

A backward analysis of simple collisions

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Motivating Introduction

- Numerical Simulations in Molecular Dynamics
 - ★ extract statistical information about trajectories of systems
 - ★ reliability of these computations is usually monitored with a combination of empirical observations and careful adjustments (i.e. thermostats, Dissipative Particle Dynamics)
 - ★ would like to develop an understanding of the reliability of this computational practice in terms of the numerical method used to integrate the ode

...Introduction

- Good Statistics from Bad Simulations?
 - ★ over finite time intervals, numerical integrators applied to ode's yield trajectories which converge to the true trajectories as the length of the time-step goes to zero
 - ★ simulations are run over very long time intervals with large time-steps
 - ★ the generated statistical information is accurate in many contexts

The problem

- Consider a system of N particles on a line (1d) interacting via a pairwise repulsive linear-spring potential

$$V(x) = \begin{cases} \frac{1}{2}kx^2 & , x < 0 \\ 0 & , x \geq 0 \end{cases} \quad (x \equiv \text{inter-particle separation})$$

- Integrate the system with the symplectic Euler method

$$\begin{aligned} q^{n+1} &= q^n + hT_p(q^n, p^{n+1}) \\ p^{n+1} &= p^n - hV_q(q^n, p^{n+1}) \end{aligned}$$

Three parts

1. **Backward Error Analysis** — obtain an analytic expression for the post-collision energy of two particles as a function of the initial conditions of the collision
2. **Equilibrium Statistical Physics** — develop a stochastic expression for the energy of a system of particles after n collisions
3. **Simulation** — compare theoretical predictions with computational experiments

Modified Equations

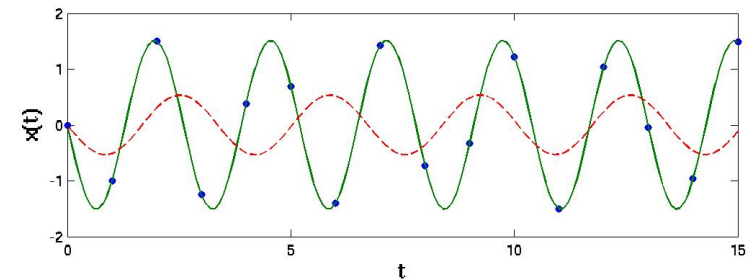
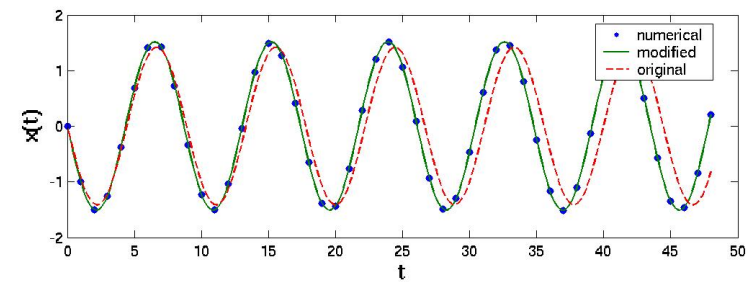
ode $\dot{y} = f(y)$

apply num. method \Downarrow

discrete map $y^{n+1} = \Phi_h(y^n)$

calculations \Downarrow

modified ode $\dot{\tilde{y}} = f_h(\tilde{y})$



Solution of the modified ode “interpolates” the discrete map.

