Kharagpur Lecture 8

microscopic reversibility and MACROSCOPIC IRREVERSIBILITY

1. What *is* microscopic reversibility ?
2. What is the stability of the motion ?
3. Macroscopic Irreversibility
4. Shockwave Structure Dynamics
5. Shockwave Structure Models

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microscopic reversibility and MACROSCOPIC IRREVERSIBILITY

What *is* microscopic reversibility ? Newtonian + Lagrangian + Hamiltonian Mechanics can all be expressed in terms of coordinates and velocities or momenta { q,p } . The momenta are derivatives of the Lagrangian , $\mathcal{L}$:

$$\mathcal{L} = \mathcal{K} - \Phi \ ; \{ p = (\partial\mathcal{L}/\partial\dot{q})_q \ ; (dp/dt) = (\partial\mathcal{L}/\partial q) \}$$

and appear in the Hamiltonian $\mathcal{H}(q,p)$. The momentum p is the partial derivative of the Lagrangian with respect to dq/dt . A "solution" of the motion equations is either a time-ordered set of coordinates { q } or a similar set of coordinate/momentum pairs { q,p } .

The "Leapfrog Algorithm", $q_+ - 2q_o + q_- = dt^2(F/m)_o$ gives coordinates { q } while the Runge-Kutta gives *pairs* of phase variables { q,p }. It is evident that Leapfrog trajectories can be extended arbitrarily into the future or past . Future and past are interchangeable . Just change the sign of { p } .

What *is* microscopic reversibility ?

Certainly the leapfrog algorithm , which generates a string of coordinates equally spaced in time , *is* time-reversible . Time enters into the motion equations as (dt)^2 . When the Lagrangian equations of motion are written In terms of the second derivatives , (d^2q/dt^2) , they too are time-reversible . The Hamiltonian equations of motion ,

$$(dq/dt) = (p/m) ; (dp/dt) = F(q) ,$$

are more problematic because the reversed trajectory breaks the usual convention that momentum is the time derivative of the coordinate . It is simpler to state that if the time-reversed movie of the motion obeys the same motion equations as those in the original forward movie , the motion is 'time-reversible" . It is my view that this is a good definition . It is evident that if there are equations describing nature well they are *not* time-reversible . Nature is definitely not reversible .

James Gleick's books , "Chaos : Making a New Science" and "Time Travel : A History" are good reading . Defining "time" has puzzled good philosophers . We will be happy to define time as "What a **Clock** Measures" .

We will make the usual choice : a particle moving to the right has a positive x velocity component .

microscopic reversibility and MACROSCOPIC IRREVERSIBILITY

It is not evident that the Leapfrog algorithm is related directly to Hamiltonian mechanics, but it is . We just give one example . If the timestep dt and the mass and the force constant are all unity the Leapfrog algorithm $q_+ - 2q_o + q_- = dt^2(F/m)_o$ gives this series of repeating coordinates for a harmonic oscillator and dt = 1 :

. . . ,+1,+1,0,-1,-1,0,+1,+1,0,-1,-1. . .

With dt = 1 the motion equation is $q_+ = q_o - q_-$. Alternatively we could use $q_+ + q_- = q_o$ which can be solved forward or back .

It is characteristic of microscopic motion equations that they have this time-reversibility property . The situation is quite different in the mesoscopic or macroscopic cases where irreversibility is the norm .

microscopic reversibility and MACROSCOPIC IRREVERSIBILITY

There is a connection linking Leapfrog to Hamiltonian dynamics !

In order to see it consider Yoshida's oscillator Hamiltonians :

$$\mathcal{H} = (1/2)(q^2 - qp\,dt + p^2) \text{ or } (1/2)(q^2 + qp\,dt + p^2) .$$

$\mathcal{H}$ generates exactly the same sequence of *coordinates* if one starts with { q,p } = { 0,1 } or { 1,0 } . The period is changed. For Yoshida's Hamiltonian approach it is $2\pi\sqrt{(4/3)}$ rather than 6 . This correspondence shows explicitly that a drift-free energy can be conserved by a finite-difference algorithm in both the future and the past . We see that the Future and Past are interchangeable for the usual types of classical mechanics .

