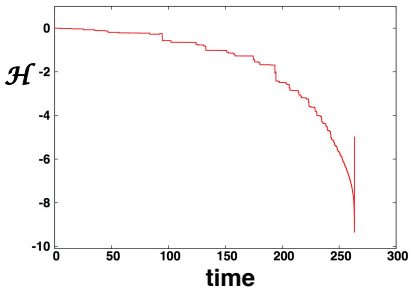
Conclusion: This algorithm is not able to integrate successfully the Nosé oscillator

Use a logarithmic scale to find the minimum values of s .

What is another check can we make on this calculation ?

We gain physical insights by checking all of the results !!





This trajectory in the time interval shown is reasonably smooth in spite of the small values of s . But notice the straight line approximations to the small radius-of-curvature loops .

The Hamiltonian is not zero !

In fact the Hamiltonian deviates from zero starting at a time of 5.0 ! Smaller time steps have not helped the numerical stability .

Conclusions

1. Always test your numerical results for errors and consistency with the physical model .

- Check the dependence of the error on the time step
- Check the dependence of the results on precision (double *versus* quadruple)
- Check the physical diagnostics (energy in this case)
- Compare the result to a known result (Nosé-Hoover)

2. The fourth-order Runge-Kutta algorithm is not useful for integrating the Nosé oscillator

3. Develop an adaptive integration routine for the Nosé oscillator and study the dependence of the stiffness on the time-scaling variable .

Student problems

1. Run Nosé-Hoover #1 trajectories with the RK4 algorithm for the chaotic initial condition (q,p,s, ζ) = (2.4, 0, $e^{-2.88}$, 0). Test all of the checks shown above. Use a simulation time longer than 264.
2. Run Nosé-Hoover #2 trajectories for the stable-torus initial condition (q,p,ζ) = (0.0, 1.55, 0.0). Test all of the checks shown above. How do these calculations differ from the chaotic solution?

An Adaptive Integration Algorithm Based on the Fourth-order Runge-Kutta Method

- **Select an error band**
  - For double precision ~ 10^{-12} to 10^{-10}
  - For quadruple precision ~ 10^{-24} to 10^{-20}
- **Calculate the root-mean-square error using the difference between two dt/2 steps and the single dt step**
- **Change the time step if outside the error band**
  - Half the time step for errors greater than the upper limit
  - Double the time step for errors less than the lower limit
- **Reset the array with the dt step to the more nearly accurate solution at the end of the time step.**

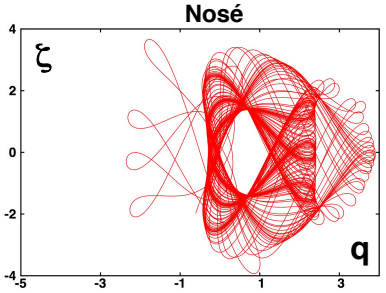
```
call rk4(x,xp,dt/2.0d00)
call rk4(x,xp,dt/2.0d00)
call rk4(y,yp,dt/1.0d00)
error2 = (x(1)-y(1))**2 + (x(2)-y(2))**2 + (x(3)-y(3))**2 +
   (x(4)-y(4))**2
error = dsqrt(error2)
if(error.gt.10.0d00**(-10)) dt = 0.5d00*dt
if(error.lt.10.0d00**(-12)) dt = 2.0d00*dt
```