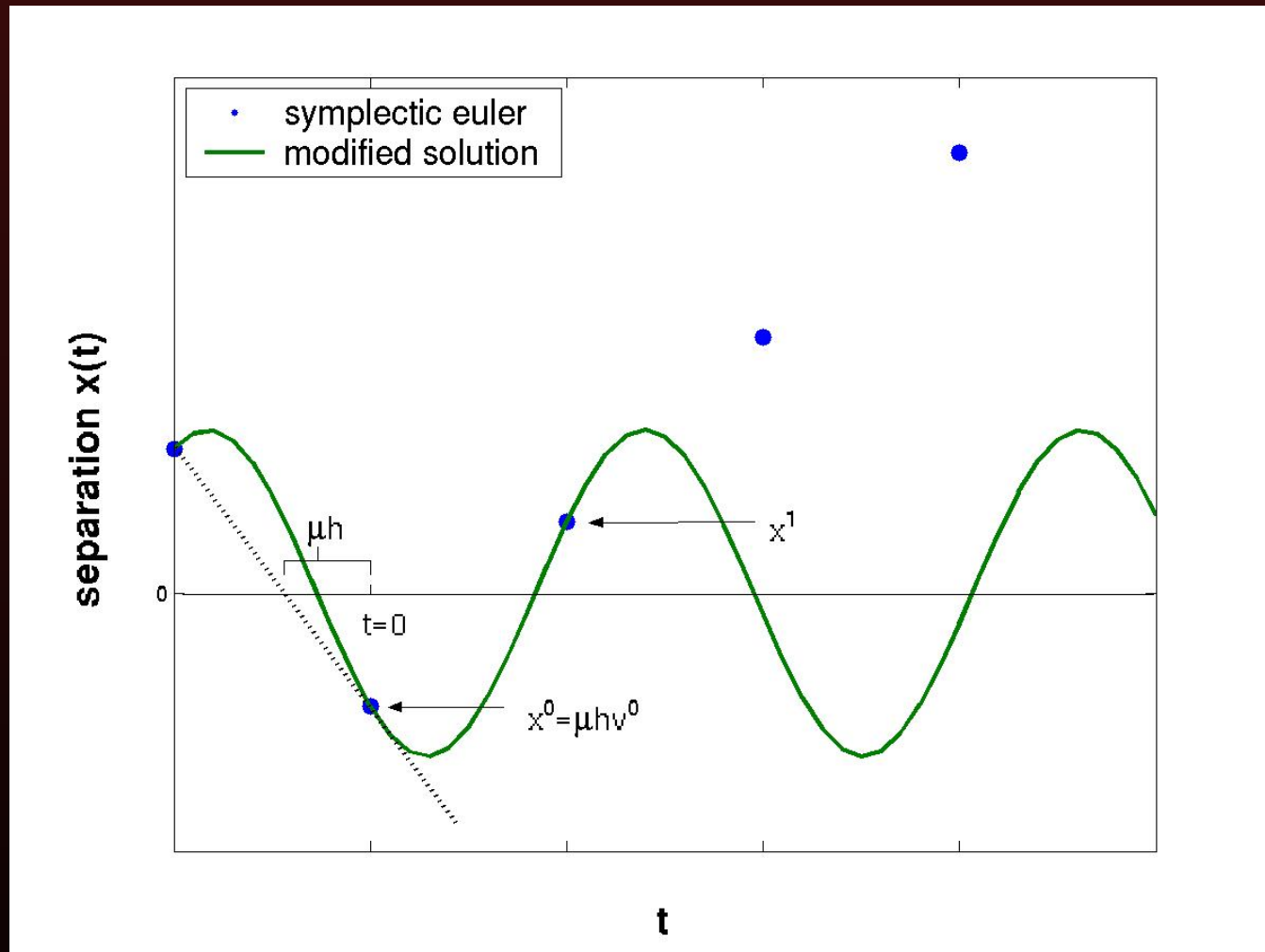
Part 1 – modified equation of a linear system

- Consider a collision between two particles with relative velocity v and separation x and let $y = (x, v)^T$.
- Suppose the particles first overlap at time $t = 0$. Then while $x < 0$ we have

$$y^{n+1} = \mathbf{A}_h y^n$$

$$\mathbf{A}_h = \begin{pmatrix} 1 - kh^2 & h \\ -kh & 1 \end{pmatrix}$$

$$y^0 = \begin{pmatrix} \mu h v^0 \\ v^0 \end{pmatrix}, \mu \in [0, 1)$$



- In this case, we can find the modified equation easily by first finding the modified solution

$$\begin{aligned}\tilde{y}(nh) &= y^n = (\mathbf{A}_h)^n y^0 \\ \Rightarrow \tilde{y}(t) &= (\mathbf{A}_h)^{\frac{t}{h}} y^0 = \exp\left(\frac{t}{h} \ln(\mathbf{A}_h)\right) y^0\end{aligned}$$

modified equation

$$\dot{\tilde{y}} = \frac{1}{h} \ln(\mathbf{A}_h) \tilde{y}$$

modified Hamiltonian

$$\begin{aligned}\tilde{\mathcal{H}}_h(x, v) &= \frac{\theta}{\sin \theta} \left(\mathcal{H}(x, v) - \frac{khxv}{2} \right) \\ (\cos \theta &= 1 - \frac{kh^2}{2})\end{aligned}$$

