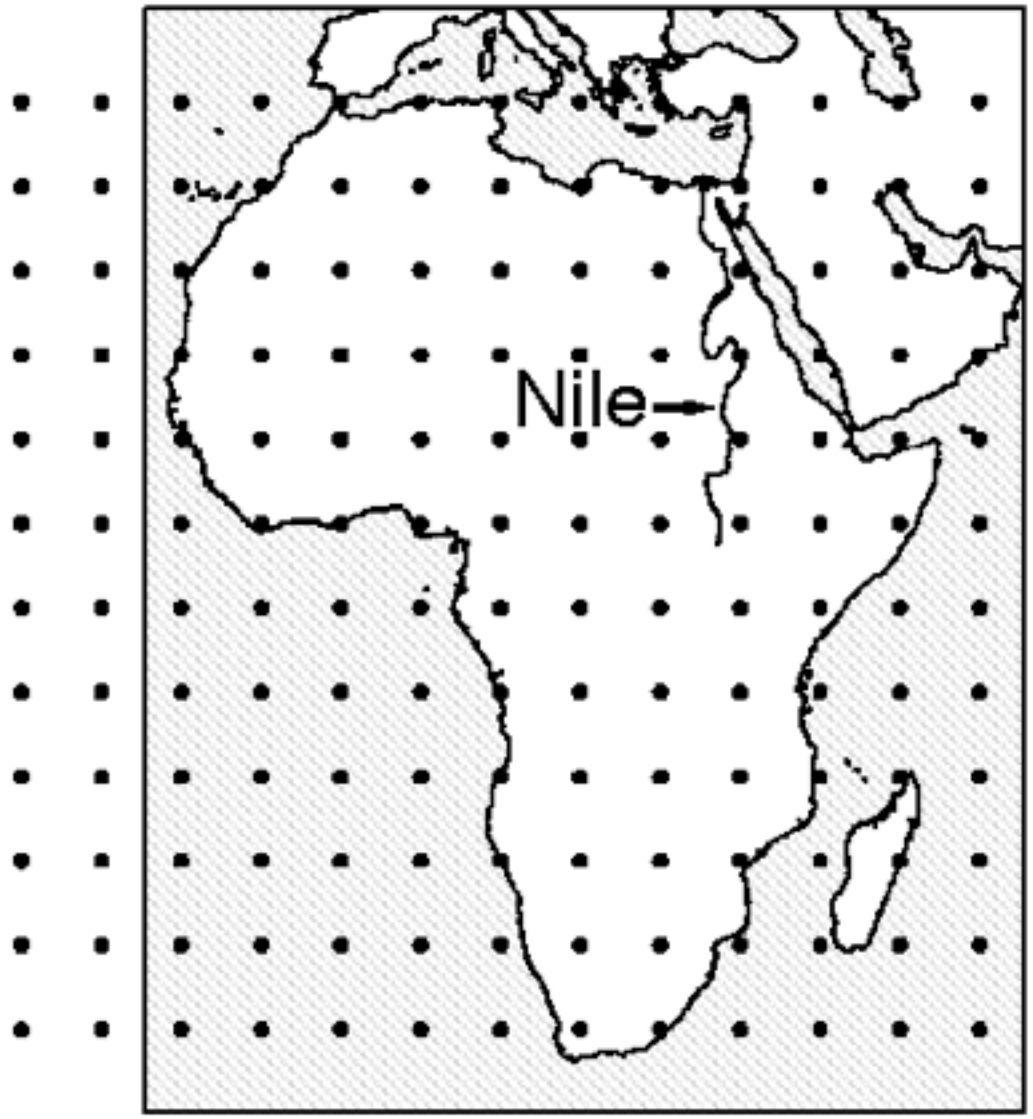
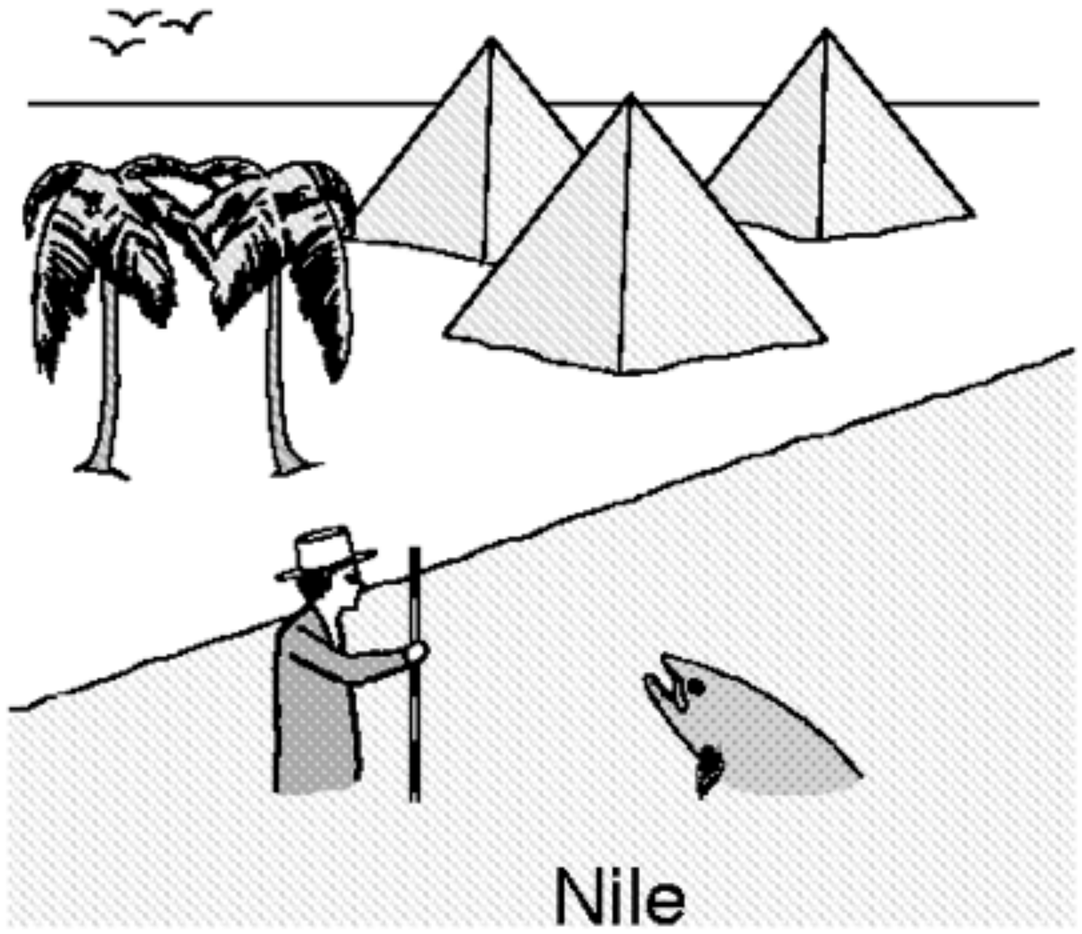
Announcements

- lecture slides online
- wireless
- account lifetime
- group photo Monday morning


Nile


Nile

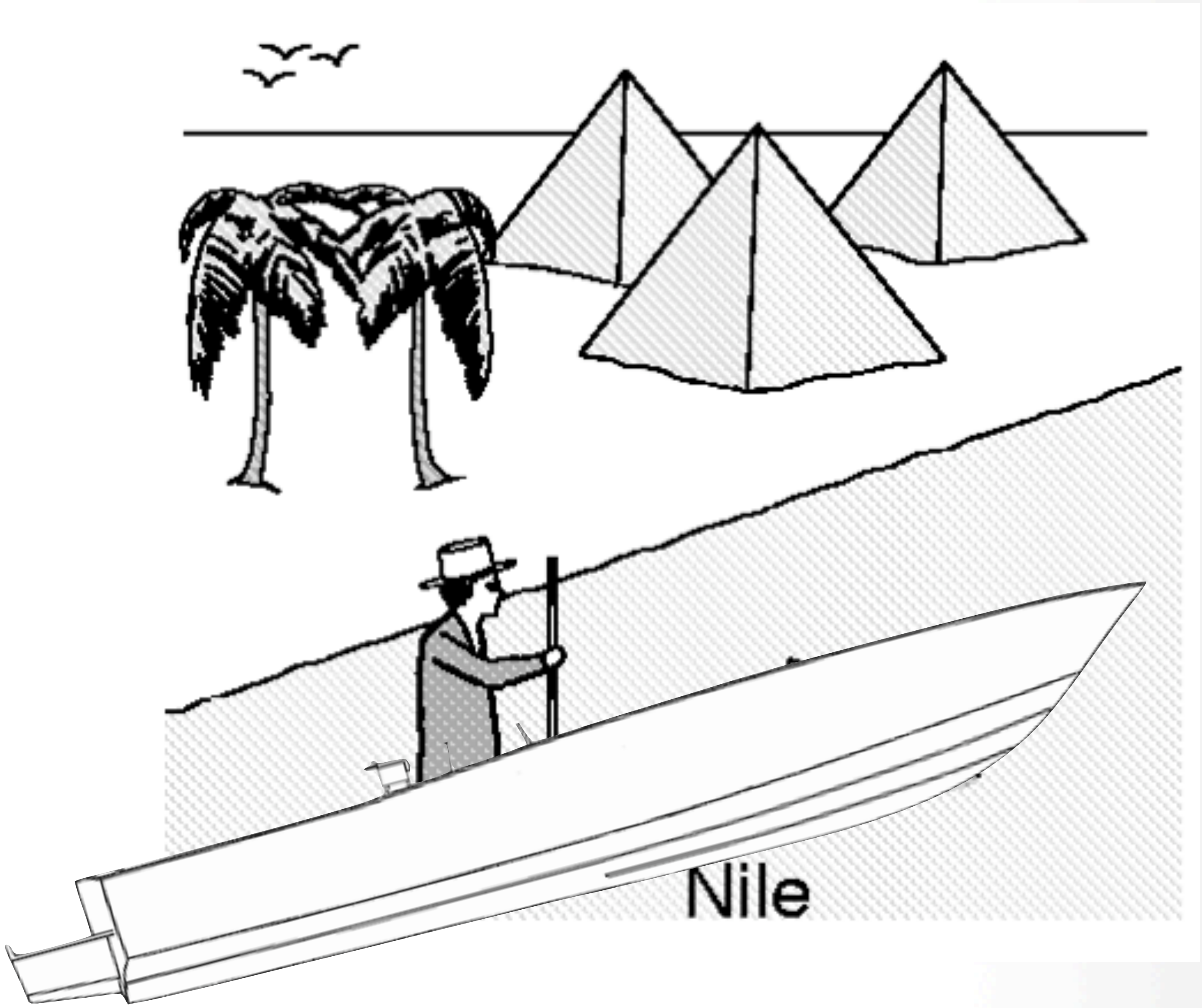
Molecular Dynamics

- Theory:

$$\mathbf{F} = m \frac{d^2\mathbf{r}}{dt^2}$$

- Compute the forces on the particles
- Solve the equations of motion
- Sample after some timesteps

MD Sampling



MD Sampling

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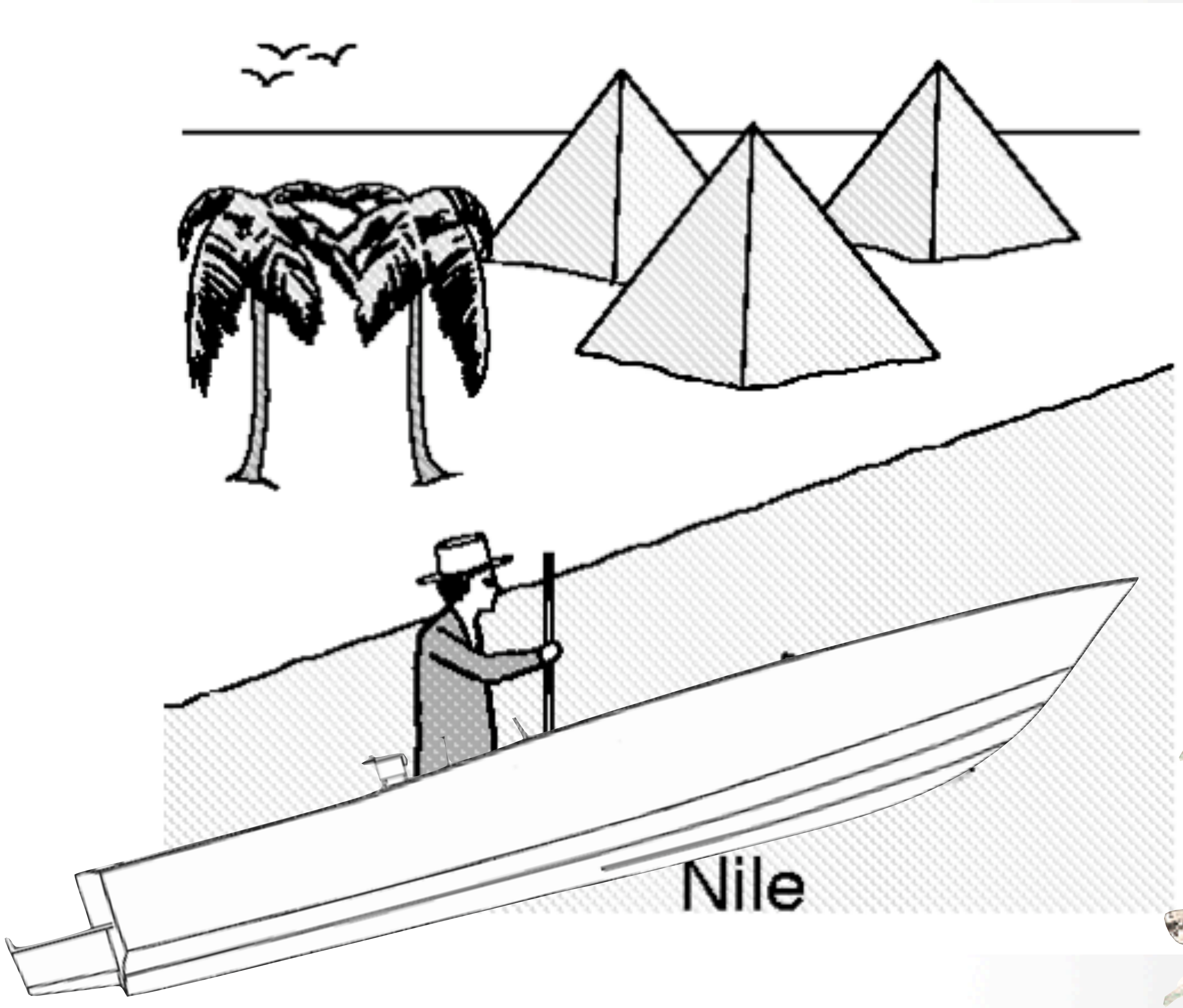