Adaptive Integration

Nosé's Oscillator is much stiffer than the Nosé-Hoover Oscillator

100, 000 Adaptive time steps

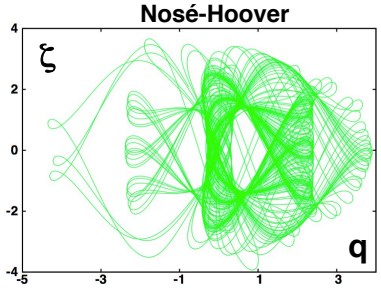
Nosé



< s > = 0.660893 < 1/s > = 3.28299

Time = 2,267,838.344

Nosé-Hoover

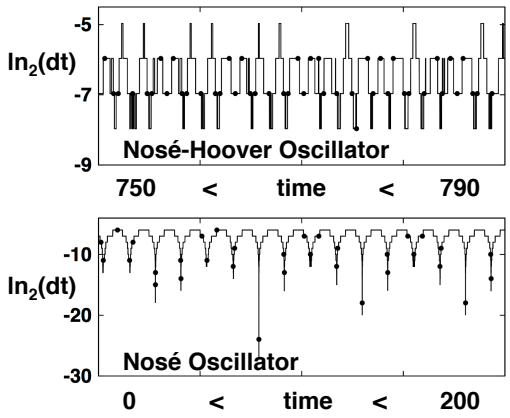


< s > = 0.3046773 < 1/s > = 964.2

Time = 9,319,142.032

We can show that the rates for the Nosé oscillator are about 3 times faster but progress along the trajectory is considerably reduced for the same number of adaptive time steps. This is evidence for the numerical stiffness for the Nosé oscillator. The trajectories are the same but progress at different rates.

Adaptive Time Step Comparisons
Nosé-Hoover Oscillator Versus Nosé Oscillator



$\dot{q} = (p/s^2)\,;\ \dot{p} = -q\,;\ \dot{s} = \zeta\ ;\ \dot{\zeta} = (p^2/s^3) - 1/s$ Nosé

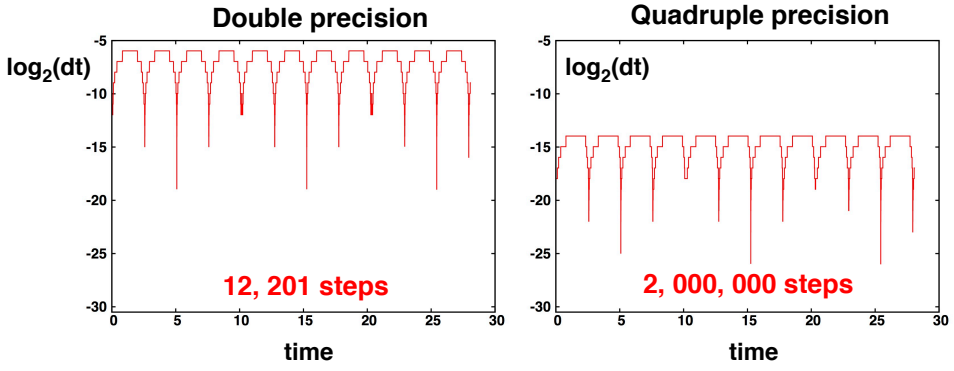
$\dot{q} = p/s\ ;\ \dot{p} = -sq\ ;\ \dot{s} = s\zeta\ ;\ \dot{\zeta} = p^2/s^2 - 1$ Nosé-Hoover

Adaptive Time Step Comparisons
Double Precision Versus Quadruple Precision

Nosé Oscillator

Initial condition: (q, p, s, z) = (2.4, 0, $e^{-2.88}$, 0) ; $\mathcal{H} = 0$.

Time = 28.1097 , 22 crossings of p = 0 section .



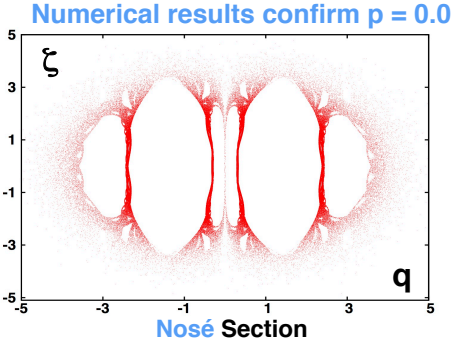
$\dot{q} = (p/s^2)\,;\ \dot{p} = -q\,;\ \dot{s} = \zeta\ ;\ \dot{\zeta} = (p^2/s^3) - 1/s$

$for\ \kappa, T, k, m = 1$.

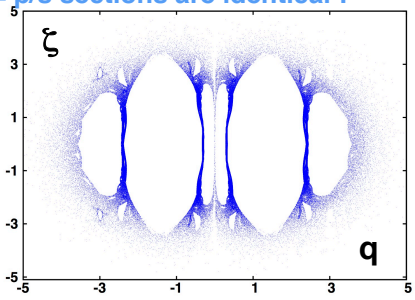
The Distance Between two p = 0 sections Measures a Length Along a Trajectory

A section is a two-dimensional set of points in the four-dimensional phase space. A section is defined by setting both of the other two variables set to 0.0 . In this special case, we look at two p = 0.0 sections and let s take on whatever values that occur along the trajectory between the two sections. This allows us to measure the rate at which the Nosé or Nosé-Hoover oscillator travels between two known points on the trajectory.