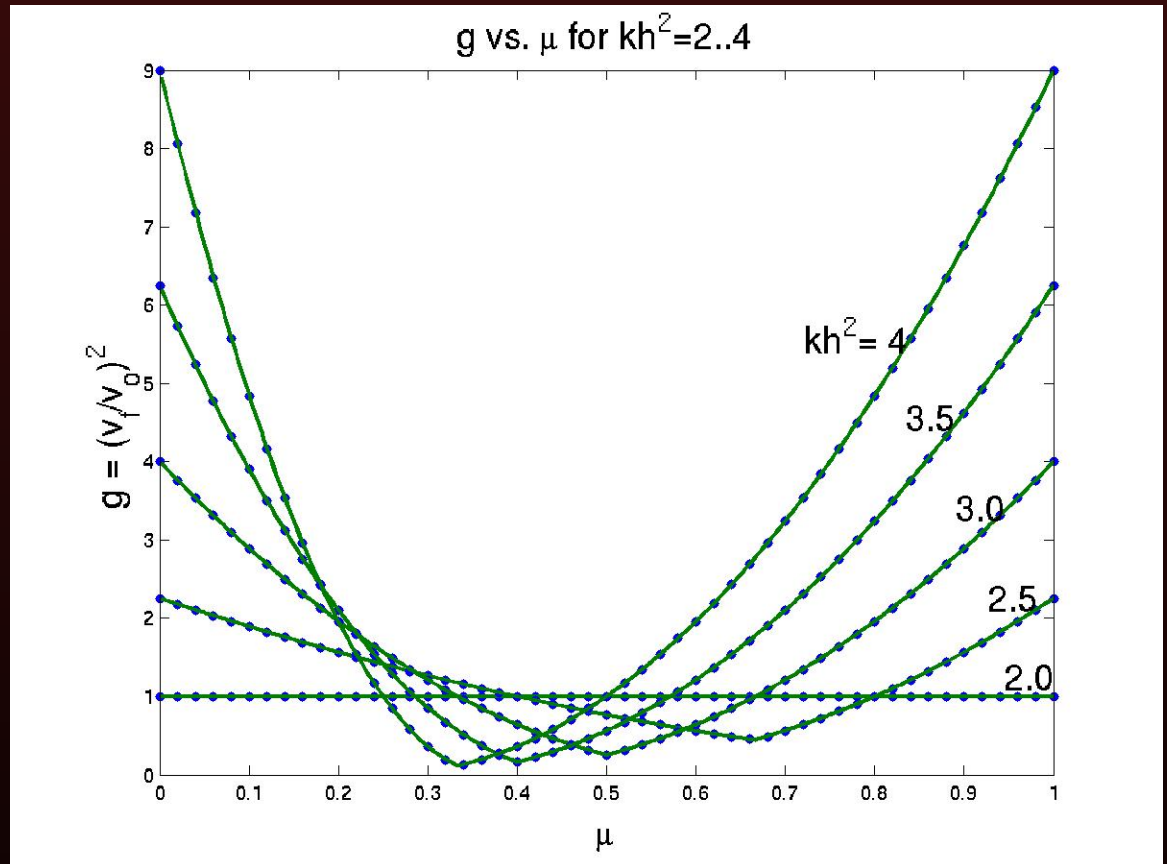
- The length of the collision, n_c , is determined by μ and kh^2

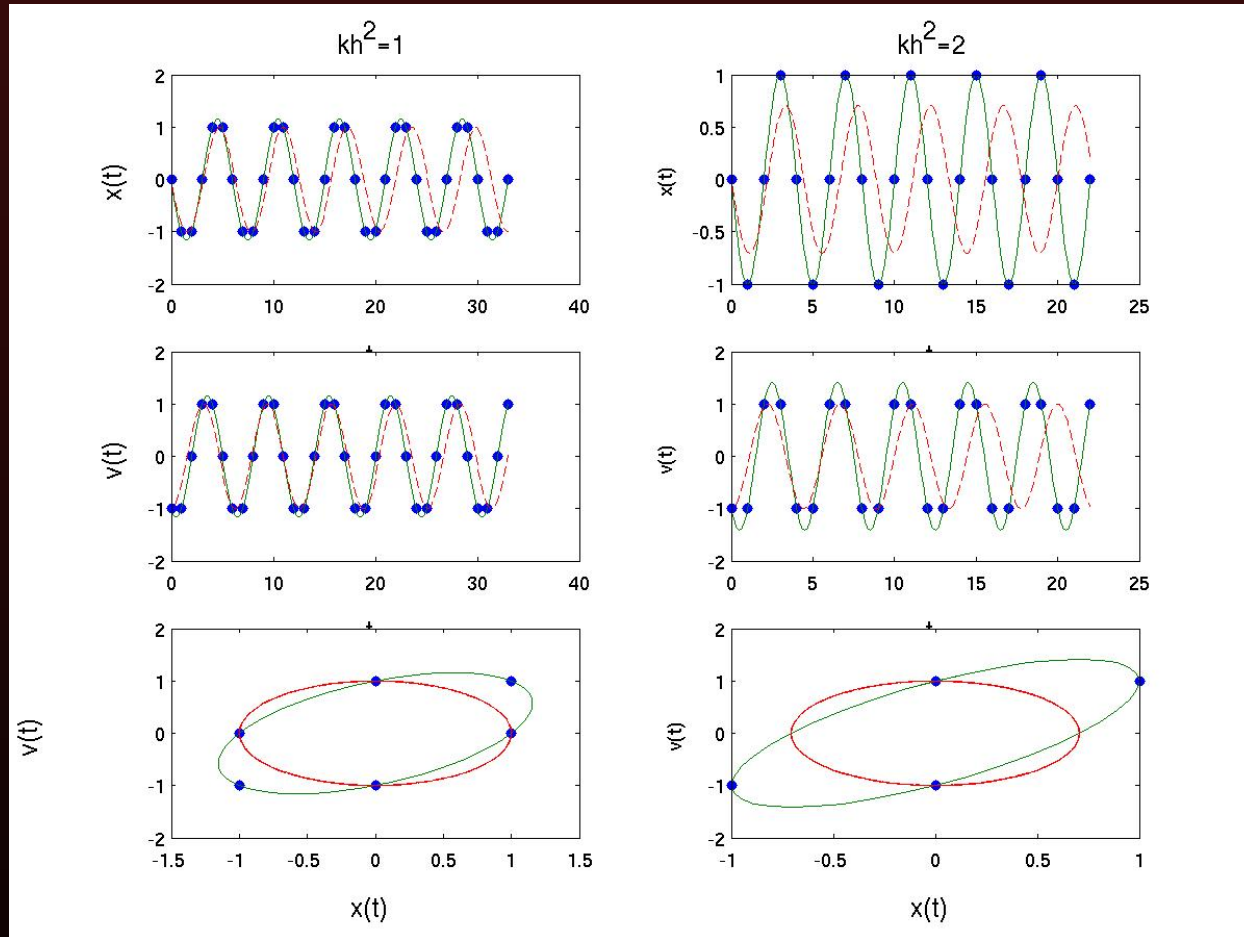
- The post-collision relative velocity is then determined by the initial conditions