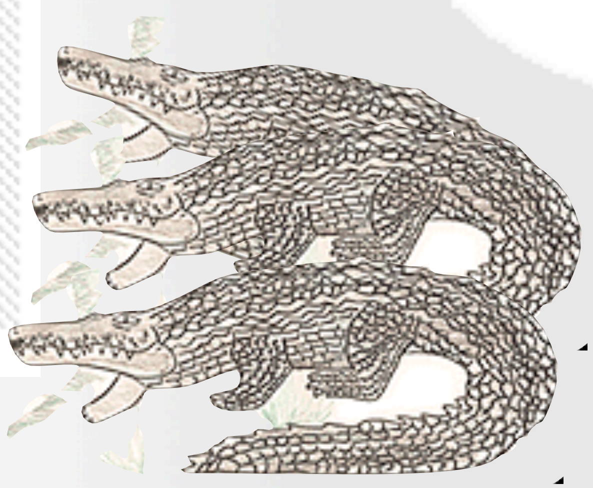

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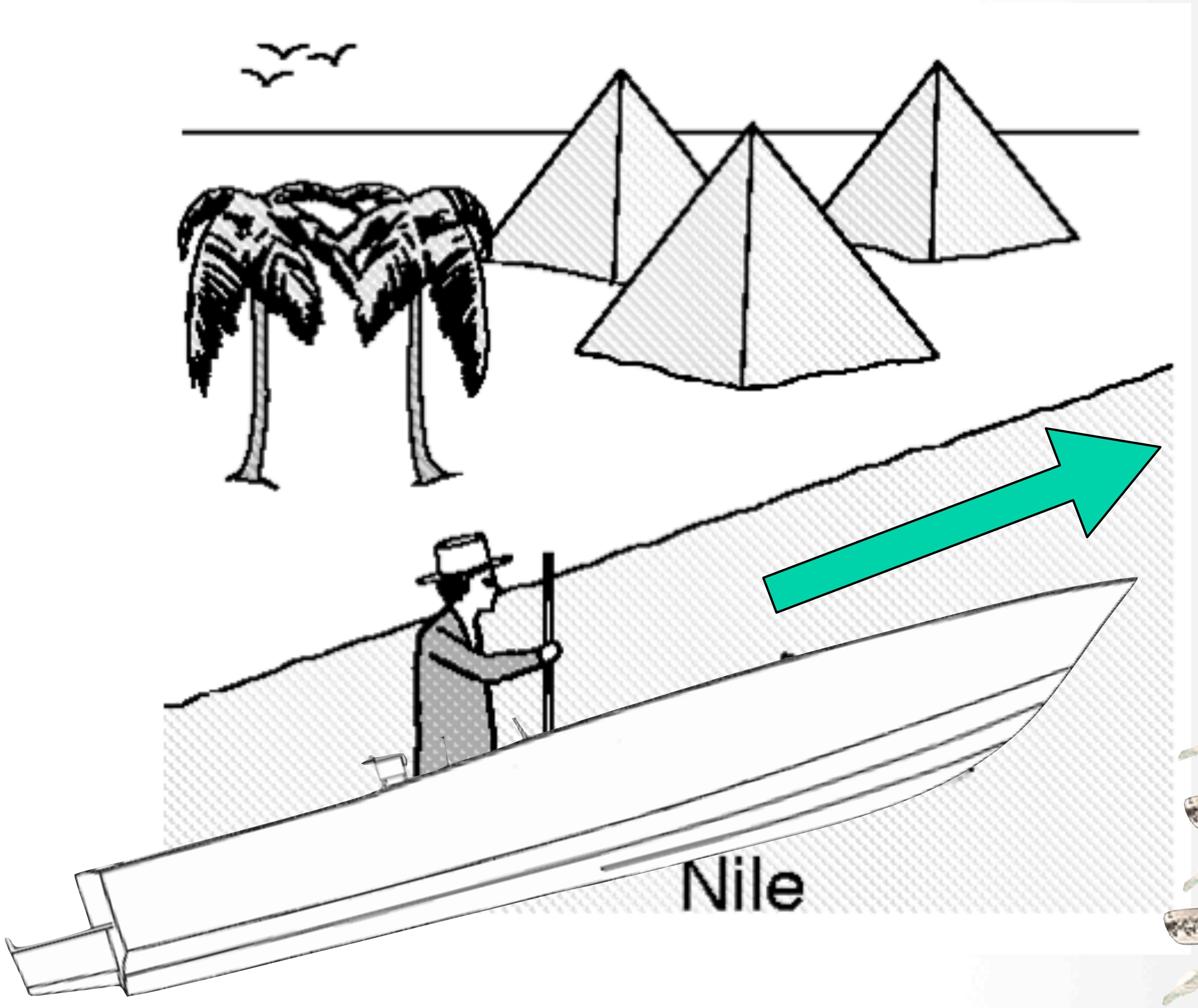
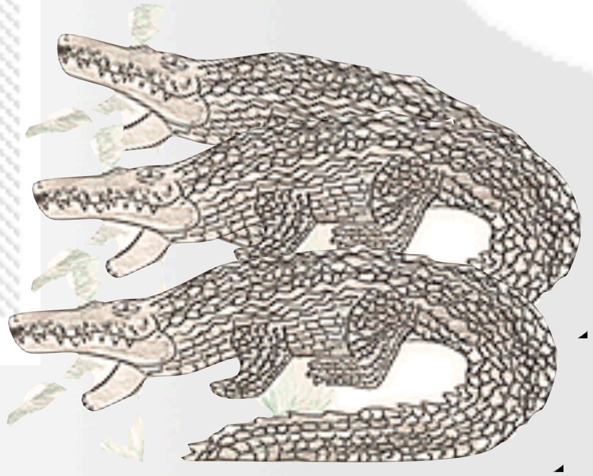
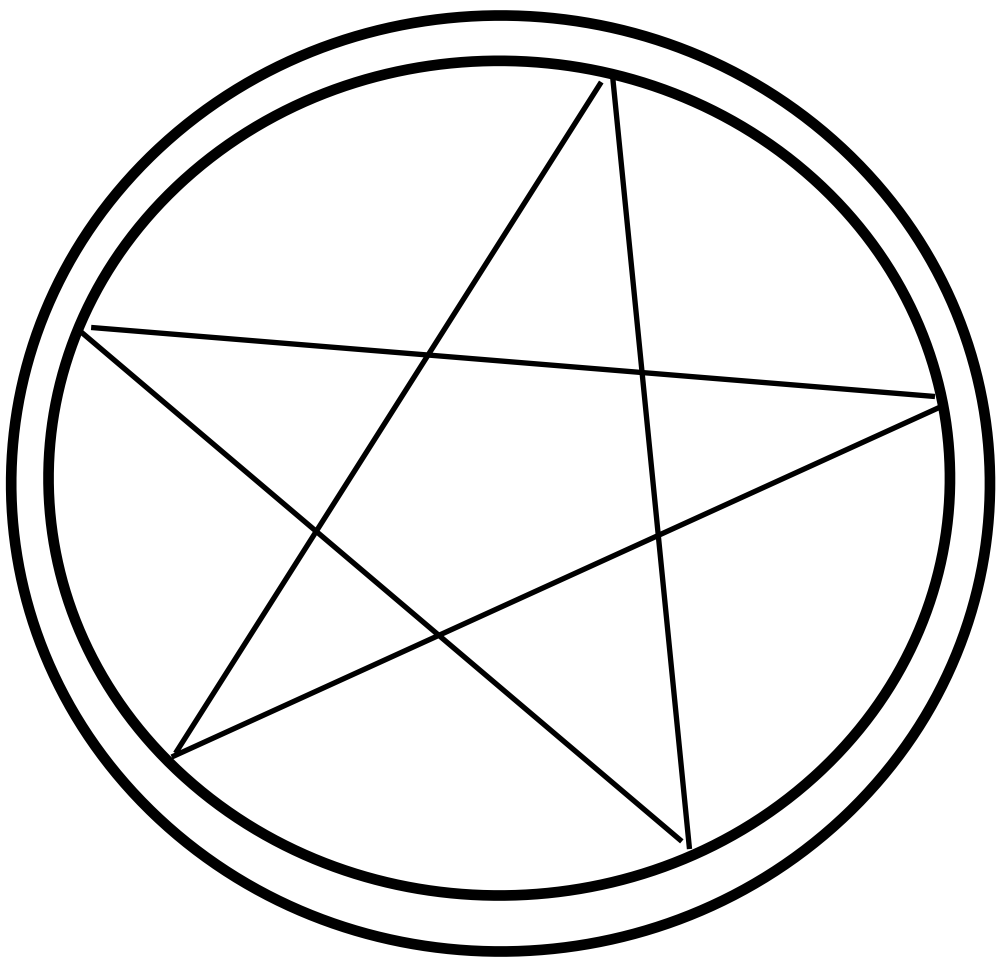
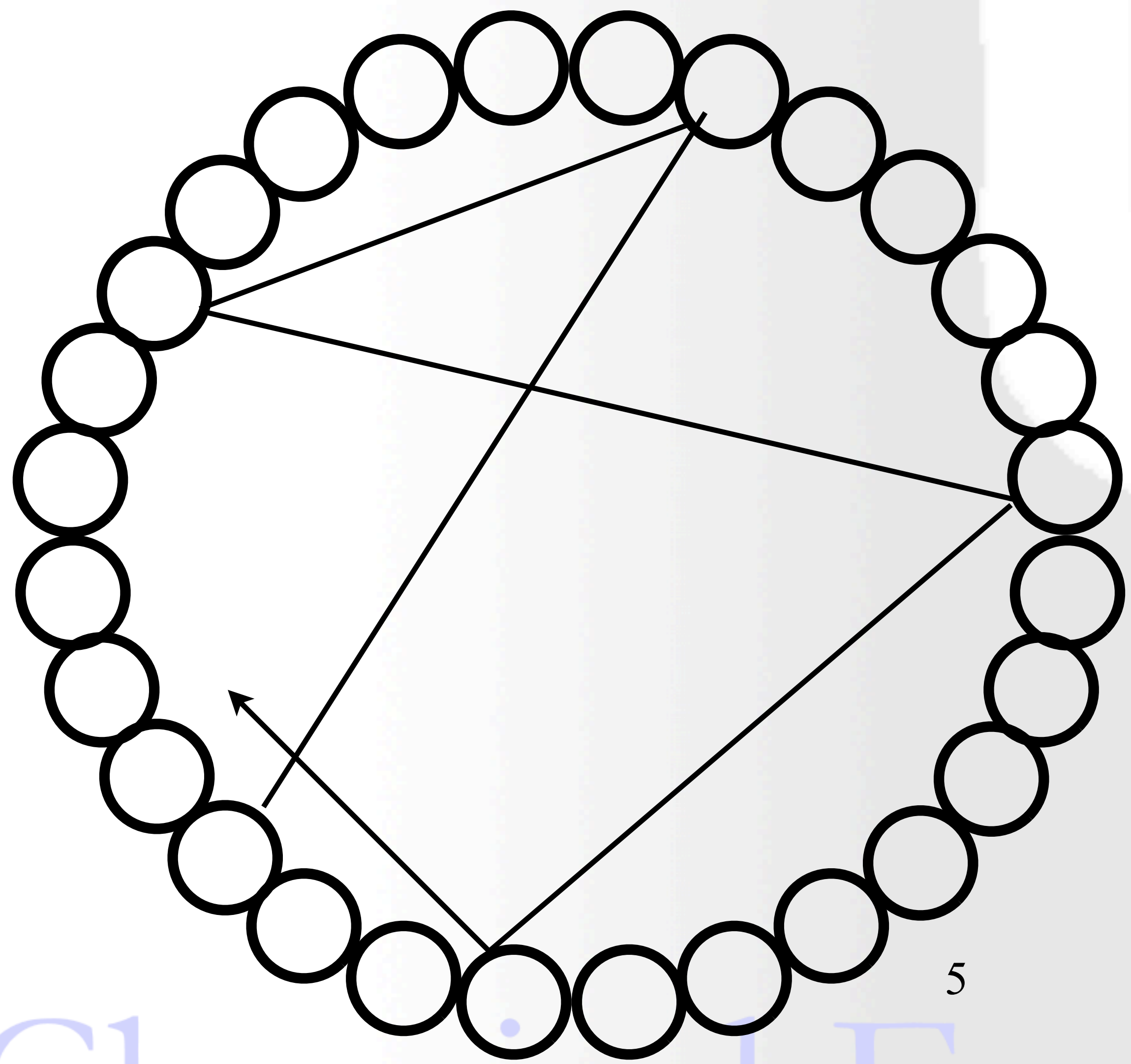




MD Sampling

- Ergodicity



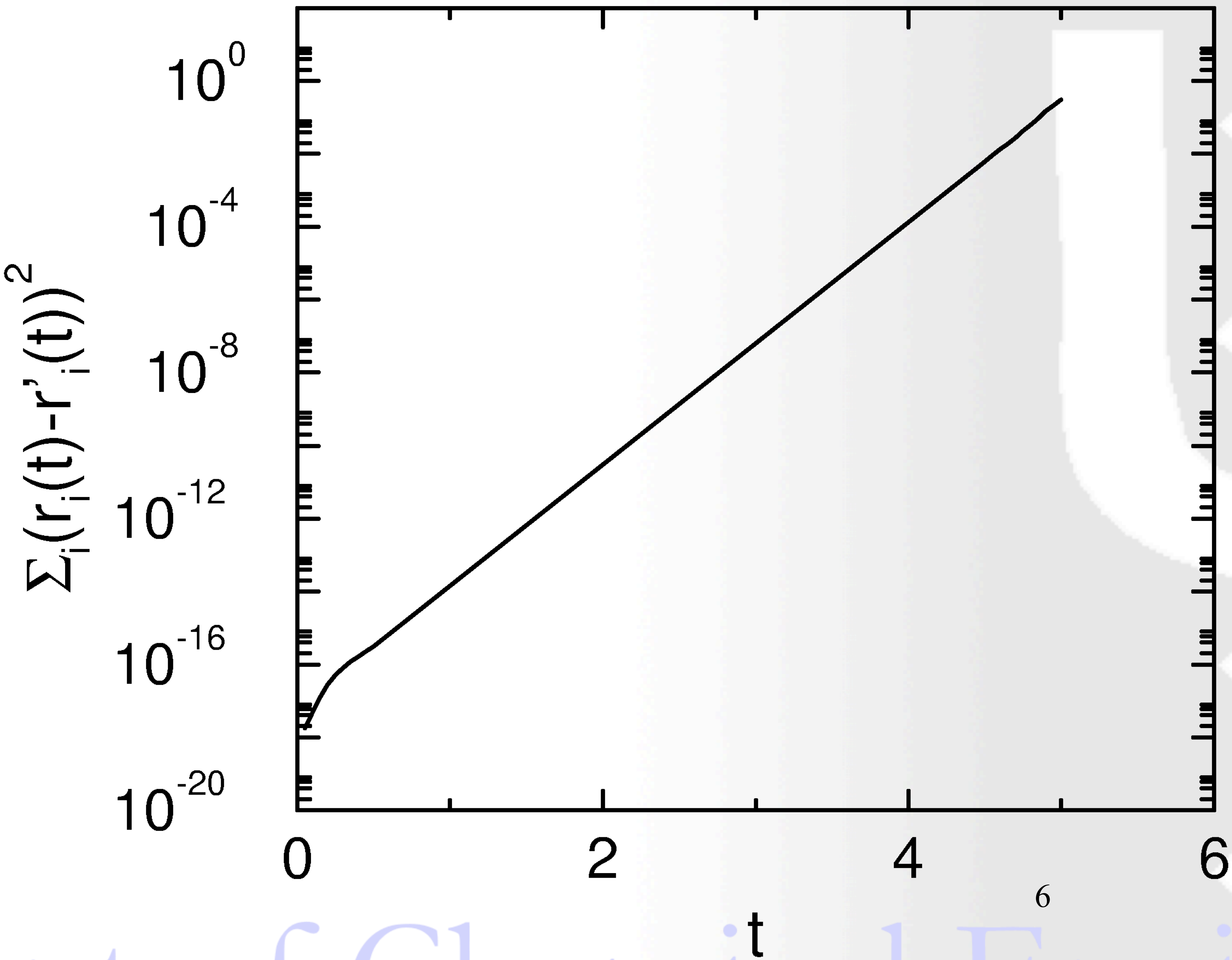


Lyaponov instability

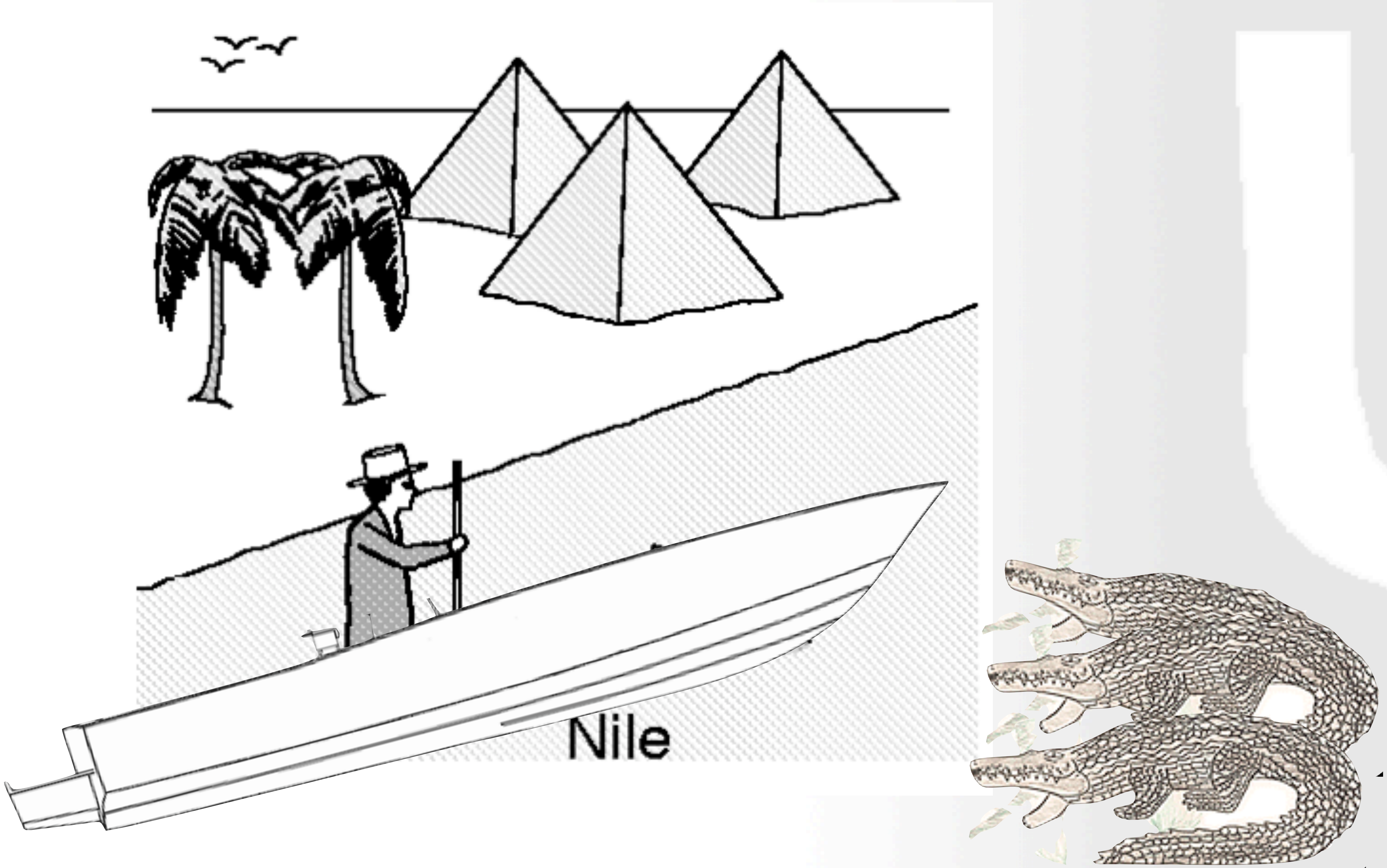
$$\left(\mathbf{r}^N(0), \mathbf{p}^N(0)\right)$$

$$\left(\mathbf{r}^N(0), \mathbf{p}_1(0), \cdots, \mathbf{p}_j(0)+\varepsilon, \mathbf{p}_i(0)-\varepsilon \cdots, \mathbf{p}_N(0)\right)$$