Numerical results confirm p = 0.0 = p/s sections are identical !



Nosé Section



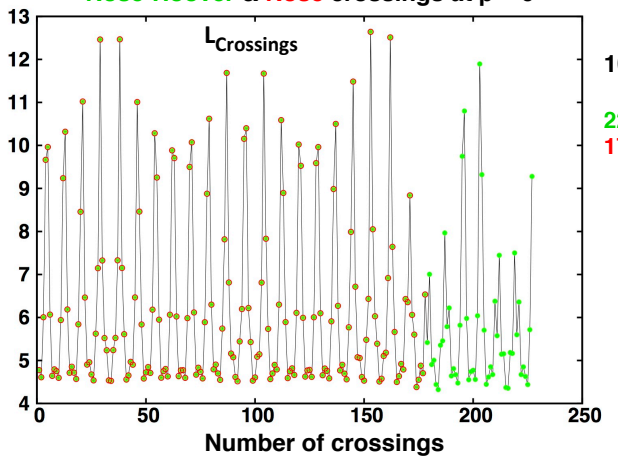
Nosé-Hoover Section

Compute the trajectory length between two crossings in a p = 0 plane

Trajectory length in a time step is $dL_I = \sqrt{\delta q_I^2 + \delta p_I^2 + \delta s_I^2 + \delta\, \zeta_I^{\,2}}$. *For N time steps the trajectory length between two crossings of a p = 0 plane is* $L_{cross} = \sum dL_I$.

For $\mathcal{H}$ = 0 the trajectories for the two oscillators are identical .

Nosé-Hoover & Nosé crossings at p = 0

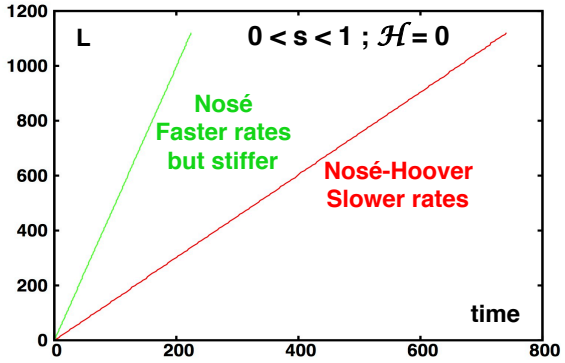


100,000 adaptive steps

227 Nosé-Hoover crossings
173 Nosé crossings

The Variable s in the Equations of Motion Scales all of the Rates

Trajectory Length :
dL_i = length between two crossings of the p = 0 plane
$L = \Sigma\, dL_i$ for 178 crossings



Initial condition
(q, p, s, ζ) = (2.4, 0, $e^{-2.88}$, 0)
Chosen to insure that
$\mathcal{H} = 0$

Notice that these equations differ by 1/s where s is the time-scaling factor .

$$\dot{q} = (p/s^2)\,;\ \dot{p} = -q\,;\ \dot{s} = \zeta\ ;\ \dot{\zeta} = (p^2/s^3) - 1/s$$ Nosé

$$\dot{q} = p/s\ ;\ \dot{p} = -sq\ ;\ \dot{s} = s\zeta\ ;\ \dot{\zeta} = p^2/s^2 - 1$$ Nosé-Hoover

Nosé Oscillator with $\mathcal{H} = 0$;
What is the Best Initial Value of *s* ?

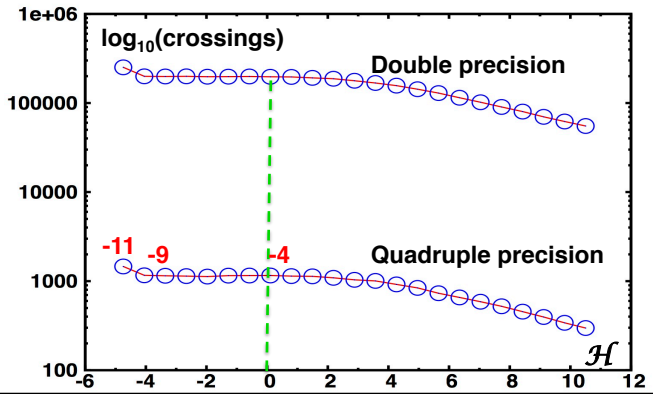
Vary s to maximize the number of crossings in 100,000,000 steps

Initial condition:
(q, p, ζ) = (2.4, 0, 0) ,

$s = 2^n$, $-11 < n < 11$

→

$s = 2^{-4} = .06250$
$s = e^{-2.88} = 0.056135$
$\mathcal{H} = 0$
$s = 2^{-5} = .03125$



One more test :
Hamiltonian Systems
Are Conservative !