1. Two methods for generating periodic oscillator orbits

Leapfrog method with a period 6 :

```
qnew = 2*qnow – qold – qnow
  → qnew + qold = qnow
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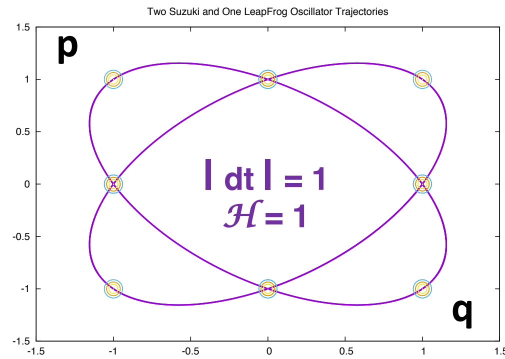
`RK4` solutions of Hamilton's motion equations* using

$$2\mathcal{H}(q,p) = p^2 \pm qpdt + q^2$$



In the Hamiltonian case the period is $(4/3)^{1/2}2\pi$ rather than 6 .

* Such an oscillator Hamiltonian was discovered by Yoshida .

1. Two methods for generating periodic oscillator orbits

$$2\mathcal{H}(q,p) = p^2 - qp + q^2 \text{ [Yoshida]}$$

$$(dq/dt) = p - (q/2) \ ; \ (dp/dt) = -q + (p/2)$$

Because the equations are linear they have an analytic solution :

$$q = \cos(\omega t) \ ; \ p = -\omega \sin(\omega t) + (1/2)\cos(\omega t) \text{ where } \omega = (3/4)^{1/2}$$

The alternative better/faster method is fourth-order Runge-Kutta .

In this Hamiltonian case the period is $(4/3)^{1/2}2\pi$ rather than 6 .
There is a "phase error" rather than an amplitude error .
Are the motion equations reversible ? Not exactly , but they could be made so by a rotation in the phase space .

1. What *is* microscopic reversibility ?

**The Nosé-Hoover oscillator , which Carol showed has Hamiltonian roots , is time-reversible .
The equations of motion, taken from the Dettmann Hamiltonian, reduce from four to three :**

$$2\mathcal{H} = p^2/s + sq^2 + s\zeta^2 + s\ln(s^2) = 0 \rightarrow$$

$$\{ dq/dt = p/s \ ; \ dp/ds = -\,sq \ ; \ ds/dt = s\zeta \ ; \ d\zeta/dt = (p/s)^2 - 1 \}$$

or $\{ (d/dt)^2 q = -\,q - \zeta(dq/dt) \ ; \ d\zeta/dt = (dq/dt)^2 - 1 \}$ where

we can ignore the motion equation for (ds/dt) .

Alternatively , $\{ dq/dt = p \ ; \ dp/dt = -\,q - \zeta p \ ; \ d\zeta/dt = p^2 - 1 \}$.

This *is* reversible with p and ζ and dt changing signs .

Is the reversed motion stable as is $\{ dq/dt = p \ ; \ dp/dt = -\,q \}$?
Linearized perturbation theory reveals robust instability !

1. What *is* microscopic reversibility ?

**The Nosé-Hoover oscillator, which Carol showed has Hamiltonian roots , is time-reversible .
The equations of motion, taken from the Dettmann Hamiltonian , reduce from four to three :**

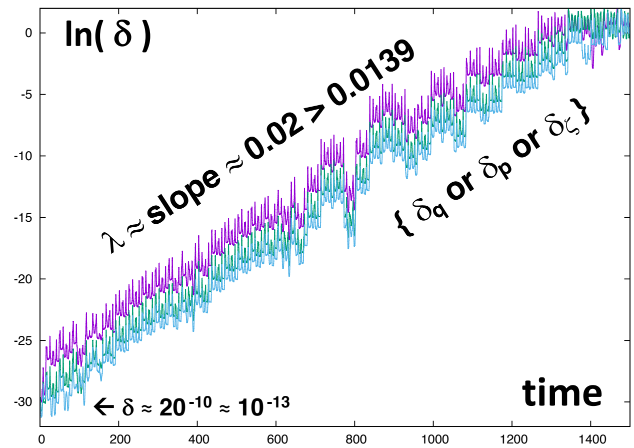
$$\{ dq/dt = p \ ; \ dp/dt = -\,q - \zeta p \ ; \ d\zeta/dt = p^2 - 1 \} .$$

This quadratic set *is* reversible . p and ζ and dt change signs .

Is the reversed motion stable ? Unlike $\{ dq/dt = p \ ; \ dp/dt = -\,q \}$
a linearized perturbation reveals robust instability !

The method involves starting with two neighboring solutions .
In the absence of Benettin's idea that neighboring solutions
be constrained , the separations soon become macroscopic .

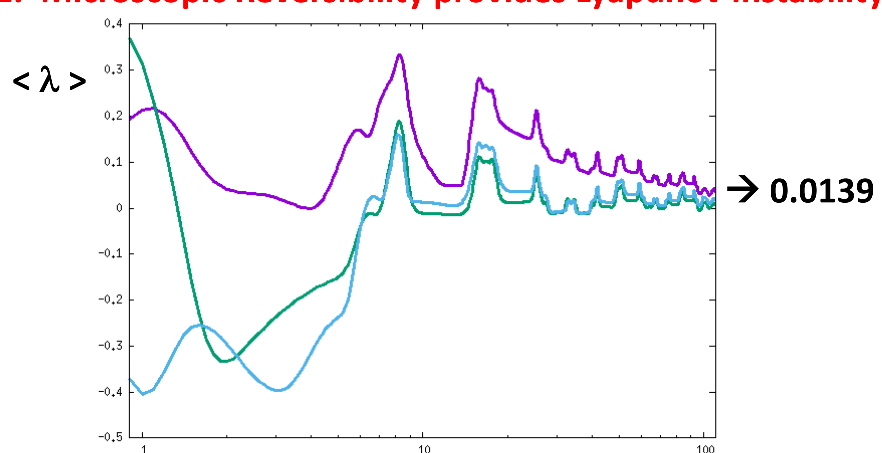
1. What *is* microscopic reversibility ?



$\{ (dq/dt) = p \; ; \; (dp/dt) = -q - \zeta p \; ; \; (d\zeta/dt) = p^2 - 1 \}$

[local] Lyapunov exponent estimates without rescaling .

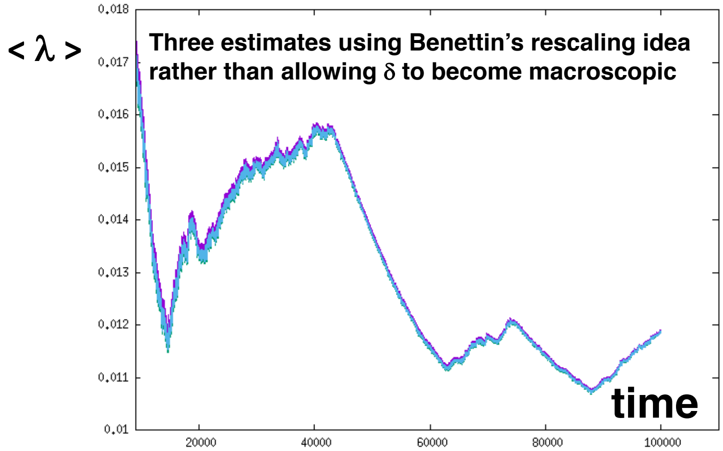
1. Microscopic Reversibility provides Lyapunov Instability



0 < log(time) < 2

Results with three initial conditions, dq or dp or dζ = 0.000001 .
The long-time-averaged Lyapunov exponent is 0.0139 .

1. Microscopic Reversibility provides Lyapunov Instability



Results with three initial conditions, dq or dp or $d\zeta = 0.000001$ have all converged to similar average values at time = 10 000 .