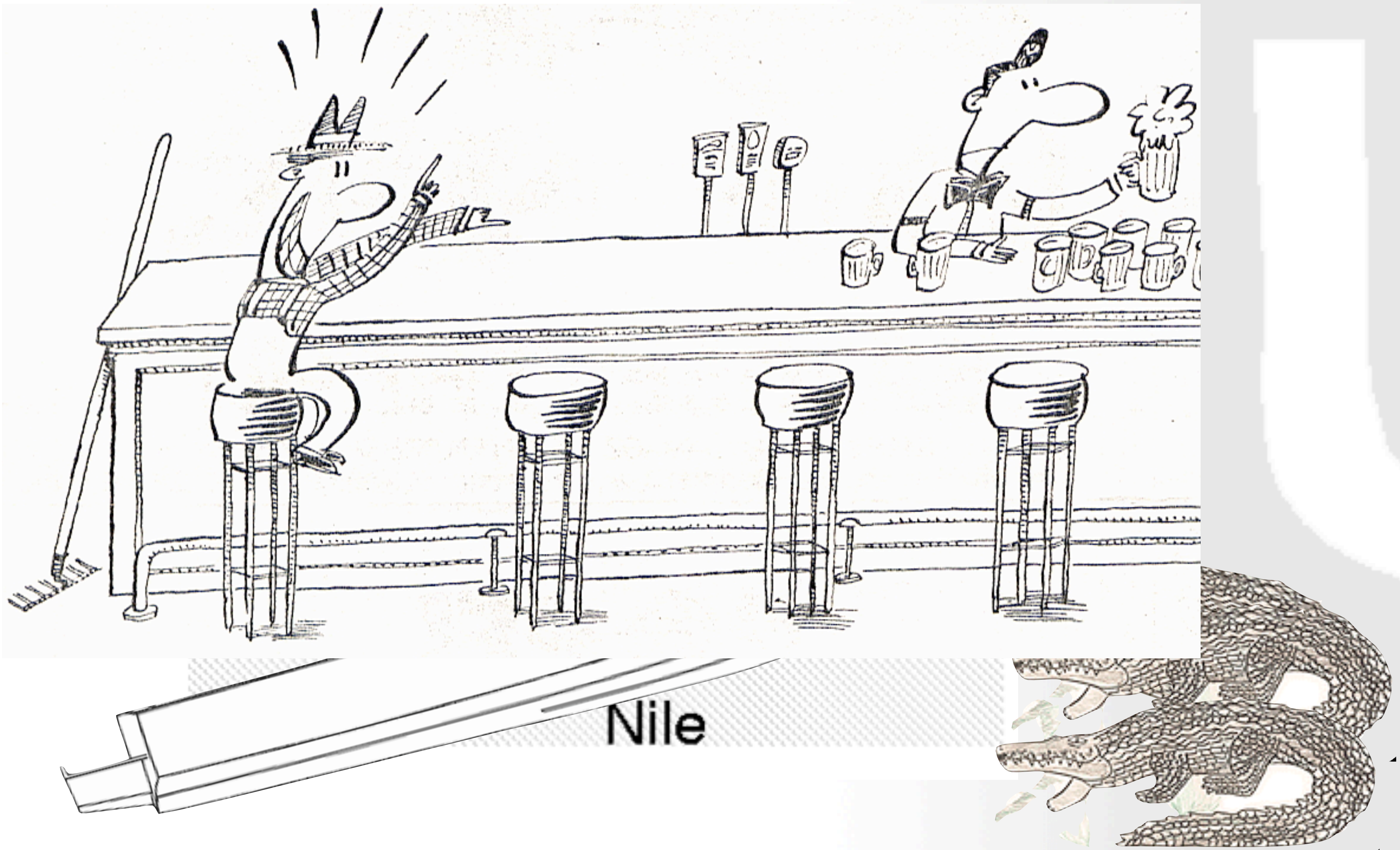
$\varepsilon = 10^{-10}$



MD Sampling



MD Sampling



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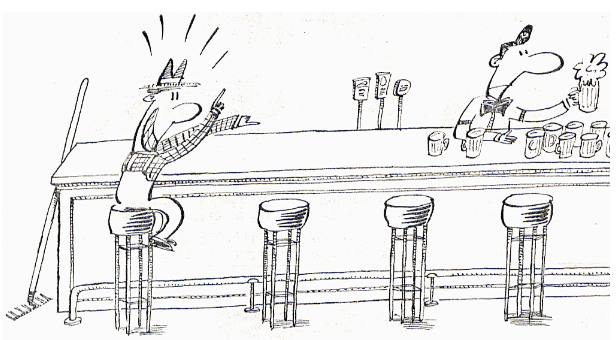
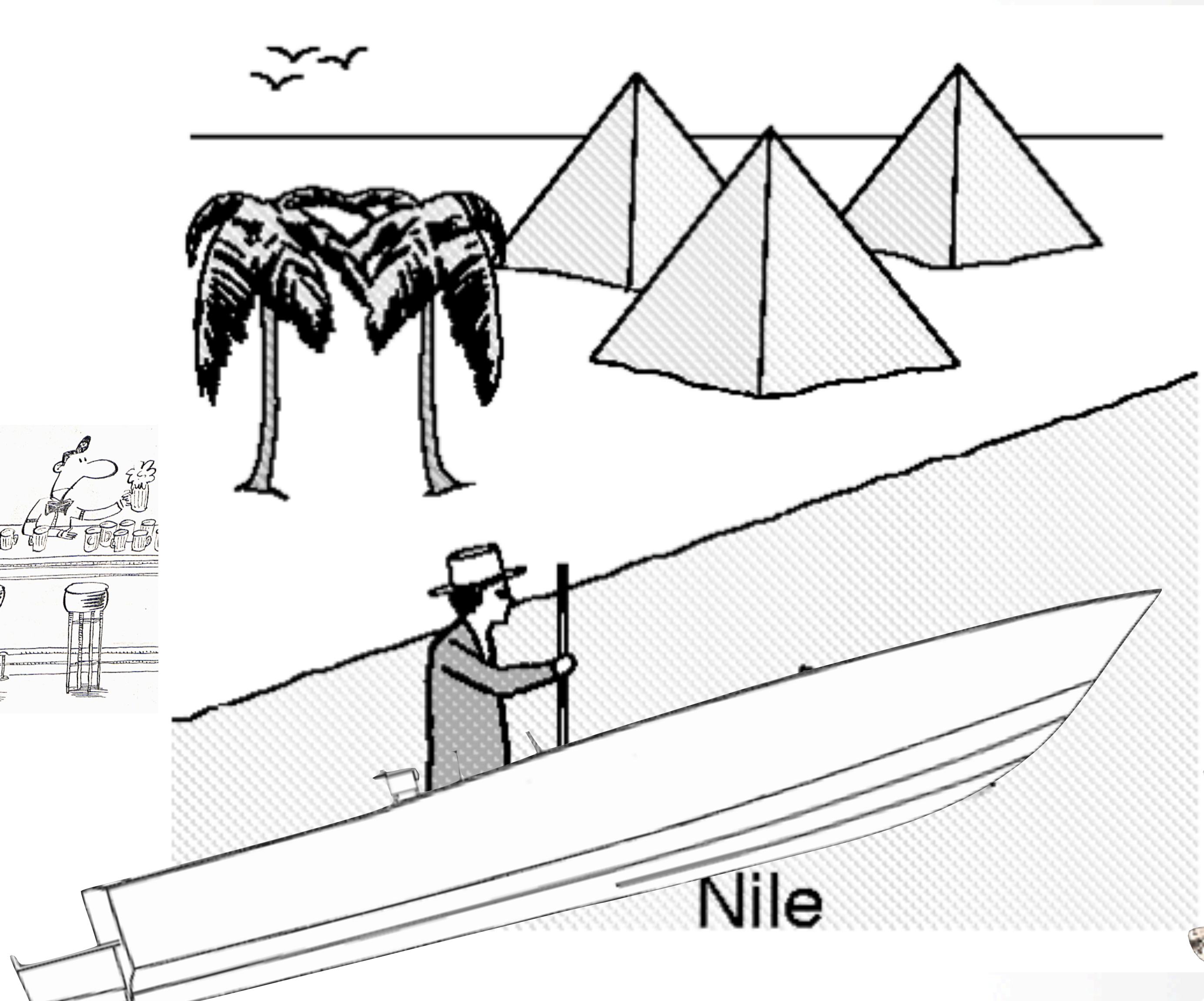
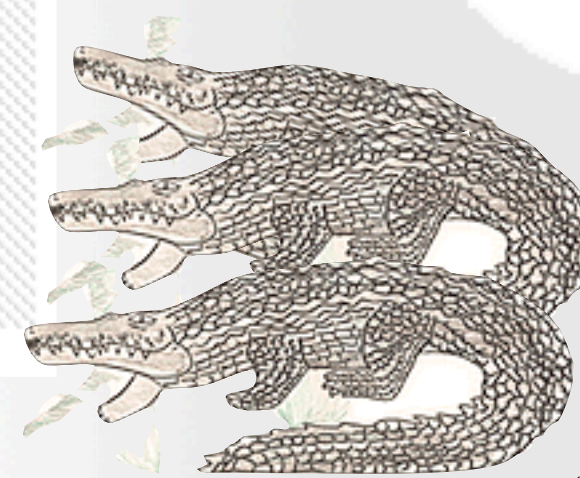
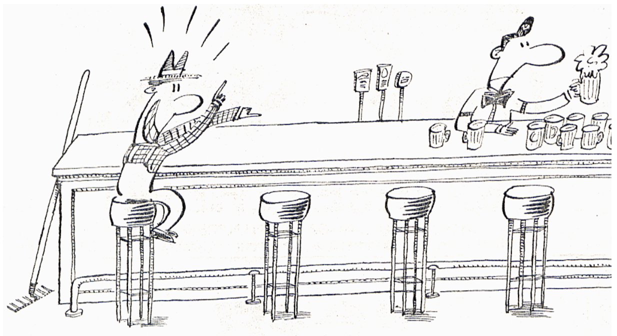
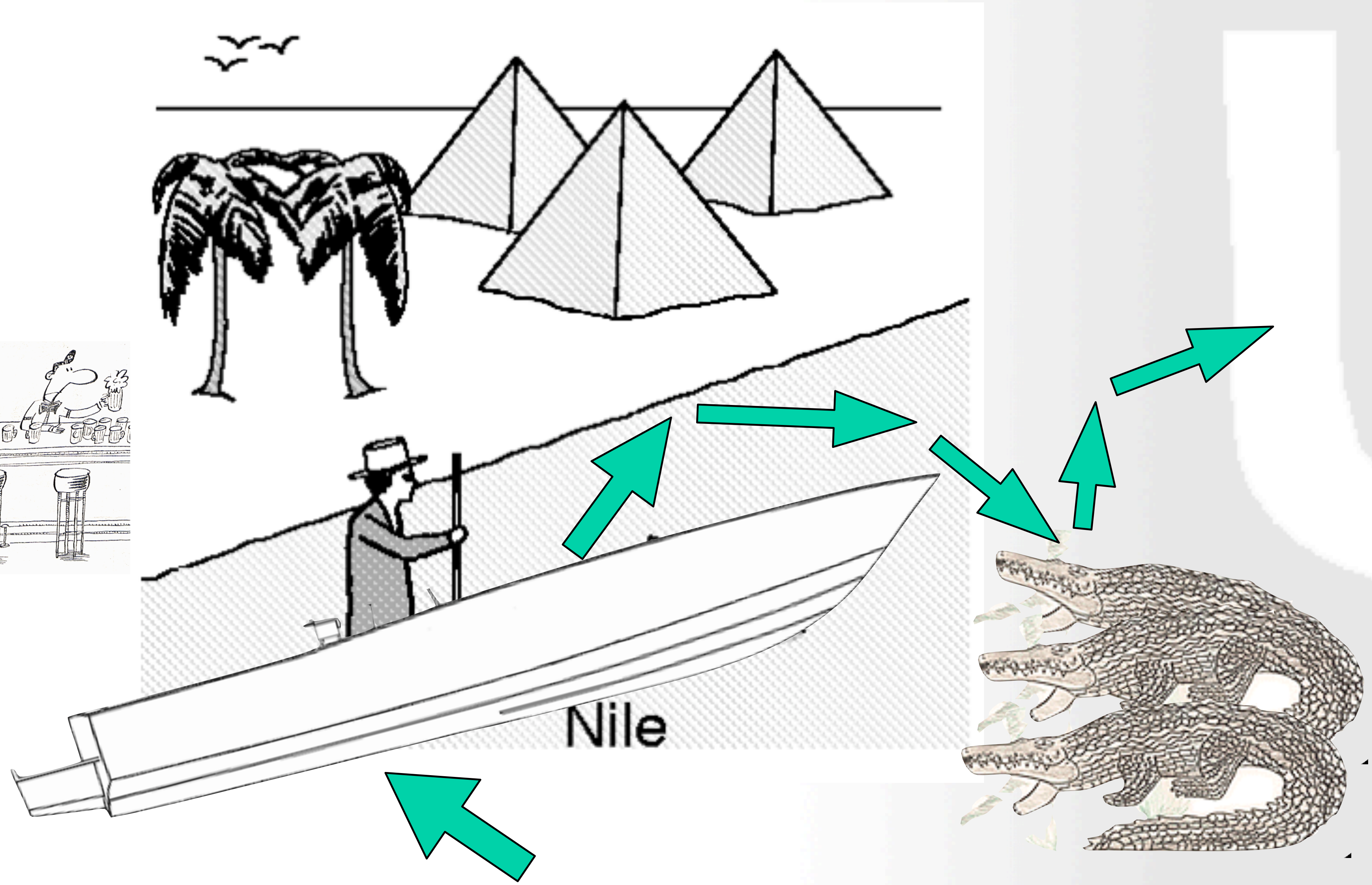




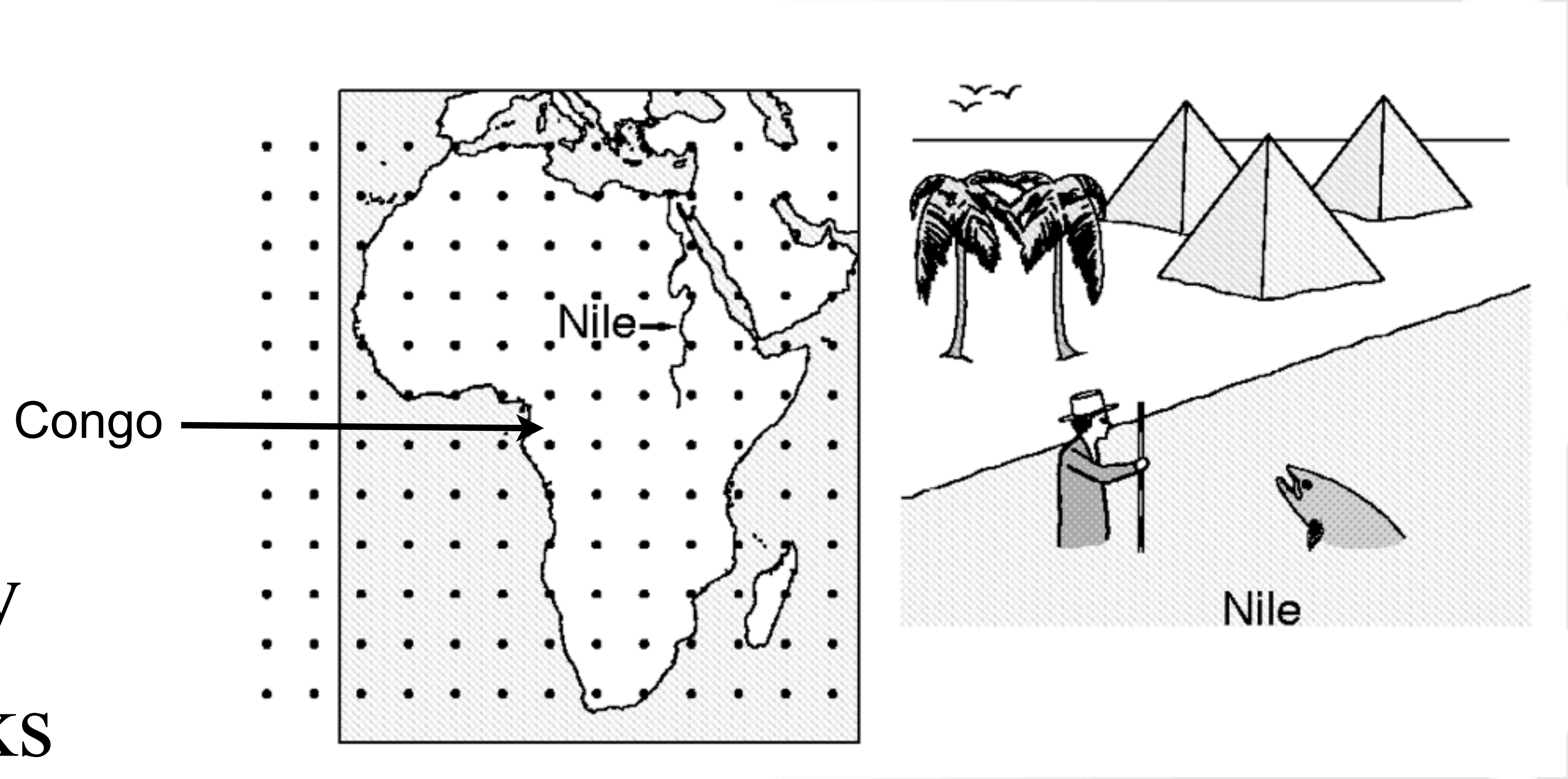


MD Sampling





MD Sampling



- Ergodicity
- bottlenecks
- time scale
- representability

short MD movie

- Ergodicity
- bottlenecks
- time scale
- representability

Molecular Dynamics

Basics (4.1, 4.2, 4.3)

