Molecular Dynamics and Monte Carlo Methods

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Classical mechanics

- Newton's equation of motion
  $$\mathbf{F} = m\mathbf{a}$$ **F**: force, *m*: mass, **a**: acceleration
  3D vectors are denoted by bold-face symbols.
  Scalar values are denoted by italic symbols.

- **a** is second-derivative of position **r** with respect to time *t*.

$$\mathbf{v} = \frac{d\mathbf{r}}{dt} = \left(\frac{dx}{dt}, \frac{dy}{dt}, \frac{dz}{dt} \right)$$

$$\mathbf{a} = \frac{d\mathbf{v}}{dt} = \frac{d^2\mathbf{r}}{dt^2} = \left(\frac{d^2 x}{dt^2}, \frac{d^2 y}{dt^2}, \frac{d^2 z}{dt^2} \right)$$

Solution of equation of motion (1)

- Fall of a body of mass *m* from height *h*

h $v = 0$

$F = -mg$

z

0
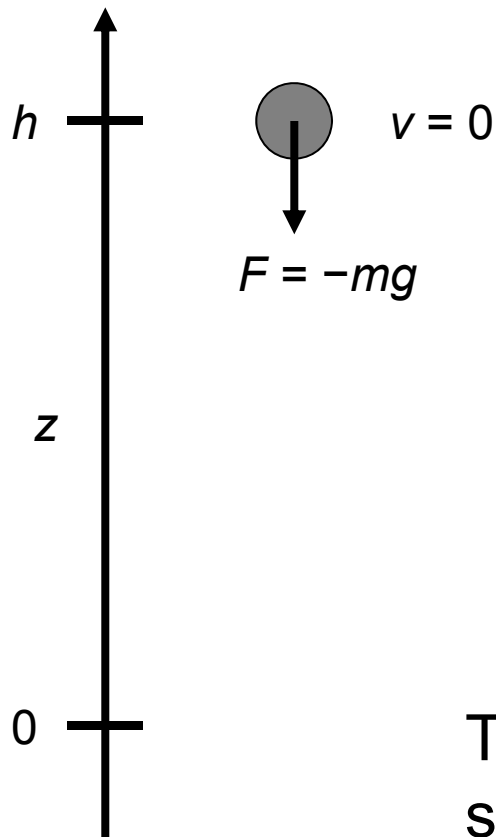
$$m\frac{d^2z}{dt^2} = -mg \quad \rightarrow \quad \frac{d^2z}{dt^2} = \frac{dv_z}{dt} = -g,$$

$$v_z(t) = -gt + C, \quad v_z(0) = 0 \quad \rightarrow \quad C = 0$$

$$\frac{dz}{dt} = v_z(t) = -gt \quad \rightarrow \quad z(t) = -\frac{1}{2}gt^2 + D$$

$$z(0) = h \quad \rightarrow \quad D = h$$

$$z(t) = -\frac{1}{2}gt^2 + h$$

Two initial conditions are required to solve second order differential equations.
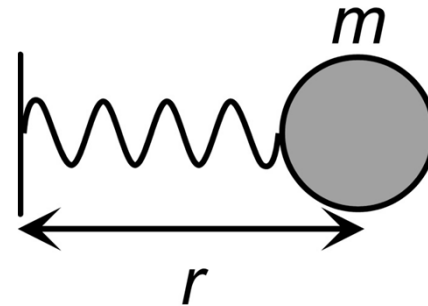
Solution of equation of motion (2)

- Harmonic oscillator
  Mass: m
  Spring length: r
  Length of unstrained spring: r_0
  Force constant: k

$$F = -k(r - r_0)$$

$$m\frac{d^2 r}{dt^2} = -k(r - r_0)$$

$$q = r - r_0$$

$$F = -kq$$

$$m\frac{d^2 q}{dt^2} = -kq$$

Solution of equation of motion (2)

$$\frac{d^2 q}{dt^2} = -\frac{k}{m} q = -\omega^2 q, \quad \omega = \sqrt{\frac{k}{m}}$$

$$q(t) = A \cos \omega t + B \sin \omega t \qquad \text{General solution}$$

$$q(0) = q_0, \quad dq/dt\big|_{t=0} = v(0) = 0 \qquad \text{Initial conditions}$$
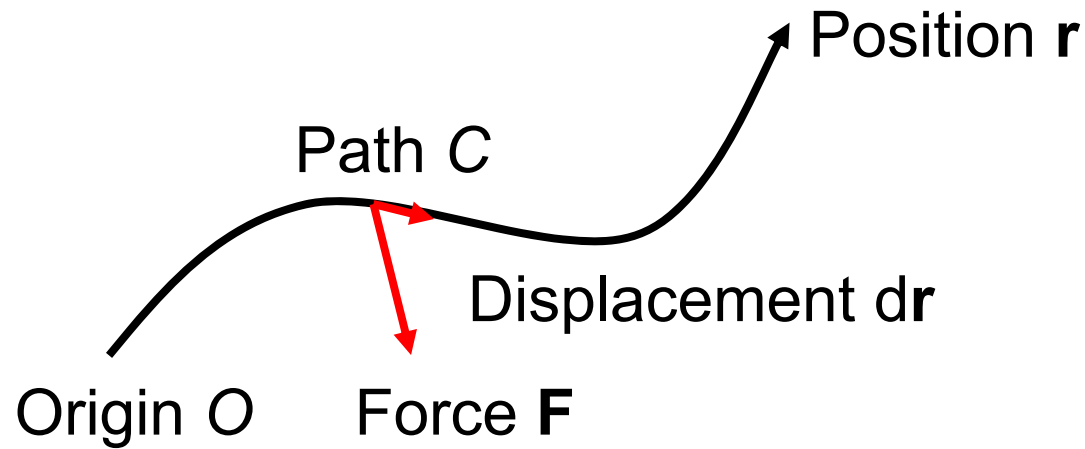
$$A = q_0, \quad B = 0$$

$$q(t) = q_0 \cos \omega t, \quad r = q_0 \cos \omega t + r_0$$

Potential energy and force (1)

Definition of potential energy $E(\mathbf{r})$ at position $\mathbf{r}$:

$$E(\mathbf{r}) = -\int_C \mathbf{F} \cdot d\mathbf{r}$$

Integrate dot-product of $\mathbf{F}$ and $d\mathbf{r}$ from O to $\mathbf{r}$ along C.

Position $\mathbf{r}$

Path C

Displacement $d\mathbf{r}$

Origin O Force $\mathbf{F}$

Potential energy and force (2)

Change in potential energy by displacement $\Delta\mathbf{r}$.

$$E(\mathbf{r}+\Delta\mathbf{r})-E(\mathbf{r}) = E(x+\Delta x, y+\Delta y, z+\Delta z)-E(x, y, z)$$

$$= E(x+\Delta x, y+\Delta y, z+\Delta z)-E(x, y+\Delta y, z+\Delta z)$$

$$+ E(x, y+\Delta y, z+\Delta z)-E(x, y, z+\Delta z)$$

$$+ E(x, y, z+\Delta z)-E(x, y, z)$$

$$= \frac{\partial E}{\partial x}\Delta x + \frac{\partial E}{\partial y}\Delta y + \frac{\partial E}{\partial z}\Delta z = \nabla E \cdot \Delta\mathbf{r}$$

Since

$$E(\mathbf{r}+\Delta\mathbf{r})-E(\mathbf{r}) = -\mathbf{F}\cdot\Delta\mathbf{r}$$

we obtain

$$\mathbf{F} = -\nabla E$$

Force can be calculated from potential energy.

Energy conservation law (1)