$< \lambda > = 0.0139$ at time = 40 000 000 using dt = 0.002 and RK4 .

Q: Why is the direction of the perturbation irrelevant ?
A: The direction of most rapid growth wins out soon !

We demonstrate with an example in which one variable is unstable and the other one is not . { dq/dt = q ; dp/dt = 0 } . We consider the evolution of a linear perturbation (δ_q, δ_p) constrained to have unit length by the Lagrange multiplier λ :

$$d\delta_q/dt = \delta_q - \lambda\delta_q \; ; \; d\delta_p/dt = -\lambda\delta_p \rightarrow \lambda = \delta_q^2 / (\delta_q^2 + \delta_p^2)$$

To solve the differential equations use $(\delta_q,\delta_p) = (+\cos(\theta), -\sin(\theta))$.

$$-\sin(\theta)\,(d\theta/dt) = +\cos(\theta) - \cos^3(\theta) \rightarrow (d\theta/dt) = -\sin(\theta)\cos(\theta)$$

which has the solution $\delta_q = [\, 1 + e^{-2t} \,]^{-1/2}$; $\delta_p = -[\, 1 + e^{+2t} \,]^{-1/2}$

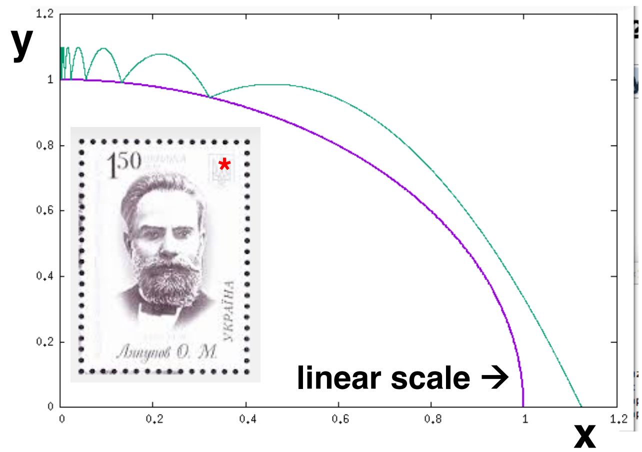
This example demonstrates that the dominant growth direction wins out over all the others exponentially fast .

2. What is the stability of the motion ?

Consider the motion of a mass point on a stationary ball .

Initially (x,y) = (10^{-6},1.1) with a gravitational field strength of 1 where the ball radius is 1 . The total number of bounces is 16 within a time of 13.92 .

*** Aleksandr Lyapunov**



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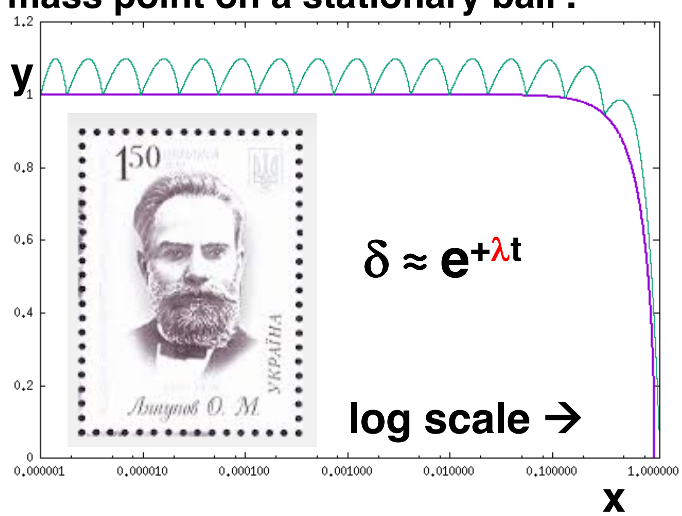
$\lambda \approx 6 \times \ln(10) / 14 \approx 1$



2. What is the stability of classical motion ?

The Bouncing Ball Problem is *typical* :

Time-reversible equations of motion ;
Logarithmic measure of instability , λ ;
λ depends on the past , *not* the future .

Many-Body Problems are more typical , but they are more difficult to treat numerically .

Lyapunov analysis provides an *Arrow* .
We consider a manybody collision in which Time's Arrow is clearly evident .
We can understand IRREVERSIBILITY !

2. What is the stability of classical motion ?

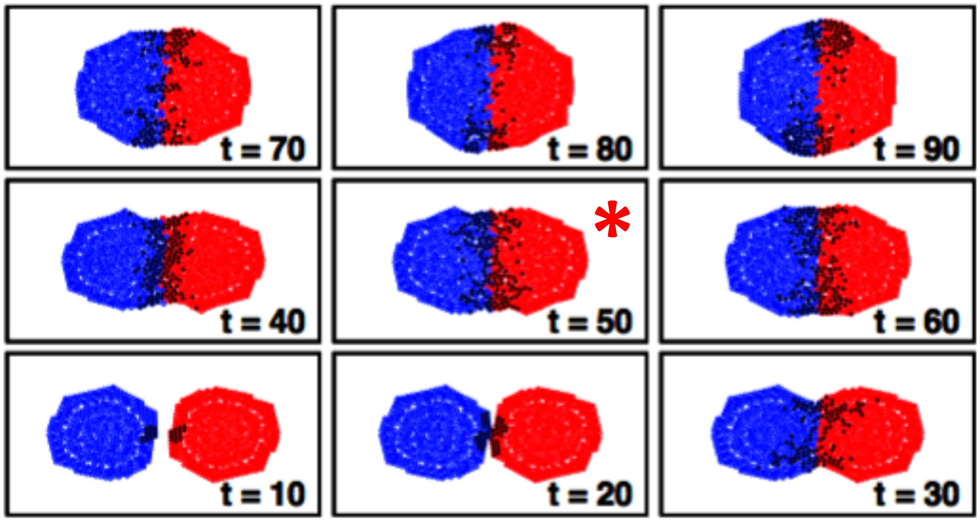
Mesoscopic motion (molecular dynamics simulations) obeys the Second Law . One way to see this is to simulate a noticeably irreversible process . Thus we consider the inelastic collision of two 400-particle balls . All 800 particles interact with a repulsive pair potential, $(1 - r^2)^4$. The attraction is furnished by an additional "embedded-atom" potential , $\Sigma (1/2)(\rho - 1)^2$, where each of the 800 terms in the sum depends on the deviation of the particle densities from unity . The particle densities are computed from Lucy's weight function with a range of h = 3.5 ; here z = r/h :

$$w(r < h = 3.5) = (5/\pi h^2)[1 + 3z] [1 - z]^3 .$$

In the continuum descriptions of macroscopic flows it is usual to use Newtonian viscosity and Fourier heat conduction to describe the irreversible processes involving dissipation and transport . *These processes are irreversible in the sense that a reversed flow no longer satisfies the same motion equations .* Fourier's Law, $Q_x = -\kappa (dT/dx)$, that heat flows from hot to cold furnishes the simplest example . If the flow is instantaneously reversed (changing the signs of all of the velocities) the heat flux will also be reversed but the temperature will remain unchanged . In the artificial reversed flow heat flows from cold to hot which would correspond to a negative heat conductivity ($\kappa < 0$) and a violation of the Second Law of Thermodynamics . Although the dynamics of a few particles can violate the "law" for a short time 800 particles are enough to be described by macroscopic phenomenological constitutive equations . We will illustrate this now .