Liouville formulation (4.3.3)

Multiple timesteps (15.3)

Algorithm 3 (A Simple Molecular Dynamics Program)

```
program md                      simple MD program

call init                       initialization
t=0
do while (t.lt.tmax)            MD loop
   call force(f,en)             determine the forces
   call integrate(f,en)         integrate equations of motion
   t=t+delt
   call sample                  sample averages
enddo
stop
end
```

Comment to this algorithm:

1. *Subroutines* `init`, `force`, `integrate`, *and* `sample` *will be described in Algorithms 4, 5, and 6, respectively. Subroutine* `sample` *is used to calculate averages like pressure or temperature.*

Algorithm 4 (Initialization of a Molecular Dynamics Program)

```
subroutine init                 initialization of MD program
sumv=0
sumv2=0
do i=1,npart
   x(i)=lattice_pos(i)          place the particles on a lattice
   v(i)=(ranf()-0.5)            give random velocities
   sumv=sumv+v(i)               velocity center of mass
   sumv2=sumv2+v(i)**2          kinetic energy
enddo
sumv=sumv/npart                 velocity center of mass
sumv2=sumv2/npart               mean-squared velocity
fs=sqrt(3*temp/sumv2)           scale factor of the velocities
do i=1,npart                    set desired kinetic energy and set
   v(i)=(v(i)-sumv)*fs          velocity center of mass to zero
   xm(i)=x(i)-v(i)*dt           position previous time step
enddo
return
end
```

Algorithm 5 (Calculation of the Forces)

```
subroutine force(f,en)                      determine the force
en=0                                        and energy
do i=1,npart
   f(i)=0                                   set forces to zero
enddo
do i=1,npart-1
  do j=i+1,npart                            loop over all pairs
     xr=x(i)-x(j)
     xr=xr-box*nint(xr/box)                 periodic boundary conditions
     r2=xr**2
     if (r2.lt.rc2) then                    test cutoff
       r2i=1/r2
       r6i=r2i**3
       ff=48*r2i*r6i*(r6i-0.5)              Lennard-Jones potential
       f(i)=f(i)+ff*xr                      update force
       f(j)=f(j)-ff*xr
       en=en+4*r6i*(r6i-1)-ecut             update energy
     endif
  enddo
enddo
return
end
```

Algorithm 6 (Integrating the Equations of Motion)

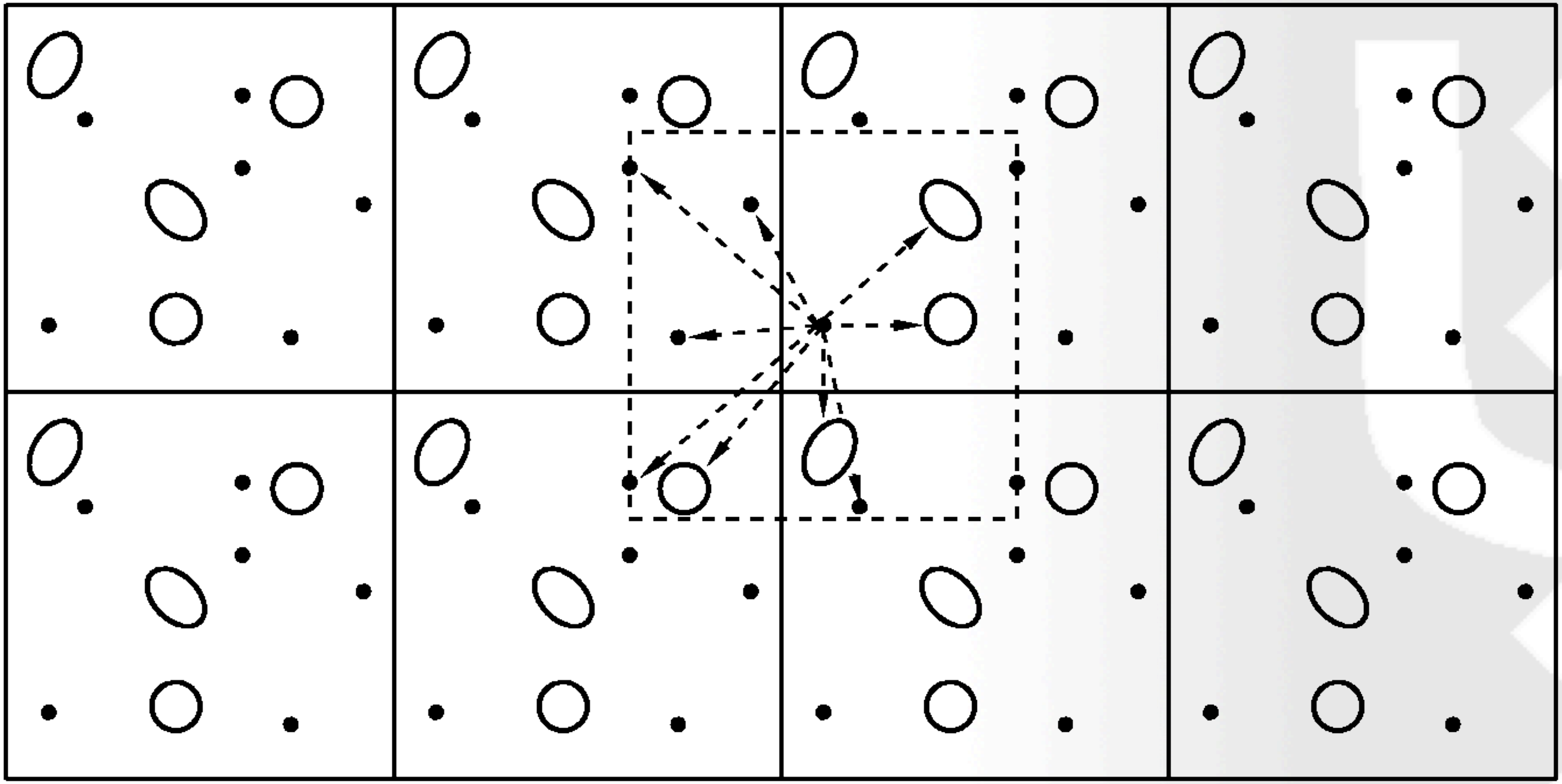
```
subroutine integrate(f,en)                integrate equations of motion
sumv=0
sumv2=0
do i=1,npart                              MD loop
   xx=2*x(i)-xm(i)+delt**2*f(i)           Verlet algorithm (4.2.3)
   vi=(xx-xm(i))/(2*delt)                 velocity (4.2.4)
   sumv=sumv+vi                           velocity center of mass
   sumv2=sumv2+vi**2                      total kinetic energy
   xm(i)=x(i)                             update positions previous time
   x(i)=xx                                update positions current time
enddo
temp=sumv2/(3*npart)                      instantaneous temperature
etot=(en+0.5*sumv2)/npart                 total energy per particle
return
end
```

Molecular Dynamics

Molecular Dynamics

- Initialization
  - Total momentum should be zero (no external forces)
  - Temperature rescaling to desired temperature
  - Particles start on a lattice
- Force calculations
  - Periodic boundary conditions
  - Order NxN algorithm,
  - Order N: neighbor lists, linked cell
  - Truncation and shift of the potential
- Integrating the equations of motion
  - Velocity Verlet
  - Kinetic energy

Periodic boundary conditions



Lennard Jones potentials

Lennard Jones potentials

- The Lennard-Jones potential

$$u^{LJ}(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

Lennard Jones potentials

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$$u^{LJ}(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

- The truncated Lennard-Jones potential

$$u(r) = \begin{cases} u^{LJ}(r) & r \leq r_c \\ 0 & r > r_c \end{cases}$$

Lennard Jones potentials

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$$u^{LJ}(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

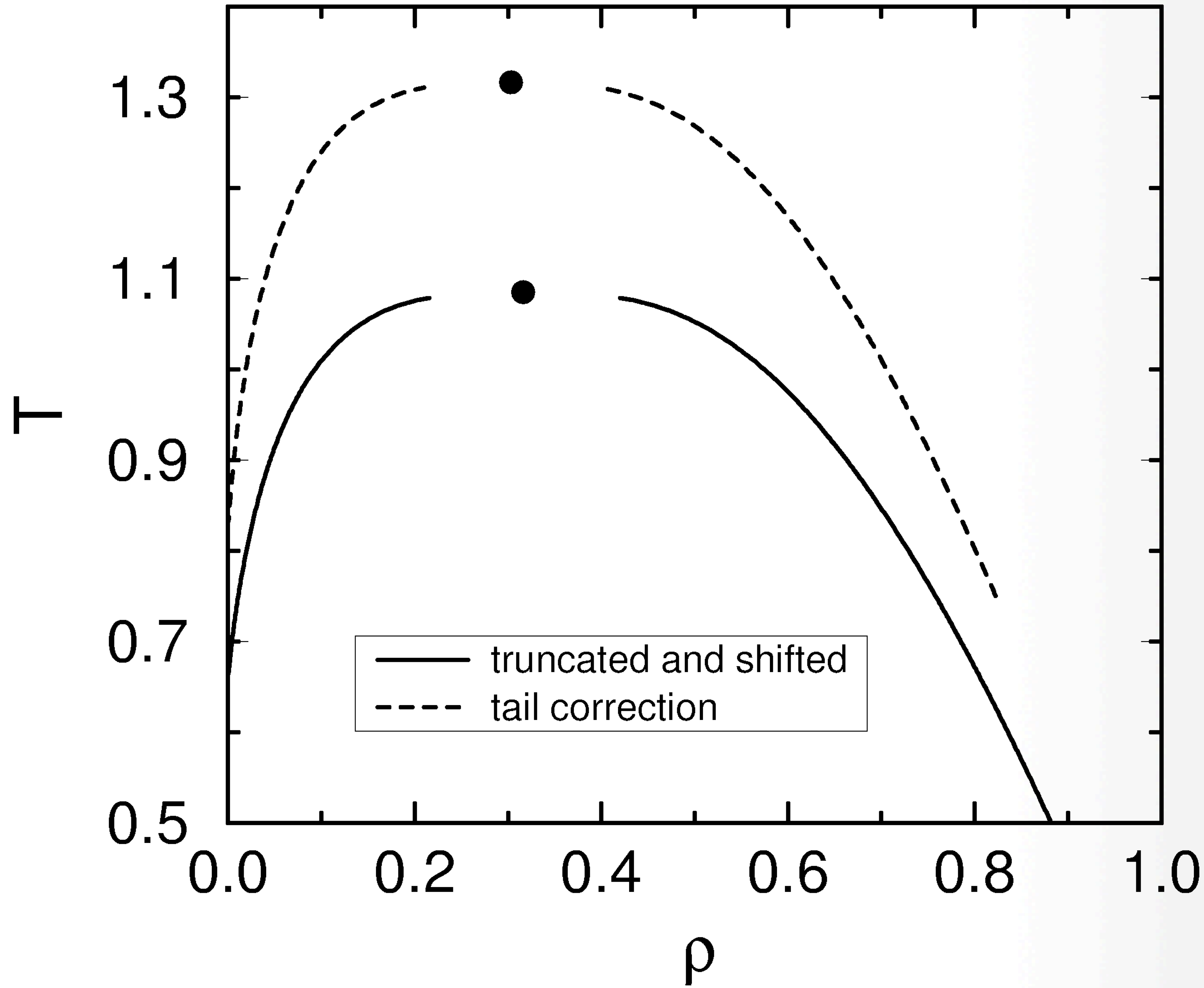
- The truncated Lennard-Jones potential

$$u(r) = \begin{cases} u^{LJ}(r) & r \le r_c \\ 0 & r > r_c \end{cases}$$

- The truncated and shifted Lennard-Jones potential

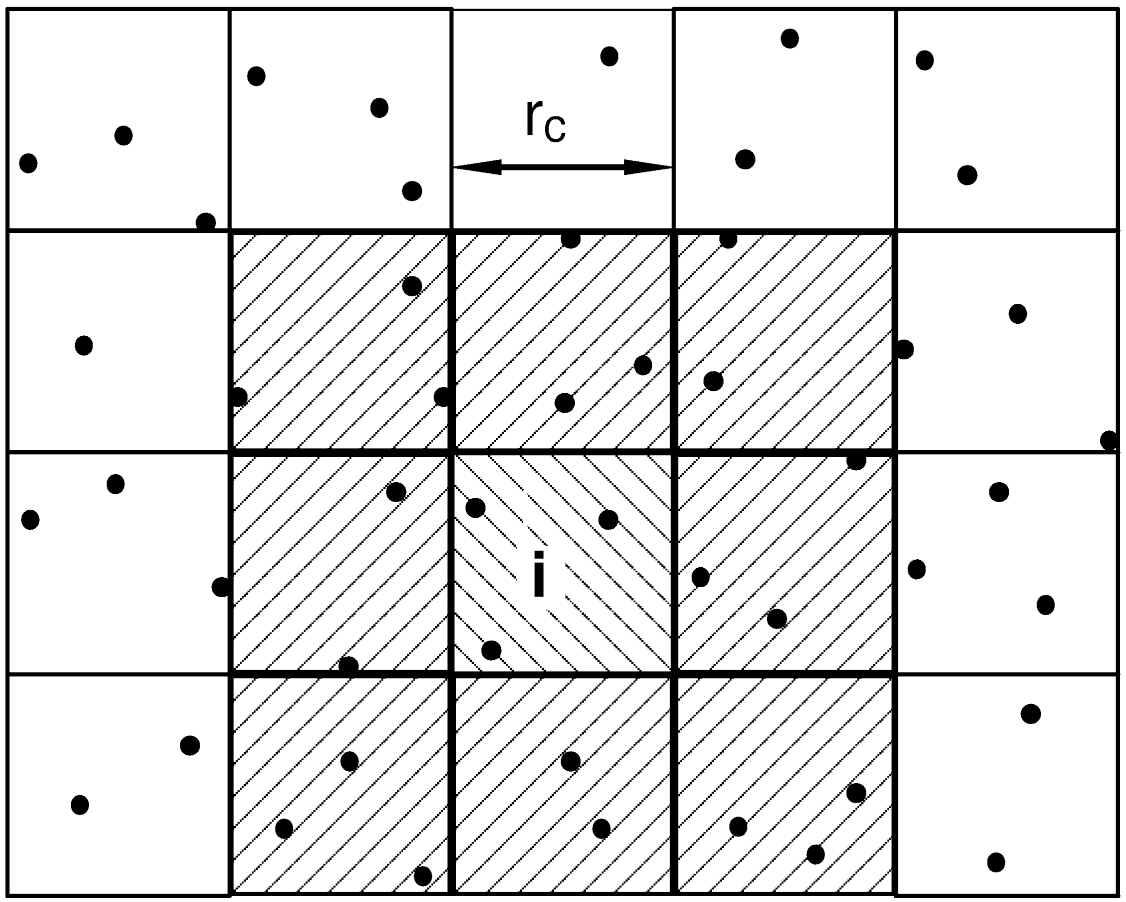
$$u(r) = \begin{cases} u^{LJ}(r) - u^{LJ}(r_c) & r \le r_c \\ 0 & r > r_c \end{cases}$$

Phase diagrams of Lennard Jones fluids

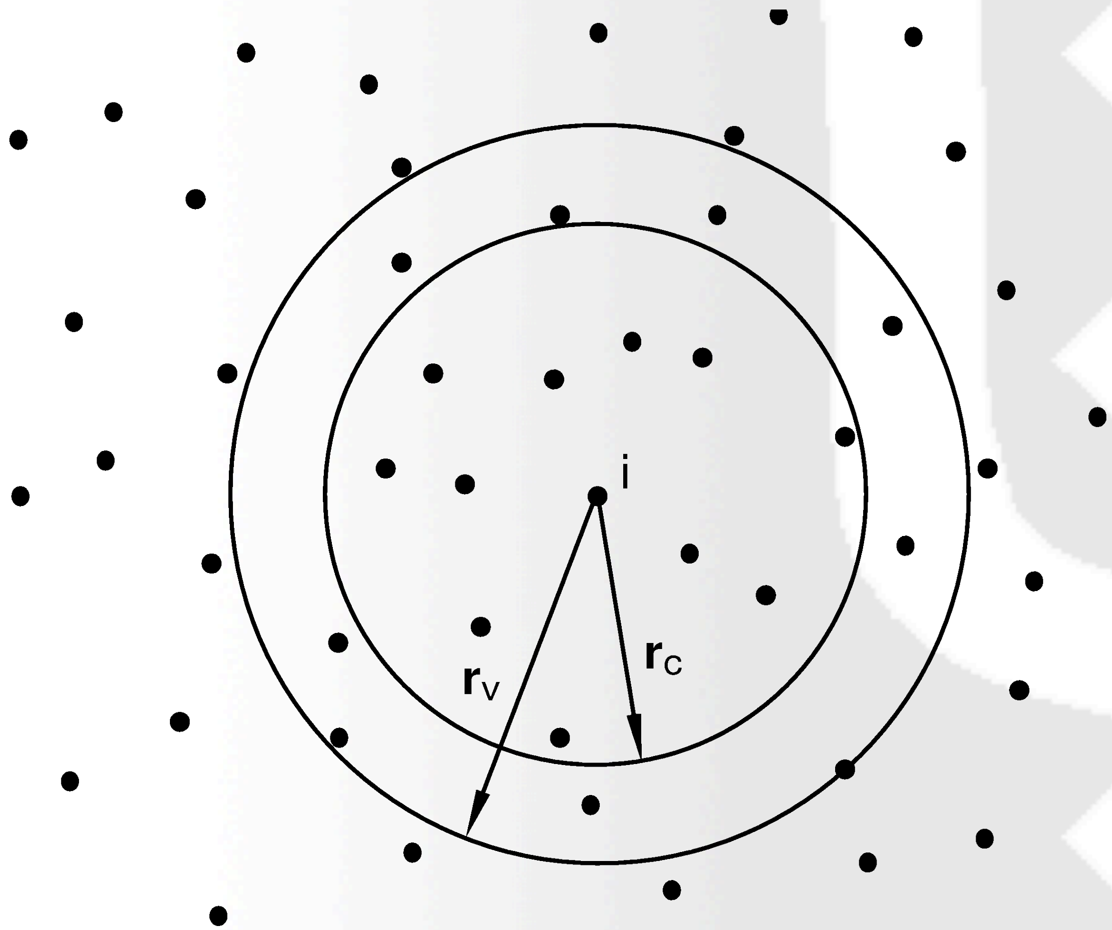


Saving cpu time

Cell list



Verlet-list



Equations of motion

Equations of motion

$$\mathbf{r}(t+\Delta t)=\mathbf{r}(t)+\mathbf{v}(t)\Delta t+\frac{\Delta t^2}{2m}\mathbf{f}(t)+\frac{\Delta t^3}{3!}\frac{d^3\mathbf{r}(t)}{dt^3}+\mathrm{O}(\Delta t^4)$$

