Random Number Generators

Pseudo–

Set of integers $\xrightarrow[\text{rule (deterministic)}]{\text{"production}}$ new set

Lit.: – Numerical Recipes

– Knuth, The Art of Computer Programming (vol. 2)

– Tausworthe, Math. Comput. 19, 201 (1965)

→ Heuer / BD / Ferrenberg, Comput. Phys. Comm. 103, 1 (1997)

– Bauke / Mertens, PRE 75, 066701 (2007)

Simplest: "linear congruential"

$$x_{n+1} = (a \cdot x_n + c) \bmod m$$

popular choice: $a = 7^5 = 16807$, $c = 0$

$m = 2^{31} - 1$ (largest integer on 32-bit, prime #)

this has maximum period

$$m - 1 = 2^{31} - 2 \simeq \underline{2 \cdot 10^9}$$

rule of thumb: # of produced RN $\ll \sqrt{\text{period}}$

3 yrs CPU time $\simeq 10^8$ sec.

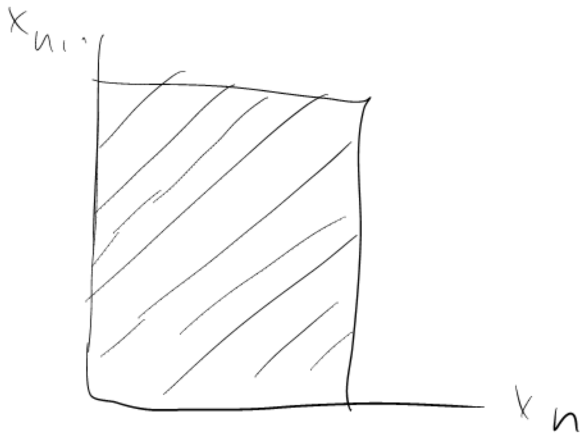
10^6 processors, one RN per machine cycle:

# of RN $\simeq 10^8 \cdot 10^9 \cdot 10^6 = \underline{\underline{10^{23}}}$

period $\gg 10^{46}$

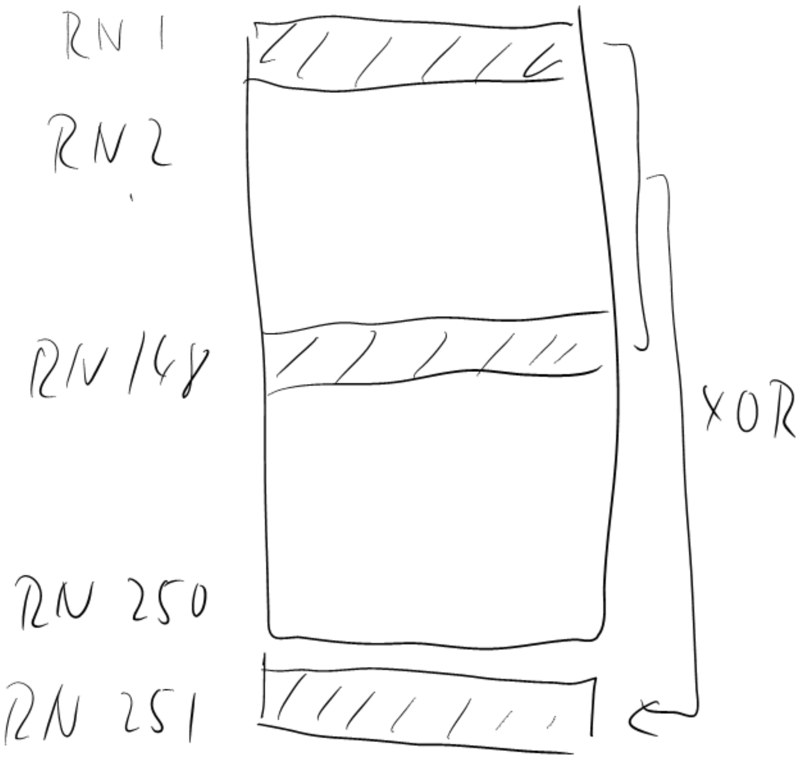
correlations "d-space non-uniformity"

d = 2



work on arrays of RNs

R250:



