Exploring factorizations in the event chain algorithm

application to particle simulations

A.C. Maggs

CNRS-ESPCI

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Werner Krauth and Ze Lei: Phys. Rev. E 99, 043301

ECMC: Replacing Monte Carlo and Molecular Dynamics

Can one find algorithms that better equilibrate for thermodynamic simulation?

However: multiple criteria:

- Single particle motion, diffusion speed
- Auto-correlation of energy/density – fluctuations near equilibrium
- Mixing times – worst case – includes nucleation

Exploit freedom to split potentials in ECMC to optimize speed

Major algorithms today

- Metropolis Monte Carlo
  - large individual steps
  - slow diffusive explorations of space
  - exact sampling
- time step driven molecular dynamics
  - propagative modes
  - small steps for stability

Event chains have the potential of : large steps, propagation, exact sampling

Hydrodynamics in simple fluids

MD: Slow modes in large systems are hydrodynamic: linked to conservation laws

- Mass
- momentum
- energy

Gives rise to

- sound: $\omega = cq$
- heat: $\omega = Dq^2$
- vorticity: $\omega = D'q^2$

Modes with dynamic exponent $z = 1$ and $z = 2$: $\tau \sim L^z$

MC: single conserved quantity: density, $\omega = D''q^2$ for $\langle \rho(r,t)\rho(0,0) \rangle$

- CF: Onsager, Talk of Masaharu Isobe
- Hydrodynamic theories of liquid crystals, multicomponent systems

Dynamics of ECMC

Very great flexibility in the formulation: There is not just one ECMC

Does this change the large scale dynamics? Lennard-Jones potential

$$U_{LJ} = \frac{1}{r^{12}} - \frac{1}{r^6}$$

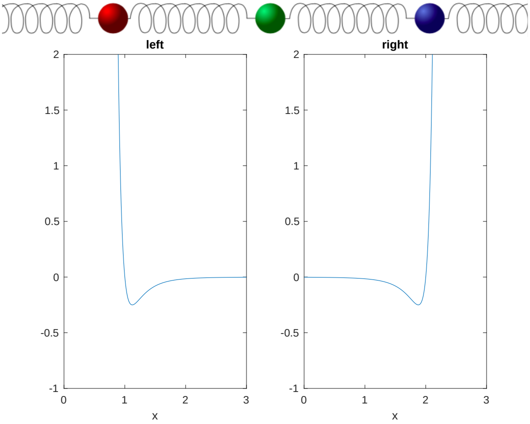
Can split LJ into components, independent management of $1/r^6$ and $1/r^{12}$.

Here: Only factors over pairs, keeping these contributions together, but will add extra "factor field "

What is the exponent z for ECMC? Reminder $\tau \sim L^z$ want z small

1D interaction with left and right particles

Green particle active, moving to the right:

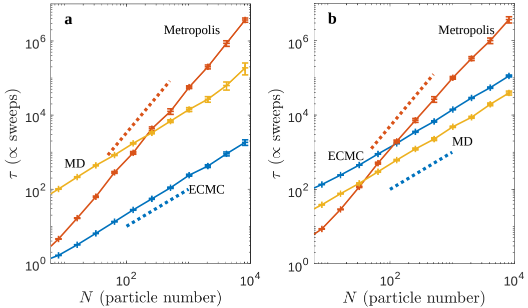


Remember: events when potential is increasing

Lifting can go left and right, even if particle motion is uni-directional

Does it work? Lennard-Jones Chains

Measure dynamics of slowest Fourier density mode
Autocorrelation time : $cpu \sim N^{z+1}$



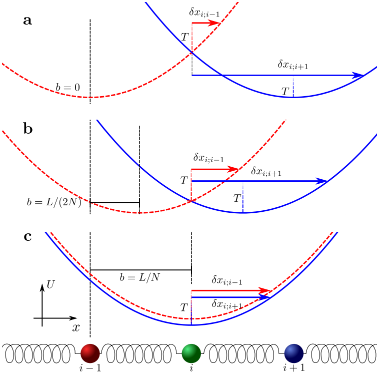
- See dynamic exponent $z = 2$ for metropolis, $z = 1$ for MD and event chain.
- High and low temperatures: it works sometimes...

Harmonic model

- Low temperature LJ is also harmonic, so why is it slow?