$$v^{n_c} = \tilde{v}(n_c h)$$

$$= \sqrt{g(\mu, kh^2)} v^0$$

$$\Rightarrow (v_f)^2 = g(\mu, kh^2) (v^0)^2$$





Two particle Energy

- Measure time in number of collisions
- Let v_i^n, v_j^n be the velocities of two colliding particles after the n th collision.
- Since momentum is conserved by the method:

$$\begin{cases} v_i^{n+1} + v_j^{n+1} &= v_i^n + v_j^n \\ v_i^{n+1} - v_j^{n+1} &= \sqrt{g(\mu, kh^2)}(v_i^n - v_j^n) \end{cases}$$

- Letting $E_{ij}^n = (v_i^n)^2 + (v_j^n)^2$ we have

$$\Rightarrow E_{ij}^{n+1} = \frac{1}{2} (1 + g(\mu, kh^2)) E_{ij}^n + \frac{1}{2} (1 - g(\mu, kh^2)) v_i^n v_j^n$$

Part 2: Energy growth in systems of particles

1. Collisions involving three or more particles are rare.
2. Velocities of non-colliding particles are constant in time.
3. Velocities are *iid* with Boltzmann Distribution

$$P(v_i \in [\nu_i, \nu_i + d\nu)) = f(\nu_i)d\nu = \frac{1}{\sqrt{2\pi\sigma_n^2}} e^{-\frac{\nu_i^2}{2\sigma_n^2}} d\nu.$$

where σ_n^2 is the variance of the velocity distribution after the n th collision.