XOR: bitwise addition without carry

$0 \text{ XOR } 0 = 0$

$1 \text{ XOR } 1 = 0$

$1 \text{ XOR } 0 = 1$

$0 \text{ XOR } 1 = 1$

$$x_n = x_{n-103} \text{ XOR } x_{n-250}$$

altern.:

$$x_n = x_{n-168} \text{ XOR } x_{n-521}$$

"shift-register RNGs"

triplet correlations

period := largest possible $\cong 2^{250} \simeq 2 \cdot 10^{75}$

$\gg 10^{46}$

combine 250 & 521 via XOR of the output

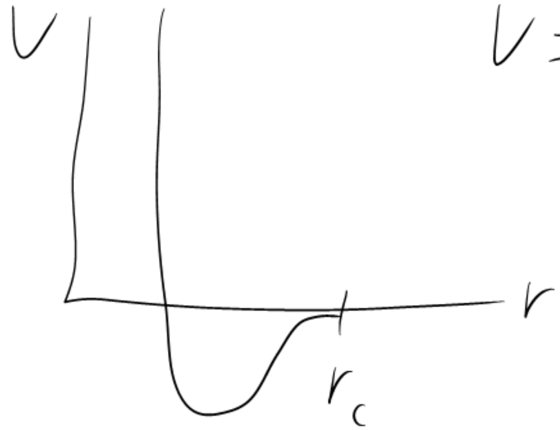
Molecular Dynamics

$$m_i \ddot{\vec{r}}_i = \vec{F}_i = -\frac{\partial U}{\partial \vec{r}_i}$$

$$V_{LJ} = \begin{cases} 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] & r < 2.5\sigma \\ 0 & \text{else} \end{cases}$$

typically:

$$U = \sum_{i<j} V(|\vec{r}_i - \vec{r}_j|)$$



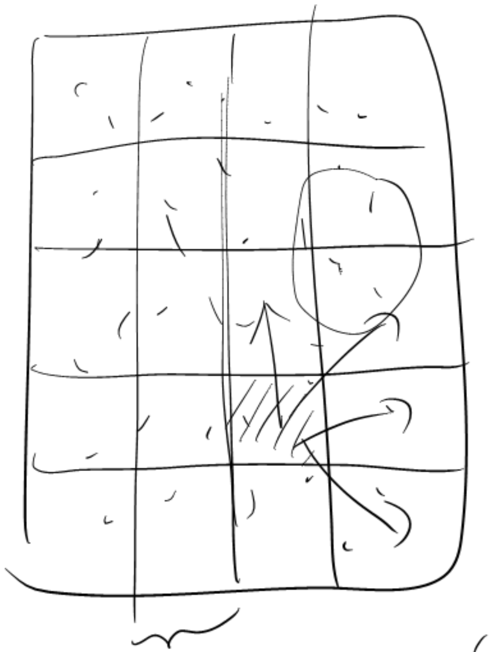
$V = 0$ for $r > r_c$

Short-range interactions

(i) how to calculate $\vec{F}_i$?

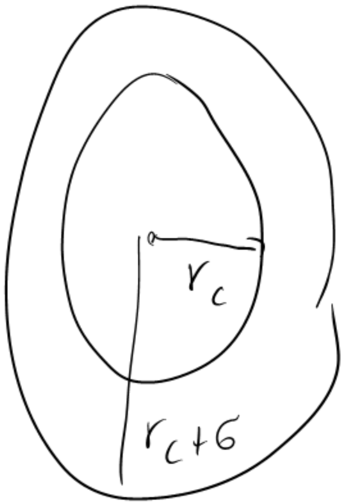
- all pairs: $O(N^2)$ $\quad \frac{N(N-1)}{2}$

boxes: $O(N)$ calculation



$r_c + \sigma \longrightarrow$ "skin" $\sigma > 0$

Verlet table:



Store all the neighbors within $r_c + \sigma$, for each particle

$$\max_i \Delta r_i^2 > \frac{\sigma^2}{4} \text{ : UPDATE}$$

$\sigma/2$ $\sigma/2$

before

$r_c + \sigma$

after:

r_c

problem (ii) Integrate Newton II !