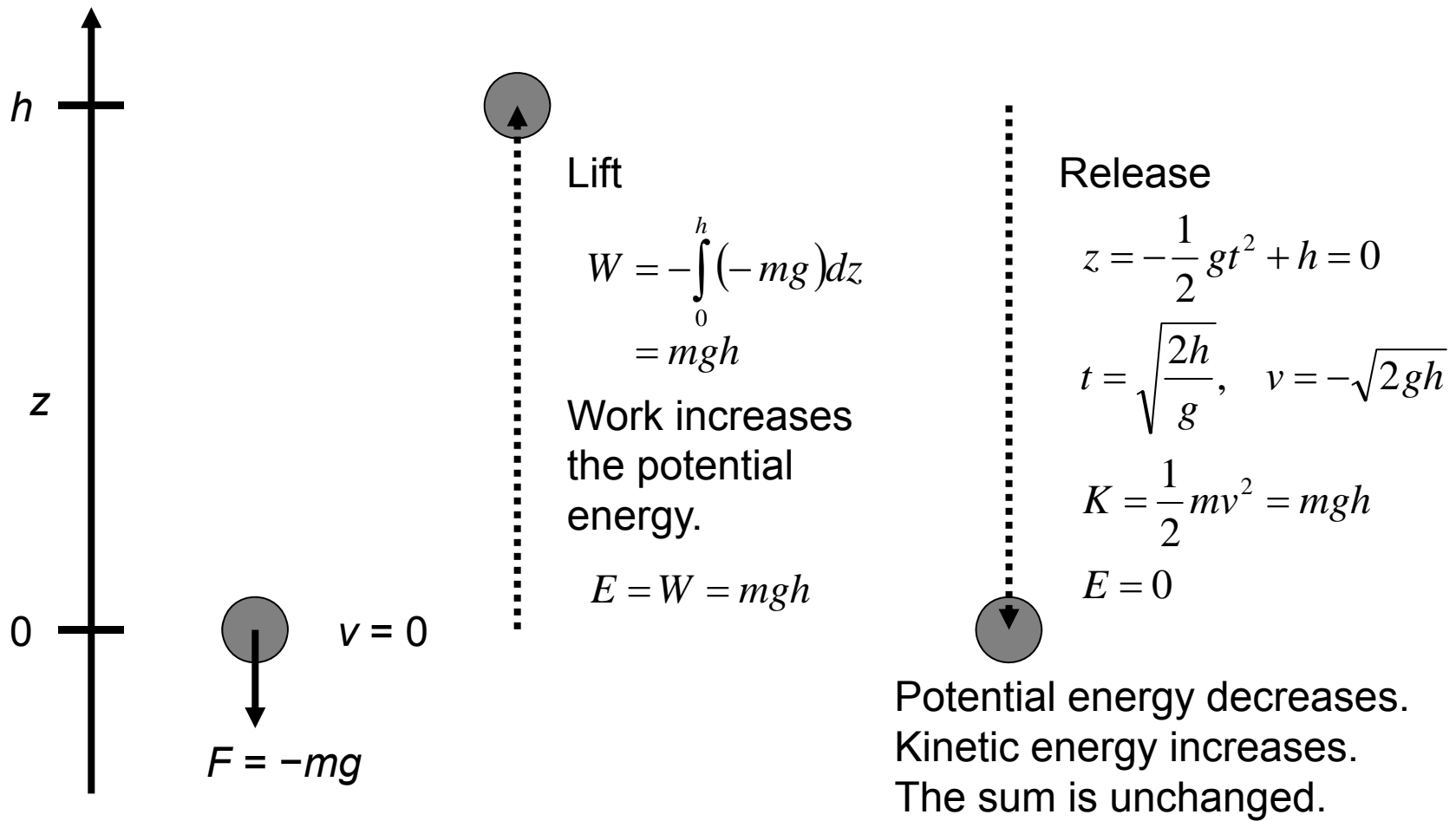- In an isolated system, the sum (denoted by *H*) of potential energy *E* and kinetic energy *K* remains constant.

- Kinetic energy

$$K = \frac{1}{2} m |\mathbf{v}|^2$$

- Proof of the conservation law

$$\frac{dH}{dt} = \frac{dK}{dt} + \frac{dE}{dt} = m\mathbf{v} \cdot \frac{d\mathbf{v}}{dt} + \frac{d\mathbf{x}}{dt} \cdot \frac{\partial E}{\partial \mathbf{x}}$$
$$= m\mathbf{v} \cdot \mathbf{a} - \mathbf{v} \cdot \mathbf{F} = \mathbf{v} \cdot (m\mathbf{a} - \mathbf{F}) = 0$$

Energy conservation law (2)

Lift

$$W = -\int_0^h (-mg)\,dz$$
$$= mgh$$

Work increases the potential energy.

$$E = W = mgh$$

Release

$$z = -\frac{1}{2}gt^2 + h = 0$$

$$t = \sqrt{\frac{2h}{g}}, \quad v = -\sqrt{2gh}$$

$$K = \frac{1}{2}mv^2 = mgh$$

$$E = 0$$

Potential energy decreases.
Kinetic energy increases.
The sum is unchanged.

h

z

0

$v = 0$

$F = -mg$
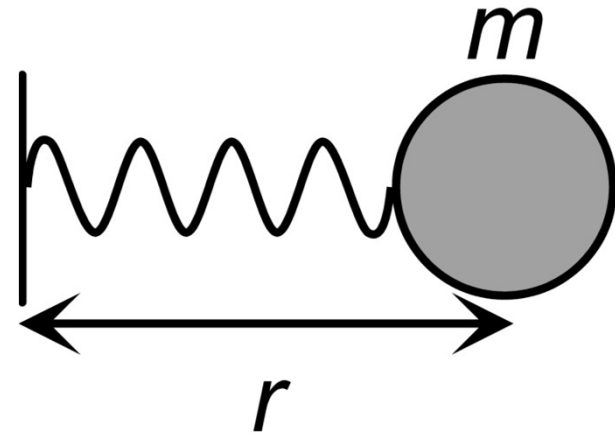
Energy conservation law (3)

Harmonic oscillator

$$r(t) = q_0 \cos \omega t + r_0$$

$$v(t) = dr(t)/dt = -q_0 \omega \sin \omega t$$

$$E(r) = -\int_{r_0}^{r} -k(r' - r_0) dr' = \frac{k}{2}(r - r_0)^2$$

$$H = \frac{m}{2}[v(t)]^2 + \frac{k}{2}[r(t) - r_0]^2$$

$$= \frac{mq_0^2 \omega^2}{2}\sin^2 \omega t + \frac{kq_0^2}{2}\cos^2 \omega t = \frac{1}{2}kq_0^2$$

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Molecular dynamics method

- Molecular dynamics (MD) method calculates the time variation of the positions and the velocities of the atoms in a molecular system, evaluating the forces from the potential energy function and integrating Newton's equations of motion.
- The equations of motion for a system composed of more than two atoms cannot be integrated analytically.
- In this case, they are integrated numerically, where the whole calculation is decomposed into a series of the calculations for a very short time period.
- Accuracy of the numerical integration is evaluated by examining the energy conservation.

Velocity Verlet integrator
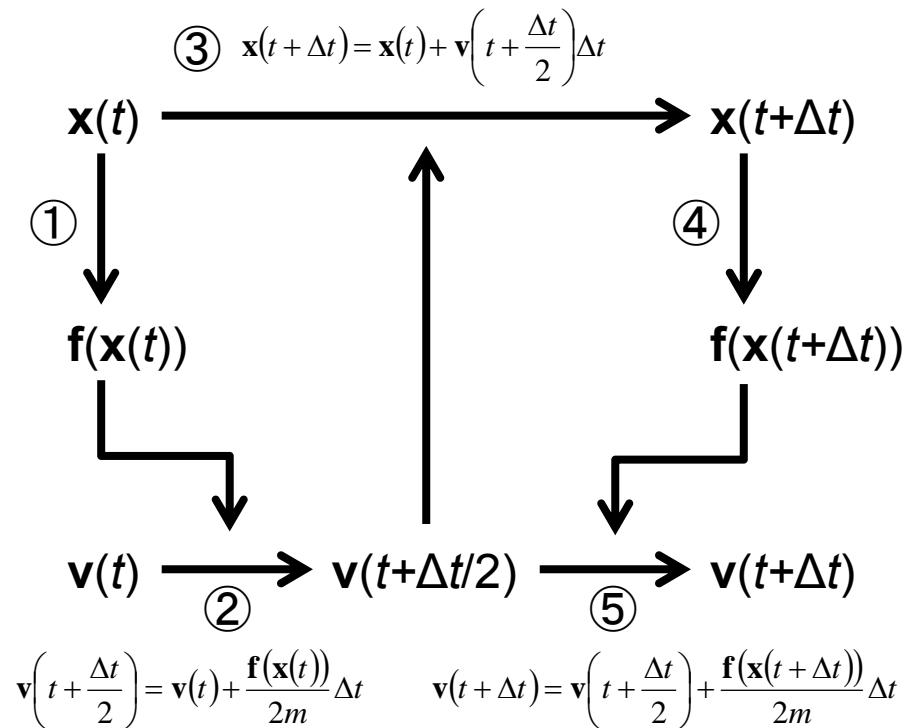
① Calculate force

② Calculate velocities at $t+\Delta t/2$

③ Calculate coordinates at $t+\Delta t$

④ Calculate force

⑤ Calculate velocities at $t+\Delta t$

⑥ Return to ② and repeat

③ $\mathbf{x}(t+\Delta t) = \mathbf{x}(t) + \mathbf{v}\left(t+\dfrac{\Delta t}{2}\right)\Delta t$

$\mathbf{x}(t) \longrightarrow \mathbf{x}(t+\Delta t)$

① $\mathbf{f}(\mathbf{x}(t))$

④ $\mathbf{f}(\mathbf{x}(t+\Delta t))$

$\mathbf{v}(t) \xrightarrow{②} \mathbf{v}(t+\Delta t/2) \xrightarrow{⑤} \mathbf{v}(t+\Delta t)$

$\mathbf{v}\left(t+\dfrac{\Delta t}{2}\right) = \mathbf{v}(t) + \dfrac{\mathbf{f}(\mathbf{x}(t))}{2m}\Delta t$

$\mathbf{v}(t+\Delta t) = \mathbf{v}\left(t+\dfrac{\Delta t}{2}\right) + \dfrac{\mathbf{f}(\mathbf{x}(t+\Delta t))}{2m}\Delta t$
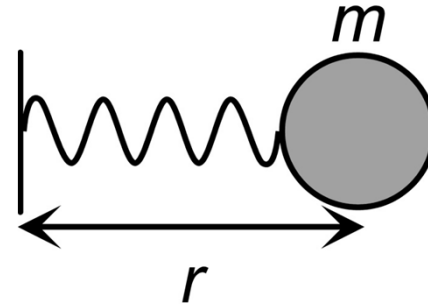
Harmonic oscillator (1)

- Harmonic oscillator
  Mass: m
  Spring length: r
  Length of unstrained spring: r_0
  Force constant: k

$$F = -k(r - r_0)$$

$$m\frac{d^2 r}{dt^2} = -k(r - r_0)$$

$$q = r - r_0$$

$$F = -kq$$

$$m\frac{d^2 q}{dt^2} = -kq$$

Harmonic oscillator (2)