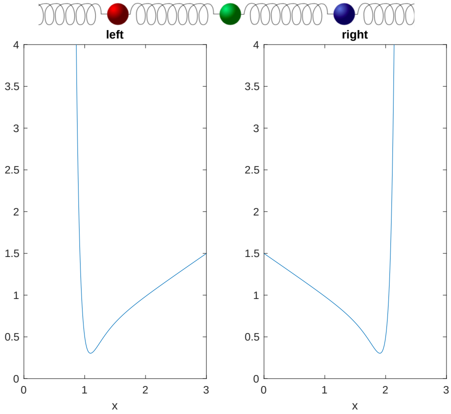
$$U \sim \sum_i (x_i - x_{i-1} - b)^2$$

Stretched chain: step sizes falls with temperature



Factor field

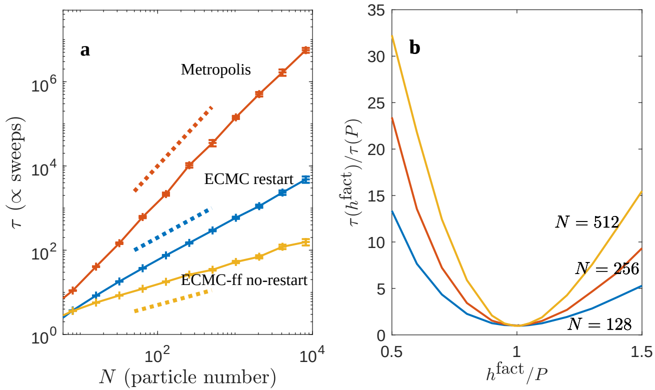
- Add in a constant to the energy: $\Delta U = -h \sum (x_{i+1} - x_i) = -hL$
- Does not change thermodynamics, only changes dynamics



Choose the special value $h = P$

Autocorrelation times

Low temperature LJ: the bad case



Super-fast relaxation: $z = 1/2$, hard-rods and LJ.

Large scale motion

- Strong change in the nature of the dynamics at the special value of h.

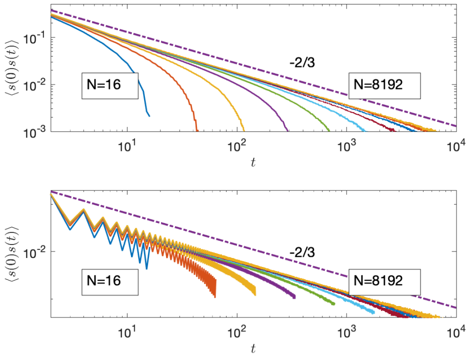
$$P \sim \frac{1}{|s - s'|} \langle x_{i(s)} - x_{i(s')} \rangle \quad \text{drift speed of activity}$$

  (Michel, Kapfer, Krauth)

- Special value of the factor-field corresponds to zero mean speed for the active position.
- Is the activity diffusing?

Lifting correlations

define $u = \pm 1$ for left/right lifting , measure $\langle u(0)u(s)\rangle$
Like a velocity-velocity correlation function



$\langle u(0)u(s)\rangle \sim s^{-\gamma}, \quad \gamma = 2/3$
(Displacement)^2: $\langle i(s)^2\rangle = \int\int \langle u(s)u(s')\rangle ds\, ds' \sim s^{2-\gamma} \sim s^{4/3}$

Exponent identities

Consider s liftings
(Index) distance explored:

$$\langle |i(s)| \rangle \sim s^{1-\gamma/2} \sim s^{2/3}$$

Hyperdiffusion law: but we can link z and γ:

In the autocorrelation time activity explores the whole chain

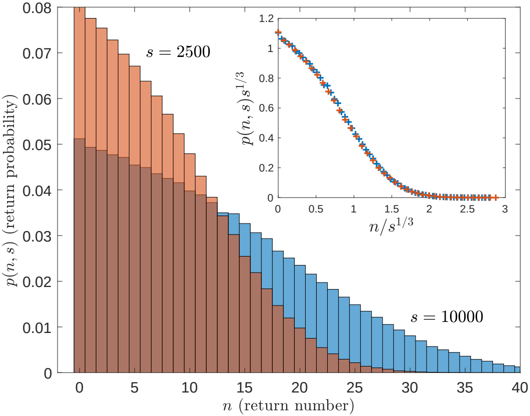
$$(N^{(1+z)})^{(1-\gamma/2)} = N, \qquad z = \gamma/(2-\gamma) = 1/2.$$

Return probability: Local time

How far does a single particle move?

It advances whenever activity returns to origin

Count returns to origin



number of steps of a given particle increases as $s^{1/3}$

Conclusions+questions

- Distinct dynamics generated by ECMC, different from MD and MC
- Factor-fields lead to acceleration, but anomalous dynamics $|i| \sim s^{2/3}$, $z = 1/2$
- Factor fields in 2 and more dimensions : is it possible to generalise?
- Soft-matter simulation with general potentials

- What is the dynamic process for the hyperdiffusive walk? We have the scaling theory
- What are the “hydrodynamic” equations of this kind of algorithm?