Energy must be conserved in a Hamiltonian System !

Error in the Hamiltonian

s	Double precision	Quadruple precision
0.062500	-3.2702049634902863E-05	-4.997996331072645417188952190057969E-13
0.056135*	-3.3960281428768724E-05	9.5100417260022603409237012759510 37E-13
0.031250	-3.3617859108492354E-05	-3.2076744813181568684207578316120 92E-11

*** This is the value that corresponds to a vanishing Hamiltonian .**

Lyapunov Exponents and Chaos

The instantaneous Lyapunov exponent measures the exponential growth of the separation of two nearby neighboring trajectories, $\dot{\delta} = \lambda\delta$. We choose a neighboring *satellite trajectory* x_s constrained a distance $\delta = 0.000001$ from a *reference trajectory* x_r . After a time step dt, the distance is rescaled to δ providing a measure of the growth of separation during that interval.

$$x_r = x_r + g(x_s - x_r) \quad where\ g = \left(\delta/\sqrt{(x_s - x_r)^2}\right) \cong e^{-\lambda dt}$$

$$\longrightarrow \lambda(t) = -ln(g)/dt$$

This instantaneous or local Lyapunov exponent averaged over a very long trajectory gives the Lyapunov exponent for the phase-space trajectory.

$$\lambda = \sum(\lambda(t)dt)/\sum(dt)$$

This Lyapunov is the maximum of the four Lyapunov exponent measuring the growth in phase space for the oscillator. Bill will present algorithms for calculating the full spectrum in a later lecture. The solutions of the thermostated oscillator are characterized by the value of the maximum exponent :

$$\lambda > 0\ chaotic\ solution\ ;\ \lambda = 0\ conservative\ tori\ .$$

Calculated Results for the Lyapunov Exponents using the time-scaling factors

λ_N = .0468 ; $d\mathcal{H}$ = 0.000197

λ_{NH} = .0140 ; $d\mathcal{H}$ = 0.000006

$< 1/s >_{Nosé}\ \lambda_{NH} = 0.0140\ (\ 3.28\ ) = 0.0460$

$< s >_{NH}\ \lambda_{Nosé} = 0.305\ (\ 0.0468\ ) = 0.0143$

Nosé	Nosé-Hoover
$< s > = 0.661$; $< 1/s > = 3.28$	$< s > = 0.305$; $< 1/s > = 964.0$

$\lambda_{Nosé} = 3.28\ \lambda_{NH}$; $t_{NH} = 3.28\ t_{Nosé}$

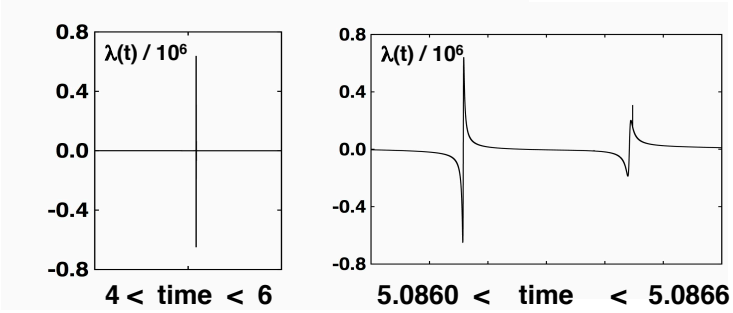
Student Problem

$< s >< 1/s > =\ (\ 0.661\ )\ 3.28 = 2.17$
which is true for all Nosé s-values calculated .

$< s >< 1/s > =\ (\ 0.\ 305\ )\ 964.0 = 294.0$
Is this true for any Nosé-Hoover s-values ?

The Nosé Oscillator Local Lyapunov Exponent Is Another Measure of Stiffness

Adaptive Integration
Quadruple precision with error band between 10^{-28} and 10^{-24}



4 < time < 6 — Time interval between 1.63×10^6 and 3.07×10^6 steps

5.0860 < time < 5.0866 — Time interval between 2.01×10^6 and 2.16×10^6 steps

The corresponding time 16.42 for the Nosé-Hoover #2 dynamics and corresponds to a broad minimum in s. The amplitudes and the required number of steps differ by about six orders of magnitude. Fixed dt = 0.001 !