2. What is the stability of classical motion ?

Here is a mesoscopic inelastic collision :



Forward Times 10 to 90 ; dt = 0.001

The stability of motion *via* "the" Lyapunov Exponent

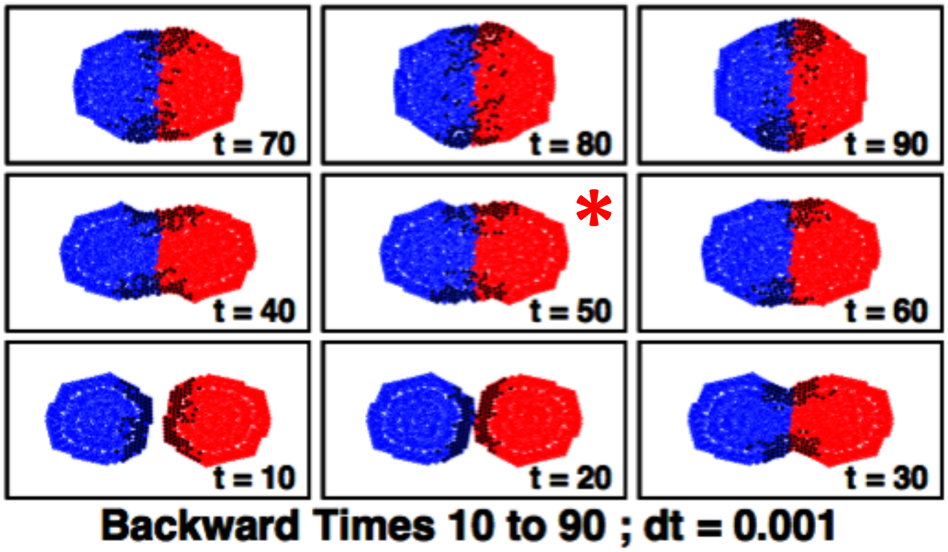
At any time the direction of the Lyapunov instability vector (satellite – reference) can be determined by following two trajectories with the separation between them constrained (this is the Benettin + Shimada + Nagashima idea of 1979-1980) . By looking at the components of the vector one can identify the "important" particles at any time . It is good manners to recognize that these "local-exponent" properties depend upon the choice of coordinate system, which causes mathematicians to fret .

In the previous (forward view) it is the leading-edge particles which contribute most to the Lyapunov instability . In the following (backward reversed-velocity view) the important particles are the surface particles undergoing plastic strain . Such a calculation could not be reversed in continuum mechanics as the flow equations are not time-reversible .

Although microscopic Newtonian mechanics *is* reversible the reversed results are completely unstable and can only be obtained by storing or using Levesque-Verlet .

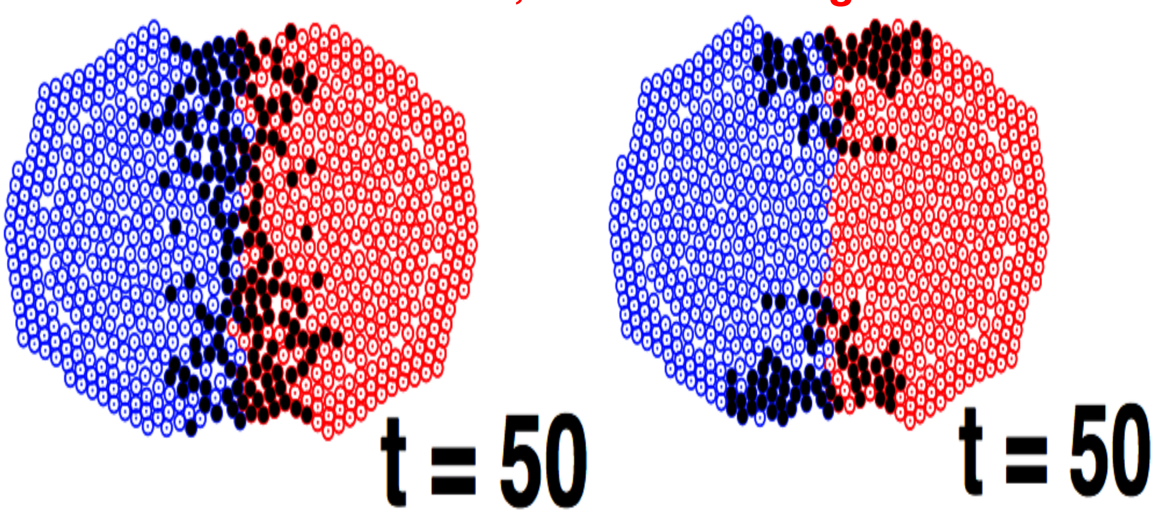
2. What is the stability of classical motion ?

Here is the mesoscopic inelastic collision :



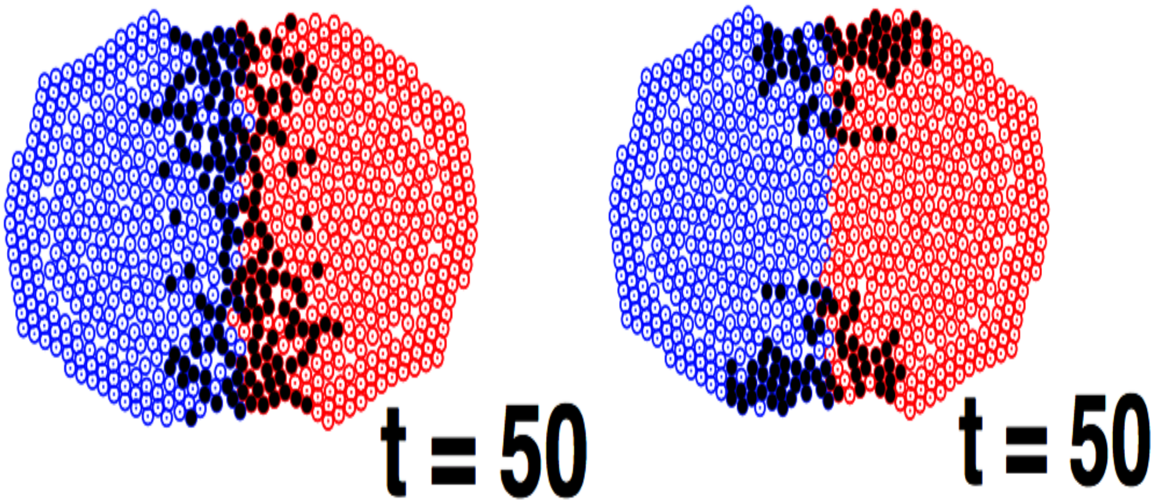
2. What is the stability of classical motion ?

Here is the mesoscopic inelastic collision
with Forward at left, Backward at right .



2. What is the stability of classical motion ?

Strain rate changes sign ;
Stress does not !



2. What is the stability of classical motion ?

The Second Law is readily apparent in these plastic flows or in shear flows or in heat flows . In a viscous fluid the shear stress is proportional to the strain rate in a thermostated isochoric flow . In a heat flow the heat flux Q is proportional to the temperature gradient :

$$-P_{xy} = \sigma_{xy} = \eta \,[\, (du/dy) + (dv/dx) \,] \;;\; Q_x = -\kappa \,(dT/dx) \,.$$

We know from the virial theorem and the heat theorem that the stress and the temperature gradient are independent of time reversal while the strain rate and the heat flux are not . Any flow which obeys the phenomenological linear laws can easily be detected by computing η and κ . If these transport coefficients are negative the motion has been reversed ! There is an obvious arrow of time with dt > 0 having normal transport coefficients and dt < 0 having abnormal ones .

3. Macroscopic Irreversibility ?

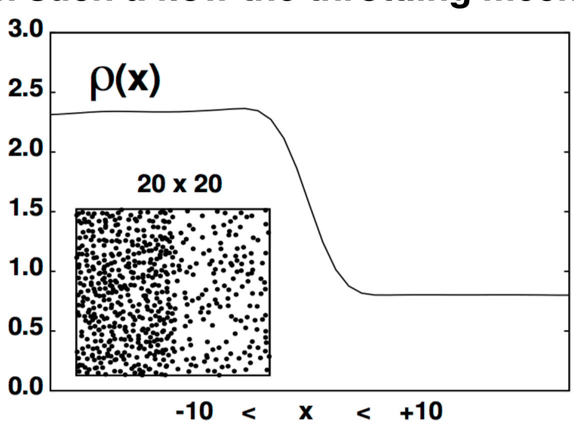
The Second Law is automatically satisfied in the phenomenological models used in shockwave simulations . Viscoelastic models of material response stress the parallel structures of homogeneous linear elasticity and fluid linear viscosity :

$$\sigma_{xx} = 2\eta(du/dx) + \lambda[\ (du/dx) + (dv/dy)\ ]$$
$$\text{and } \sigma_{xy} = \eta[\ (du/dy) + (dv/dx)\ ] \text{ and}$$
