

Multiresolution coarse-graining of polymer models

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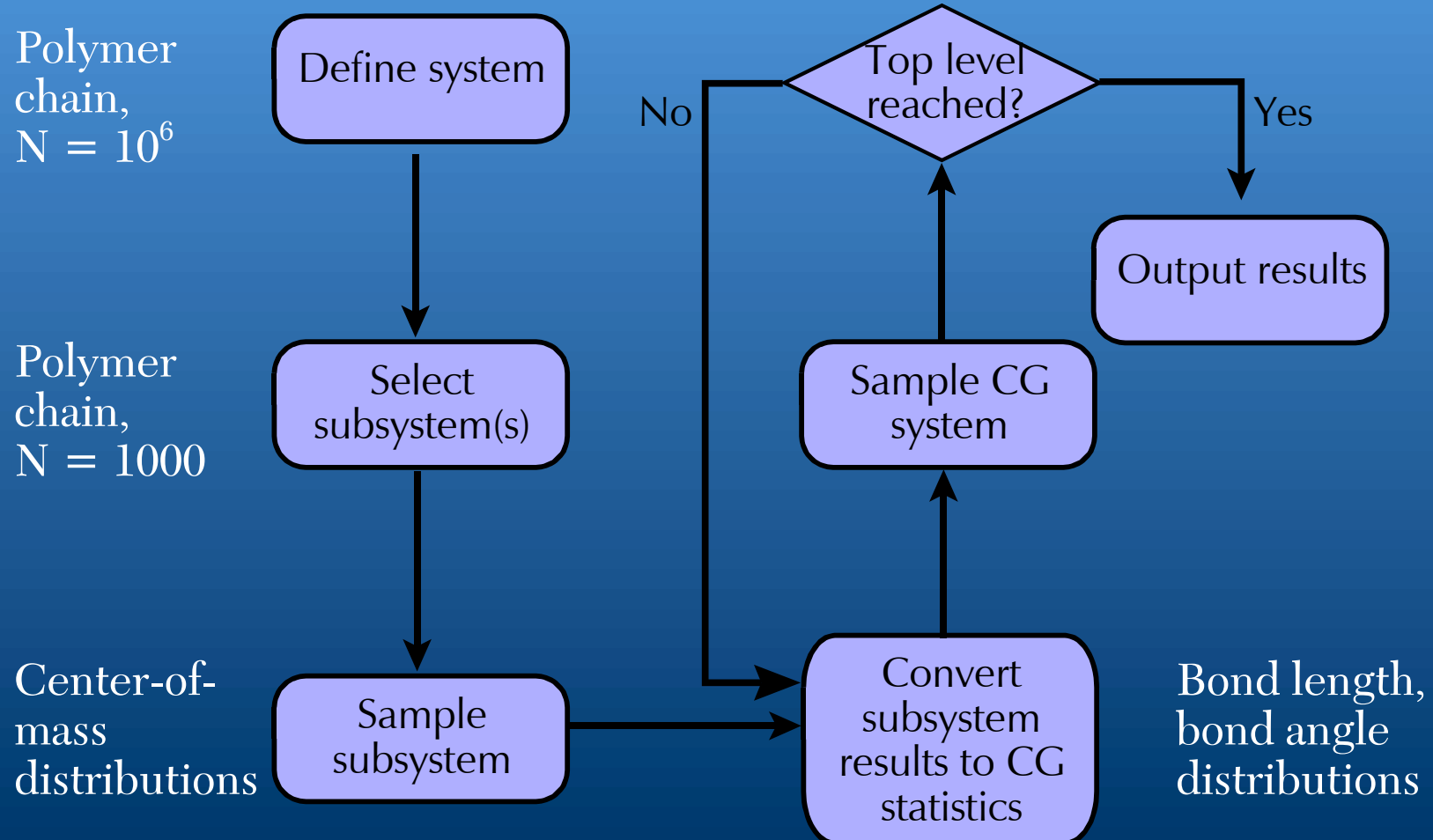
Motivations

Why?