- A Perl program (osc.pl) that numerically integrates the equation of motion of harmonic oscillator with velocity Verlet method

- Initial position: $q(0)=1$, initial velocity: $v(0)=0$

```perl
$q=1.0;$v=0.0;
$m=1.0;$k=1.0;
$dt=0.01;$nstep=100;
sub calc_force {
  my $q=$_[0];
  my $f=-$k*$q;
  my $e=0.5*$k*$q**2;
  return ($e,$f);
}
open(OUT,">osc$dt.csv");
```

```perl
($e,$f)=calc_force($q);
for($i=1;$i<=$nstep;$i++) {
  $v+=0.5*$f/$m*$dt;
  $q+=$v*$dt;
  ($e,$f)=calc_force($q);
  $v+=0.5*$f/$m*$dt;
  $H=0.5*$m*$v**2+$e;
  print OUT $i*$dt,",",$q,
    ",",$v,",",$H,"¥n";
}
```
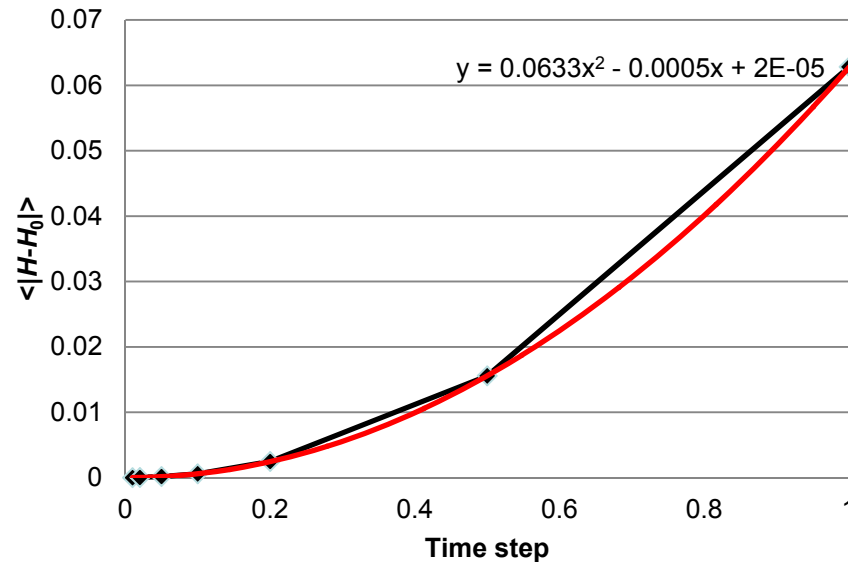
Exercise 1

- Calculate the averages of the absolute differences of total energies and its initial value $<|H-H_0|>$, changing the time steps as $dt=0.01, 0.02, 0.05, 0.1, 0.2, 0.5,$ and 1 in osc.pl.

- Plot $<|H-H_0|>$ against the time step in the Excel sheet osc.xlsx.

- Briefly discuss the result.

Error depends on time step

$y = 0.0633x^2 - 0.0005x + 2E\text{-}05$
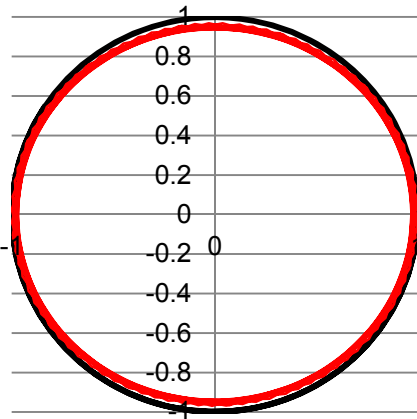
Plots of q against v calculated with $dt = 0.1$ (black), 0.5 (red).

Plot of $<|H-H_0|>$ against dt.

$$H = \frac{mv^2}{2} + \frac{kq^2}{2} = 0.5 \quad \Rightarrow \quad v^2 + q^2 = 1$$

$|H-H_0|$ corresponds deviation from the circle.

Choice of appropriate time step

- The smaller time step causes the smaller error in the total energy.

- In general, 1/10 – 1/20 of the cycle of the fastest motion is used for the time step.

- In the case of a protein, the fastest motion is the bond-stretching motion (3000 cm^{-1}; 10 fs) of X–H bonds (X=C, N, O, or S).

- Therefore, 0.5 – 1.0 fs is appropriate.

A system with many atoms (1)

- A system composed of atoms with van der Waals interactions (vdw.pl)
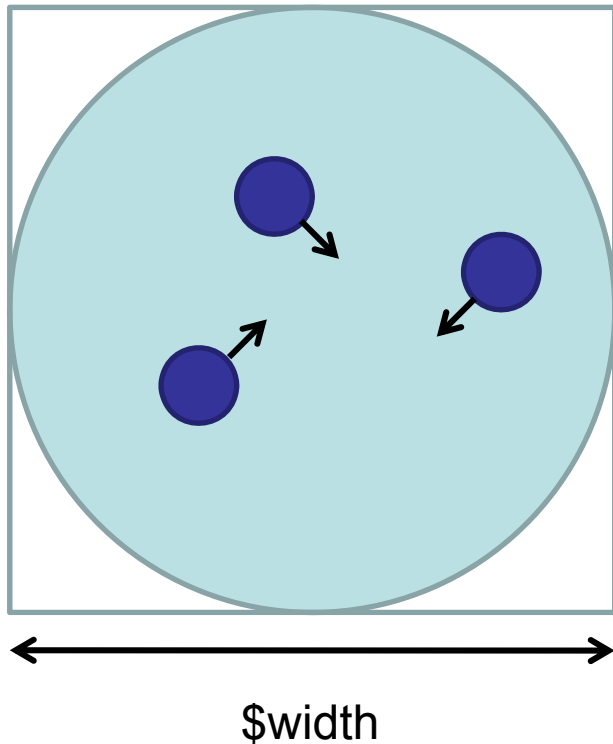
$width

```
$natom=3;          # Number of particles
$width=10.0;       # Width of initial
                     particle distribution
$scale=1.0;        # Scaling factor for
                     initial velocity
$fcap=1.0;         # Force constant for
                     spherical boundary
$sigma=1.0;        # Atom radius
$epsilon=1.0;      # Well depth
$mass=1.0;         # Atomic mass
$nstep=100000;     # Number of MD steps
$nsave=100;        # Frequency of saving
                     trajectory
$dt=0.001;         # Time step
$seed=110601;      # Random seed
```

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A system with many atoms (2)

- Initial arrangement
  - Atoms are randomly placed with in a cube with the edge length of $width.
- Initial velocities
  - Randomly assigned. Their magnitude can be changed by $scale parameter.
- Potential energy function:

$$E = \sum_{i=1}^{N} \sum_{j=i+1}^{N} 4\varepsilon \left(\frac{\sigma^{12}}{r_{ij}^{12}} - \frac{\sigma^{6}}{r_{ij}^{6}} \right) + \sum_{i=1}^{N} E_{\text{cap}}(r_i)$$

$$E_{\text{cap}}(r_i) = \begin{cases} 0 & r_i < r_{\text{cut}} \\ f_{\text{cap}}(r_i - r_{\text{cut}})^2 & r_i \geq r_{\text{cut}} \end{cases}$$

r_i is distance from origin.
r_{cut} is set to the half of $width.

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A system with many atoms (3)

- Result can be visualized by using UCSF Chimera.
1. Double-click the icon of Chimera 1.5.2.
2. Choose "Tools" → "MD/Ensemble Analysis" → "MD Movie." Set Trajectory format to "PDB", PDB frames contained in to "Single file", and "vdw.pdb" to the file. Then, click "OK."
3. Choose "Actions" → "Atoms/Bonds" → "stick" to show atoms.
4. Click playback button to start animation.
- Examine the effect on the dynamics of the parameters.

Comparison with experimental data

- Integration of Newton's equations of motion corresponds to the simulation of the dynamics of an isolated system.

- Experimentally observed data are the averages over a huge number (say 10^{23}) of molecules.

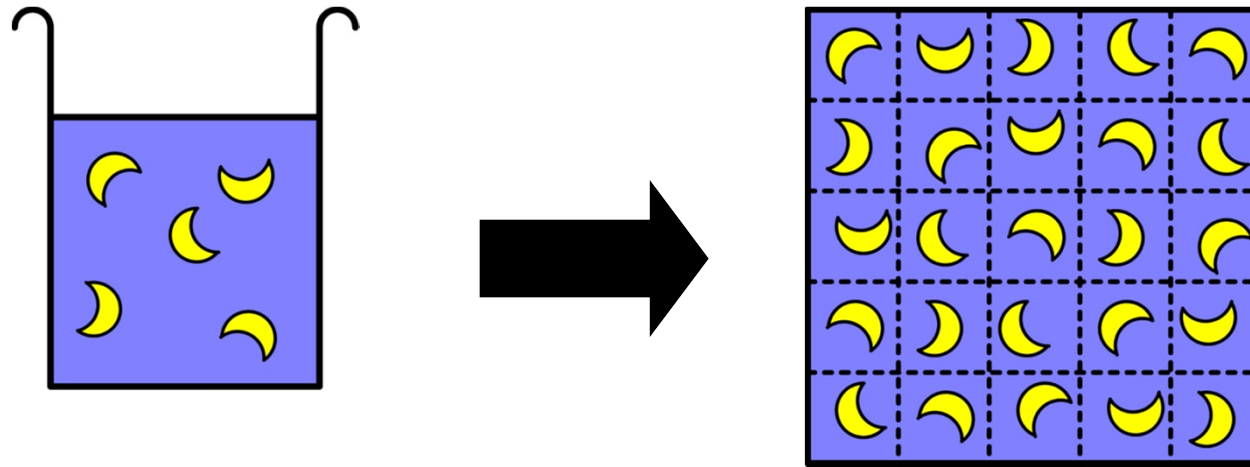- Are the results from molecular simulations comparable with the experimental data?

