Approach of molecular dynamic simulation (MDS):

* Prepare a sample (model) w/ N particles
* Solve Newton equations for this system till system properties are independent from time (equilibriate)
* Actual measurement:
  + Express each observable in function (x, p) of the particles in system
  + Illustrate a number of important features of MDS
    - Read parameters that specify the conditions (temp, N, density, etc)
    - Initialize system w/ selected initial x & v, for instance.
    - Compute forces on all particles
    - Repeat integrating Newton equation until time is up
    - Averaged measure quantities and stop
* Initialization
  + Place particle
  + V0 (might be random)
  + Set desired parameters
* Calculation
  + Utilize information of present and previous time steps
  + Bootstrap procedure by generating approximate previous positions
  + Select appropriate approximation (rounding might apply) for potential and take derivatives. Ek, Ep and Etotal are related to instantaneous temperature and v should be used with caution of floating.
  + Integration always involve errors. Just be aware of the order of function and the integration we may apply.
  + Should we save the previous-calculated info (position, energy, etc) to keep track of the trajectory?
* Equation of motion: good algorithm
  + Speed and efficiency: last thing to consider
  + Always obey the conservation of linear momenta and energy
  + Accuracy matters. Avoid exponential errors during large time-scale simulation. Keep an eye on the floats, although it seems not matter much.
  + Statistical prediction works: get the average behavior of system.
  + Time asymmetry of many algorithms: not reversible. OOP might help us design algorithm without assigning new variables (preservation), and avoid energy drift.
* Other algorithm
  + Verlet: fast, not accurate for long time steps, less memory usage, energy conservation is good in both long and short-term. Time reversible and area conserved.
  + Leap Frog: first-ordered
  + Beeman: second-ordered term revised, more accurate velocity description, time asymmetry
  + Acquiring higher order terms: more accurate for longer time-scale, slower
  + Liouville Formulation: it reminds me of angular momenta of hydrogen atom… are they the same?
  + Lyapunov Instability: linear segment of each time period, where its coefficient diverges exponentially (decrease, from the graph?). We are able to test our initial condition to shrink the error by tmax.
* Computer Experiments

Var(E) vs dt

Add Langeuin thermostat to the energy