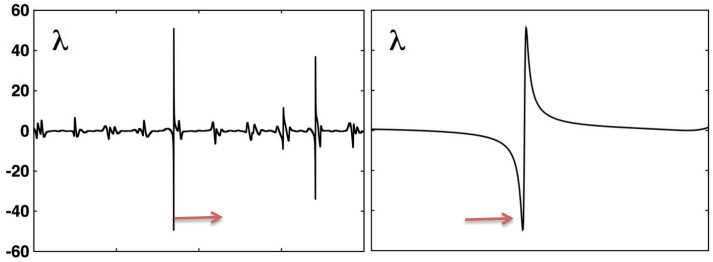
Nosé Oscillator $\dot{q} = (p/s^2)\ ;\ \dot{p} = -q\ ;\ \dot{s} = \zeta\ ;\ \dot{\zeta} = (p^2/s^3) - 1/s$

$(\ q, p, s, \zeta\ )_0 = (\ 2.4, 0, e^{-2.88}, 0\ )$; $\delta = 10^{-6}$

The Nosé-Hoover #1 Oscillator Local Lyapunov Exponent Is Orders of Magnitude Smaller

Adaptive Integration
Double precision with error band between 10^{-16} and 10^{-14}

Typical Local Lyapunov Peaks for the Nosé-Hoover Oscillator | **Resolution of Lyapunov Peak for the Nosé-Hoover Oscillator**



$(q, p, \zeta)_0 = (2.4, 0, 0)$; $\delta = 10^{-6}$

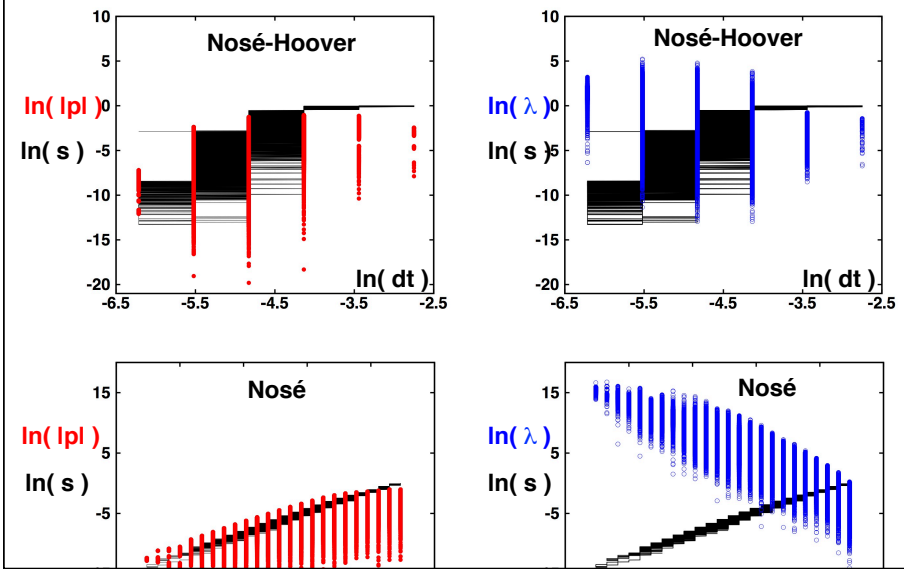
Nosé-Hoover Oscillator Equations

$$\dot{q} = p/s \;;\; \dot{p} = -sq \;;\; \dot{s} = s\zeta \;;\; \dot{\zeta} = p^2/s^2 - 1 \qquad \#\,1$$

$$p/s \rightarrow p \;;\; \dot{q} = p \;;\; \dot{p} = -q - \zeta p \;;\; \dot{\zeta} = p^2 - 1\,. \qquad \#\,2$$

Correlation of lpl, λ, and s with dt

Linear correlation on the log-log plot for all 3 variables and both oscillators !



Analyzing the Results With Histograms

We can understand better the motion of the oscillators by looking at the probability density for the logarithm of the time scaling variable and the time steps.