4. The system is at all times near equilibrium (Boltzmann distribution) and satisfies the thermodynamic relation

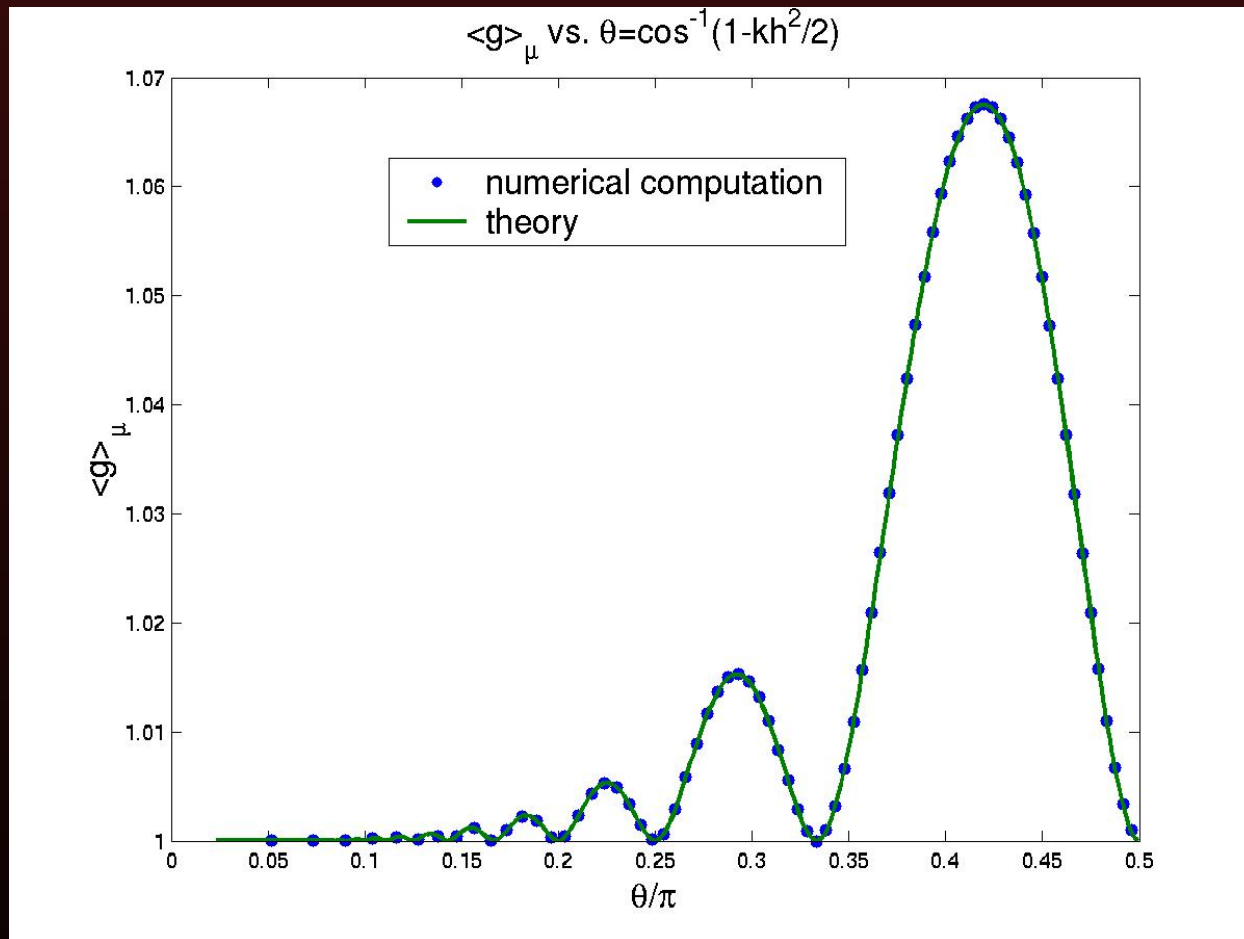
$$\frac{\langle E^n \rangle}{N} = \sigma_n^2.$$

5. Positions of colliding particles are independent of their velocities (i.e. μ is independent of $v_i, i = 1, \dots, N$).

- For a system of particles it is reasonable to consider μ^n to be independent uniformly distributed random variables
- Each collision changes the relative velocity of the particles by a random factor, $\sqrt{g(\mu^n, kh^2)}$

$$\begin{aligned}
 E_{total}^{n+1} &= \sum_{k \neq i, j}^N E_k^{n+1} + E_{ij}^{n+1} \\
 &= \sum_{k \neq i, j}^N E_k^n + \frac{1}{2} (1 + g) E_{ij}^n + \frac{1}{2} (1 - g) v_i^n v_j^n \\
 &= E_{total}^n + \frac{1}{2} (1 - g(\mu^n, kh^2)) (v_i^n v_j^n - E_{ij}^n)
 \end{aligned}$$

- Averaging over μ^n is easy, but averaging over v_i^n, v_j^n requires knowledge of the joint pdf of the velocities of colliding particles.



- The joint pdf (for a billiard system) is given by Sigurgeirsson (2001):

$$f(\nu_i, \nu_j) = \frac{1}{4\sqrt{\pi}\sigma^3} f(\nu_i) f(\nu_j) |\nu_i - \nu_j|.$$

$$\Rightarrow \langle E_{ij}^n \rangle = \int \int (\nu_i^2 + \nu_j^2) f(\nu_i, \nu_j) d\nu_i d\nu_j = 3\sigma_n^2 = 3 \frac{\langle E^n \rangle}{N}$$

$$\langle v_i^n v_j^n \rangle = \int \int \nu_i \nu_j f(\nu_i, \nu_j) d\nu_i d\nu_j = -\frac{\sigma_n^2}{2} = \frac{\langle E^n \rangle}{2N}$$