Real system
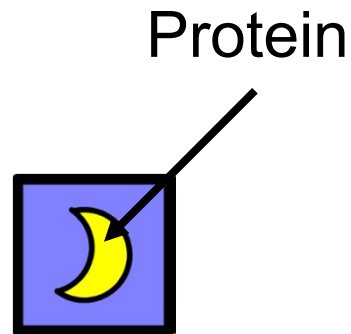
Protein

An isolated system
(Constant-*NVE)*
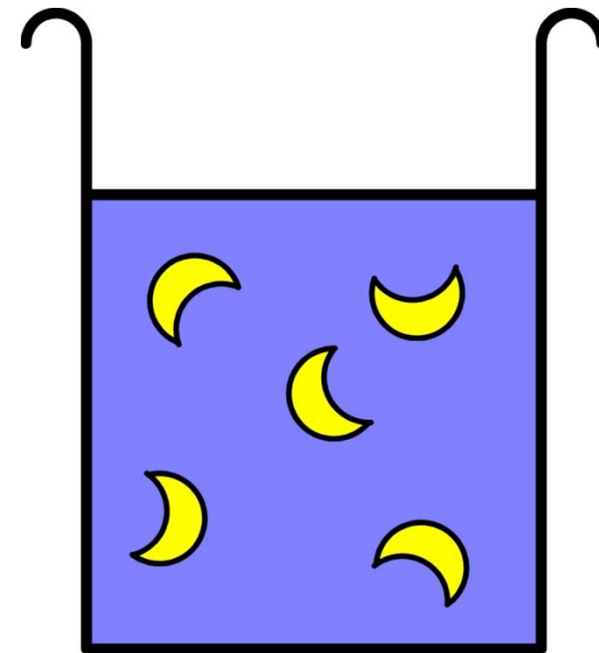
A constant-temperature and constant-volume (constant-*NVT*) system composed of 10^{23} protein molecules

Constant-*NVT* system (1)

- The system is composed of many identical sub-systems.
- Each sub-system is composed of a protein molecule and its surrounding water molecules.
- Each sub-system can exchange heat with its neighbors.
- Number of the unit system and the total energy of the whole system are constant.

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Constant-*NVT* system (2)

- Experimentally observed data are the averages of the observables of each state weighted by its probability of existence.

$$\langle A \rangle = A_i \rho_i, \quad \sum_i \rho_i = 1 \qquad \rho_i\text{: probability of existence}$$

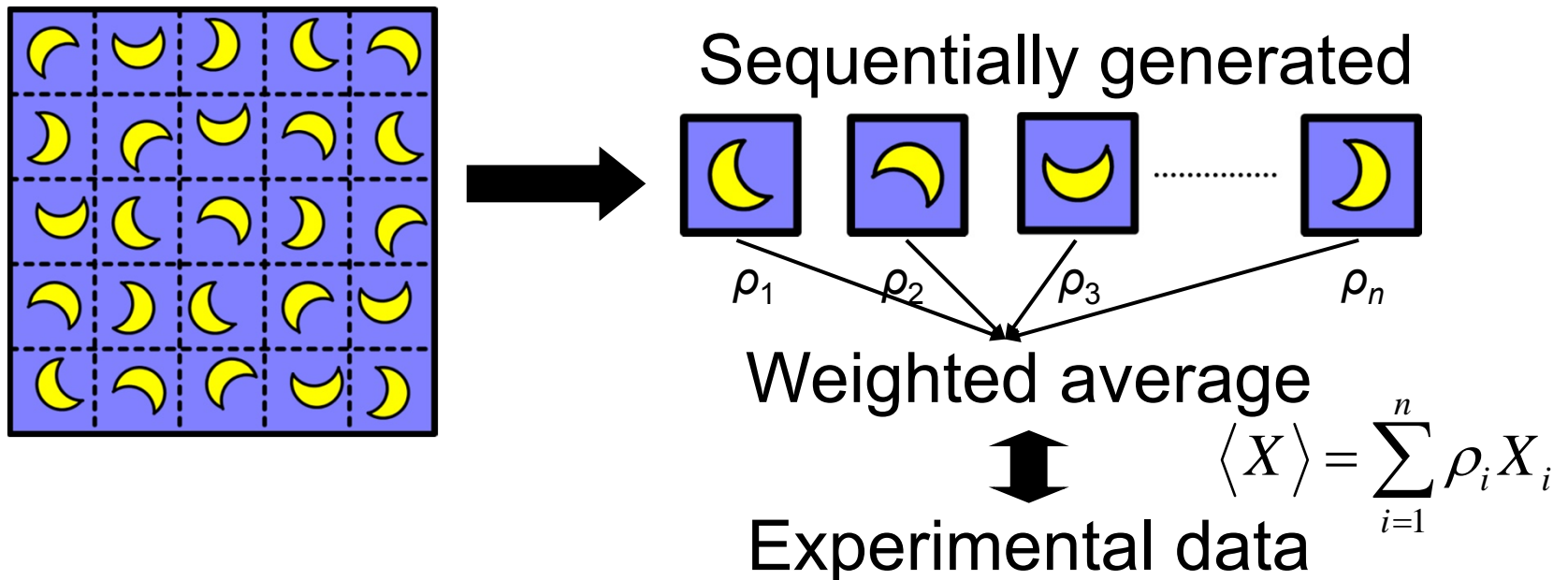- Distribution with maximum entropy
  = canonical distribution

$$\rho_i = Z^{-1} \exp\left(-e_i / k_B T\right)$$
$$Z = \sum_i \exp\left(-e_i / k_B T\right)$$

e_i: energy of state *i*

Z: partition function

Constant-*NVT* system (3)

- In a molecular simulation, each state in the whole system is generated sequentially.

Sequentially generated

ρ_1 ρ_2 ρ_3 ρ_n

Weighted average

$$\langle X \rangle = \sum_{i=1}^{n} \rho_i X_i$$

Experimental data

Ensemble average

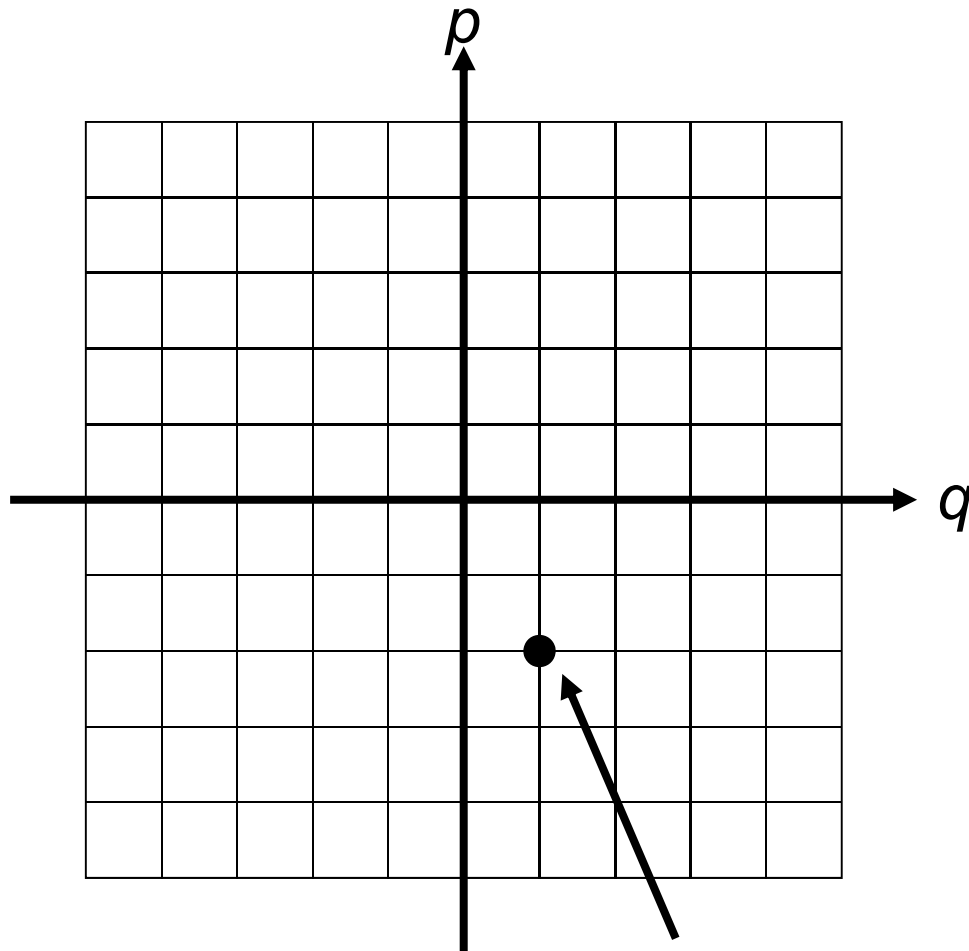- Evaluate the ensemble average of the total energy of a harmonic oscillator

$$H(q,p) = \frac{p^2}{2m} + \frac{k}{2}q^2, \quad \rho(q,p) = \frac{\exp\left[-\dfrac{H(q,p)}{k_B T}\right]}{\displaystyle\int \exp\left[-\dfrac{H(q,p)}{k_B T}\right] dq\,dp}$$

$$\langle H \rangle = \int H(q,p)\rho(q,p)\,dq\,dp = k_B T \qquad \text{Exact value}$$