useful: so-called "symplectic integrators"

based on Hamiltonian formalism

[Leimkuhler / Reich, Simulating Hamiltonian Dynamics]

$$\dot{q}_i = \frac{\partial \mathcal{H}}{\partial p_i} \qquad \dot{p}_i = -\frac{\partial \mathcal{H}}{\partial q_i}$$

Liouville operator

$$\frac{d}{dt} A = \sum_i \Big(\underbrace{\frac{\partial \mathcal{H}}{\partial p_i} \frac{\partial}{\partial q_i}}_{i\mathcal{L}_q} - \underbrace{\frac{\partial \mathcal{H}}{\partial q_i} \frac{\partial}{\partial p_i}}_{i\mathcal{L}_p} \Big) A = i\mathcal{L} A$$

$$i\mathcal{L} = i\mathcal{L}_q + i\mathcal{L}_p$$

specialization:

$$\mathcal{H} = T(\{p_i\}) + U(\{q_i\})$$

$$i\mathcal{L}_q = \sum_i \frac{\partial T}{\partial p_i}\frac{\partial}{\partial q_i} \qquad i\mathcal{L}_p = \sum_i \left(-\frac{\partial U}{\partial q_i}\right)\frac{\partial}{\partial p_i}$$

$$= \sum_i \frac{\partial}{\partial q_i}\frac{\partial T}{\partial p_i} \qquad = -\sum_i \frac{\partial}{\partial p_i}\frac{\partial U}{\partial q_i}$$

$\mathcal{L}$ is self-adjoint, but also $\mathcal{L}_q$ and $\mathcal{L}_p$ separately

$$(A|\mathcal{L}_q B) = \frac{1}{i}(A|i\mathcal{L}_q B) = \frac{1}{i}\int d\Gamma\, A^*(\Gamma)\sum_i \frac{\partial T}{\partial p_i}\frac{\partial}{\partial q_i} B(\Gamma)$$

$$= -\frac{1}{i}\int d\Gamma\, B(\Gamma)\sum_i \frac{\partial T}{\partial p_i}\frac{\partial}{\partial q_i} A^*(\Gamma) = -\frac{1}{i}\int d\Gamma\, B(\Gamma)\, i\mathcal{L}_q A^*(\Gamma)$$

$$= \int d\Gamma\, B(\Gamma)\underbrace{(-\mathcal{L}_q)}_{\mathcal{L}_q^*} A^*(\Gamma) = \int d\Gamma\, B(\Gamma)\left[\mathcal{L}_q A\right]^* = (\mathcal{L}_q A|B)$$

$\mathcal{L}_p$: analogous!

e^{iLt} unitary, $e^{iL_q t}$ unitary, $e^{iL_p t}$ unitary

would <u>like</u> to know:

$e^{iLt} q_i$, $e^{iLt} p_i = ?$ HARD!

$e^{iL_q t} q_i = ?$ $e^{iL_p t} q_i = ?$

$e^{iL_q t} p_i = ?$ $e^{iL_p t} p_i = ?$ EASY!

$$\exp(i L_q t) = \sum_{n=0}^{\infty} \frac{t^n}{n!} (i L_q)^n = \sum_{n=0}^{\infty} \frac{t^n}{n!} \left\{ \sum_j \frac{\partial T}{\partial p_j} \frac{\partial}{\partial q_j} \right\}^n$$

$$\exp(i L_q t)\, q_i = q_i + t \frac{\partial T}{\partial p_i} = q_i + v_i t$$

$$\exp(i L_q t)\, p_i = p_i$$

$$\exp(i L_p t)\, q_i = q_i$$

$$\exp(i L_p t)\, p_i = p_i - \frac{\partial U}{\partial q_i} t = p_i + F_i t$$

operator-splitting

time step h, $h \to 0$

$$\exp[i(L_q + L_p)h] \simeq \exp\{iL_p \tfrac{h}{2}\} \exp\{iL_q h\} \exp\{iL_p \tfrac{h}{2}\}$$

