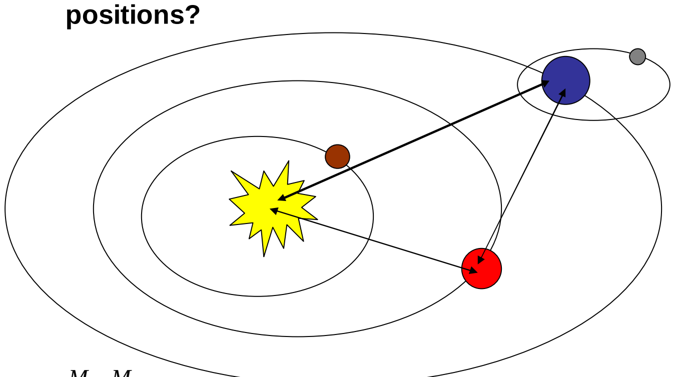
Dynamics Simulations
COMP3320/6464

Dynamics (N-Body Problem)

How do we calculate future positions?

$$E_{sun-earth} = G\frac{M_{sun}M_{earth}}{r_{sun-earth}}$$



$$E_{sun-venus} = G\frac{M_{sun}M_{venus}}{r_{sun-venus}}$$

$$E_{venus-earth} = G\frac{M_{venus}M_{earth}}{r_{venus-earth}}$$

Interactions

- Total interaction (potential) energy is sum of pairwise interactions
  - Total energy is sum of potential plus kinetic energy
- Each pairwise interaction gives rise to a pairwise force
  - The derivative of the potential with respect to distance
- Total force on a body is sum of all pairwise forces
- Given an applied force each body will respond according to Newtonian mechanics (F=ma)
  - But total energy is conserved

Code Kernel

```
for body1 in solar_system
  for body2 in solar_system

    if (body1 != body2){
      r2 = (x_body1 – x_body2)^2 +
           (y_body1 – y_body2)^2 +
           (z_body1 – z_body2)^2
      r  = sqrt(r2)
      PE += G*M1*M2/r
      force_x_body1 -= (G*M1*M2/r^3)*(x_body1 – x_body2)
      force_y_body1 -= (G*M1*M2/r^3)*(y_body1 – y_body2)
      force_z_body1 -= (G*M1*M2/r^3)*(z_body1 – z_body2)
    }

  next body2
next body1
```

Equations of Motion

- Taylor's series expansion:

$$r(t+\Delta t) = r(t) + \Delta t \frac{\partial r}{\partial t} + \frac{1}{2}\Delta t^2 \frac{\partial^2 r}{\partial t^2} + \frac{1}{6}\Delta t^3 \frac{\partial^3 r}{\partial t^3} + \cdots$$

$$r(t-\Delta t) = r(t) - \Delta t \frac{\partial r}{\partial t} + \frac{1}{2}\Delta t^2 \frac{\partial^2 r}{\partial t^2} - \frac{1}{6}\Delta t^3 \frac{\partial^3 r}{\partial t^3} + \cdots$$

- Adding gives

$$r(t+\Delta t) = 2r(t) - r(t-\Delta t) + \Delta t^2 \frac{\partial^2 r}{\partial t^2} + \cdots$$

- What about $(t\text{-}\Delta t)$? Use velocity

$$v(t) = [r(t+\Delta t) - r(t-\Delta t)]/(2\Delta t) \quad \Rightarrow \quad r(t-\Delta t) = r(t+\Delta t) - 2v(t)\Delta t$$

- To second order gives

$$r(t+\Delta t) = 2r(t) - r(t+\Delta t) + 2v(t)\Delta t + \Delta t^2 \frac{\partial^2 r}{\partial t^2}$$

Velocity Verlat

$$r(t+\Delta t) = r(t) + v(t)\Delta t + \frac{1}{2}\Delta t^2 \frac{\partial^2 r}{\partial t^2}$$

$$r(t+\Delta t) = r(t) + v(t)\Delta t + \frac{1}{2}\Delta t^2 a(t)$$

- Where a(t) is the acceleration at time t
- Similarly for the velocity we obtain

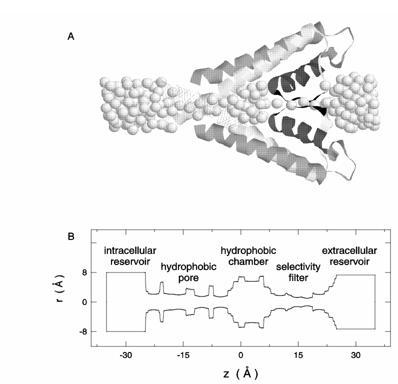
$$v(t+\Delta t) = v(t) + \frac{1}{2}\Delta t[a(t) + a(t+\Delta t)]$$

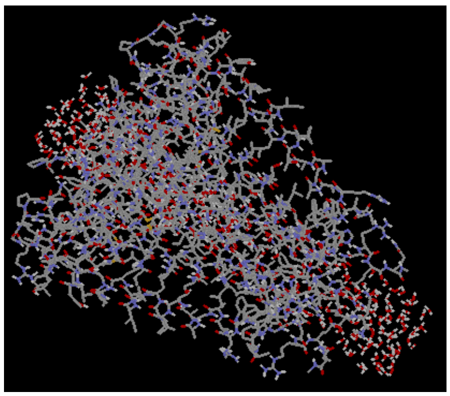
- Using F=ma we can replace a with force
- Requires r(t), v(t) and a(t) to generate new position

Molecular Dynamics

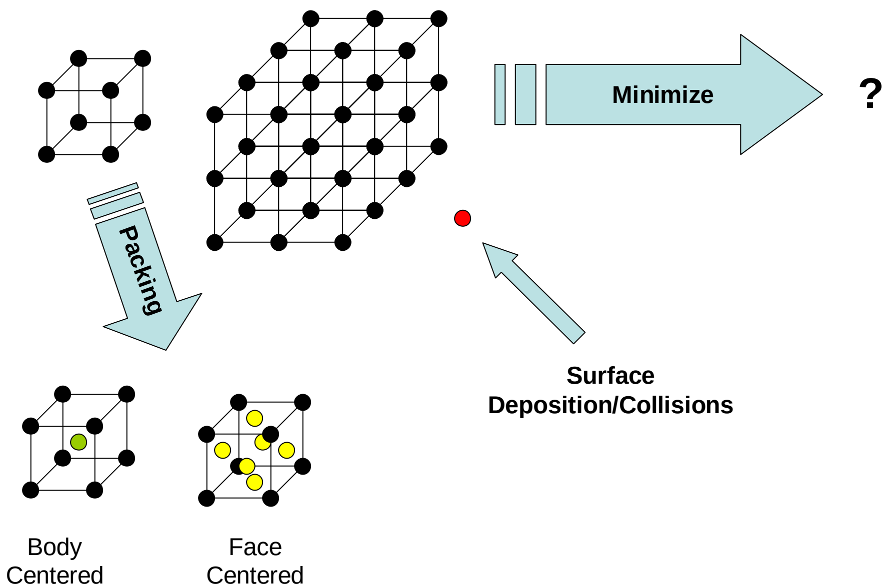
- Replace planets by atoms
- Replace gravity by some empirical (i.e. guessed!) function
- Use many thousands of atoms
- Timestep corresponds to 10^{-15} seconds
  - Require a lot of timesteps to simulate for 1 second of real time!

Ion Channel with Water Simulation





Assignment and Relevance



Discussion

- What approximations have we made?
- What performance do you expect?
  - As function of input parameters (which are)
  - Absolute performance