- Method 1: Numerical integration with grid
- Method 2: Monte Carlo integration
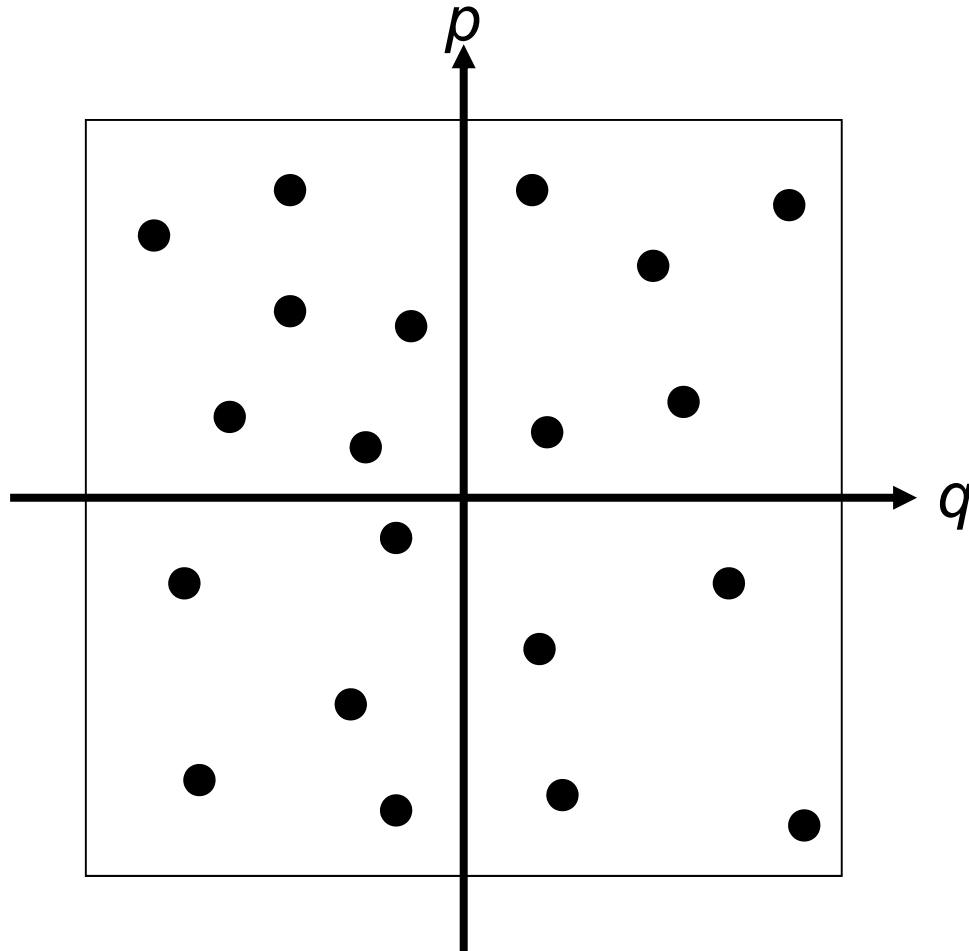- Method 3: Importance sampling

1: Numerical integration with grid

p

q

- Evaluate $\exp(-H/k_BT)$ at each grid point and compute its sum and the sum of the product with H.
- Only the grid points within $-10 \le q \le 10$ and $-10 \le p \le 10$ are considered.
- Plot the ratio of the sums (*i.e. <H>*) against the number of grid points.

Evaluate H and $\exp(-H/k_BT)$.

2: Monte Carlo integration

- Draw q and p from a uniform distribution within $-10 \le q \le 10$ and $-10 \le p \le 10$.

- Evaluate $\exp(-H/k_{\mathrm{B}}T)$ at each point and compute its sum and the sum of the product with H.

- Plot the ratio of the sums (*i.e.* <H>) against the number of the sample points.

Comparison of the results (1)

Black: Grid
Red: Monte Carlo

$\langle H \rangle$

$k_B T = 1.0$

Number of points
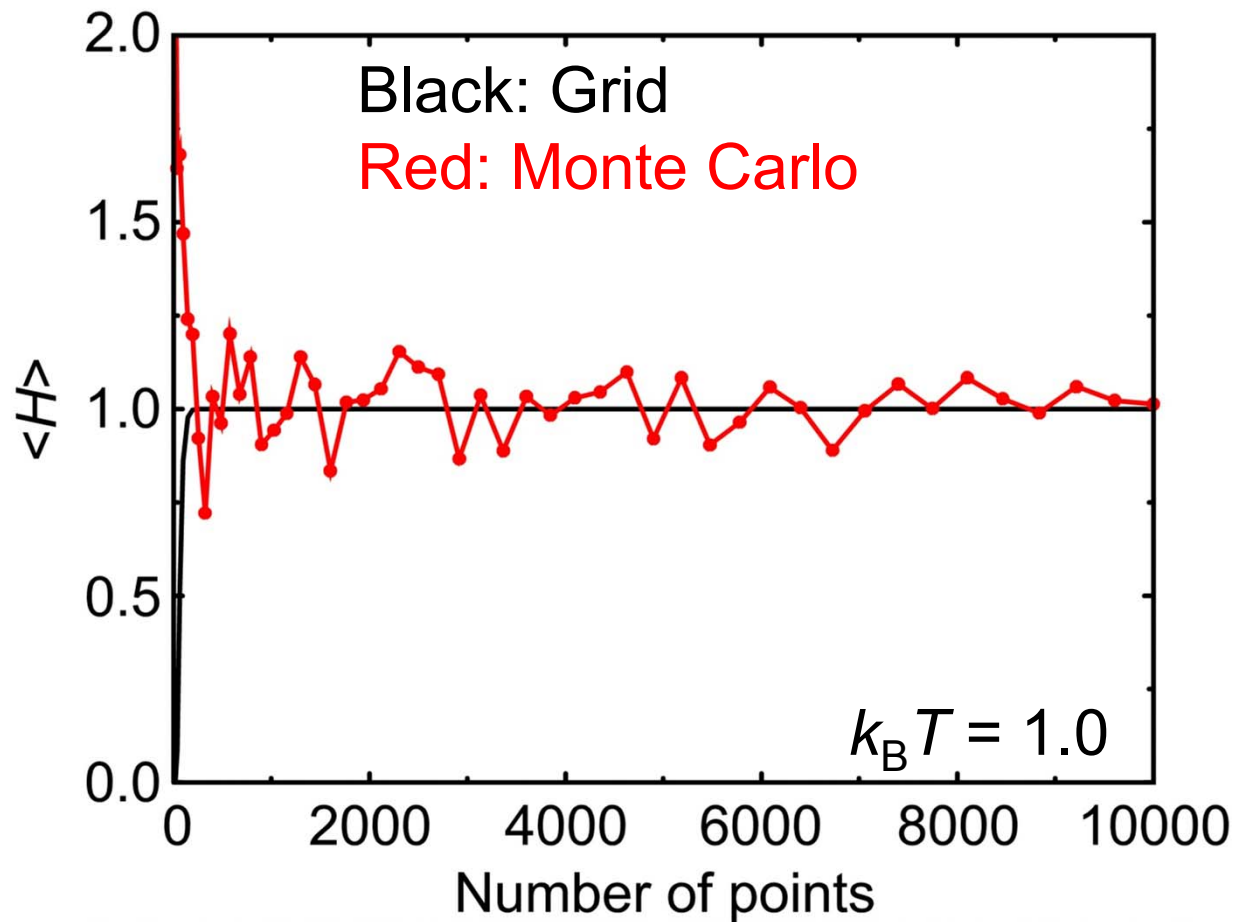
Monte Carlo integration is slow to converge.

Problem of Monte Carlo integration

- Error is inversely proportional to the square root of the number of samples→To decrease the error by a factor of 10, 100 times larger samples are required.

- However, grid approach is not applicable to biomacromolecules due to their large internal degrees of freedom. A 100-residue protein has more than $2^{100} \fallingdotseq 10^{30}$ different conformations.

- It is necessary to improve the accuracy of the Monte Carlo method.
  →importance sampling

Importance sampling

- The Monte Carlo integration calculates the weighted sum of H with the weighting factors of $\exp(-H/k_\mathrm{B}T)$.

- At $(q, p) = (0, 0)$, the weighting factor is one, whereas at $(q, p) = (10, 10)$, it is 3.7×10^{-44}.

- The contributions to the average are different between sample points, which decreases computational efficiency.