Equations of motion

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$$\mathbf{r}(t-\Delta t)=\mathbf{r}(t)-\mathbf{v}(t)\Delta t+\frac{\Delta t^2}{2m}\mathbf{f}(t)-\frac{\Delta t^3}{3!}\frac{d^3\mathbf{r}(t)}{dt^3}+\mathrm{O}(\Delta t^4)$$

Equations of motion

$$\mathbf{r}(t+\Delta t) = \mathbf{r}(t) + \mathbf{v}(t)\Delta t + \frac{\Delta t^2}{2m}\mathbf{f}(t) + \frac{\Delta t^3}{3!}\frac{d^3\mathbf{r}(t)}{dt^3} + \mathrm{O}(\Delta t^4)$$

$$\mathbf{r}(t-\Delta t) = \mathbf{r}(t) - \mathbf{v}(t)\Delta t + \frac{\Delta t^2}{2m}\mathbf{f}(t) - \frac{\Delta t^3}{3!}\frac{d^3\mathbf{r}(t)}{dt^3} + \mathrm{O}(\Delta t^4)$$

$$\mathbf{r}(t+\Delta t) + \mathbf{r}(t-\Delta t) = 2\mathbf{r}(t) + \frac{\Delta t^2}{m}\mathbf{f}(t) + \mathrm{O}(\Delta t^4)$$

Equations of motion

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$$\mathbf{r}(t+\Delta t) + \mathbf{r}(t-\Delta t) = 2\mathbf{r}(t) + \frac{\Delta t^2}{m}\mathbf{f}(t) + O(\Delta t^4)$$

Verlet algorithm

$$\mathbf{r}(t+\Delta t) \approx 2\mathbf{r}(t) - \mathbf{r}(t-\Delta t) + \frac{\Delta t^2}{m}\mathbf{f}(t)$$

Equations of motion

$$\mathbf{r}(t+\Delta t)=\mathbf{r}(t)+\mathbf{v}(t)\Delta t+\frac{\Delta t^2}{2m}\mathbf{f}(t)+\frac{\Delta t^3}{3!}\frac{d^3\mathbf{r}(t)}{dt^3}+\mathrm{O}(\Delta t^4)$$

$$\mathbf{r}(t-\Delta t)=\mathbf{r}(t)-\mathbf{v}(t)\Delta t+\frac{\Delta t^2}{2m}\mathbf{f}(t)-\frac{\Delta t^3}{3!}\frac{d^3\mathbf{r}(t)}{dt^3}+\mathrm{O}(\Delta t^4)$$

$$\mathbf{r}(t+\Delta t)+\mathbf{r}(t-\Delta t)=2\mathbf{r}(t)+\frac{\Delta t^2}{m}\mathbf{f}(t)+\mathrm{O}(\Delta t^4)$$

Verlet algorithm

$$\mathbf{r}(t+\Delta t)\approx 2\mathbf{r}(t)-\mathbf{r}(t-\Delta t)+\frac{\Delta t^2}{m}\mathbf{f}(t)$$

Velocity Verlet algorithm

$$\mathbf{r}(t+\Delta t)\approx\mathbf{r}(t)+\mathbf{v}(t)\Delta t+\frac{\Delta t^2}{2m}\mathbf{f}(t)$$

$$\mathbf{v}(t+\Delta t)\approx\mathbf{v}(t)+\frac{\Delta t}{2m}\left[\mathbf{f}(t+\Delta t)+\mathbf{f}(t)\right]$$

Liouville formulation

Liouville formulation

$$f\left(\mathbf{p}^N, \mathbf{r}^N\right)$$

Liouville formulation

$$f\left(\mathbf{p}^N,\mathbf{r}^N\right)$$

Depends implicitly on t

Liouville formulation

$$f\left(\mathbf{p}^N, \mathbf{r}^N\right)$$

Liouville formulation

$$f\left(\mathbf{p}^N,\mathbf{r}^N\right)$$

$$\dot{f} = \dot{\mathbf{r}}\frac{\partial f}{\partial \mathbf{r}} + \dot{\mathbf{p}}\frac{\partial f}{\partial \mathbf{p}}$$

Liouville formulation

$$f\left(\mathbf{p}^N, \mathbf{r}^N\right)$$

$$\dot{f} = \dot{\mathbf{r}} \frac{\partial f}{\partial \mathbf{r}} + \dot{\mathbf{p}} \frac{\partial f}{\partial \mathbf{p}}$$

$$\mathrm{i}L \equiv \dot{\mathbf{r}} \frac{\partial}{\partial \mathbf{r}} + \dot{\mathbf{p}} \frac{\partial}{\partial \mathbf{p}}$$

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$$\mathrm{i}L \equiv \dot{\mathbf{r}}\frac{\partial}{\partial \mathbf{r}} + \dot{\mathbf{p}}\frac{\partial}{\partial \mathbf{p}}$$

Liouville operator

Liouville formulation

$$f\left(\mathbf{p}^N, \mathbf{r}^N\right)$$

$$\dot{f} = \dot{\mathbf{r}} \frac{\partial f}{\partial \mathbf{r}} + \dot{\mathbf{p}} \frac{\partial f}{\partial \mathbf{p}}$$

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$$\frac{\mathrm{d}f}{\mathrm{d}t} = \mathrm{i}Lf$$

Liouville formulation

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$$\dot{f} = \dot{\mathbf{r}} \frac{\partial f}{\partial \mathbf{r}} + \dot{\mathbf{p}} \frac{\partial f}{\partial \mathbf{p}}$$

$$\mathrm{i}L \equiv \dot{\mathbf{r}} \frac{\partial}{\partial \mathbf{r}} + \dot{\mathbf{p}} \frac{\partial}{\partial \mathbf{p}}$$

$$\frac{\mathrm{d}f}{\mathrm{d}t} = \mathrm{i}Lf$$

Solution

$$f(t) = \exp(\mathrm{i}Lt) f(0)$$

Liouville formulation

$$f\left(\mathbf{p}^N,\mathbf{r}^N\right)$$

$$\dot{f}=\dot{\mathbf{r}}\frac{\partial f}{\partial \mathbf{r}}+\dot{\mathbf{p}}\frac{\partial f}{\partial \mathbf{p}}$$

$$\mathrm{i}L\equiv\dot{\mathbf{r}}\frac{\partial}{\partial \mathbf{r}}+\dot{\mathbf{p}}\frac{\partial}{\partial \mathbf{p}}$$

$$\frac{\mathrm{d}f}{\mathrm{d}t}=\mathrm{i}Lf$$

Solution

$$f(t)=\exp(\mathrm{i}Lt)f(0)$$

Beware: this solution is equally useless as the differential equation!

$$i\mathcal{L} \equiv i\mathcal{L}_r + i\mathcal{L}_p = \dot{\mathbf{r}}\frac{\partial}{\partial \mathbf{r}} + \dot{\mathbf{p}}\frac{\partial}{\partial \mathbf{p}}$$

$$i\mathcal{L} \equiv i\mathcal{L}_r + i\mathcal{L}_p = \dot{\mathbf{r}}\frac{\partial}{\partial \mathbf{r}} + \dot{\mathbf{p}}\frac{\partial}{\partial \mathbf{p}}$$

Let us look at them separately

$$i\mathcal{L} \equiv i\mathcal{L}_r + i\mathcal{L}_p = \dot{\mathbf{r}}\frac{\partial}{\partial \mathbf{r}} + \dot{\mathbf{p}}\frac{\partial}{\partial \mathbf{p}}$$

$$f(t) = \exp(i\mathcal{L}_r t) f(0)$$

$$i\mathcal{L} \equiv i\mathcal{L}_r + i\mathcal{L}_p = \dot{\mathbf{r}}\frac{\partial}{\partial \mathbf{r}} + \dot{\mathbf{p}}\frac{\partial}{\partial \mathbf{p}}$$

$$f(t) = \exp(i\mathcal{L}_r t) f(0)$$

$$= \exp\left(\dot{\mathbf{r}}(0)t\frac{\partial}{\partial \mathbf{r}} f(0)\right)$$

Taylor expansion

$$i\mathcal{L} \equiv i\mathcal{L}_r + i\mathcal{L}_p = \dot{\mathbf{r}}\frac{\partial}{\partial \mathbf{r}} + \dot{\mathbf{p}}\frac{\partial}{\partial \mathbf{p}}$$

$$f(t) = \exp(i\mathcal{L}_r t) f(0)$$

$$= \exp\left(\dot{\mathbf{r}}(0)t\frac{\partial}{\partial \mathbf{r}} f(0)\right)$$

$$= \sum_{n=0}^{\infty} \frac{(\dot{\mathbf{r}}(0)t)^n}{n!}\frac{\partial^n}{\partial \mathbf{r}^n} f(0)$$

$$i\mathcal{L} \equiv i\mathcal{L}_r + i\mathcal{L}_p = \dot{\mathbf{r}}\frac{\partial}{\partial \mathbf{r}} + \dot{\mathbf{p}}\frac{\partial}{\partial \mathbf{p}}$$

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$$= f\left(\mathbf{p}^N(0), (\mathbf{r}(0) + \dot{\mathbf{r}}(\mathbf{0})t)^N\right)$$

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Shift of coordinates

$$\mathbf{r}(0) \rightarrow \mathbf{r}(0) + \dot{\mathbf{r}}(\mathbf{0})t$$

$$i\mathcal{L} \equiv i\mathcal{L}_r + i\mathcal{L}_p = \dot{\mathbf{r}}\frac{\partial}{\partial \mathbf{r}} + \dot{\mathbf{p}}\frac{\partial}{\partial \mathbf{p}}$$

$$f(t) = \exp(i\mathcal{L}_r t) f(0)$$

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$$f(t) = \exp(i\mathcal{L}_p t) f(0)$$

Shift of coordinates

$$\mathbf{r}(0) \rightarrow \mathbf{r}(0) + \dot{\mathbf{r}}(\mathbf{0})t$$

$$i\mathcal{L} \equiv i\mathcal{L}_r + i\mathcal{L}_p = \dot{\mathbf{r}}\frac{\partial}{\partial \mathbf{r}} + \dot{\mathbf{p}}\frac{\partial}{\partial \mathbf{p}}$$

$$\begin{aligned} f(t) &= \exp(i\mathcal{L}_r t) f(0) \\ &= \exp\left(\dot{\mathbf{r}}(0)t\frac{\partial}{\partial \mathbf{r}} f(0)\right) \\ &= \sum_{n=0}^{\infty} \frac{(\dot{\mathbf{r}}(0)t)^n}{n!}\frac{\partial^n}{\partial \mathbf{r}^n} f(0) \\ &= f\left(\mathbf{p}^N(0), (\mathbf{r}(0) + \dot{\mathbf{r}}(\mathbf{0})t)^N\right) \end{aligned}$$

$$\begin{aligned} f(t) &= \exp(i\mathcal{L}_p t) f(0) \\ &= \exp\left(\dot{\mathbf{p}}(0)t\frac{\partial}{\partial \mathbf{p}} f(0)\right) \end{aligned}$$

Shift of coordinates

$$\mathbf{r}(0) \to \mathbf{r}(0) + \dot{\mathbf{r}}(\mathbf{0})t$$

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Shift of coordinates

$$\mathbf{r}(0) \rightarrow \mathbf{r}(0) + \dot{\mathbf{r}}(\mathbf{0})t$$

$$i\mathcal{L} \equiv i\mathcal{L}_r + i\mathcal{L}_p = \dot{\mathbf{r}}\frac{\partial}{\partial \mathbf{r}} + \dot{\mathbf{p}}\frac{\partial}{\partial \mathbf{p}}$$

$$f(t) = \exp(i\mathcal{L}_r t) f(0)$$

$$= \exp\left(\dot{\mathbf{r}}(0) t \frac{\partial}{\partial \mathbf{r}} f(0)\right)$$

$$= \sum_{n=0}^{\infty} \frac{(\dot{\mathbf{r}}(0)t)^n}{n!} \frac{\partial^n}{\partial \mathbf{r}^n} f(0)$$

$$= f\left(\mathbf{p}^N(0), (\mathbf{r}(0) + \dot{\mathbf{r}}(\mathbf{0})t)^N\right)$$

$$f(t) = \exp(i\mathcal{L}_p t) f(0)$$

$$= \exp\left(\dot{\mathbf{p}}(0) t \frac{\partial}{\partial \mathbf{p}} f(0)\right)$$

$$= \sum_{n=0}^{\infty} \frac{(\dot{\mathbf{p}}(0)t)^n}{n!} \frac{\partial^n}{\partial \mathbf{p}^n} f(0)$$

$$= f\left((\mathbf{p}(0) + \dot{\mathbf{p}}(\mathbf{0})t)^N, \mathbf{r}^N(0)\right)$$

Shift of coordinates

$$\mathbf{r}(0) \rightarrow \mathbf{r}(0) + \dot{\mathbf{r}}(\mathbf{0})t$$

$$i\mathcal{L} \equiv i\mathcal{L}_r + i\mathcal{L}_p = \dot{\mathbf{r}}\frac{\partial}{\partial \mathbf{r}} + \dot{\mathbf{p}}\frac{\partial}{\partial \mathbf{p}}$$

$$\begin{aligned} f(t) &= \exp(i\mathcal{L}_r t) f(0) \\ &= \exp\left(\dot{\mathbf{r}}(0)t\frac{\partial}{\partial \mathbf{r}} f(0)\right) \\ &= \sum_{n=0}^{\infty} \frac{(\dot{\mathbf{r}}(0)t)^n}{n!}\frac{\partial^n}{\partial \mathbf{r}^n} f(0) \\ &= f\left(\mathbf{p}^N(0), (\mathbf{r}(0) + \dot{\mathbf{r}}(\mathbf{0})t)^N\right) \end{aligned}$$

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Shift of coordinates

$$\mathbf{r}(0) \rightarrow \mathbf{r}(0) + \dot{\mathbf{r}}(\mathbf{0})t$$

Shift of momenta

$$\mathbf{p}(0) \rightarrow \mathbf{p}(0) + \dot{\mathbf{p}}(\mathbf{0})t$$

$$i\mathcal{L}_r \Rightarrow \mathbf{r}(0) \rightarrow \mathbf{r}(0) + \dot{\mathbf{r}}(\mathbf{0})t$$
$$i\mathcal{L}_p \Rightarrow \mathbf{p}(0) \rightarrow \mathbf{p}(0) + \dot{\mathbf{p}}(\mathbf{0})t$$

$$i\mathcal{L}_r \Rightarrow \mathbf{r}(0) \rightarrow \mathbf{r}(0) + \dot{\mathbf{r}}(\mathbf{0})t$$
$$i\mathcal{L}_p \Rightarrow \mathbf{p}(0) \rightarrow \mathbf{p}(0) + \dot{\mathbf{p}}(\mathbf{0})t$$

$$f\left(\mathbf{p}^N(t), (\mathbf{r}(t)\right) = e^{(i\mathcal{L}t)} f\left(\mathbf{p}^N(0), (\mathbf{r}^N(0)\right)$$

$$i\mathcal{L}_r \Rightarrow \mathbf{r}(0) \rightarrow \mathbf{r}(0) + \dot{\mathbf{r}}(\mathbf{0})t$$
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$$i\mathcal{L}_r \Rightarrow \mathbf{r}(0) \rightarrow \mathbf{r}(0) + \dot{\mathbf{r}}(\mathbf{0})t$$

$$i\mathcal{L}_p \Rightarrow \mathbf{p}(0) \rightarrow \mathbf{p}(0) + \dot{\mathbf{p}}(\mathbf{0})t$$

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$$i\mathcal{L}_r \Rightarrow \mathbf{r}(0) \rightarrow \mathbf{r}(0) + \dot{\mathbf{r}}(\mathbf{0})t$$

$$i\mathcal{L}_p \Rightarrow \mathbf{p}(0) \rightarrow \mathbf{p}(0) + \dot{\mathbf{p}}(\mathbf{0})t$$