$$\sigma_{yy} = 2\eta(dv/dy) + \lambda[\ (du/dx) + (dv/dy)\ ]\ .$$

In two dimensions η is shear viscosity or shear modulus while $\lambda + \eta$ is the bulk viscosity or bulk modulus . (u,v) are displacements or velocities . The products of stress times strain or strainrate correspond to work done in the elastic case and rate of heating in the viscous case . The elastic λ and η are the Lamé constants .

4. Irreversibility in Joule-Thomson Expansion ? *

The Second Law is likewise satisfied in adiabatic throttling , which will cool or heat the fluid through energy conservation . In such a flow the throttling mechanism is a potential barrier .



In this simulation we use a quartic pair potential :

$$\phi(\ r < 1) = (\ 1 - r^2\ )^4$$

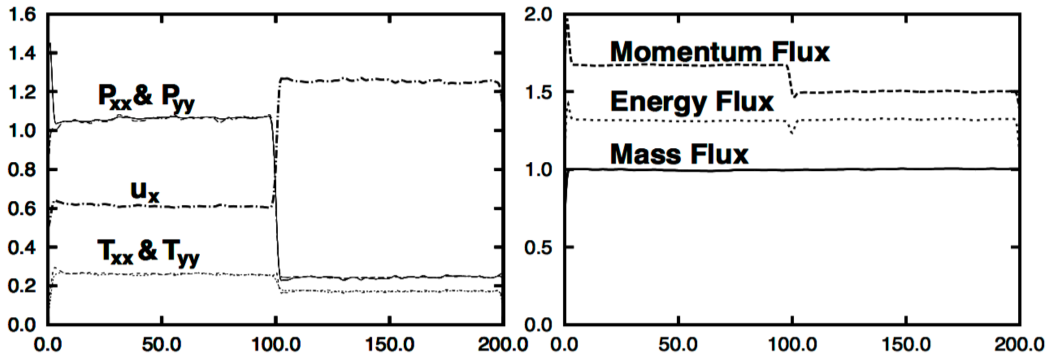
and a quartic barrier :

$$\phi(\ |\ x\ |\ < 1) = (\ 1 - x^2\ )^4$$

The system is 200 x 40 .

* Hoovers and Travis, PRL 112 (2014)

4. Irreversibility in Joule-Thomson Expansion ?

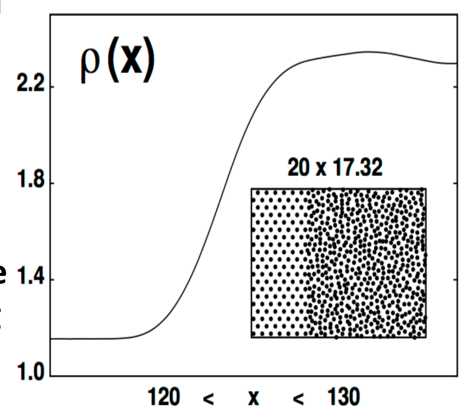


Interpretation of the irreversibility is tricky . Evidently the irreversible process occurs in the vicinity of the potential barrier at x = 100 . The flow is strictly Newtonian everywhere . We simply notice that the entropies of the equilibrium states entering and leaving are not the same . But the details depend upon the structure of the potential barrier . In the shock the structure of the wave is furnished by the fluid itself without any external influences .

4. Irreversibility in Shockwaves ?

The Second Law is satisfied in shockwaves , which are ideal for study because they require no special boundary conditions . From the standpoint of simulation it is easy to add displacements or velocities to particles as they enter the system . Likewise the particles about to leave can be given the exit velocity as they near the boundary .

One can look locally at the stress and the heat flux and see that the corresponding transport coefficients are positive .

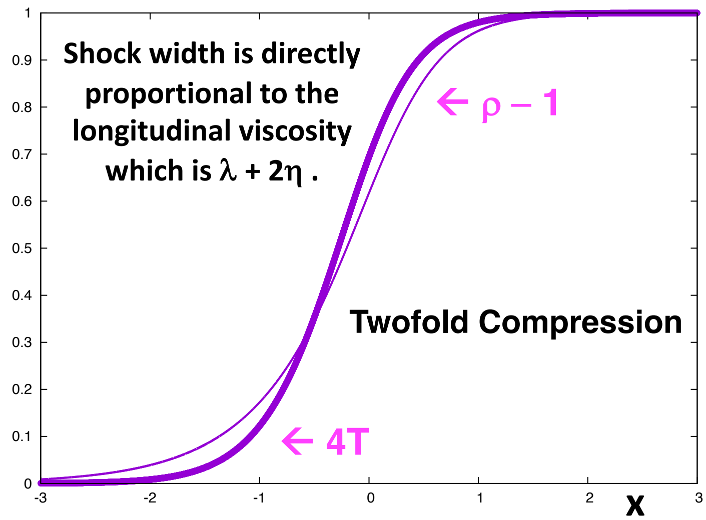


5. Back to Stationary Shockwave Structure with Unit Viscosity *

$P_{xx} = P - \lambda(du/dx + dv/dy) - 2\eta(du/dx)$;
$P_{yy} = P - \lambda(du/dx + dv/dy) - 2\eta(dv/dy)$.

ρu , $P_{xx} + \rho u^2$, and $\rho u[e + (u^2/2) + (P_{xx}/\rho)]$, are the fluxes , of mass , momentum , and energy , are constant throughout .

Elimination of the cold and hot speeds gives the Hugoniot relation :
$\Delta e = \langle P \rangle \Delta V$.



* η and λ are the first and second viscosity coefficients, with η the "shear viscosity" .

5. Back to Stationary Shockwave Structure with Unit Viscosity *

Let us consider the simplest possible fluid shockwave . We imagine a fluid with a weak repulsive energy proportional to ρ and a thermal energy T so that the thermomechnical equation of state is : $P = \rho e = (\rho^2/2) + \rho T$ with $e = (\rho/2) + T$. These relations , as well as the entropy S follow from the corresponding Gibbs' canonical partition function :

$$Z^{1/N} = e^{[- A/NkT]} = e^{[+ S/Nk]} e^{[- E/NkT]} = (VT/N) e^{[- N/2VT]}$$

A steady shockwave necessarily has constant fluxes of mass, momentum, and energy . We choose to study a wave with twofold compression from the cold T = 0 state :

$$\rho : 1 \rightarrow 2 ; u : 2 \rightarrow 1 ; P : (1/2) \rightarrow (5/2) ; e : (1/2) \rightarrow (5/4) ; T : 0 \rightarrow (1/4) .$$