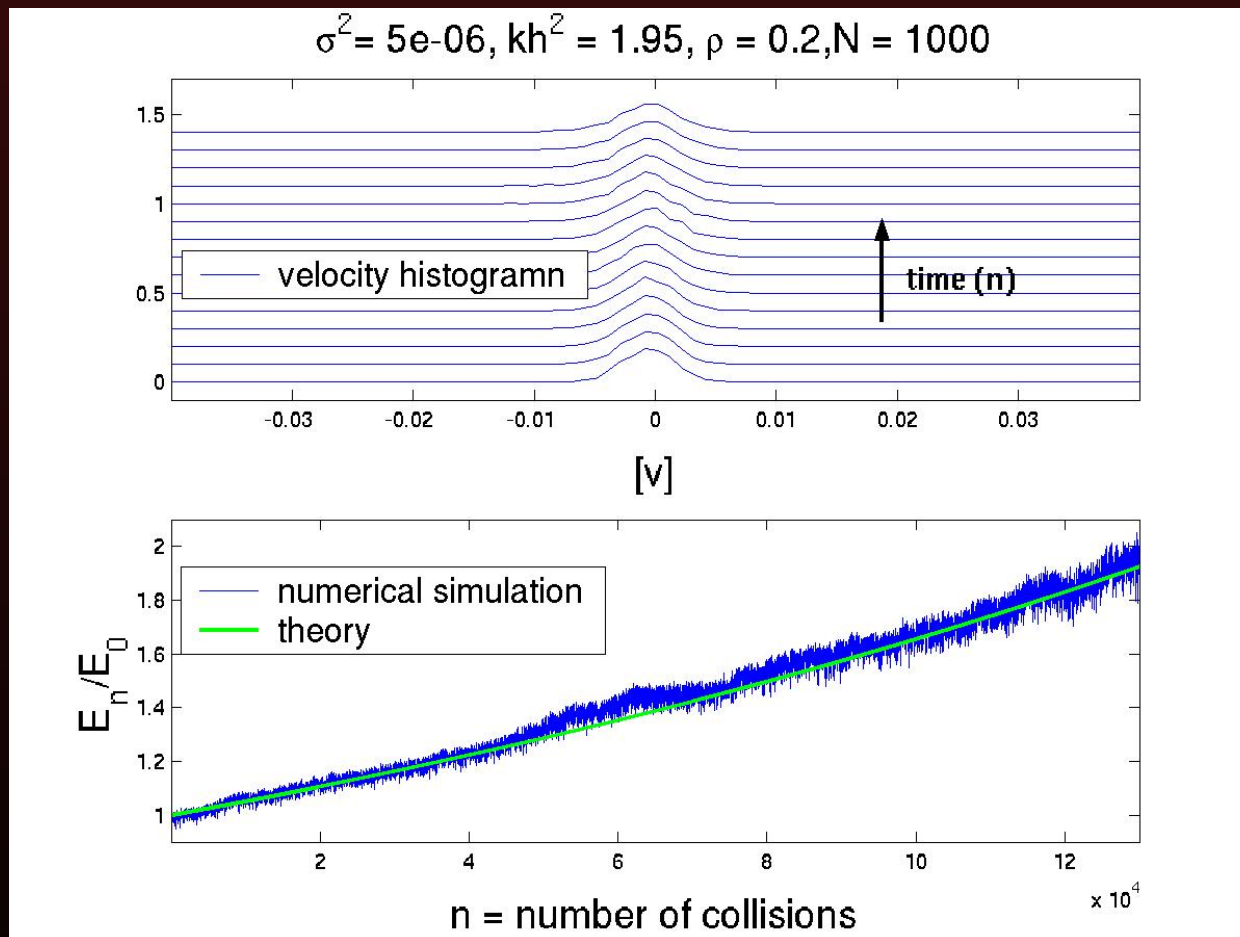
- Taking averages over μ^n and $v_i^n, i = 1 \dots N$ and using assumptions 4 and 5 yields

$$\langle E^{n+1} \rangle = \left[1 + \frac{7}{4N} (\langle g \rangle - 1) \right] \langle E^n \rangle$$