$\Downarrow$ + error: $O(h^3)$ or smaller

Taylor w.r.t. h:

agreement up to $O(h^2)$ inclusively

$\to$ conserves the phase-space volume

$\to$ $h \to -h$: time-reversal symmetric algorithm:

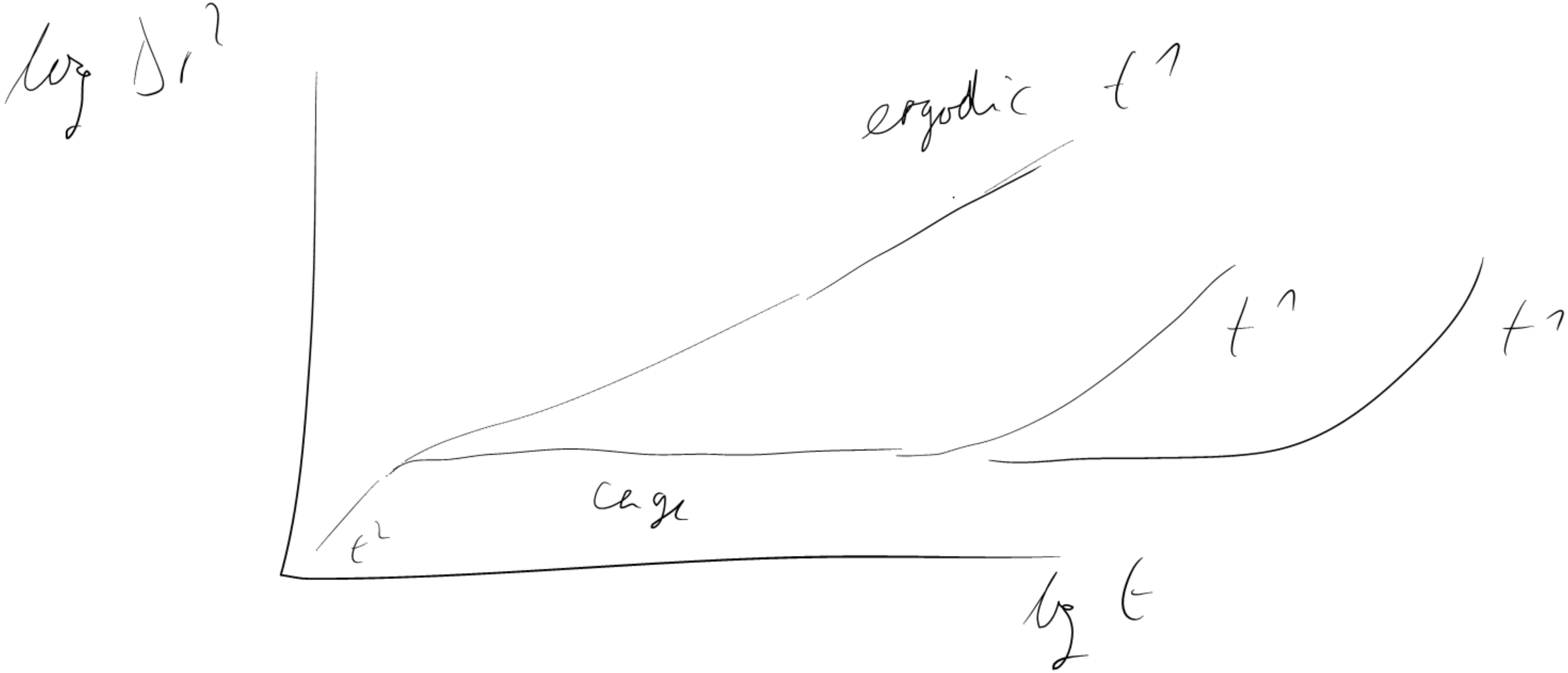
$$p_i\left(\frac{h}{2}\right) = p_i(0) + F_i(0)\,\frac{h}{2}$$

$$q_i(h) = q_i(0) + v_i\left(\frac{h}{2}\right) h$$

$$p_i(h) = p_i\left(\frac{h}{2}\right) + F_i(h)\,\frac{h}{2}$$

velocity Verlet

time step: 10^{-2} x shortest oscillation time



log Δr²
ergodic t¹
t¹
t¹
cage
t²
log t