- The efficiency is maximized when the number of sample points from a region is proportional to the weighting factor, $\exp(-H/k_\mathrm{B}T)$, of the region.→importance sampling

3: Importance sampling
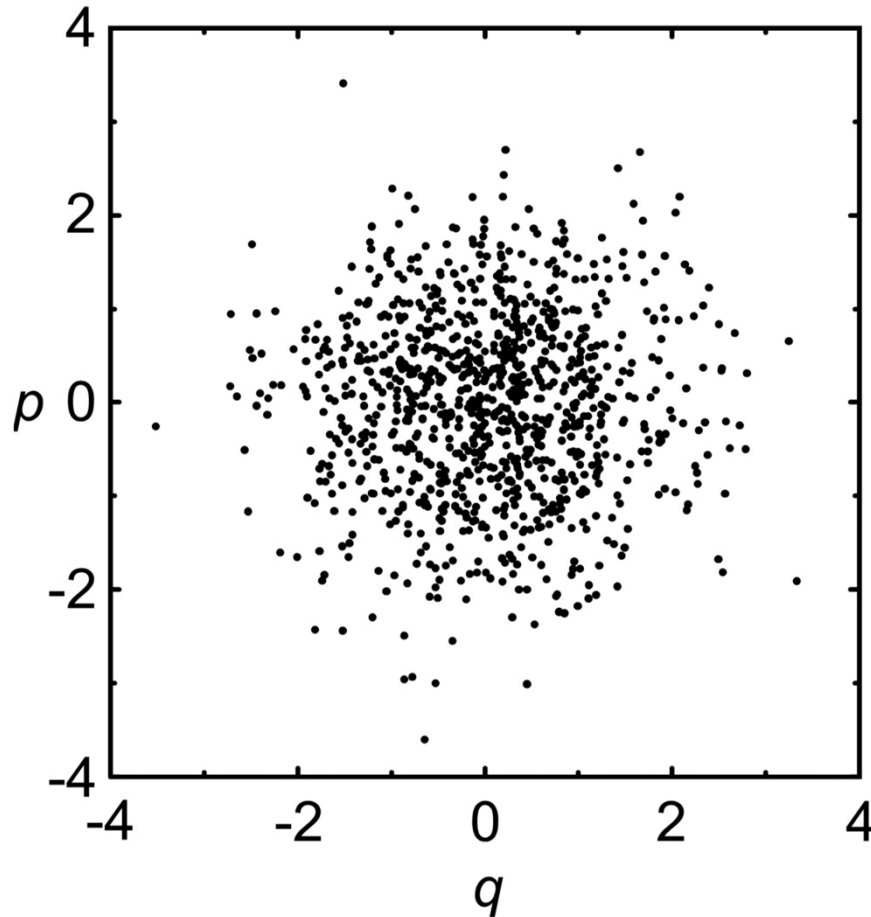
- Draw samples from a distribution proportional to the weight $\exp(-H/k_BT)$.

- Evaluate H at each sample point and calculate the average.

- Plot the average $<H>$ against the number of samples.

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A Perl program

```perl
$kT=1.0;
$pi=atan2(1.0,1.0)*4.0;
$max_npt=100;

for($npt=2;$npt<=$max_npt;$npt+=2) {
  $val1=0.0;
  for($i=0;$i<$npt**2;++$i) {
    $x1=rand;
    $x2=rand;
#Convert uniform distribution into normal distribution.
    $q=sqrt(-2.0*$kT*log($x1))*cos(2.0*$pi*$x2);
    $p=sqrt(-2.0*$kT*log($x1))*sin(2.0*$pi*$x2);
    $H=0.5*$q**2+0.5*$p**2;
    $val1+=$H;                #Sum of total energy
  }
  printf("%d %f¥n",$npt**2,$val1/($npt**2));
}
```
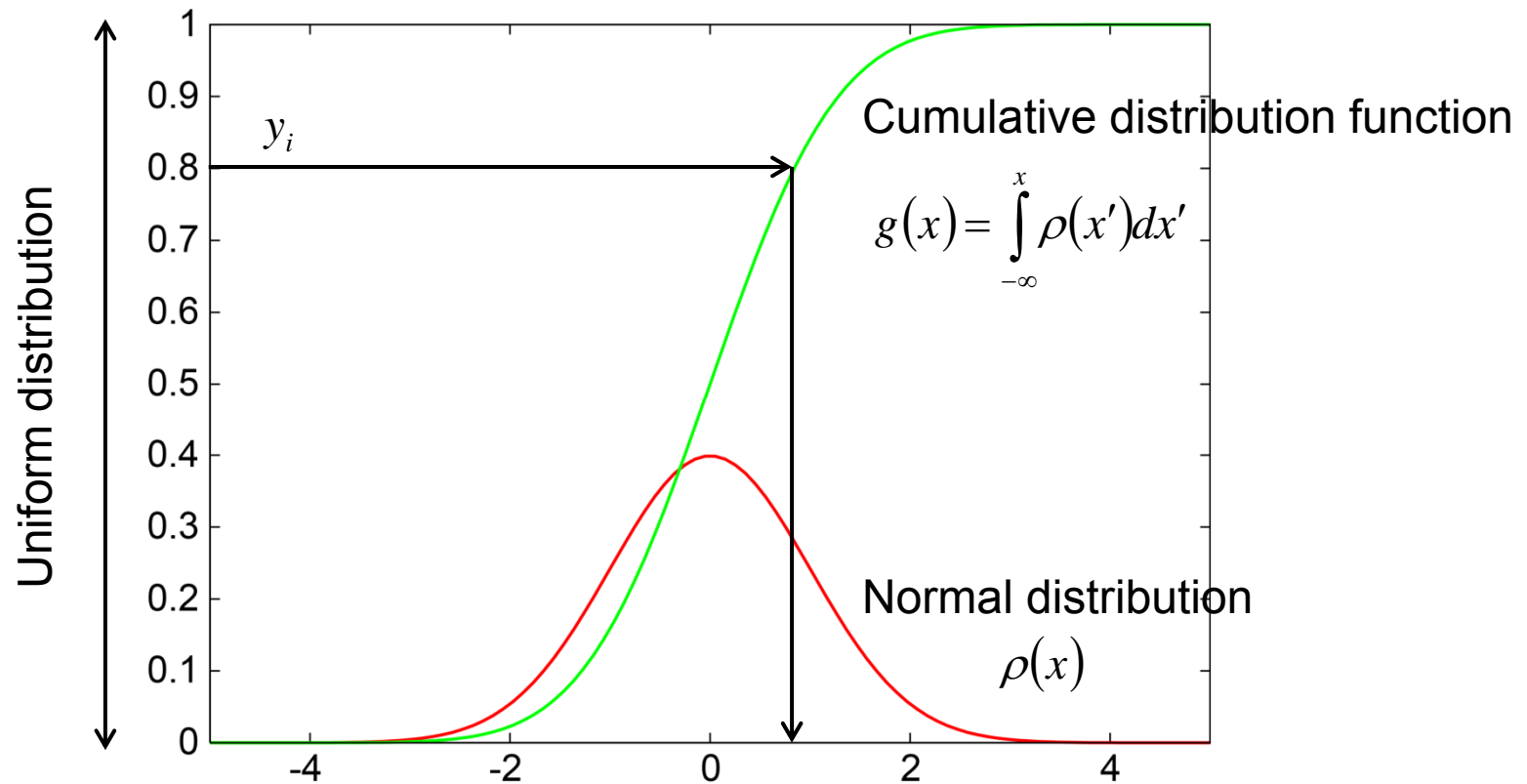
Comparison of the results (2)

Black: grid
Red: Monte Carlo
Green: Importance sampling

$k_B T = 1.0$
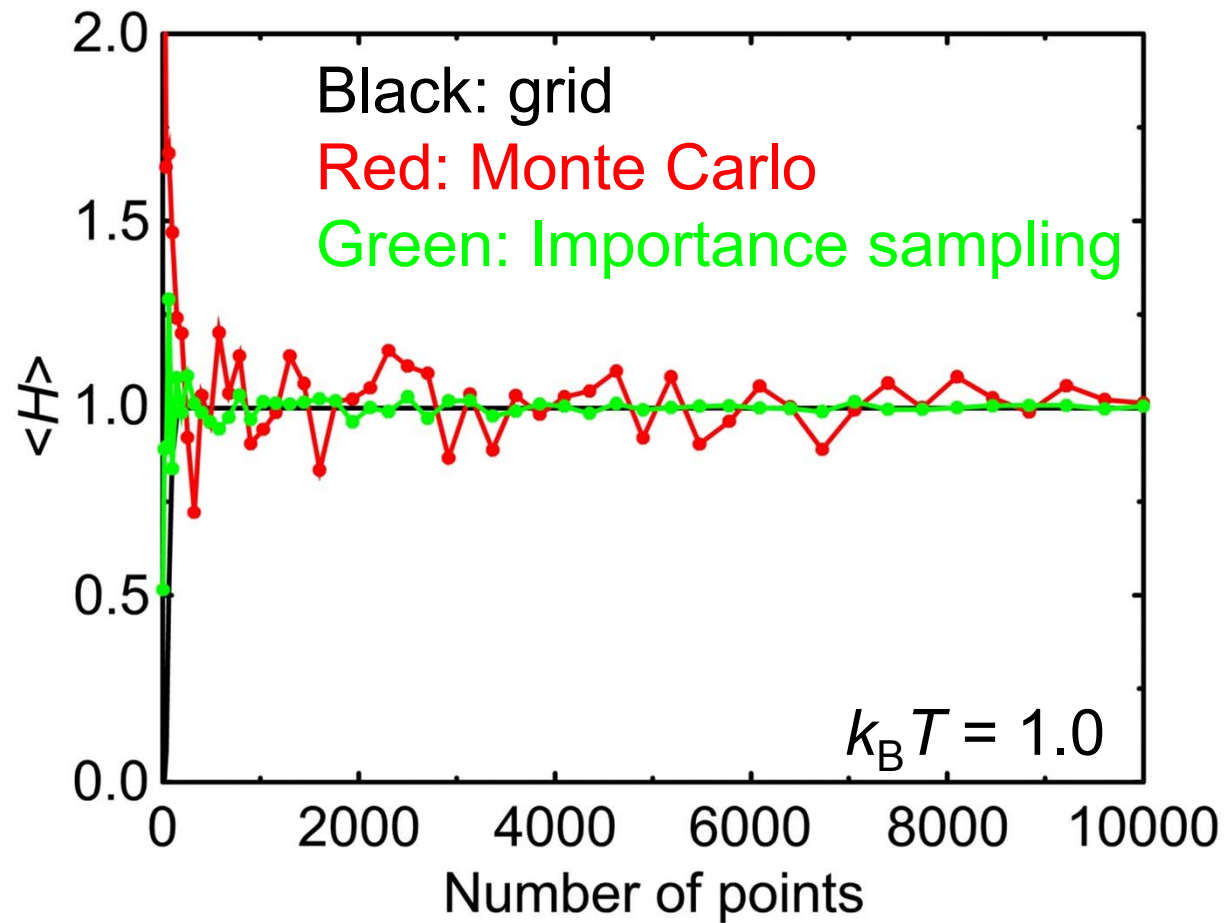
Accuracy and efficiency are improved.