- Better materials design requires a detailed understanding of polymer properties
 - ▶ Examples: size distributions, rigidity, density, morphology
- Atomistic simulations with current computational capabilities are still not feasible
 - ▶ Current limits: approximately 200,000 “atoms”
 - ▶ Moore’s law won’t help much: algorithms still $O(N^3)$

Coarse-graining paradigm

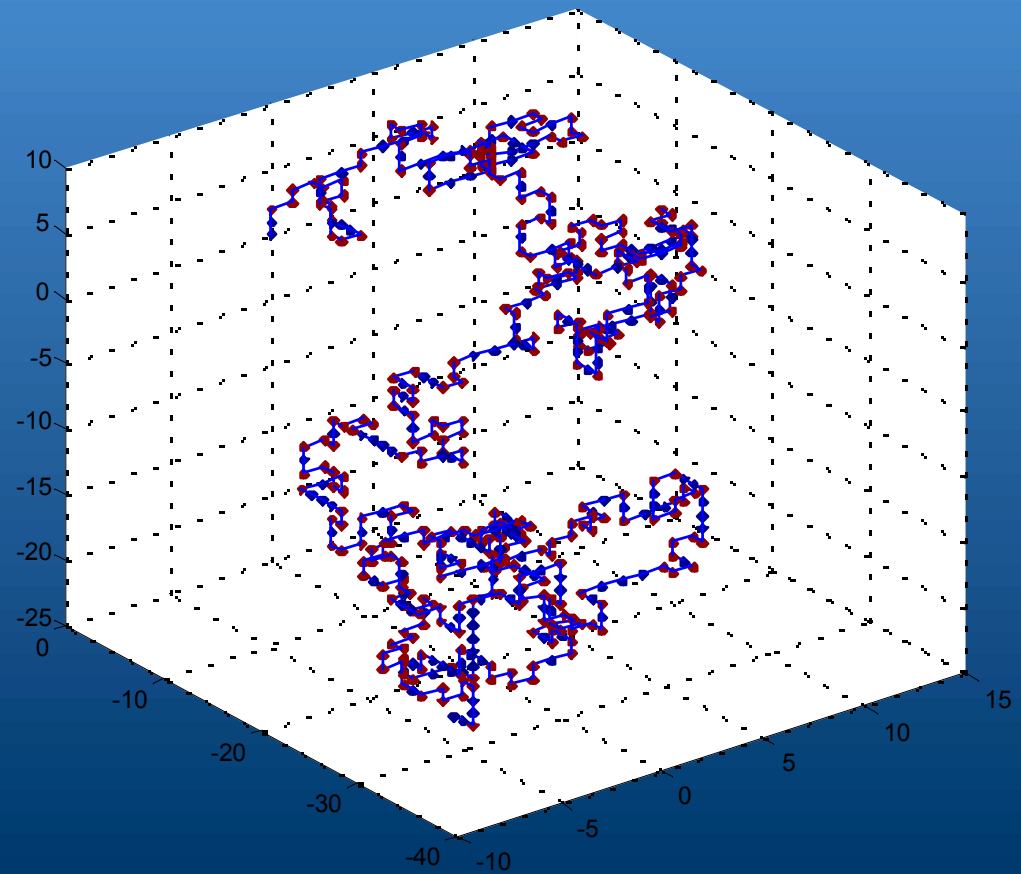
A “divide and conquer” hierarchical modeling scheme