- **With a variable time step care must be taken in computing the probability density for the time scaling variable s . A trajectory value, $\ln(s_{traj})$, is associated with the ith bin if**

$$ln(s)_i \le ln(s_{traj}) < ln(s)_{i+1} .$$

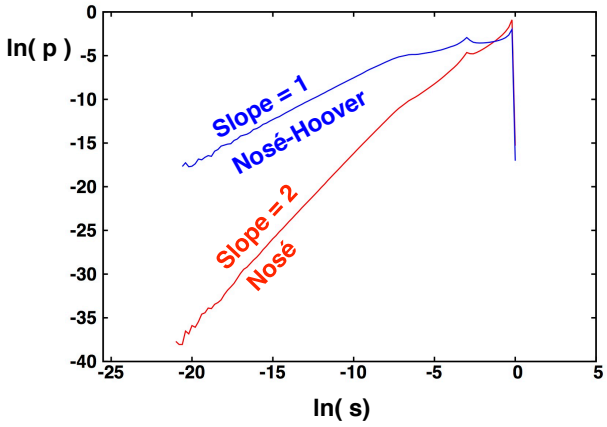
However, the probability that the trajectory values will fall into the bin is equal to the fraction of the time that the trajectory spends within the bin. Thus, the probability density in the ith bin is given by

$$p(ln(s)_i \le ln(s_{traj}) < ln(s_{i+1}) = \sum_{i=1}^{N} \Delta t_i \; / \; \Sigma \; \Delta t_j$$

for 4 000,000,000 time steps .

The time-step histograms show that there were three values of dt used for the smooth Nosé-Hoover equations and more than 20 values of dt (a factor of a million) for the Nosé oscillator. All these time steps are adaptive .

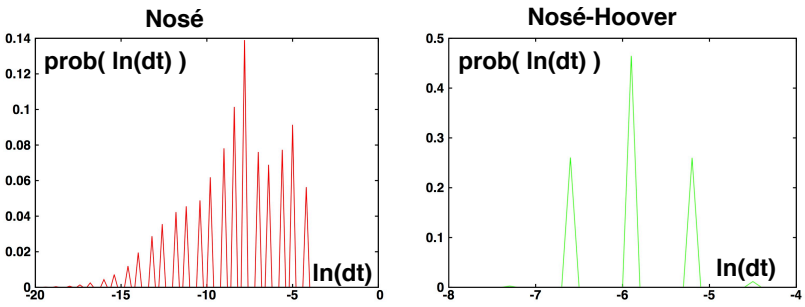
Probability Distribution for the Time-Scaling Variable



$$p_{NH} \propto s \; ; \; p_{Nosé} \propto s^2$$

Histograms for the Probability of dt Show Differences in the Slow and Fast Rates !

100,000,000 steps



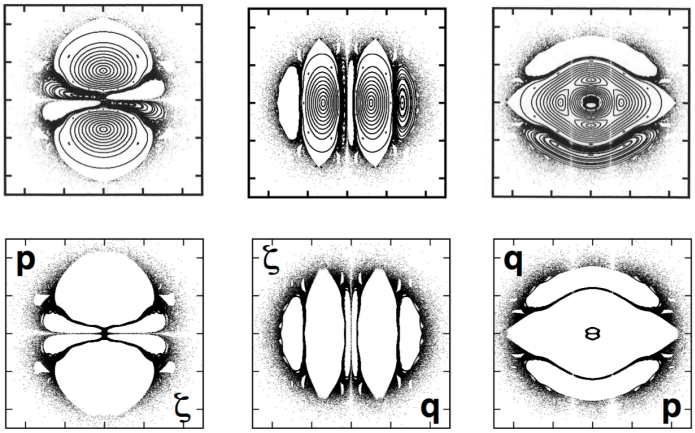
The time-step histograms show that there were three different time intervals used for the smooth Nosé-Hoover equations and there are about twenty different time intervals used for the Nosé oscillator. Keep in mind that in each interval the timestep is halved and doubled in the adaptive method.

