Computational Physics
Lecture 6

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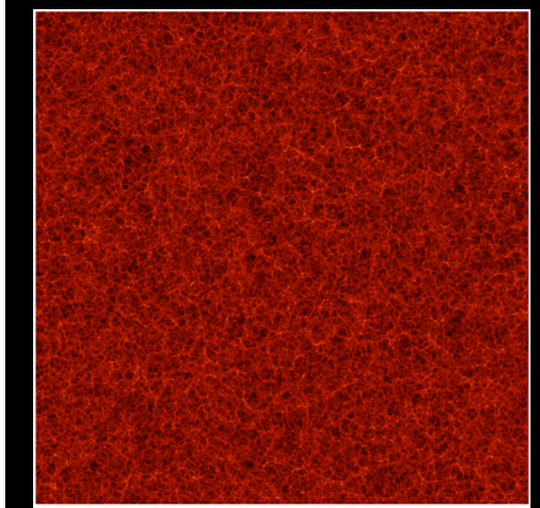
git clone https://github.com/ukzncompphys/lecture6.git
wget www.cita.utoronto.ca/~sievers/compphys/lecture6.tar.gz
(followed by tar -xzf lecture6.tar.gz)

N-Body

- Dominant force in the universe on large scales is gravity.
- Physical systems often too complex to deal with analytically. Computer simulations often key to understanding.
- Wide variety of problems in e.g. astrophysics involve matter fields evolving with gravity.
- Evolution of 2 masses is called the "2-body problem." With many (many) objects, called the "n-body problem," or just n-body.
- N-body simulations are key to understanding the universe around us. Also useful in chemistry, economics…

Cosmology

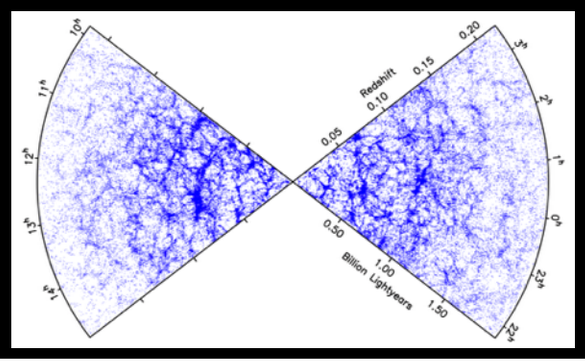


MacFarland, Colberg, White (München), Jenkins, Pearce, Frenk (Durham), Evrard (Michigan), Couchman (London, CA), Thomas (Sussex), Efstathiou (Cambridge), Peacock (Edinburgh)

$2000 \times 2000 \times 20\,(\mathrm{Mpc}/h)^3$

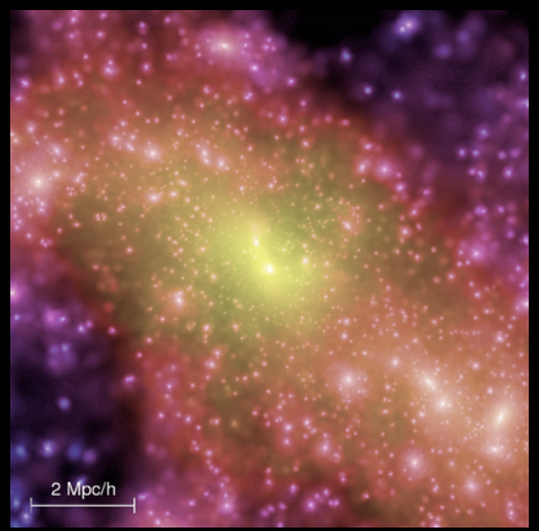
Simulation (left) dark matter, bottom is galaxy data.

We use simulations like this to interpret observations of galaxy clustering.



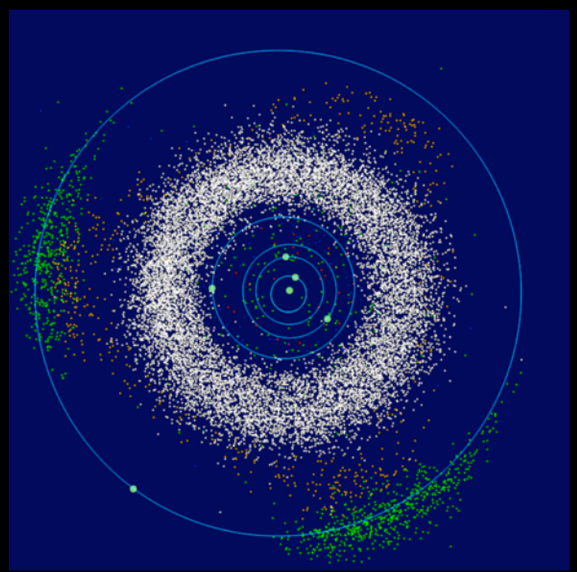
Galaxy Clusters

- Galaxy clusters are biggest objects in universe - 10^{15} solar masses.
- Picture from millenium simulation, total of 10^{10} particles.
- Need simulations to interpret galaxy cluster data.



Solar System

- more than 2 bodies usually unstable, systems kick out lightest objects.
- Is the solar system stable? Could Earth get kicked out of its orbit and become inhospitable to life?



Classical n-body

- We'll approximate system as a collection of masses, interact only through gravity.
- What is the minimum information we need per particle?

Classical n-body

- We'll approximate system as a collection of masses, interact only through gravity.
- What is the minimum information we need per particle?
- Each particle needs its own mass, position, and velocity.