Polymer models

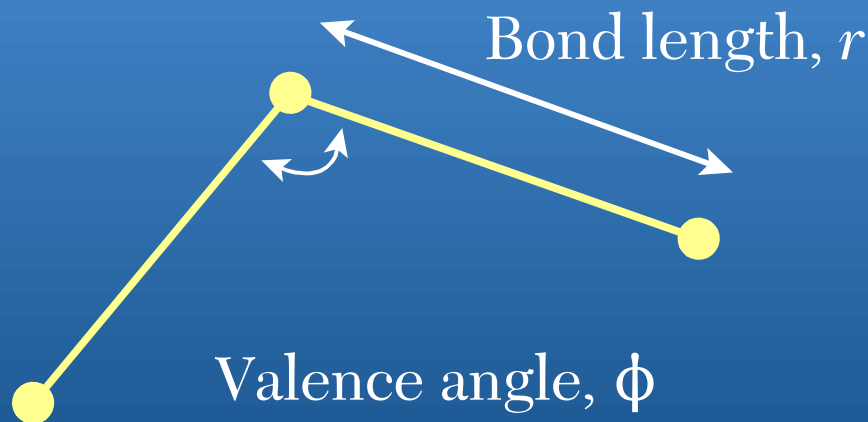
Lattice (random walk) models

- Beads are restricted to the sites of a simple cubic lattice.
- Stiffness “penalty” associated with changes in direction.
- Non-bonded interactions also possible.



Properties to pass between scales

Distributions of bond lengths and dihedral angles

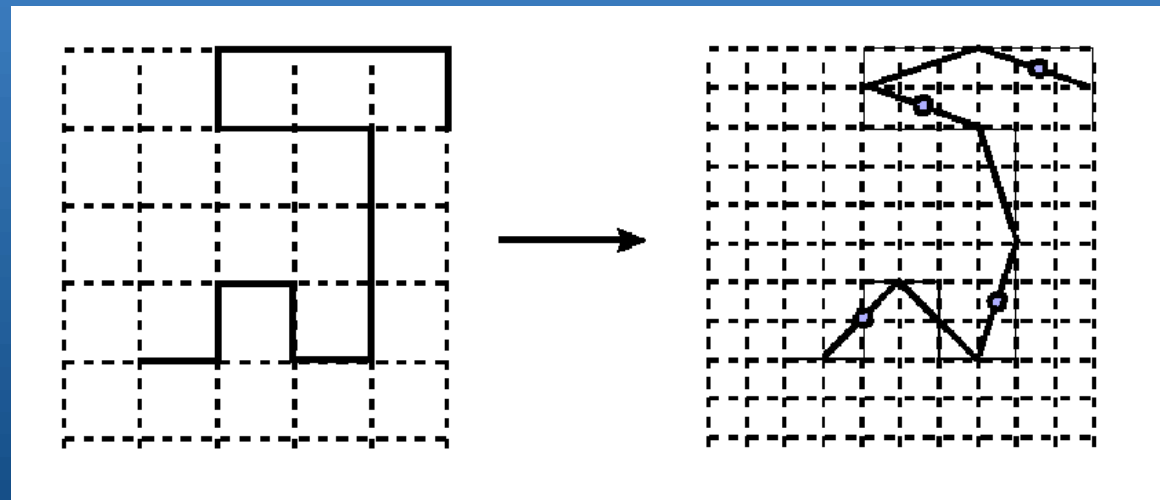
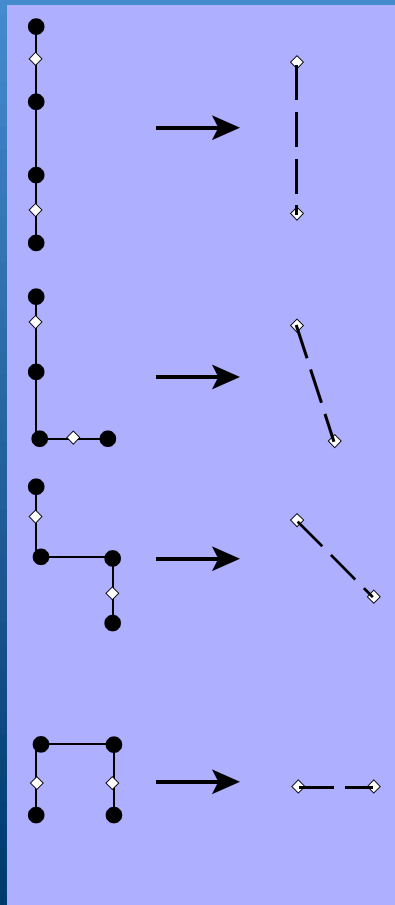