$f\left(\mathbf{p}\right.$ … $\left.0)\right)\Big)$

… $\left(\mathbf{r}^N(0)\right)$

… $), \left(\mathbf{r}^N(0)\right)$

We have *noncommuting* operators!

$$e^{\mathrm{A+B}} \neq e^{\mathrm{A}} e^{\mathrm{B}}$$

Trotter identity

$$e^{\mathrm{A+B}} = \lim_{P\rightarrow\infty} \left(e^{\mathrm{A/2P}} e^{\mathrm{B/P}} e^{\mathrm{A/2P}}\right)^P$$

$$e^{\mathrm{A+B}} \approx \left(e^{\mathrm{A/2P}} e^{\mathrm{B/P}} e^{\mathrm{A/2P}}\right)^P$$

$$i\mathcal{L}_r \Rightarrow \mathbf{r}(0) \rightarrow \mathbf{r}(0) + \dot{\mathbf{r}}(\mathbf{0})t$$

$$i\mathcal{L}_p \Rightarrow \mathbf{p}(0) \rightarrow \mathbf{p}(0) + \dot{\mathbf{p}}(\mathbf{0})t$$

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$$\frac{A}{P} = \frac{i\mathcal{L}_p t}{P} \qquad \frac{B}{P} = \frac{i\mathcal{L}_r t}{P} \qquad \Delta t = \frac{t}{P}$$

$f\,(\mathbf{p}$ … $0))$

… $(\mathbf{r}^N(0))$

… $), (\mathbf{r}^N(0))$

$$i\mathcal{L}_r \Rightarrow \mathbf{r}(0) \rightarrow \mathbf{r}(0) + \dot{\mathbf{r}}(\mathbf{0})t$$

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$$\begin{aligned} f\left(\mathbf{p}^N(t), (\mathbf{r}(t)\right) &= e^{(i\mathcal{L}t)} f\left(\mathbf{p}^N(0), (\mathbf{r}^N(0)\right) \\ &= e^{(i\mathcal{L}_r t + i\mathcal{L}_p t)} f\left(\mathbf{p}^N(0), (\mathbf{r}^N(0)\right) \\ &\neq e^{(i\mathcal{L}_r t)} e^{(i\mathcal{L}_p t)} f\left(\mathbf{p}^N(0), (\mathbf{r}^N(0)\right) \end{aligned}$$

$$i\mathcal{L}_r \Rightarrow \mathbf{r}(0) \rightarrow \mathbf{r}(0) + \dot{\mathbf{r}}(\mathbf{0})t$$
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$$= \left(e^{(i\mathcal{L}_p \Delta t/2)} e^{(i\mathcal{L}_r \Delta t)} e^{(i\mathcal{L}_p \Delta t/2)}\right)^P f\left(\mathbf{p}^N(0), (\mathbf{r}^N(0)\right)$$

$$i\mathcal{L}_r \Delta t \Rightarrow \mathbf{r} \rightarrow \mathbf{r} + \dot{\mathbf{r}}\Delta t$$

$$i\mathcal{L}_p \Delta t \Rightarrow \mathbf{p} \rightarrow \mathbf{p} + \dot{\mathbf{p}}\Delta t$$

$$\left(e^{(i\mathcal{L}_p \Delta t/2)} e^{(i\mathcal{L}_r \Delta t)} e^{(i\mathcal{L}_p \Delta t/2)}\right)^P$$

$$i\mathcal{L}_r \Delta t \Rightarrow \mathbf{r} \rightarrow \mathbf{r} + \dot{\mathbf{r}}\Delta t$$

$$i\mathcal{L}_p \Delta t \Rightarrow \mathbf{p} \rightarrow \mathbf{p} + \dot{\mathbf{p}}\Delta t$$

$$\left(e^{(i\mathcal{L}_p \Delta t/2)} e^{(i\mathcal{L}_r \Delta t)} e^{(i\mathcal{L}_p \Delta t/2)}\right)^P$$

$$e^{(i\mathcal{L}_p \Delta t/2)} f\left(\mathbf{p}^N(0), (\mathbf{r}^N(0)\right) = f\left(\left[\mathbf{p}(0) + \frac{\Delta t}{2}\dot{\mathbf{p}}(0)\right]^N, \mathbf{r}^N(0)\right)$$

$$i\mathcal{L}_r \Delta t \Rightarrow \mathbf{r} \rightarrow \mathbf{r} + \dot{\mathbf{r}}\Delta t$$

$$i\mathcal{L}_p \Delta t \Rightarrow \mathbf{p} \rightarrow \mathbf{p} + \dot{\mathbf{p}}\Delta t$$

$$\left(e^{(i\mathcal{L}_p \Delta t/2)} e^{(i\mathcal{L}_r \Delta t)} e^{(i\mathcal{L}_p \Delta t/2)}\right)^P$$

$$e^{(i\mathcal{L}_p \Delta t/2)} f\left(\mathbf{p}^N(0), (\mathbf{r}^N(0)\right) = f\left(\left[\mathbf{p}(0) + \frac{\Delta t}{2}\dot{\mathbf{p}}(0)\right]^N, \mathbf{r}^N(0)\right)$$

$$e^{(i\mathcal{L}_r \Delta t)} f' = f\left(\left[\mathbf{p}(0) + \frac{\Delta t}{2}\dot{\mathbf{p}}(0)\right]^N, \left[\mathbf{r}(0) + \Delta t\dot{\mathbf{r}}(\frac{\Delta t}{2})\right]^N\right)$$

$$i\mathcal{L}_r \Delta t \Rightarrow \mathbf{r} \rightarrow \mathbf{r} + \dot{\mathbf{r}} \Delta t$$

$$i\mathcal{L}_p \Delta t \Rightarrow \mathbf{p} \rightarrow \mathbf{p} + \dot{\mathbf{p}} \Delta t$$

$$\left(e^{(i\mathcal{L}_p \Delta t/2)} e^{(i\mathcal{L}_r \Delta t)} e^{(i\mathcal{L}_p \Delta t/2)} \right)^P$$

$$e^{(i\mathcal{L}_p \Delta t/2)} f\left(\mathbf{p}^N(0), (\mathbf{r}^N(0)\right) = f\left(\left[\mathbf{p}(0) + \frac{\Delta t}{2} \dot{\mathbf{p}}(0) \right]^N, \mathbf{r}^N(0) \right)$$

$$e^{(i\mathcal{L}_r \Delta t)} f' = f\left(\left[\mathbf{p}(0) + \frac{\Delta t}{2} \dot{\mathbf{p}}(0) \right]^N, \left[\mathbf{r}(0) + \Delta t \dot{\mathbf{r}}(\frac{\Delta t}{2}) \right]^N \right)$$

$$e^{(i\mathcal{L}_p \Delta t/2)} f'' = f\left(\left[\mathbf{p}(0) + \frac{\Delta t}{2} \dot{\mathbf{p}}(0) + \frac{\Delta t}{2} \dot{\mathbf{p}}(\Delta t) \right]^N, \left[\mathbf{r}(0) + \Delta t \dot{\mathbf{r}}(\frac{\Delta t}{2}) \right]^N \right)$$

$$i\mathcal{L}_r \Delta t \Rightarrow \mathbf{r} \rightarrow \mathbf{r} + \dot{\mathbf{r}}\Delta t$$

$$i\mathcal{L}_p \Delta t \Rightarrow \mathbf{p} \rightarrow \mathbf{p} + \dot{\mathbf{p}}\Delta t$$

$$\left(e^{(i\mathcal{L}_p \Delta t/2)} e^{(i\mathcal{L}_r \Delta t)} e^{(i\mathcal{L}_p \Delta t/2)}\right)^P$$

$$e^{(i\mathcal{L}_p \Delta t/2)} f\left(\mathbf{p}^N(0), (\mathbf{r}^N(0)\right) = f\left(\left[\mathbf{p}(0) + \frac{\Delta t}{2}\dot{\mathbf{p}}(0)\right]^N, \mathbf{r}^N(0)\right)$$

$$e^{(i\mathcal{L}_r \Delta t)} f' = f\left(\left[\mathbf{p}(0) + \frac{\Delta t}{2}\dot{\mathbf{p}}(0)\right]^N, \left[\mathbf{r}(0) + \Delta t\dot{\mathbf{r}}(\frac{\Delta t}{2})\right]^N\right)$$

$$e^{(i\mathcal{L}_p \Delta t/2)} f'' = f\left(\left[\mathbf{p}(0) + \frac{\Delta t}{2}\dot{\mathbf{p}}(0) + \frac{\Delta t}{2}\dot{\mathbf{p}}(\Delta t)\right]^N, \left[\mathbf{r}(0) + \Delta t\dot{\mathbf{r}}(\frac{\Delta t}{2})\right]^N\right)$$

$$\mathbf{p}(0) \rightarrow \mathbf{p}(0) + \frac{\Delta t}{2}\left[\dot{\mathbf{p}}(0) + \dot{\mathbf{p}}(\Delta t)\right]$$

$$\mathbf{r}(0) \rightarrow \mathbf{r}(0) + \Delta t\dot{\mathbf{r}}(\frac{\Delta t}{2}) = \mathbf{r}(0) + \Delta t\dot{\mathbf{r}}(0) + \frac{\Delta t^2}{2m}\mathbf{F}(\mathbf{0})$$

$$i\mathcal{L}_r\Delta t \Rightarrow \mathbf{r} \rightarrow \mathbf{r} + \dot{\mathbf{r}}\Delta t$$

$$i\mathcal{L}_p\Delta t \Rightarrow \mathbf{p} \rightarrow \mathbf{p} + \dot{\mathbf{p}}\Delta t$$

$$\left(e^{(i\mathcal{L}_p\Delta t/2)}e^{(i\mathcal{L}_r\Delta t)}e^{(i\mathcal{L}_p\Delta t/2)}\right)^P$$

$$e^{(i\mathcal{L}_p\Delta t/2)} f\left(\mathbf{p}^N(0), (\mathbf{r}^N(0)\right) = f\left(\left[\mathbf{p}(0) + \frac{\Delta t}{2}\dot{\mathbf{p}}(0)\right]^N, \mathbf{r}^N(0)\right)$$

$$\ldots t\dot{\mathbf{r}}\left(\frac{\Delta t}{2}\right)\Big]^N\Big)$$

$$\ldots \mathbf{r}(0) + \Delta t\dot{\mathbf{r}}\left(\frac{\Delta t}{2}\right)\Big]^N\Big)$$

Velocity Verlet!

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

$$\mathbf{v}(t+\Delta t) = \mathbf{v}(t) + \frac{\Delta t}{2m}\left[\mathbf{F}(t) + \mathbf{F}(t+\Delta t)\right]$$

$$\mathbf{p}(0) \rightarrow \mathbf{p}(0) + \frac{\Delta t}{2}\left[\dot{\mathbf{p}}(0) + \dot{\mathbf{p}}(\Delta t)\right]$$

$$\mathbf{r}(0) \rightarrow \mathbf{r}(0) + \Delta t\dot{\mathbf{r}}\left(\frac{\Delta t}{2}\right) = \mathbf{r}(0) + \Delta t\dot{\mathbf{r}}(0) + \frac{\Delta t^2}{2m}\mathbf{F}(\mathbf{0})$$

Velocity Verlet:

$$e^{(i\mathcal{L}_p \Delta t/2)} e^{(i\mathcal{L}_r \Delta t)} e^{(i\mathcal{L}_p \Delta t/2)}$$

Velocity Verlet:

$$e^{(i\mathcal{L}_p \Delta t/2)} e^{(i\mathcal{L}_r \Delta t)} e^{(i\mathcal{L}_p \Delta t/2)}$$

```
Call force(fx)
```

Velocity Verlet:

$$e^{(i\mathcal{L}_p \Delta t/2)} e^{(i\mathcal{L}_r \Delta t)} e^{(i\mathcal{L}_p \Delta t/2)}$$

```
Call force(fx)
Do while (t<tmax)



enddo
```

Velocity Verlet:

$$e^{(i\mathcal{L}_p \Delta t/2)} e^{(i\mathcal{L}_r \Delta t)} e^{(i\mathcal{L}_p \Delta t/2)}$$

```
Call force(fx)
Do while (t<tmax)
```

$$e^{(i\mathcal{L}_p \Delta t/2)} : \mathbf{v}\left(t + \frac{\Delta t}{2}\right) \rightarrow \mathbf{v}(t) + \frac{\Delta t}{2m}\mathbf{f}(\mathbf{t})$$

```
enddo
```

Velocity Verlet:

$$e^{(i\mathcal{L}_p \Delta t/2)} e^{(i\mathcal{L}_r \Delta t)} e^{(i\mathcal{L}_p \Delta t/2)}$$

```
Call force(fx)
Do while (t<tmax)
```

$$e^{(i\mathcal{L}_p \Delta t/2)} : \mathbf{v}\left(t + \frac{\Delta t}{2}\right) \rightarrow \mathbf{v}(t) + \frac{\Delta t}{2m}\mathbf{f}(\mathbf{t})$$

```
vx=vx+delt*fx/2
```

```
enddo
```

Velocity Verlet:

$$e^{(i\mathcal{L}_p \Delta t/2)} e^{(i\mathcal{L}_r \Delta t)} e^{(i\mathcal{L}_p \Delta t/2)}$$

```
Call force(fx)
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```

$$e^{(i\mathcal{L}_p \Delta t/2)} : \mathbf{v}\left(t + \frac{\Delta t}{2}\right) \rightarrow \mathbf{v}(t) + \frac{\Delta t}{2m}\mathbf{f}(\mathbf{t})$$

```
vx=vx+delt*fx/2
```

$$e^{(i\mathcal{L}_r \Delta t/2)} : \mathbf{r}\left(t + \Delta t\right) \rightarrow \mathbf{r}(t) + \Delta t \mathbf{v}(t + \Delta t/2)$$

```
enddo
```

Velocity Verlet:

$$e^{(i\mathcal{L}_p \Delta t/2)} e^{(i\mathcal{L}_r \Delta t)} e^{(i\mathcal{L}_p \Delta t/2)}$$

```
Call force(fx)
Do while (t<tmax)
```

$$e^{(i\mathcal{L}_p \Delta t/2)} : \mathbf{v}\left(t + \frac{\Delta t}{2}\right) \rightarrow \mathbf{v}(t) + \frac{\Delta t}{2m}\mathbf{f}(\mathbf{t})$$

```
vx=vx+delt*fx/2
```

$$e^{(i\mathcal{L}_r \Delta t/2)} : \mathbf{r}\,(t + \Delta t) \rightarrow \mathbf{r}(t) + \Delta t \mathbf{v}(t + \Delta t/2)$$

```
x=x+delt*vx
Call force(fx)
```



```
enddo
```

Velocity Verlet:

$$e^{(i\mathcal{L}_p \Delta t/2)} e^{(i\mathcal{L}_r \Delta t)} e^{(i\mathcal{L}_p \Delta t/2)}$$

```
Call force(fx)
Do while (t<tmax)
```

$$e^{(i\mathcal{L}_p \Delta t/2)} : \mathbf{v}\left(t + \frac{\Delta t}{2}\right) \rightarrow \mathbf{v}(t) + \frac{\Delta t}{2m}\mathbf{f}(\mathbf{t})$$

```
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```

$$e^{(i\mathcal{L}_r \Delta t/2)} : \mathbf{r}\left(t + \Delta t\right) \rightarrow \mathbf{r}(t) + \Delta t \mathbf{v}(t + \Delta t/2)$$

```
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```

$$e^{(i\mathcal{L}_p \Delta t/2)} : \mathbf{v}\left(t + \Delta t\right) \rightarrow \mathbf{v}(t + \Delta t/2) + \frac{\Delta t}{2m}\mathbf{f}(\mathbf{t} + \mathbf{\Delta t})$$


```
enddo
```

Velocity Verlet:

$$e^{(i\mathcal{L}_p \Delta t/2)} e^{(i\mathcal{L}_r \Delta t)} e^{(i\mathcal{L}_p \Delta t/2)}$$

```
Call force(fx)
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```

$$e^{(i\mathcal{L}_p \Delta t/2)} : \mathbf{v}\left(t + \frac{\Delta t}{2}\right) \rightarrow \mathbf{v}(t) + \frac{\Delta t}{2m}\mathbf{f}(\mathbf{t})$$

```
vx=vx+delt*fx/2
```

$$e^{(i\mathcal{L}_r \Delta t/2)} : \mathbf{r}\,(t + \Delta t) \rightarrow \mathbf{r}(t) + \Delta t \mathbf{v}(t + \Delta t/2)$$

```
x=x+delt*vx
Call force(fx)
```

$$e^{(i\mathcal{L}_p \Delta t/2)} : \mathbf{v}\,(t + \Delta t) \rightarrow \mathbf{v}(t + \Delta t/2) + \frac{\Delta t}{2m}\mathbf{f}(\mathbf{t} + \boldsymbol{\Delta}\mathbf{t})$$

```
vx=vx+delt*fx/2
```



```
enddo
```

Liouville Formulation

Velocity Verlet algorithm:

$$\mathbf{p}(t+\Delta t) = \mathbf{p}(t) + \frac{\Delta t}{2}\left[\dot{\mathbf{p}}(t) + \dot{\mathbf{p}}(t+\Delta t)\right]$$

$$\mathbf{r}(t+\Delta t) = \mathbf{r}(t) + \Delta t\,\dot{\mathbf{r}}(t) + \frac{\Delta t^2}{2m}\mathbf{F}(t)$$

Three subsequent coordinate transformations in either **r** or **p** of which the *Jacobian* is one: *Area preserving*