Results and Conclusions: Adaptive Integration for Nosé and Nosé-Hoover Oscillators

- **Nosé Oscillator can be treated with the Adaptive 4th-Order Runge-Kutta Algorithm**
- **The trajectories for the Nosé and Nosé-Hoover oscillators are the same but progress at different rates**
- **Trajectory intervals measured between two p = 0 sections show that the sections are identical for the two oscillators**
- **The time scaling variable provides the connection between the Lyapunov exponents for the two oscillators**
- **The local Lyapunov exponent is an important measure of stiffness**
- **We find linear correlations on log-log plots of the the momentum and time scaling versus time.**

The Three Sections of the Nosé & NH Generate Conservative Tori and Points in the Chaotic Sea

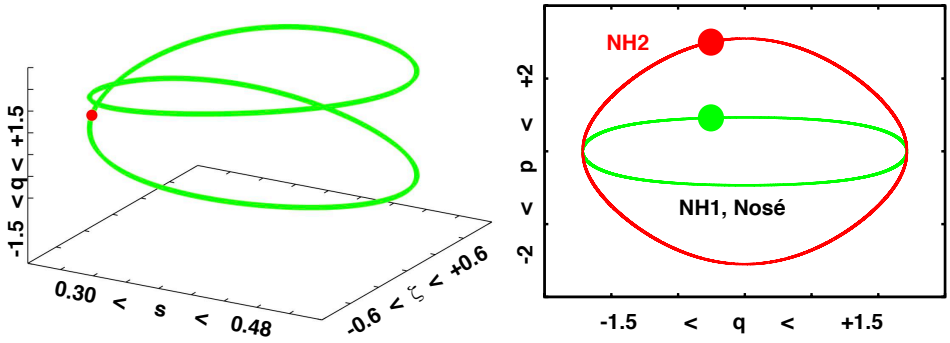
Initial periodic orbits $\{q, p, \zeta\} = (\pm 1.2144, 0, 0)$ *incremented by* ± 0.1. *The* $12th$ *increment* $(2.4144, 0, 0)$ *lies in the chaotic sea.*



Time Scaling in Nosé and Nosé-Hoover Mechanics

Initial condition for a periodic orbit

$$\{q, p, s, \zeta\}_o = \left(1.2145, 0, e^{-q^2/2}, 0\right)$$

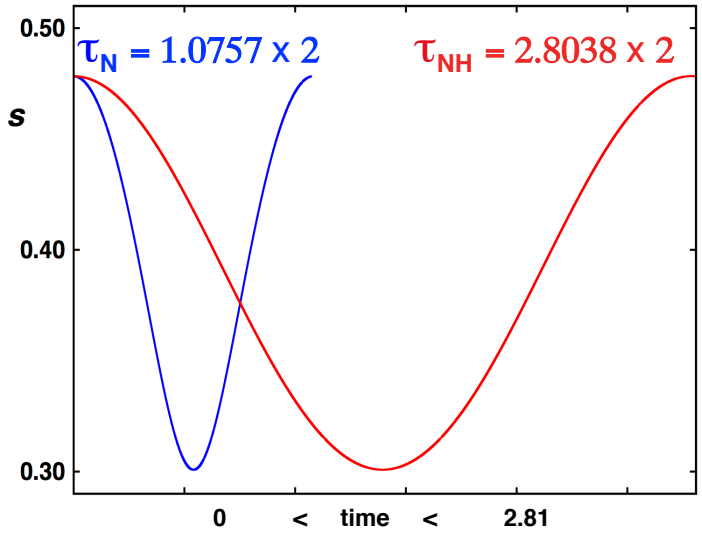


$$At\ time\ t_{NH2} = \mathbf{4.018}$$

$$\{q, p, s, \zeta\} = \{-0.2538, \mathbf{1.5000}, 0.3066, -0.2237\ \}$$

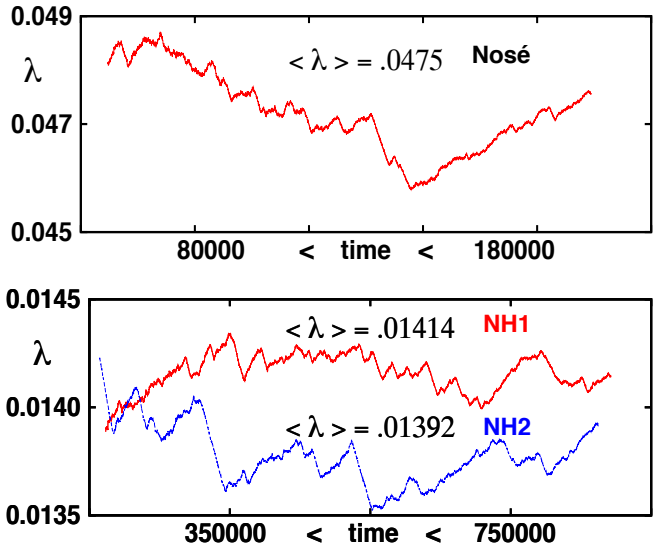
$$\boldsymbol{p_{NH2}} = \{\boldsymbol{p_{Nose}}/s\}\ ;\ \boldsymbol{p_{Nose}} = p_{NH2}s = 0.4599$$