Notice that the three fluxes are constant where we omit Q_x for simplicity :

$$\rho u = 2 ; P_{xx} + \rho u^2 = (9/2) ; (\rho u)[e + (P_{xx}/\rho) + (u^2/2)] = 6 .$$

The Hugoniot equation, which results from eliminating the cold and hot velocities , is the overall energy conservation relation for shocks :

$$\Delta e = (1/2)(P_{hot} + P_{cold})\Delta V = (3/4) = (1/2)3(1/2) .$$

5. Back to Stationary Shockwave Structure with Unit Viscosity, $P_{xx} = \rho e - (du/dx)$

Further, we imagine that the viscosity coefficient is equal to unity. We can find a single ordinary differential equation to solve for the shockwave profile by eliminating temperature from the two equations for the fluxes of momentum and energy :

$$(\rho^2/2) + \rho T - (du/dx) + (4/\rho) = (9/2)\ ;\ \rho + 2T - (du/dx)/\rho + (2/\rho^2) = 3\ .$$

With the substitution $(du/dx) = (-2/\rho^2)(d\rho/dx)$ * the elimination of the temperature from the flux relations provides a single differential equation for the density as a function of the coordinate x :

$$(d\rho/dx) = (3/2)\rho(\rho - 1)(2 - \rho)\ .$$

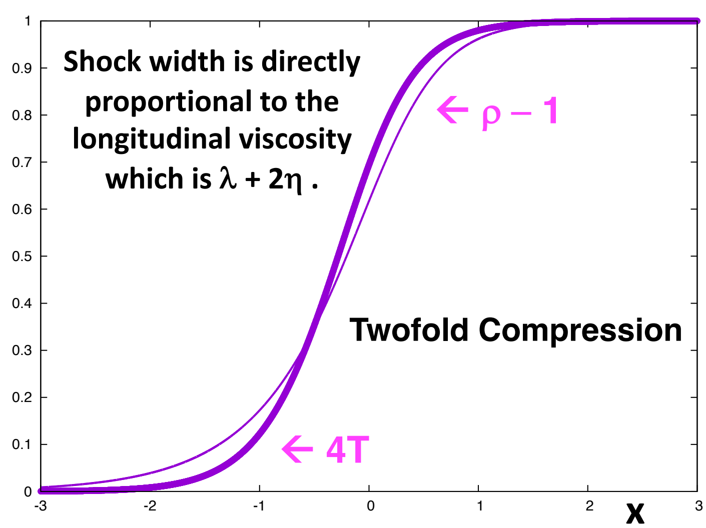
As is usual, the numerical solution converges easily (starting at the "hot" end with $dx = -0.001$) using our standby integrator, fourth-order Runge-Kutta . Starting at the cold end is not at all tempting as the entropy diverges there ! * Remember $\rho u = 2$.

5. Back to Stationary Shockwave Structure with Unit Viscosity *

$P_{xx} = P - \lambda(du/dx + dv/dy) - 2\eta(du/dx)$;
$P_{yy} = P - \lambda(du/dx + dv/dy) - 2\eta(dv/dy)$.

ρu , $P_{xx} + \rho u^2$, and $\rho u[e + (u^2/2) + (P_{xx}/\rho)]$, are the fluxes , of mass , momentum , and energy , are constant throughout .

Elimination of the cold and hot speeds gives the Hugoniot relation : $\Delta e = \langle P \rangle \Delta V$.



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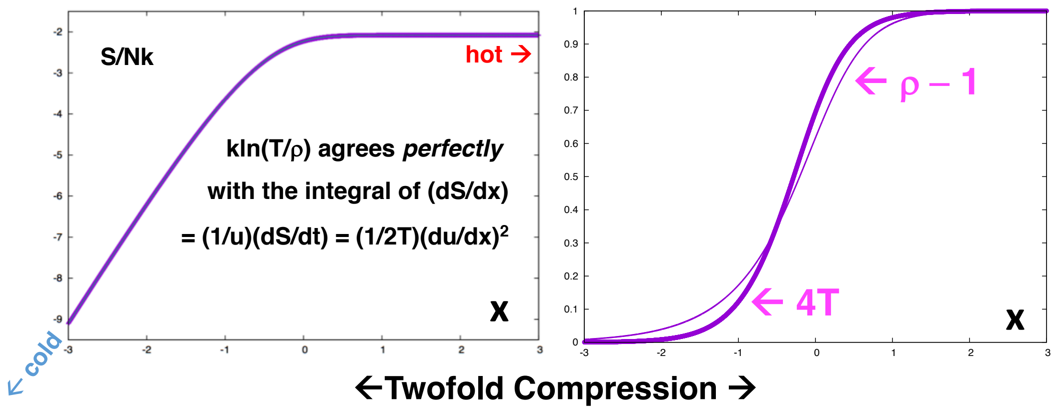
5. Back to Stationary Shockwave Structure with Unit Viscosity *



The hot entropy is ln(1/8) = -2.079 and the cold entropy is – ∞ .

5. Solving the Navier-Stokes-Fourier equations for shockwave structure *

The solution of the Navier-Stokes-Fourier equations is only a little more complicated. We illustrate for a shockwave structure worked out in 1980 for the Lennard-Jones liquid, compressed twofold with a temperature increase of about 10 000 kelvins , enough to begin the ionization process for argon , the fluid being modeled . Bulk and shear viscosity , as well as heat conductivity , were included in the modeling . * As a result one can solve two simultaneous differential equations , one for $(d\rho/dx)$ coming from the momentum flux , and one involving both $(d\rho/dx)$ and (dT/dx) , coming from the energy flux . Alternatively one can divide and solve the resulting equation for $(d\rho/dT)$. In order to complete this calculation molecular dynamics simulations for the viscosity coefficients and the thermal conductivity were carried out and fitted with convenient functions of density and temperature . For this shockwave the maximum value of T_{xx} was about 50% larger than the transverse temperatures T_{yy} and T_{zz} .

* Holian, Hoover, Moran, and Straub in the December 1980 Physical Review A .

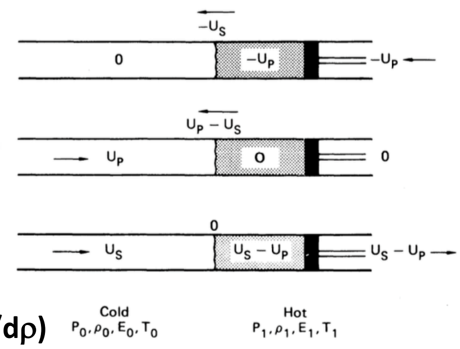