Sample generation (1)

Uniform distribution

y_i

Cumulative distribution function

$$g(x) = \int\limits_{-\infty}^{x} \rho(x')dx'$$

Normal distribution
$\rho(x)$

Conversion into normal distribution
$$g(x_i) = y_i, \quad x_i = g^{-1}(y_i)$$

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Sample generation (2)

- This method is possible only when the cumulative distribution function (CDF) can be calculated.
- It is impossible to obtain an analytical form of the CDF for a system of biomacromolecules, because the relation between bonded and non-bonded interactions is quite complicated.
- It is also impossible to calculate it numerically due to the huge internal degrees of freedom.

Use Markov chain

Markov chain

Transition probability π_{ij}
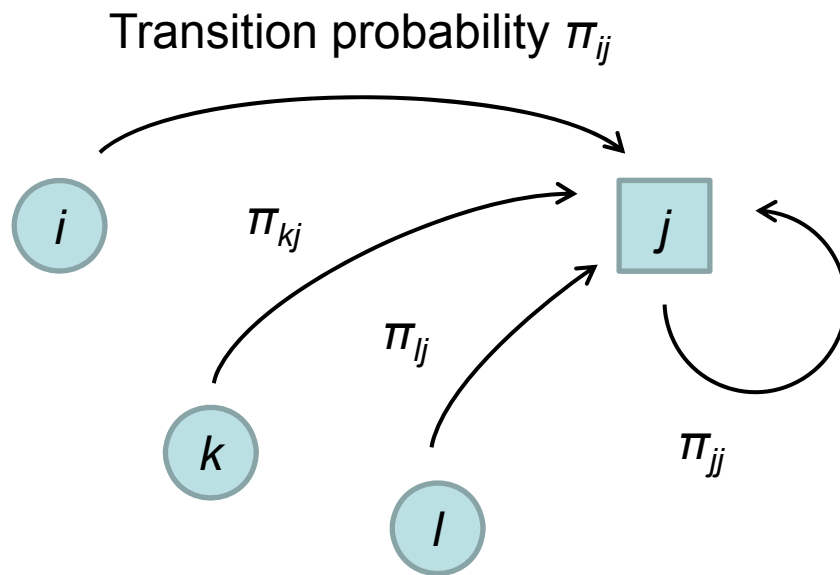
- Let the probability of transition from state i to state j be π_{ij}.
- Let the probability of existence of state i before transition be ρ^0_i, the probability of existence of state j after transition is given by,

$$\rho^1_j = \sum_i \rho^0_i \pi_{ij}$$

- Transition probability satisfies the following:
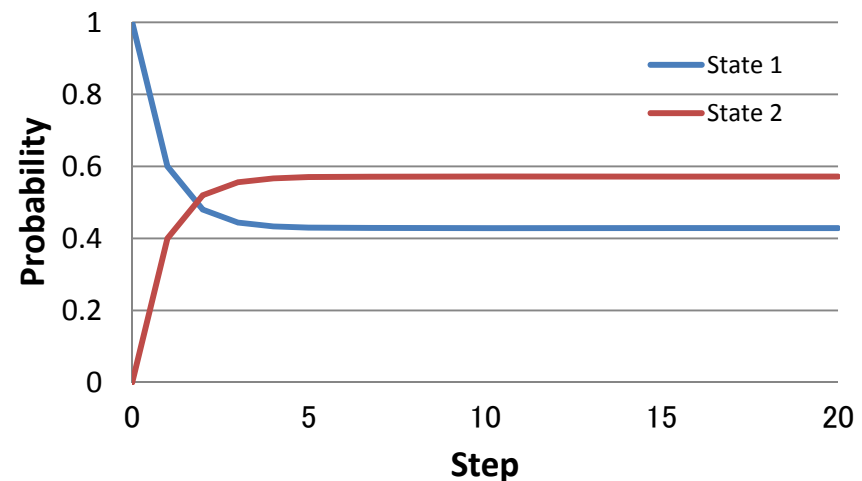
$$\sum_j \pi_{ij} = 1$$

Example of Markov chain (1)

- Consider two states.

- Let transition probabilities be:

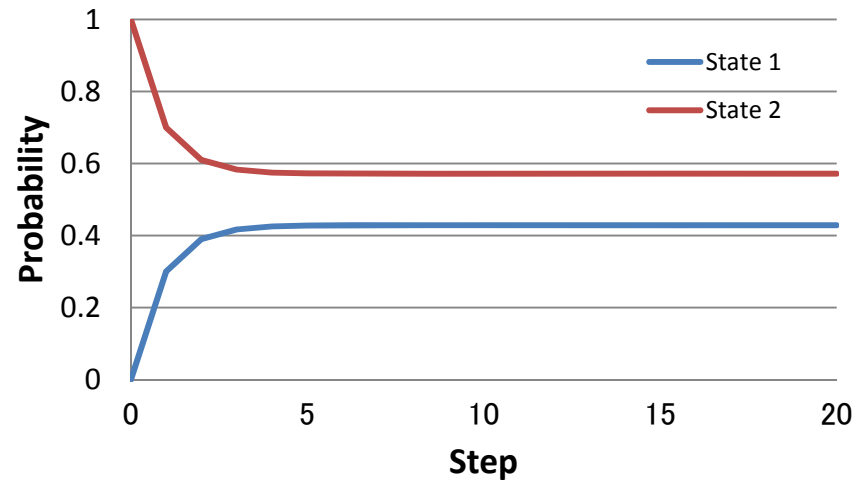| π_{11} = 0.6	π_{12} = 0.4
π_{21} = 0.3	π_{22} = 0.7

- Start with state 1

Step	State 1	State 2
0	1	0
1	0.6	0.4
2	0.48	0.52
3	0.444	0.556

Example of Markov chain (2)

- When stating with state 2, the probabilities converge to the same values.

- After convergence, **ρ** = **ρπ**.

- **ρ** is a eigenvector of matrix **π**.
  → **ρ** is uniquely determined by **π**.

Metropolis method (1)

- We want to derive transition matrix from probability distribution.

- The detailed balance condition is the sufficient condition for **ρ** = **ρπ**.

$$\rho_i \pi_{ij} = \rho_j \pi_{ji} \quad \Rightarrow \quad \sum_i \rho_i \pi_{ij} = \sum_i \rho_j \pi_{ji} = \rho_j \sum_i \pi_{ji} = \rho_j$$

- Metropolis method:

$$\begin{cases} \pi_{ij} = \alpha_{ij} & \text{if } \rho_j \geq \rho_i \text{ and } i \neq j \\ \pi_{ij} = \alpha_{ij}\left(\rho_j / \rho_i\right) & \text{if } \rho_j < \rho_i \text{ and } i \neq j \end{cases}$$
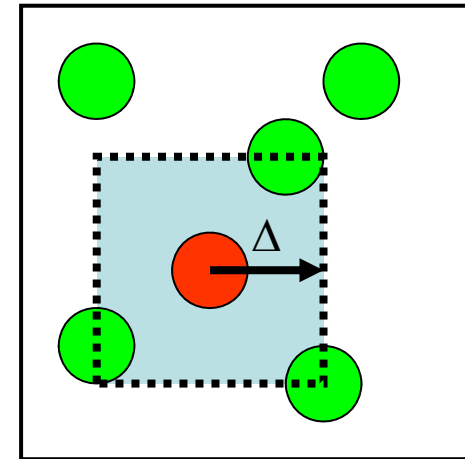
$$\alpha_{ij} = \alpha_{ji}, \quad \sum_{j \neq i} \alpha_{ij} = 1, \quad \pi_{ii} = 1 - \sum_{j \neq i} \pi_{ij} = \sum_{\substack{j \neq i \text{ and} \\ \rho_j < \rho_i}} \alpha_{ij}\left(1 - \rho_j / \rho_i\right)$$

Metropolis method (2)

- Randomly move an atom within a cube centered at the atom with the edge length of 2Δ to generate a new state.

$$\alpha_{ij} = \frac{1}{N_\Delta} \quad \text{Within the cube}$$

$$\alpha_{ij} = 0 \quad \text{Outside the cube}$$

- The move is accepted if the energy of the new state, e_j, is lower than that of the original state, e_i. Otherwise, the move is accepted with the following probability:

$$\rho_j / \rho_i = \exp\left[-\left(e_j - e_i\right)/k_B T\right] = \exp\left(-\Delta e_{ji}/k_B T\right)$$