Bond length: distance between adjacent centers-of-mass of N_p consecutive particles along original chain

Valence angle: Spherical angle formed by two adjacent center-of-mass bonds

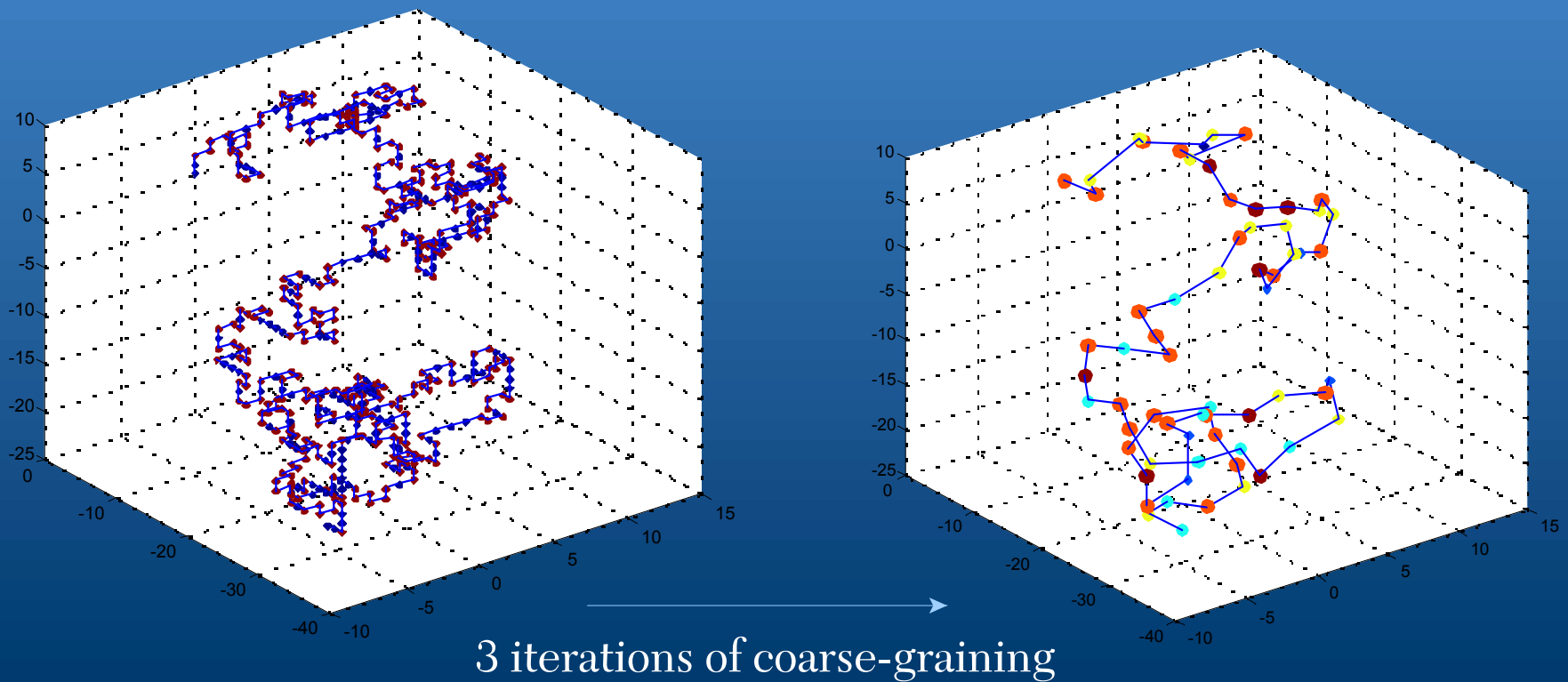