5. Solving the Navier-Stokes-Fourier equations for shockwave structure *

There is a longstanding tradition of solving the Navier-Stokes equations . The three equations for mass , momentum , and energy can be solved by eliminating the entrance and exit velocities giving ΔE = < P > ΔV , the "Hugoniot Equation" .

$$\rho u = 40.9 \; ,$$

$$P_{\mathrm{eq}} - (\eta_v + \tfrac{4}{3}\eta)\,\frac{du}{dx} + \rho u^2 = 1980 = P_{xx} + \rho u^2 \; ,$$

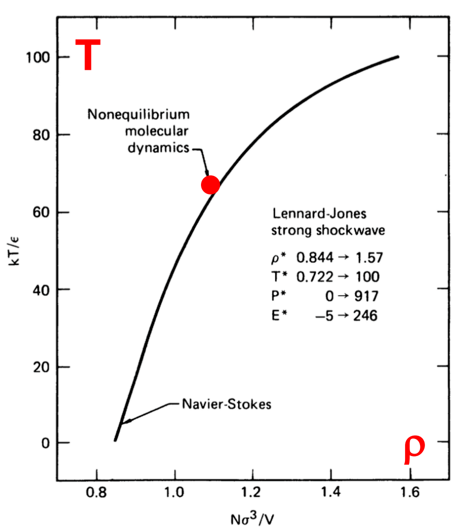
$$\rho u \left(E_{\mathrm{eq}} + \frac{P_{xx}}{\rho} + \frac{u^2}{2} \right) - \kappa \frac{dT}{dx} = 47\,900 \; .$$



Traditionally one divides and computes (dT/du) or (dT/dρ) though it is easy to solve *two* simultaneous differential equations with fourth-order Runge-Kutta , giving the shock profile , the space dependence of all the variables .

* Holian, Hoover, Moran, and Straub December 1980 Physical Review A .

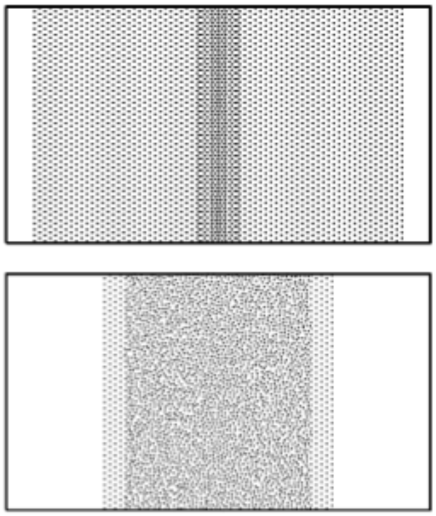
5. Solving the Navier-Stokes-Fourier equations for shockwave structure



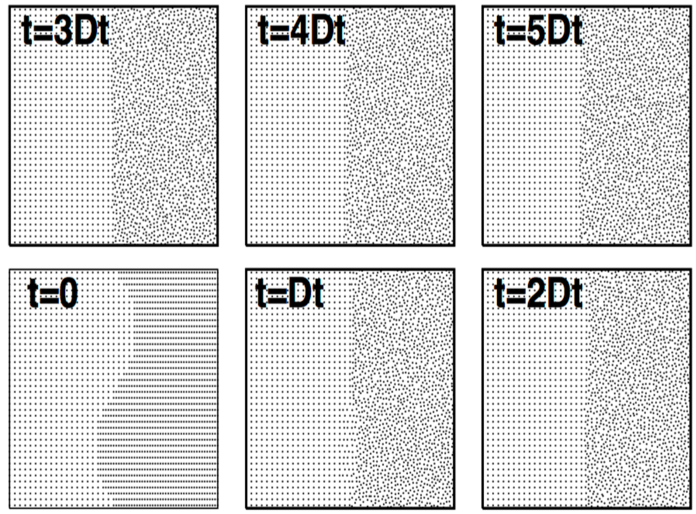
Here is temperature *versus* density from the Navier-Stokes equations using the transport coefficients determined from molecular dynamics solutions . The red point comes from the center of the shock profile from this nonequilibrium molecular dynamics simulation . The Navier-Stokes equations cannot be used to understand the difference between T_{xx} and T_{yy} , which here are different by a factor of 3/2 . This shock → twofold Lennard-Jones ρ change .

5. Planar shockwaves *are* stable in one dimension

Twofold Compression of two blocks



$\phi(r < 1) = (10/\pi)(1 - r)^3$



5. Lucy Function averages provide smooth continuum fields from molecular dynamics

$$F(r) = \Sigma\, F_i\, w(r_i - r) \,/\, \Sigma\, F_i\, w(r_i - r)$$

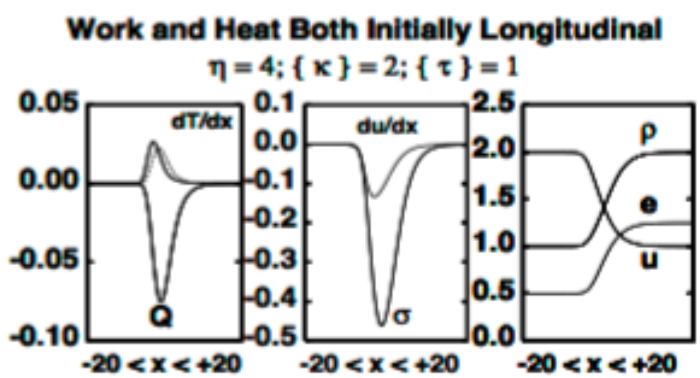


FIG. 8: Stationary profiles showing the longitudinal and transverse temperature gradients $[(dT_{xx}/dx)$ is solid; (dT_{yy}/dx) is dashed] as well as the velocity gradients. Notice that the heat flux and shear stress lag behind the gradients which "cause" them.

microscopic reversibility and MACROSCOPIC IRREVERSIBILITY

1. What is microscopic reversibility ?
   Remember Leapfrog
2. What is the stability of the motion ?
   Remember Lyapunov
3. Macroscopic Irreversibility
   Remember the Second Law
4. Shockwave Structure Dynamics
   Comoving Frame Dynamics is stationary
5. Shockwave Structure Models
   Time delay, work/heat tensor $T_{xx} \neq T_{yy}$

[Shockwaves are an ideal test of nonlinear ideas]

microscopic reversibility and MACROSCOPIC IRREVERSIBILITY

1. What is microscopic reversibility ?
   $q_+ - 2q_o + q_- = (dt)^2 (F/m)_o$
2. What is the stability of the motion ?
   Remember that Lyapunov lives in the past .
3. Macroscopic Irreversibility
   P_{xy} and (du/dx) *versus* Q_x and (dT/dx)
4. Shockwave Structure Dynamics
   Entropy Production certainly works !
5. Shockwave Structure Models
   Time delay, work/heat tensor $T_{xx} \neq T_{yy}$

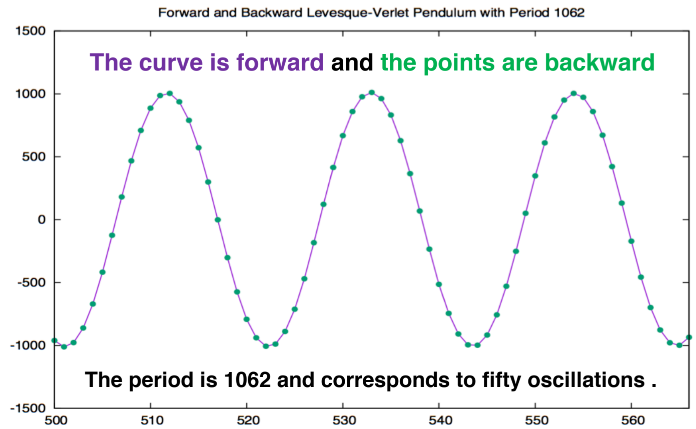
[Shockwaves are an ideal test of nonlinear ideas]

6. Addendum : What sorts of simulations can be run *in perpetuity* ? And , are they *Reversible* ? What about Loschmidt and Poincaré ? Levesque + Verlet Leapfrog (forward/backward with finite precision) .