- If not accepted, the atom does not move.

$$\pi_{ii} = 1 - \sum_{j \neq i} \pi_{ij} = \sum_{j \neq i} \left(\alpha_{ij} - \pi_{ij}\right) = \sum_{\substack{j \neq i \text{ and} \\ \rho_j < \rho_i}} \alpha_{ij}\left(1 - \rho_j / \rho_i\right)$$

An application

- A harmonic oscillator
- Initial condition: $(q, p) = (0, 0)$
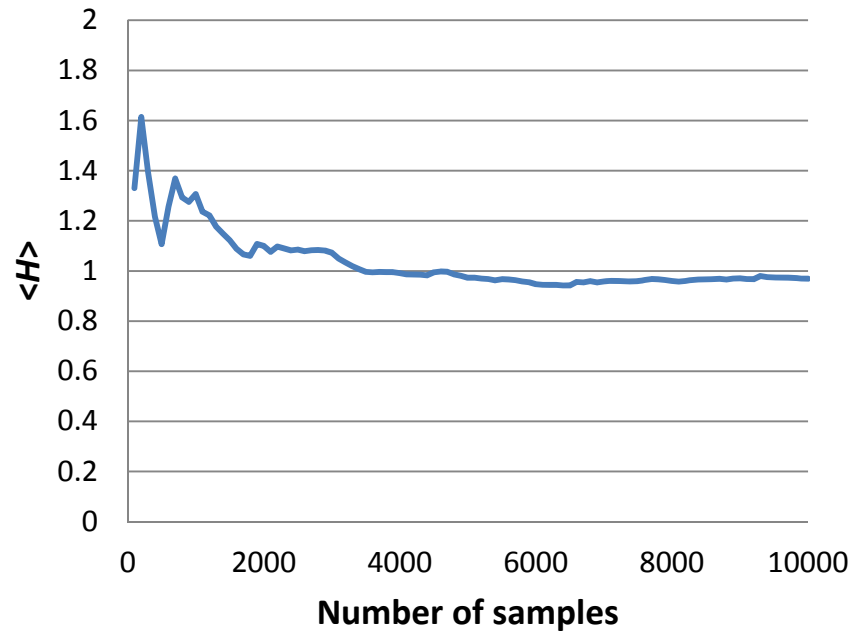
A Perl program

```perl
$nstep=10000;                                       #Number of steps
($q,$p)=(0.0,0.0);                                  #Initial states
$delta=1.0;                                         #Maximum displacement
$kT=1.0;$m=1.0;$k=1.0;                              #kT, mass, force constant
$delta_q=$delta/sqrt($k);
$delta_p=$delta*sqrt($m);


open(OUT,">metropolis$delta.csv");                  #Output file


$ave=0.0;
$H=&calc_H($q,$p);                                  #Initial energy
for($i=1;$i<=$nstep;$i++) {
  $q_new=$q+2.0*$delta_q*(rand()-0.5);              #Trial move
  $p_new=$p+2.0*$delta_p*(rand()-0.5);              #Trial move
  $H_new=&calc_H($q_new,$p_new);
  $probability=exp(($H-$H_new)/$kT);
  if($probability >= 1.0 || $probability >= rand()) {       #Metropolis criterion
    $q=$q_new;$p=$p_new;$H=$H_new;
  }
  $ave+=$H;
  printf(OUT "%d,%f¥n",$i,$ave/$i) if($i % 100 == 0);
}
close(OUT);


sub calc_H {                                        #Energy function
  my ($q,$p)=@_;
  return 0.5*$p*$p/$m+0.5*$k*$q*$q;
}
```

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Exercise 2

- Download metropolis.pl from the web page of this lecture and double-click the icon of the downloaded file to execute it.

  – Plot *<H>* against the sample number. Check whether *<H>* converges to 1.

- Check the convergence changing the value for $delta.

  – Try $delta=0.1.

- Discuss why the convergence depends on $delta.

Application to biomacromolecules

- Metroplis method can be realized by choosing an atom randomly and moving the atom to a random position.

- However, such a move changes the bond length and causes increase of energy. →Probability of acceptance is very small.

- To avoid this problem, only dihedral angles are changed. But, this has following drawbacks. →It is difficult to handle multiple molecules. →In the region where atoms are closely packed, such as protein cores, change in the dihedral angle will cause steric clashes.

Constant-temperature MD (1)

- Constant-temperature MD can generate a canonical ensemble.
- This can be more easily applied to the systems of biomacromolecules than Monte Carlo method.
- The ensemble average is given by the time average.
- Temperature is regulated by modifying the velocity.

$$\frac{3}{2}NkT = \sum_{i=1}^{N}\frac{m_i|\mathbf{v}_i|^2}{2}$$

Constant-temperature MD (2)

- Nosé method
- Nosé-Hoover chain method ⎤
- Constraint method

  – Only the coordinate part follows the canonical distribution.

- Langevin dynamics

  – Temperature is regulated by friction and random force.

- Berendsen weak-coupling method

  – Does not generate a canonical ensemble.
  – Simple and easy to use.

Degrees of freedom of the heat bath are explicitly considered.
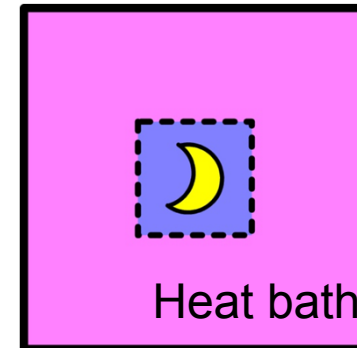
Heat bath

Langevin dynamics

- The physical system exchanges heat with the heat bath through collisions with fictitious particles of the heat bath.

- Equations of motion

$$m\mathbf{a} = \mathbf{F}(\mathbf{x}) - \gamma\mathbf{v} + \mathbf{R}(t)$$

Friction   Random force caused by the collisions

- Random force **R** satisfies the following:

$$\langle\mathbf{R}(t)\rangle = 0, \quad \langle\mathbf{R}(t)\cdot\mathbf{R}(t')\rangle = 6k_{\mathrm{B}}T\gamma\delta(t-t')$$

Average   Variance and covariance

An application

- A system composed of atoms with van der Waals interactions (vdw_langevin.pl)

```
$natom=4;          # Number of particles
$width=10.0;       # Width of initial
                   #   particle distribution
$fcap=1.0;         # Force constant for
                   #   spherical boundary
$sigma=1.0;        # Atom radius
$epsilon=1.0;      # Well depth
$mass=1.0;         # Atomic mass
$nstep=100000;     # Number of MD steps
$nsave=100;        # Frequency of saving
                   #   trajectory
$dt=0.001;         # Time step
$seed=120528;      # Random seed
$gamma=10.0;       # friction coefficient
$kT=1.0;
```
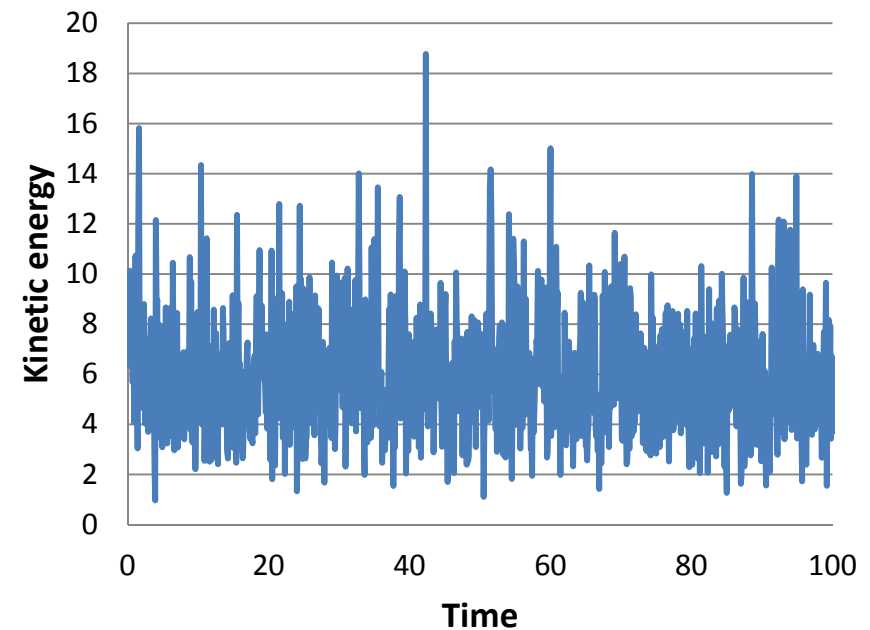
Average: 5.91 (exact value: 6)

Berendsen weak-coupling method

1. Calculate instantaneous temperature T' at every step of velocity Verlet.

$$\frac{3}{2}NkT' = \sum_{i=1}^{N} \frac{m_i |\mathbf{v}_i|^2}{2}$$

2. Scale velocities by a factor of χ. Constant τ controls the speed of adjustment.

$$\chi = \left[1 + \frac{\Delta t}{\tau}\left(\frac{T}{T'} - 1 \right) \right]^{1/2}$$

How to send your report

- Use PowerPoint to create your report.

- Report should include the results and discussion of exercises 1 and 2.

- Send the PowerPoint file to tterada@iu.a.u-tokyo.ac.jp.

- Subject of the e-mail should be "Molecular modeling" and write your name and ID card number in the body of the e-mail.