Coarse-graining of bonds

Beads are replaced by centers-of-mass; differences stored



Recursive coarse-graining

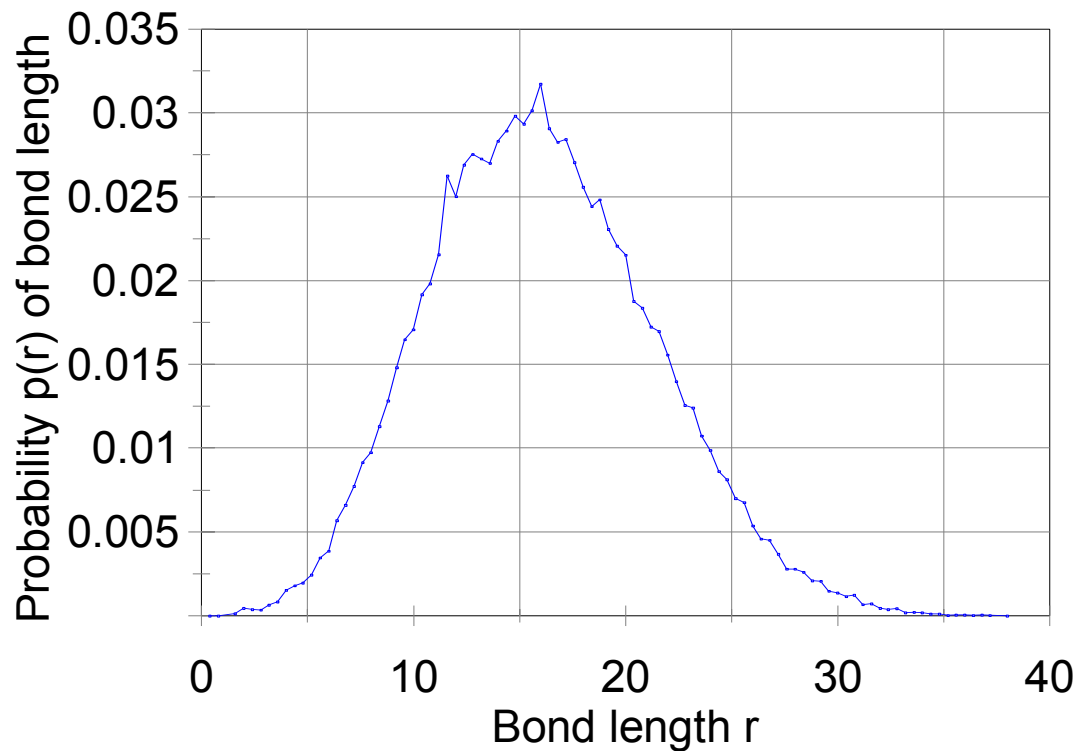
Repeated application yields increasingly coarse description