```
iqnow = 1 034
iqold = 1 024
do i = 1,1063 ! GOING FORWARD
iFdtdt = -100*dsin(iqnow/1000.0d00)
iqnew = iqnow + iqnow - iqold + iFdtdt
write(8,*) i,iqold,iqnow,iqnew
iqold = iqnow
iqnow = iqnew
Enddo

iold = iqnow ! REVERSING THE VELOCITY
inow = iqold
iqnow = iold
iqold = inow

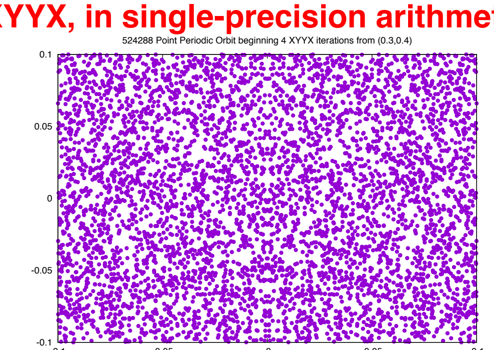
do i = 2,1064 ! GOING BACKWARD
iFdtdt = -100*dsin(iqnow/1000.0d00)
iqnew = iqnow + iqnow - iqold + iFdtdt
write(9,*) i,iqold,iqnow,iqnew
iqold = iqnow
iqnow = iqnew
enddo
```



6. Addendum : What sorts of simulations can be run *in perpetuity* ? And, are they *Reversible* ? What about Loschmidt and Poincaré ? Here we consider 4 unit shears, XYYX, in single-precision arithmetic .

```
subroutine xit(xin,yin,xout,yout)
xout = xin + 2*yin
if(xout.gt.+1) xout = xout - 2
if(xout.lt.-1) xout = xout + 2
yout = yin
return
end ! This is the X shear map

subroutine yit(xin,yin,xout,yout)
yout = yin + 2*xin
if(yout.gt.+1) yout = yout - 2
if(yout.lt.-1) yout = yout + 2
xout = xin
return
end ! This is the Y shear map
```



Here is the central 1% of the 2x2 square . Evidently The XYYX mapping is ergodic . Notice the symmetry ! On the fourth iteration * , beginning with (0.3,0.4) the Map enters into the periodic orbit of 524 288 points . A portion of the complete 2x2 mapping is shown above .

* This is worth investigating !

microscopic reversibility and MACROSCOPIC IRREVERSIBILITY

Notice that all of the motion equations which we have considered are time-reversible . This includes equilibria as well as shear flows , heat flows , and stationary shockwaves . These systems and these flows are typically time-reversible stationary states . How can such flows be "irreversible" ?

The simplest irreversibility can occur if there is the possibility of phase-volume change , as In the nonequilibrium Baker Map which will be much discussed in the next lecture . If parts of the comoving phase-space volume expand while other parts contract the time-averaged volume change cannot be positive , producing a strange attractor in the nonequilibrium case .

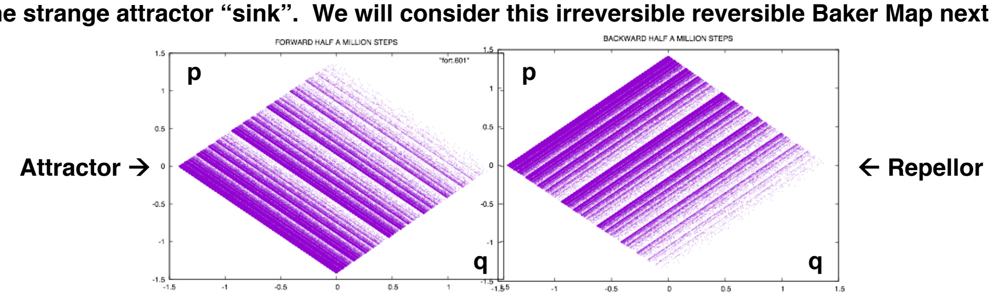
What are the characteristics of nonequilibrium steady states ? They generate with vanishing phase volume . The sum of the Lyapunov exponents describing the flow must be negative , corresponding to contraction , with $d\ln\oplus/dt = -d(S/k)/dt = \sum\zeta$, where the sum includes all of the thermostated degrees of freedom . Suppose that we wish to characterize a nonequilibrium strange attractor with 10^6 points in a two-dimensional space . 10^{12} points should be enough because the logarithm of the probability of finding 10^6 nonoverlapping points is :

$$\ln(1 - 1/N) + \ln(1 - 2/N) + \ldots + \ln(1 - n/N) \approx \int^n dk(-k/N) = -n^2/(2N) \rightarrow n \approx \sqrt{N} \;. \;*$$

*** it is a good exercise to show that taking additional terms in the expansion of $\ln(1 - \delta)$ does not change the reasoning for large N .**

microscopic reversibility and MACROSCOPIC IRREVERSIBILITY

Typically the transient and periodic parts of a forward trajectory are of the same average length . One can imagine going "backward" to the strange repellor or "source" and going "forward" to the strange attractor "sink". We will consider this irreversible reversible Baker Map next time :



FORWARD BAKER MAP **REVERSED BAKER MAP**

Although the flow is reversible with the attractor and repellor mirror images of one another the stability of the two fractals is different : the flow in the neighborhood of the attractor collapses and flow in the neighborhood of the repellor expands . The net flow is from "source" to "sink" .

microscopic reversibility and MACROSCOPIC IRREVERSIBILITY

Before leaving this subject let us consider the difference between equilibrium and nonequilibrium steady states . In both cases fluctuations obey the Central Limit Theorem in time and space. An equilibrium system has no heat flow and no viscous forces. On the other hand it can have mass , momentum , and energy gradients of the kinds typical of gravitational forces , configurational temperature gradients caused by rotation . Notice that a two-dimensional particle circling the origin has a centrifugal force + $m\omega^2 r$ which can be offset by a spring force $-\kappa(r - 1)$ so that even a situation of steady rotation and constant angular momentum would produce an apparent gradient in temperature for a rotating solid held together by Hooke's Law forces .

Nonequilibrium steady states would give rise to heat flux , gradients , dimensionality loss in phase space, strange attractors . Notice that the continuity equation is the only one of the three conservation laws which is time reversible, $(\partial\rho/\partial t) = -(\partial/\partial x)(\rho v_x)$, with both sides of the equation changing sign if the clock runs backwards . The equations in two or three dimensions have this same form . If the velocities are reversed in a Rayleigh-Bénard problem or a shockwave it is easy to see that the continuum pressure tensor , $P = P(\rho,e) - \eta[(\partial v_x/\partial y) + (\partial v_y/\partial x)]$ is typically mixed . Likewise , in a heat flow problem the heat flux is odd in the time while the temperature is even.

An interesting aspect of Hamiltonian Thermostats is that they cannot generate heat flow . There are several examples in our paper "Hamiltonian Systems Fail to Promote Heat Flows", available in the arXiv 1303.6190 .

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