The time scaling variable *s* oscillates *twice* during a single period of the oscillator



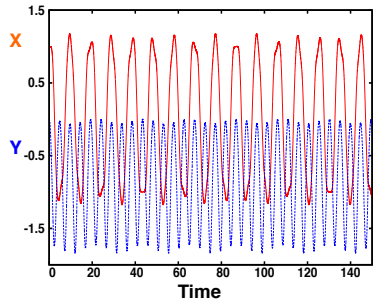
Lyapunov Exponents for Nosé & Nosé-Hoover Mechanics

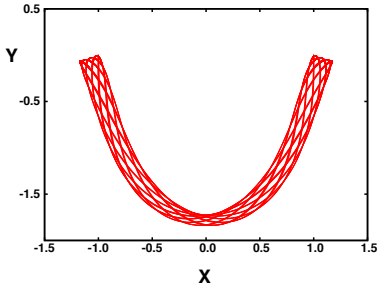
$< \lambda >_{Nosé}$ *differs from* $< \lambda >_{NH}$ *by a factor of* $< s >_{NH}$.



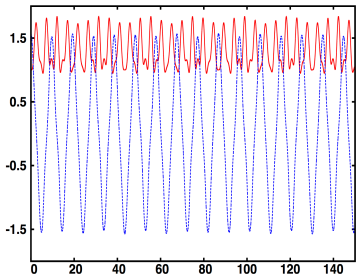
"Springy Pendulum" with a Regular Orbit

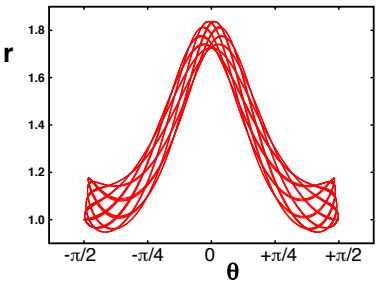
$\{ x , y , p_x , p_y \}_0 = \{ 1 , 0 , 0 , 0 \}$





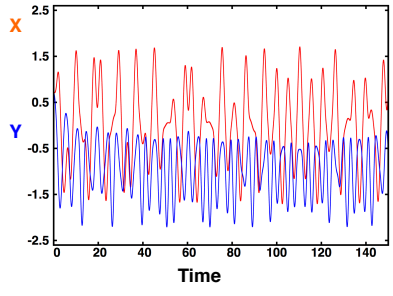
$\{ r , \theta , p_r , p_\theta \}_0 = \{ 1 , \pi / 2 , 0 , 0 \}$

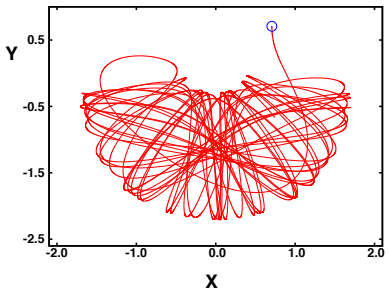




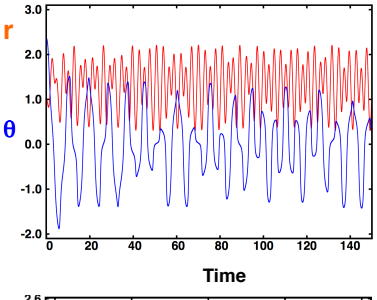
"Springy Pendulum" with a Chaotic Orbit

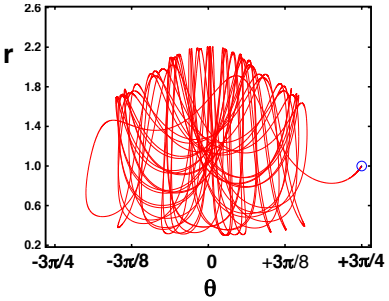
$\{ x , y , p_x , p_y \}_0 = \{ 2^{-1/2} , 2^{-1/2} , 0 , 0 \}$





$\{ r , \theta , p_r , p_\theta \}_0 = \{ 1 , 3\pi /4 , 0 , 0 \}$





Non-Ergodicity of the Springy Pendulum