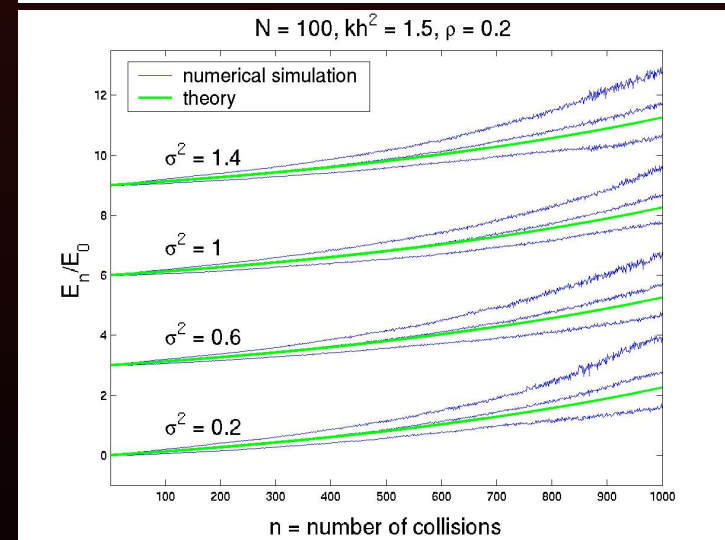
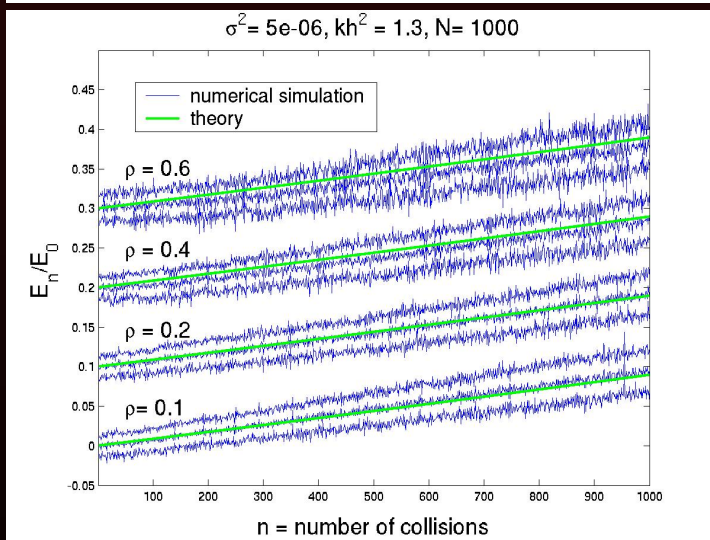
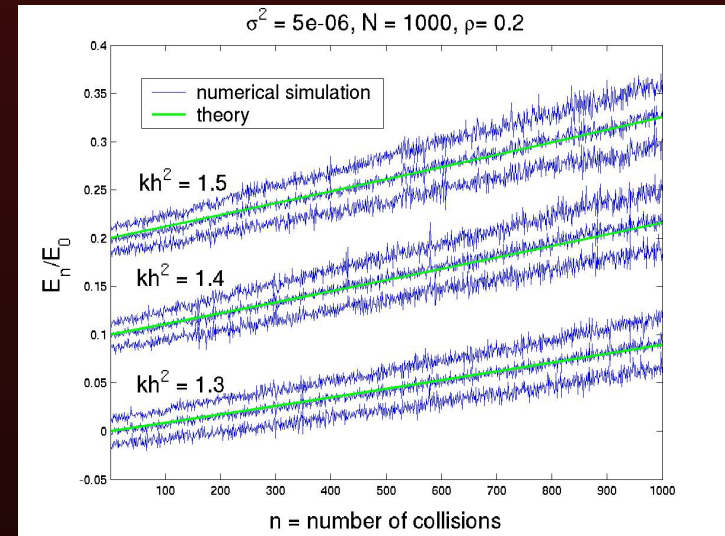
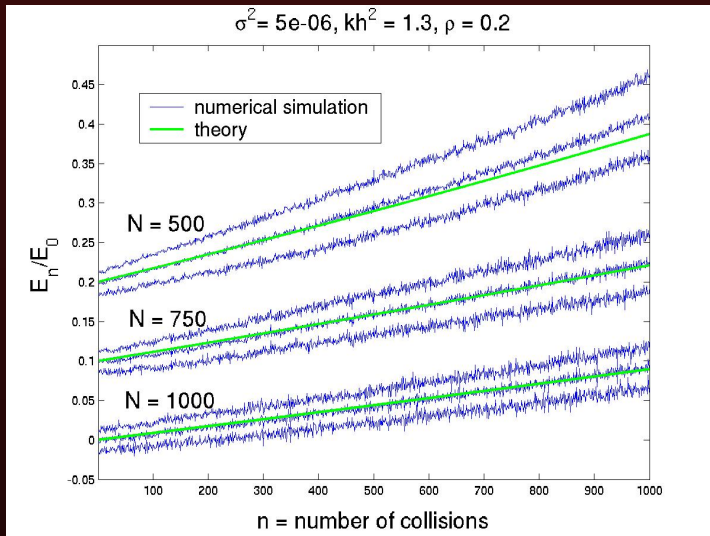
- Thus the expected energy of the system grows exponentially in collision time

$$\Rightarrow \langle E^n \rangle = \left[1 + \frac{7}{4N} (\langle g \rangle - 1) \right]^n \langle E^0 \rangle$$