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Three subsequent coordinate transformations in either **r** or **p** of which the *Jacobian* is one: *Area preserving*

$$\mathbf{p}(t+\Delta t/2) = \mathbf{p}(t) + \frac{\Delta t}{2}\mathbf{F}(\mathbf{r})$$

$$\mathbf{r}(t) = \mathbf{r}(t)$$

$$J_1 = \det\begin{vmatrix} 1 & \frac{\Delta t}{2}\frac{\partial \mathbf{F}(\mathbf{r})}{\partial \mathbf{r}} \\ 0 & 1 \end{vmatrix} = 1$$

$$\mathbf{p}(t+\Delta t/2) = \mathbf{p}(t+\Delta t/2)$$

$$\mathbf{r}(t+\Delta t) = \mathbf{r}(t) + \frac{\Delta t}{m}\mathbf{p}(t+\Delta t/2)$$

$$J_2 = \det\begin{vmatrix} 1 & 0 \\ \Delta t/m & 1 \end{vmatrix} = 1$$

$$\mathbf{p}(t+\Delta t) = \mathbf{p}(t+\Delta t/2) + \frac{\Delta t}{2}\mathbf{F}(\mathbf{r}(t))$$

$$\mathbf{r}(t) = \mathbf{r}(t)$$

$$J_3 = \det\begin{vmatrix} 1 & \frac{\Delta t}{2}\frac{\partial \mathbf{F}(\mathbf{r})}{\partial \mathbf{r}} \\ 0 & 1 \end{vmatrix} = 1$$

Liouville Formulation

Velocity Verlet algorithm:

$$\mathbf{p}(t+\Delta t) = \mathbf{p}(t) + \frac{\Delta t}{2}\left[\dot{\mathbf{p}}(t) + \dot{\mathbf{p}}(t+\Delta t)\right]$$

$$\mathbf{r}(t+\Delta t) = \mathbf{r}(t) + \Delta t\,\dot{\mathbf{r}}(t) + \frac{\Delta t^2}{2m}\mathbf{F}(t)$$

Three subsequent coordinate transformations in either **r** or **p** of which the *Jacobian* is one: *Area preserving*

$$\mathbf{p}(t+\Delta t/2) = \mathbf{p}(t) + \frac{\Delta t}{2}\mathbf{F}(\mathbf{r})$$

$$\mathbf{r}(t) = \mathbf{r}(t)$$

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$$\mathbf{p}(t+\Delta t/2) = \mathbf{p}(t+\Delta t/2)$$

$$\mathbf{r}(t+\Delta t) = \mathbf{r}(t) + \frac{\Delta t}{m}\mathbf{p}(t+\Delta t/2)$$

$$J_2 = \det\begin{vmatrix} 1 & 0 \\ \Delta t/m & 1 \end{vmatrix} = 1$$

$$\mathbf{p}(t+\Delta t) = \mathbf{p}(t+\Delta t/2) + \frac{\Delta t}{2}\mathbf{F}(\mathbf{r}(t))$$

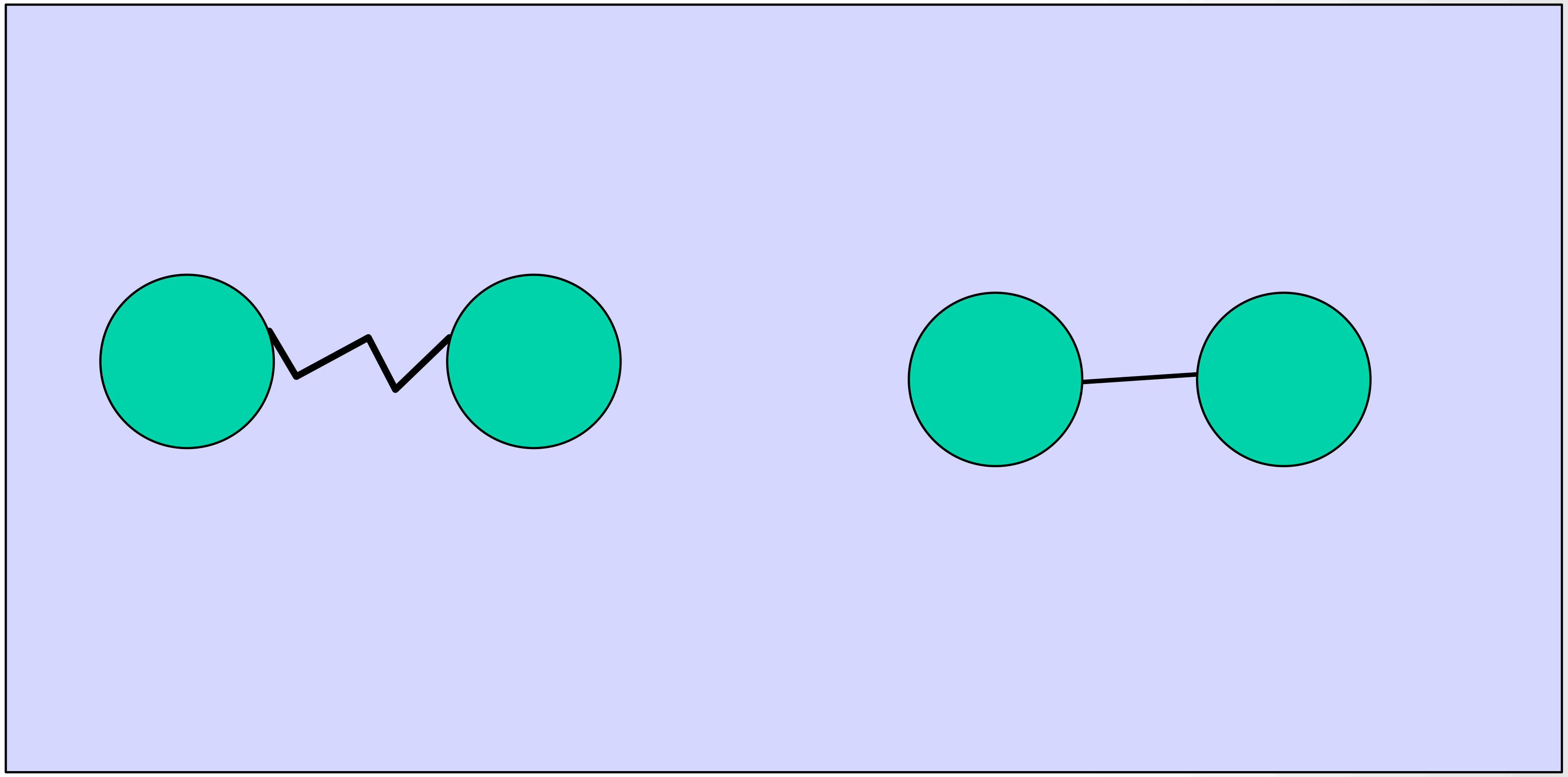
$$\mathbf{r}(t) = \mathbf{r}(t)$$

$$J_3 = \det\begin{vmatrix} 1 & \frac{\Delta t}{2}\frac{\partial \mathbf{F}(\mathbf{r})}{\partial \mathbf{r}} \\ 0 & 1 \end{vmatrix} = 1$$

Other Trotter decompositions are possible!

Multiple time steps

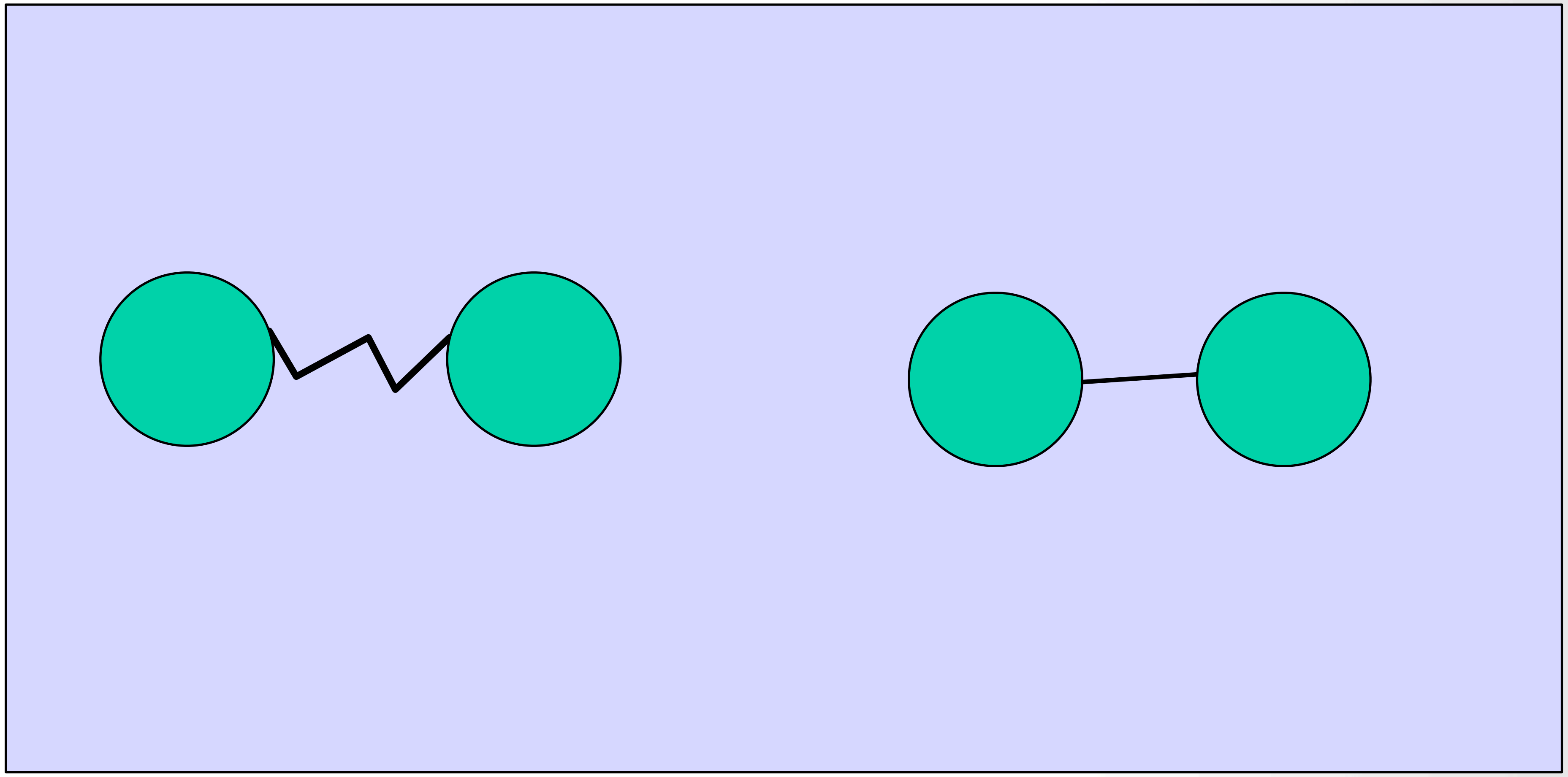
- What to use for stiff potentials:



  – Fixed bond-length: constraints (Shake)
  – Very small time step

Multiple Time steps

$$\mathbf{F} = \mathbf{F}_{short} + \mathbf{F}_{long}$$



Multiple Time steps

$$\mathbf{F} = \mathbf{F}_{\text{short}} + \mathbf{F}_{\text{long}}$$

$$i\mathcal{L} \equiv i\mathcal{L}_r + i\mathcal{L}_p = \mathbf{v}\frac{\partial}{\partial \mathbf{r}} + \frac{\mathbf{F}}{m}\frac{\partial}{\partial \mathbf{v}}$$

Multiple Time steps

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$$i\mathcal{L} \equiv i\mathcal{L}_r + i\mathcal{L}_p = \mathbf{v}\frac{\partial}{\partial \mathbf{r}} + \frac{\mathbf{F}}{m}\frac{\partial}{\partial \mathbf{v}}$$

$$i\mathcal{L} \equiv i\mathcal{L}_{\text{short}} + i\mathcal{L}_{\text{long}}$$

$$i\mathcal{L}_{\text{short}} = \frac{\mathbf{F}_{\text{short}}}{m}\frac{\partial}{\partial \mathbf{v}} \qquad i\mathcal{L}_{\text{long}} = \frac{\mathbf{F}_{\text{long}}}{m}\frac{\partial}{\partial \mathbf{v}}$$

Multiple Time steps

$$\mathbf{F} = \mathbf{F}_{\text{short}} + \mathbf{F}_{\text{long}}$$

$$i\mathcal{L} \equiv i\mathcal{L}_r + i\mathcal{L}_p = \mathbf{v}\frac{\partial}{\partial \mathbf{r}} + \frac{\mathbf{F}}{m}\frac{\partial}{\partial \mathbf{v}}$$

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$$i\mathcal{L}_{\text{short}} = \frac{\mathbf{F}_{\text{short}}}{m}\frac{\partial}{\partial \mathbf{v}} \qquad i\mathcal{L}_{\text{long}} = \frac{\mathbf{F}_{\text{long}}}{m}\frac{\partial}{\partial \mathbf{v}}$$

Trotter expansion:

$$e^{i(\mathcal{L}_{\text{long}}+\mathcal{L}_{\text{short}}+\mathcal{L}_r)\Delta t} \approx e^{i\mathcal{L}_{\text{long}}\Delta t/2} e^{i(\mathcal{L}_{\text{short}}+\mathcal{L}_r)\Delta t} e^{i\mathcal{L}_{\text{long}}\Delta t/2}$$

Multiple Time steps

$$\mathbf{F} = \mathbf{F}_{\text{short}} + \mathbf{F}_{\text{long}}$$

$$i\mathcal{L} \equiv i\mathcal{L}_r + i\mathcal{L}_p = \mathbf{v}\frac{\partial}{\partial \mathbf{r}} + \frac{\mathbf{F}}{m}\frac{\partial}{\partial \mathbf{v}}$$

$$i\mathcal{L} \equiv i\mathcal{L}_{\text{short}} + i\mathcal{L}_{\text{long}}$$

$$i\mathcal{L}_{\text{short}} = \frac{\mathbf{F}_{\text{short}}}{m}\frac{\partial}{\partial \mathbf{v}} \qquad i\mathcal{L}_{\text{long}} = \frac{\mathbf{F}_{\text{long}}}{m}\frac{\partial}{\partial \mathbf{v}}$$

Trotter expansion:

$$e^{i(\mathcal{L}_{\text{long}}+\mathcal{L}_{\text{short}}+\mathcal{L}_r)\Delta t} \approx e^{i\mathcal{L}_{\text{long}}\Delta t/2} e^{i(\mathcal{L}_{\text{short}}+\mathcal{L}_r)\Delta t} e^{i\mathcal{L}_{\text{long}}\Delta t/2}$$

Introduce: $\delta t = \Delta t / n$

$$\approx e^{i\mathcal{L}_{\text{long}}\Delta t/2} \left[e^{i\mathcal{L}_{\text{short}}\delta t/2} e^{i\mathcal{L}_r \delta t} e^{i\mathcal{L}_{\text{short}}\delta t/2} \right]^n e^{i\mathcal{L}_{\text{long}}\Delta t/2}$$

$$e^{i(\mathcal{L}_{\text{long}}+\mathcal{L}_{\text{short}}+\mathcal{L}_r)\Delta t} \approx e^{i\mathcal{L}_{\text{long}}\Delta t/2}\left[e^{i\mathcal{L}_{\text{short}}\delta t/2}e^{i\mathcal{L}_r\delta t}e^{i\mathcal{L}_{\text{short}}\delta t/2}\right]^n e^{i\mathcal{L}_{\text{long}}\Delta t/2}$$

$$e^{i(\mathcal{L}_{\text{long}}+\mathcal{L}_{\text{short}}+\mathcal{L}_r)\Delta t} \approx e^{i\mathcal{L}_{\text{long}}\Delta t/2} \left[e^{i\mathcal{L}_{\text{short}}\delta t/2} e^{i\mathcal{L}_r \delta t} e^{i\mathcal{L}_{\text{short}}\delta t/2} \right]^n e^{i\mathcal{L}_{\text{long}}\Delta t/2}$$

$$i\mathcal{L}_{\text{long}}\Delta t/2 \Rightarrow v \rightarrow v + F_{\text{long}}\Delta t/2m$$

$$i\mathcal{L}_{\text{short}}\delta t/2 \Rightarrow v \rightarrow v + F_{\text{short}}\delta t/2m$$

$$i\mathcal{L}_r \delta t \Rightarrow r \rightarrow r + v\delta t$$

$$e^{i(\mathcal{L}_{\text{long}}+\mathcal{L}_{\text{short}}+\mathcal{L}_r)\Delta t} \approx e^{i\mathcal{L}_{\text{long}}\Delta t/2}\left[e^{i\mathcal{L}_{\text{short}}\delta t/2}e^{i\mathcal{L}_r\delta t}e^{i\mathcal{L}_{\text{short}}\delta t/2}\right]^n e^{i\mathcal{L}_{\text{long}}\Delta t/2}$$

$$i\mathcal{L}_{\text{long}}\Delta t/2 \Rightarrow v \rightarrow v + F_{\text{long}}\Delta t/2m$$

$$i\mathcal{L}_{\text{short}}\delta t/2 \Rightarrow v \rightarrow v + F_{\text{short}}\delta t/2m$$

$$i\mathcal{L}_r\delta t \Rightarrow r \rightarrow r + v\delta t$$

First

$$e^{(i\mathcal{L}_{\text{long}}\Delta t/2)}f\left[r(0), v(0)\right] = f\left[r(0), v(0) + F_{\text{long}}(0)\Delta t/2m\right]$$

$$e^{i(\mathcal{L}_{\text{long}}+\mathcal{L}_{\text{short}}+\mathcal{L}_r)\Delta t} \approx e^{i\mathcal{L}_{\text{long}}\Delta t/2}\left[e^{i\mathcal{L}_{\text{short}}\delta t/2}e^{i\mathcal{L}_r\delta t}e^{i\mathcal{L}_{\text{short}}\delta t/2}\right]^n e^{i\mathcal{L}_{\text{long}}\Delta t/2}$$

$$i\mathcal{L}_{\text{long}}\Delta t/2 \Rightarrow v \rightarrow v + F_{\text{long}}\Delta t/2m$$

$$i\mathcal{L}_{\text{short}}\delta t/2 \Rightarrow v \rightarrow v + F_{\text{short}}\delta t/2m$$

$$i\mathcal{L}_r\delta t \Rightarrow r \rightarrow r + v\delta t$$

First

$$e^{(i\mathcal{L}_{\text{long}}\Delta t/2)} f\left[r(0), v(0)\right] = f\left[r(0), v(0) + F_{\text{long}}(0)\Delta t/2m\right]$$