Gravity

- $F=Gm_1m_2/r^2$. $F=ma$. For many particles, $dv/dt=-\sum Gm_2/r_{12}^2$.
- $dx/dt=v$. Definition of velocity.
- Leaves us with coupled system:
  $d/dt[x_i,v_i\ \ ]\ \ =[v, -\sum Gm_j/r_{ij}^2.]$
- Solve system of equations, and we're done!

How do we solve?

- if $dx/dt=v$, and $x_t=v_0$, then $x_{t+\delta}\approx x_0+\delta_t v$ from some "average" value of v.
- So, take discrete steps in time. Then take each particle, and use its velocity to update positions
- Also have to update velocities using accelerations: $dv_i/dt=-\sum Gm_j/r_{ij}^2$ for $i\neq j$. Note the force is a vector, so we rewrite $1/r^2$ as $r/|r|^3$
- For sufficiently small time step, we should have an accurate solution.

Let's look at two particles: two_particles_simple.py

```
import numpy
from matplotlib import pyplot as plt
#let's start two partcles in what should be a circular orbit
x0=0;y0=0;vx0=0;vy0=0.5
x1=1;y1=0;vx1=0;vy1=-0.5;

#for simplicity, let's assume G&m are all equal to 1
dt=0.01
tmax=5
```

Code to do two bodies. First, set initial conditions, integration time, and step size.

```
for t in numpy.arange(0,tmax,dt):
    dx=x0-x1
    dy=y0-y1
    rsquare=dx*dx+dy*dy
    r=numpy.sqrt(rsquare)
    r3=r*r*r
    #calculate the x and y  force components
    fx0=dx/r3;
    fy0=dy/r3
    #forces on particle 1 must be opposite of particle 0
    fx1 =-fx0
    fy1 =-fy0
    #update particle positions
    x0 +=dt*vx0
    y0 +=dt*vy0
    vx0 +=-dt*fx0
    vy0 +=-dt*fy0

    x1+= dt*vx1
    y1+=dt*vy1
    vx1 -= dt*fx1
    vy1 -= dt*fy1
```

```
plt.clf()
plt.plot(x0,y0,'rx')
plt.plot(x1,y1,'b*')
plt.ylim(-1.5,1.5)
plt.xlim(-1,2)

plt.draw()
pot=-1.0/r
kin=0.5*(vx0*vx0+vy0*vy0+vx1*vx1+vy1*vy1)
print 'kin and pot are '  + repr(kin) + '    ' + repr(pot) + '   ' + repr(pot+kin)
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Now let's loop over time steps. First calculate force with r/r^3, then update positions and velocities.

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Finally, plot particle positions, calculate the kinetic and potential energy, and print the energies to the screen.

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Higher Order

- The force changes during a timestep. We will build up inaccuracy due to ignoring this.
- We could be more accurate - what if we take a trial step, then calculate the force there and replace the effective force by the average of the two forces?
- Likewise, we can get a trial final velocity, why not use the average of the initial and final?
- This will give us higher accuracy

Leapfrog

- Another simple scheme for higher order is *leapfrog*.
- If I say my positions and velocities are half a step out of sync then the velocity is the average velocity over the position timestep.
- Likewise, position is the average position over the next velocity timestep
- Get 2nd order for no extra work!
- Downside - can't change timestep size.

Softening

- How big should a timestep be?
- Depends on forces. If force is big enough that velocity changes by a lot, then method will be inaccurate.
- for $f=1/r^2$, force can get arbitrarily big. Bad!
- Solution is to use *softening* - particles are really fuzzy balls, so once they get close enough, force *drops*.
- Possible solutions: $F\sim r/((r^2+eps^2)^{3/2}$. Or, $a=r^3$, if $a<a_0$, $a=a_0$. $F=r/a$.
- Then for large distances, force is unchanged, but goes to zero for small distances.

Many Particles

- We can do the same thing for many particles. Particles should collapse together into a ball.
- Softening is key!
- Let's watch:

How Much Work Does This Take?

- Right now, we calculate the forces on every pair of particles. Total work scales like n^2 - running big simulations is a problem!
- Instead, let's look at potential from a distribution of many particles. If the potential of 1 particle is P(r), then what is the potential from a field?
- $P_{tot}(r') = \int P(r-r')\rho(r)d^3r$.
- Wait, have we seen this operation before?

Modern N-body

- We have! Global potential is just potential from a single particle convolved with the density field.
- Force is just the gradient of the potential
- FFT takes $n\log n$, for billions of particles, $n\log n <<< n^2$.
- So, a scheme is to have a grid on which we will calculate the density, then sum particles into their nearest grid cell, and convolve with the desired potential.
- Once have potential, for each particle, calculate gradient of potential at its position. Now we can run for millions of particles on a desktop instead of thousands!

Tutorial

- Let's add some methods to the class from the last tutorial so we can use it in an n-body simulation. First, add a method to initialize # of particles witih random positions in 2-D (numpy.random.randn() will get gaussian random numbers). (5)
- Next, write a method that calculates the forces on the particles using a softened potential (10)
- Now write a method that will update the particle positions and velocities using a timestep. (5)
- Finally, plot the total kinetic and potential energies as a function of time, and show that the total energy is approximately conserved (5)

Tutorial bonus

- Write a 2nd order integrator for your n-body class. You'll need to make copies of your particles. When you look at the total energy, is conservation better or worse? (10)

Final Project

- One possible final project is to write an *nlogn* nbody simulator (the other will be to write a fluid simulator, which we will see next week). If you think you would like to do this, you can start working on it.
- I will pass out handouts with more details next week, when we meet fluids as well, but you can start now. Core routines will be to calculate the 2-d density field from particle positions, to calculate the global potential from the distribution, and to calculate the particle forces from the potential field.
- There will be some more parts, but they will all sit on top of these basic routines.