Part 3: Simulations



Varying parameters — some more plots

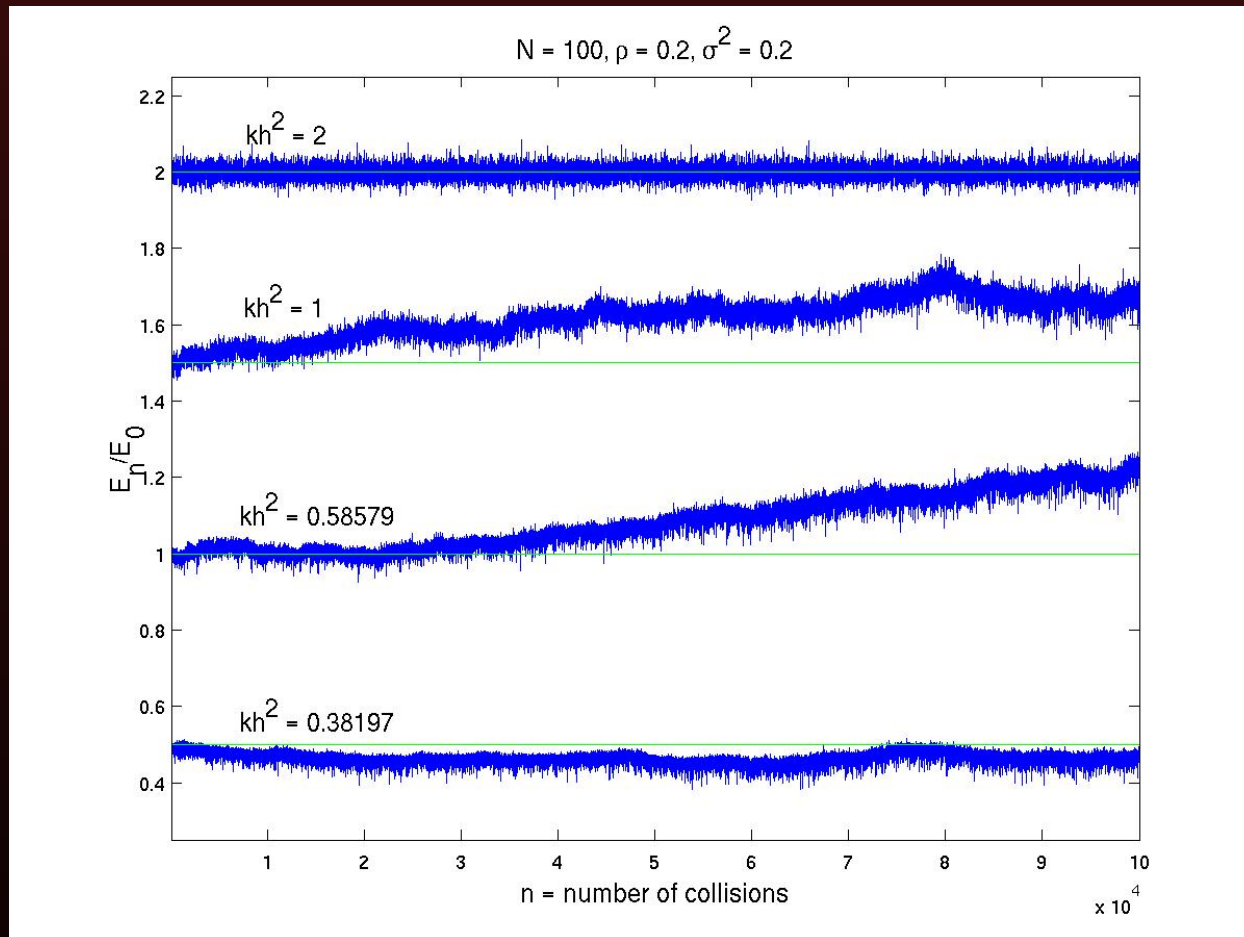


Problems

- many systems are in theory not ergodic - hard sphere systems can even have neutrally stable periodic orbits
- the empirical measure calculated from computations appears to be largely independent of initial conditions → systems appear to be ergodic
- the “random” forcing of particles through collisions may lead to non-Boltzmann equilibrium
- over short time intervals and for small changes in energy the equilibrium assumptions provide reasonable results and may be extended to non-Boltzmann systems in future work

Future Work

- Extend the analysis to systems in more than one dimension
- Other potentials (i.e. Lennard-Jones)
- post-collision velocity correction
- Higher densities



Behaviour of damped system in $(kh^2, \gamma h)$ parameter space