Now *n* times:

$$\left[e^{i\mathcal{L}_{\text{short}}\delta t/2}e^{i\mathcal{L}_r\delta t}e^{i\mathcal{L}_{\text{short}}\delta t/2}\right]^n f\left[r(0), v(0) + F_{\text{long}}(0)\Delta t/2m\right]$$

$$e^{iL_{\text{long}}\,\Delta t/2}\left[e^{iL_{\text{short}}\,\delta t/2}e^{iL_r\delta t}e^{iL_{\text{short}}\,\delta t/2}\right]^{n}e^{iL_{\text{long}}\,\Delta t/2}$$

$$iL_{\text{long}}\,\Delta t/2 \Rightarrow v \rightarrow v + F_{\text{long}}\,\Delta t/2m$$

$$iL_{\text{short}}\,\delta t/2 \Rightarrow v \rightarrow v + F_{\text{short}}\,\delta t/2m$$

$$iL_r\delta t \Rightarrow r \rightarrow r + v\delta t$$

$$e^{(i\mathcal{L}_{long}\Delta t/2)} : \mathbf{v}\left(t + \frac{\Delta t}{2}\right) \rightarrow \mathbf{v}(t) + \frac{\Delta t}{2m}\mathbf{f}_{\mathrm{long}}(t)$$

$$e^{iL_{\mathrm{long}}\Delta t/2}\left[e^{iL_{\mathrm{short}}\delta t/2}e^{iL_r\delta t}e^{iL_{\mathrm{short}}\delta t/2}\right]^{n}e^{iL_{\mathrm{long}}\Delta t/2}$$

$$iL_{\mathrm{long}}\Delta t/2 \Rightarrow v \rightarrow v + F_{\mathrm{long}}\Delta t/2m$$

$$iL_{\mathrm{short}}\delta t/2 \Rightarrow v \rightarrow v + F_{\mathrm{short}}\delta t/2m$$

$$iL_r\delta t \Rightarrow r \rightarrow r + v\delta t$$

$$e^{(i\mathcal{L}_{long}\Delta t/2)} : \mathbf{v}\left(t+\frac{\Delta t}{2}\right) \rightarrow \mathbf{v}(t) + \frac{\Delta t}{2m}\mathbf{f}_{\text{long}}(t)$$

```
Call force(fx_long,f_short)
```

$$e^{iL_{\text{long}}\Delta t/2}\left[e^{iL_{\text{short}}\delta t/2}e^{iL_r\delta t}e^{iL_{\text{short}}\delta t/2}\right]^n e^{iL_{\text{long}}\Delta t/2}$$

$$iL_{\text{long}}\,\Delta t/2 \Rightarrow v \rightarrow v + F_{\text{long}}\,\Delta t/2m$$

$$iL_{\text{short}}\,\delta t/2 \Rightarrow v \rightarrow v + F_{\text{short}}\,\delta t/2m$$

$$iL_r\delta t \Rightarrow r \rightarrow r + v\delta t$$

$$e^{(i\mathcal{L}_{long}\Delta t/2)} : \mathbf{v}\left(t+\frac{\Delta t}{2}\right) \rightarrow \mathbf{v}(t) + \frac{\Delta t}{2m}\mathbf{f}_{\text{long}}(t)$$

```
Call force(fx_long,f_short)
```

$$e^{iL_{\text{long}}\Delta t/2}\left[e^{iL_{\text{short}}\delta t/2}e^{iL_r\delta t}e^{iL_{\text{short}}\delta t/2}\right]^n e^{iL_{\text{long}}\Delta t/2}$$

$$iL_{\text{long}}\,\Delta t/2 \Rightarrow v \rightarrow v + F_{\text{long}}\,\Delta t/2m$$

$$iL_{\text{short}}\,\delta t/2 \Rightarrow v \rightarrow v + F_{\text{short}}\,\delta t/2m$$

$$iL_r\delta t \Rightarrow r \rightarrow r + v\delta t$$

$$e^{(i\mathcal{L}_{long}\Delta t/2)} : \mathbf{v}\left(t+\frac{\Delta t}{2}\right) \rightarrow \mathbf{v}(t) + \frac{\Delta t}{2m}\mathbf{f}_{\text{long}}(t)$$

```
Call force(fx_long,f_short)

vx=vx+delt*fx_long/2
```

$$e^{iL_{\text{long}}\Delta t/2}\left[e^{iL_{\text{short}}\delta t/2}e^{iL_r\delta t}e^{iL_{\text{short}}\delta t/2}\right]^n e^{iL_{\text{long}}\Delta t/2}$$

$$iL_{\text{long}}\,\Delta t/2 \Rightarrow v \rightarrow v + F_{\text{long}}\,\Delta t/2m$$

$$iL_{\text{short}}\,\delta t/2 \Rightarrow v \rightarrow v + F_{\text{short}}\,\delta t/2m$$

$$iL_r\delta t \Rightarrow r \rightarrow r + v\delta t$$

$$e^{(i\mathcal{L}_{long}\Delta t/2)}: \mathbf{v}\left(t+\frac{\Delta t}{2}\right) \rightarrow \mathbf{v}(t) + \frac{\Delta t}{2m}\mathbf{f}_{\text{long}}(t)$$

```
Call force(fx_long,f_short)

vx=vx+delt*fx_long/2

Do ddt=1,n



enddo
```

$$e^{iL_{\text{long}}\Delta t/2}\left[e^{iL_{\text{short}}\delta t/2}e^{iL_r\delta t}e^{iL_{\text{short}}\delta t/2}\right]^{\text{n}} e^{iL_{\text{long}}\Delta t/2}$$

$$iL_{\text{long}}\,\Delta t/2 \Rightarrow v \rightarrow v + F_{\text{long}}\,\Delta t/2m$$

$$iL_{\text{short}}\,\delta t/2 \Rightarrow v \rightarrow v + F_{\text{short}}\,\delta t/2m$$

$$iL_r\delta t \Rightarrow r \rightarrow r + v\delta t$$

$$e^{(i\mathcal{L}_{long}\Delta t/2)} : \mathbf{v}\left(t + \frac{\Delta t}{2}\right) \rightarrow \mathbf{v}(t) + \frac{\Delta t}{2m}\mathbf{f}_{\text{long}}(t)$$

```
Call force(fx_long,f_short)

vx=vx+delt*fx_long/2

Do ddt=1,n
```

$$e^{(i\mathcal{L}_{short}\delta t/2)} : \mathbf{v}\left(t + \frac{\Delta t}{2} + \frac{\delta t}{2}\right) \rightarrow \mathbf{v}(t + \frac{\Delta t}{2}) + \frac{\delta t}{2m}\mathbf{f}_{\text{short}}(t)$$

```
enddo
```

$$e^{iL_{\text{long}}\Delta t/2}\left[e^{iL_{\text{short}}\delta t/2} e^{iL_r \delta t} e^{iL_{\text{short}}\delta t/2}\right]^n e^{iL_{\text{long}}\Delta t/2}$$

$$iL_{\text{long}}\,\Delta t/2 \Rightarrow v \rightarrow v + F_{\text{long}}\,\Delta t/2m$$

$$iL_{\text{short}}\,\delta t/2 \Rightarrow v \rightarrow v + F_{\text{short}}\,\delta t/2m$$

$$iL_r \delta t \Rightarrow r \rightarrow r + v\delta t$$

$$e^{(i\mathcal{L}_{long}\Delta t/2)} : \mathbf{v}\left(t+\frac{\Delta t}{2}\right) \rightarrow \mathbf{v}(t) + \frac{\Delta t}{2m}\mathbf{f}_{\mathrm{long}}(t)$$

```
Call force(fx_long,f_short)

vx=vx+delt*fx_long/2

Do ddt=1,n
```

$$e^{(i\mathcal{L}_{short}\delta t/2)} : \mathbf{v}\left(t+\frac{\Delta t}{2}+\frac{\delta t}{2}\right) \rightarrow \mathbf{v}(t+\frac{\Delta t}{2}) + \frac{\delta t}{2m}\mathbf{f}_{\mathrm{short}}(t)$$

```
    vx=vx+ddelt*fx_short/2

enddo
```

$$e^{iL_{\mathrm{long}}\Delta t/2}\left[e^{iL_{\mathrm{short}}\delta t/2}e^{iL_r\delta t}e^{iL_{\mathrm{short}}\delta t/2}\right]^n e^{iL_{\mathrm{long}}\Delta t/2}$$

$$iL_{\mathrm{long}}\ \Delta t/2 \Rightarrow v \rightarrow v + F_{\mathrm{long}}\ \Delta t/2m$$

$$iL_{\mathrm{short}}\ \delta t/2 \Rightarrow v \rightarrow v + F_{\mathrm{short}}\ \delta t/2m$$

$$iL_r\delta t \Rightarrow r \rightarrow r + v\delta t$$

$$e^{(i\mathcal{L}_{long}\Delta t/2)}: \mathbf{v}\left(t +\right.$$

$$\mathrm{e}^{\mathrm{i}L_{\mathrm{long}}\Delta t/2}\left[\mathrm{e}^{\mathrm{i}L_{\mathrm{short}}\delta t/2}\mathrm{e}^{\mathrm{i}L_r\delta t}\mathrm{e}^{\mathrm{i}L_{\mathrm{short}}\delta t/2}\right]^{\mathrm{n}}\mathrm{e}^{\mathrm{i}L_{\mathrm{long}}\Delta t/2}$$

$$\mathrm{i}L_{\mathrm{long}}\,\Delta t/2 \Rightarrow v \rightarrow v + F_{\mathrm{long}}\,\Delta t/2m$$

$$\mathrm{i}L_{\mathrm{short}}\,\delta t/2 \Rightarrow v \rightarrow v + F_{\mathrm{short}}\,\delta t/2m$$

$$\mathrm{i}L_r\delta t \Rightarrow r \rightarrow r + v\delta t$$

```
Call force(fx_l
vx=vx+delt*fx_l
Do ddt=1,n
```

$$e^{(i\mathcal{L}_{short}\delta t/2)}: \mathbf{v}\left(t + \frac{}{2} + \frac{}{2}\right) \rightarrow \mathbf{v}(t + \frac{}{2}) + \frac{}{2m}\mathbf{f}_{\mathrm{short}}(t)$$

```
    vx=vx+ddelt*fx_short/2
```

$$e^{(i\mathcal{L}_r\Delta t)}: \mathbf{r}\left(t+\delta t\right) \rightarrow \mathbf{r}(t) + \delta t\mathbf{v}(t + \Delta t/2 + \delta t/2)$$

```
enddo
```

$$e^{(i\mathcal{L}_{long}\Delta t/2)} : \mathbf{v}\left(t + \right.$$

$$e^{iL_{\text{long}}\Delta t/2}\left[e^{iL_{\text{short}}\delta t/2}e^{iL_r\delta t}e^{iL_{\text{short}}\delta t/2}\right]^{n} e^{iL_{\text{long}}\Delta t/2}$$

$$iL_{\text{long}}\,\Delta t/2 \Rightarrow v \rightarrow v + F_{\text{long}}\,\Delta t/2m$$

$$iL_{\text{short}}\,\delta t/2 \Rightarrow v \rightarrow v + F_{\text{short}}\,\delta t/2m$$

$$iL_r\delta t \Rightarrow r \rightarrow r + v\delta t$$

```
Call force(fx_l
vx=vx+delt*fx_l
Do ddt=1,n
```

$$e^{(i\mathcal{L}_{short}\delta t/2)} : \mathbf{v}\left(t + \frac{\quad}{2} + \frac{\quad}{2}\right) \rightarrow \mathbf{v}(t + \frac{\quad}{2}) + \frac{\quad}{2m}\mathbf{f}_{\text{short}}(t)$$

```
    vx=vx+ddelt*fx_short/2
```

$$e^{(i\mathcal{L}_r\Delta t)} : \mathbf{r}\left(t + \delta t\right) \rightarrow \mathbf{r}(t) + \delta t\mathbf{v}(t + \Delta t/2 + \delta t/2)$$

```
    x=x+ddelt*vx
    Call force_short(fx_short)

enddo
```

$$e^{(i\mathcal{L}_{long}\Delta t/2)} : \mathbf{v}\left(t + \right.$$

```
Call force(fx_l
vx=vx+delt*fx_l
Do ddt=1,n
```

$$e^{iL_{long}\,\Delta t/2}\left[e^{iL_{short}\,\delta t/2}e^{iL_r\delta t}e^{iL_{short}\,\delta t/2}\right]^{n} e^{iL_{long}\,\Delta t/2}$$

$$iL_{long}\;\Delta t/2 \Rightarrow v \rightarrow v + F_{long}\;\Delta t/2m$$

$$iL_{short}\;\delta t/2 \Rightarrow v \rightarrow v + F_{short}\;\delta t/2m$$

$$iL_r\delta t \Rightarrow r \rightarrow r + v\delta t$$

$$e^{(i\mathcal{L}_{short}\delta t/2)} : \mathbf{v}\left(t + \frac{\quad}{2} + \frac{\quad}{2}\right) \rightarrow \mathbf{v}(t + \frac{\quad}{2}) + \frac{\quad}{2m}\mathbf{f}_{short}(t)$$

```
    vx=vx+ddelt*fx_short/2
```

$$e^{(i\mathcal{L}_r\Delta t)} : \mathbf{r}\left(t + \delta t\right) \rightarrow \mathbf{r}(t) + \delta t\mathbf{v}(t + \Delta t/2 + \delta t/2)$$

```
    x=x+ddelt*vx
    Call force_short(fx_short)
```

$$e^{(i\mathcal{L}_{short}\delta t/2)} : \mathbf{v}\left(t + \frac{\Delta t}{2} + \delta t\right) \rightarrow \mathbf{v}\left(t + \frac{\Delta t}{2} + \frac{\delta t}{2}\right) + \frac{\delta t}{2m}\mathbf{f}_{short}(t + \delta t)$$

```
enddo
```

$$e^{(i\mathcal{L}_{long}\Delta t/2)} : \mathbf{v}\left(t + \ldots\right.$$

```
Call force(fx_l
vx=vx+delt*fx_l
Do ddt=1,n
```

$$e^{iL_{\text{long}}\Delta t/2}\left[e^{iL_{\text{short}}\delta t/2}e^{iL_r\delta t}e^{iL_{\text{short}}\delta t/2}\right]^n e^{iL_{\text{long}}\Delta t/2}$$

$$iL_{\text{long}}\,\Delta t/2 \Rightarrow v \rightarrow v + F_{\text{long}}\,\Delta t/2m$$

$$iL_{\text{short}}\,\delta t/2 \Rightarrow v \rightarrow v + F_{\text{short}}\,\delta t/2m$$

$$iL_r\delta t \Rightarrow r \rightarrow r + v\delta t$$

$$e^{(i\mathcal{L}_{short}\delta t/2)} : \mathbf{v}\left(t + \frac{\quad}{2} + \frac{\quad}{2}\right) \rightarrow \mathbf{v}(t + \frac{\quad}{2}) + \frac{\quad}{2m}\mathbf{f}_{short}(t)$$

```
    vx=vx+ddelt*fx_short/2
```

$$e^{(i\mathcal{L}_r\Delta t)} : \mathbf{r}\left(t + \delta t\right) \rightarrow \mathbf{r}(t) + \delta t\mathbf{v}(t + \Delta t/2 + \delta t/2)$$

```
    x=x+ddelt*vx
    Call force_short(fx_short)
```

$$e^{(i\mathcal{L}_{short}\delta t/2)} : \mathbf{v}\left(t + \frac{\Delta t}{2} + \delta t\right) \rightarrow \mathbf{v}\left(t + \frac{\Delta t}{2} + \frac{\delta t}{2}\right) + \frac{\delta t}{2m}\mathbf{f}_{short}(t + \delta t)$$

```
    vx=vx+ddelt*fx_short/2
enddo
```

Algorithm 29 (Multiple Time Step)

`subroutine`	Multiple time step, `f_long` is
`+    multi(f_long,f_short)`	the long-range part and `f_short` the short-range part of the force
`vx=vx+0.5*delt*f_long`	velocity Verlet with time step Δt
`do it=1,n`	loop for the small time step
`   vx=vx+0.5*(delt/n)*f_short`	velocity Verlet with timestep $\Delta t/n$
`   x=x+(delt/n)2*vx`	
`   call force_short(f_short)`	short-range forces
`   vx=vx+0.5*(delt/n)*f_short`	
`enddo`	
`call force_all(f_long,f_short)`	all forces
`vx=vx+0.5*delt*f_long`	
`return`	
`end`	