Moving between scales

Distributions, not complete data, required

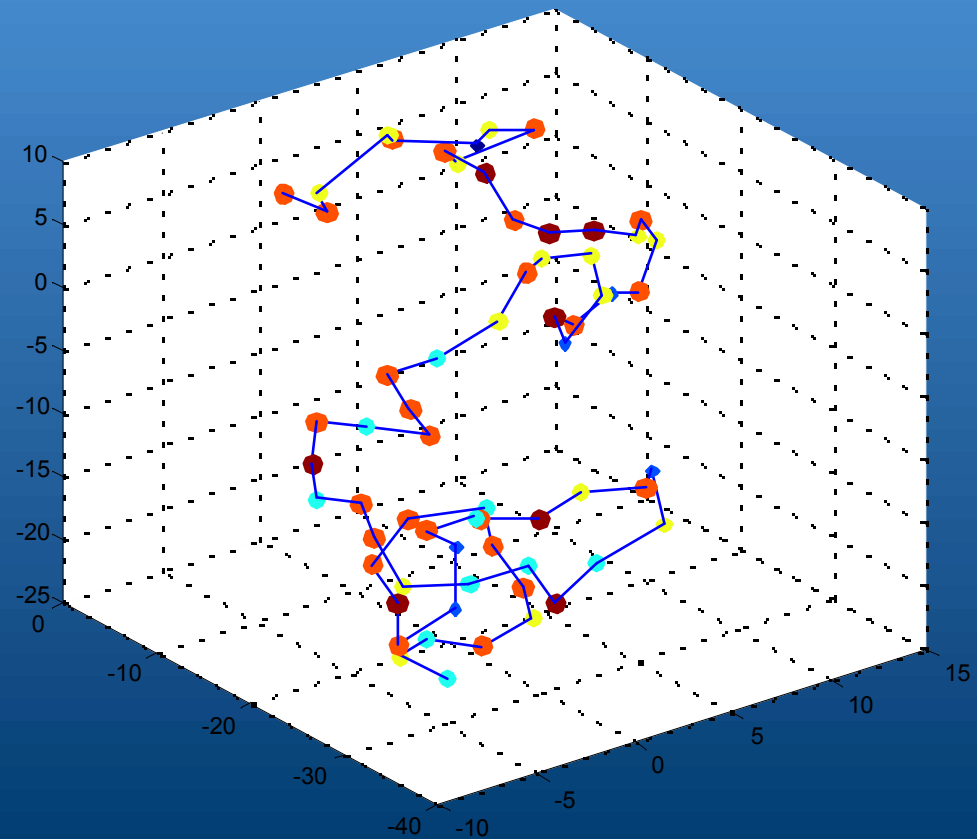
- It is not necessary to keep track of all of the details of the bond lengths of the system; just the overall probability distribution.



Polymer models

Bead-and-chain model

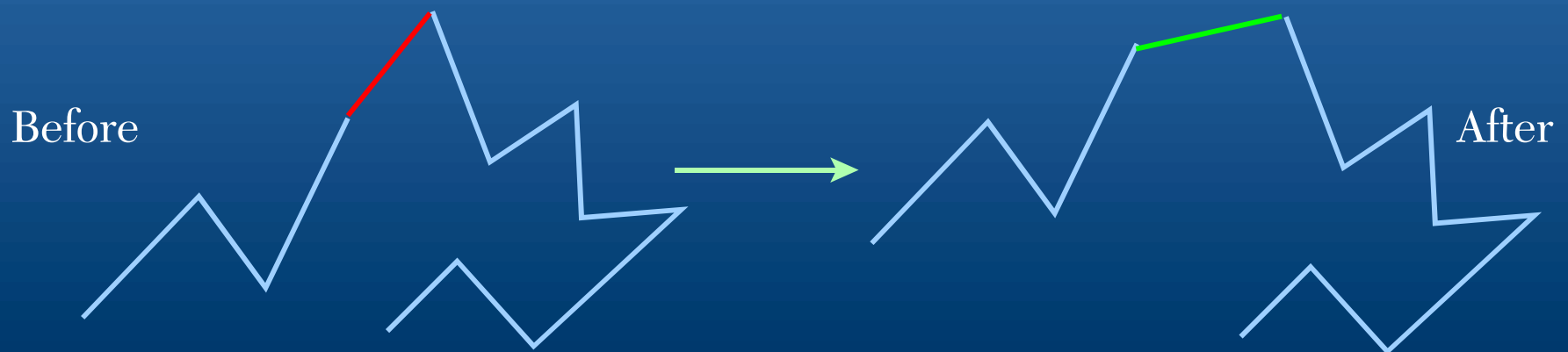
- Beads are connected to one another via flexible or rigid chains
- Energies function of distance between beads
- Particles have “excluded volume”



Coarse-grained algorithm

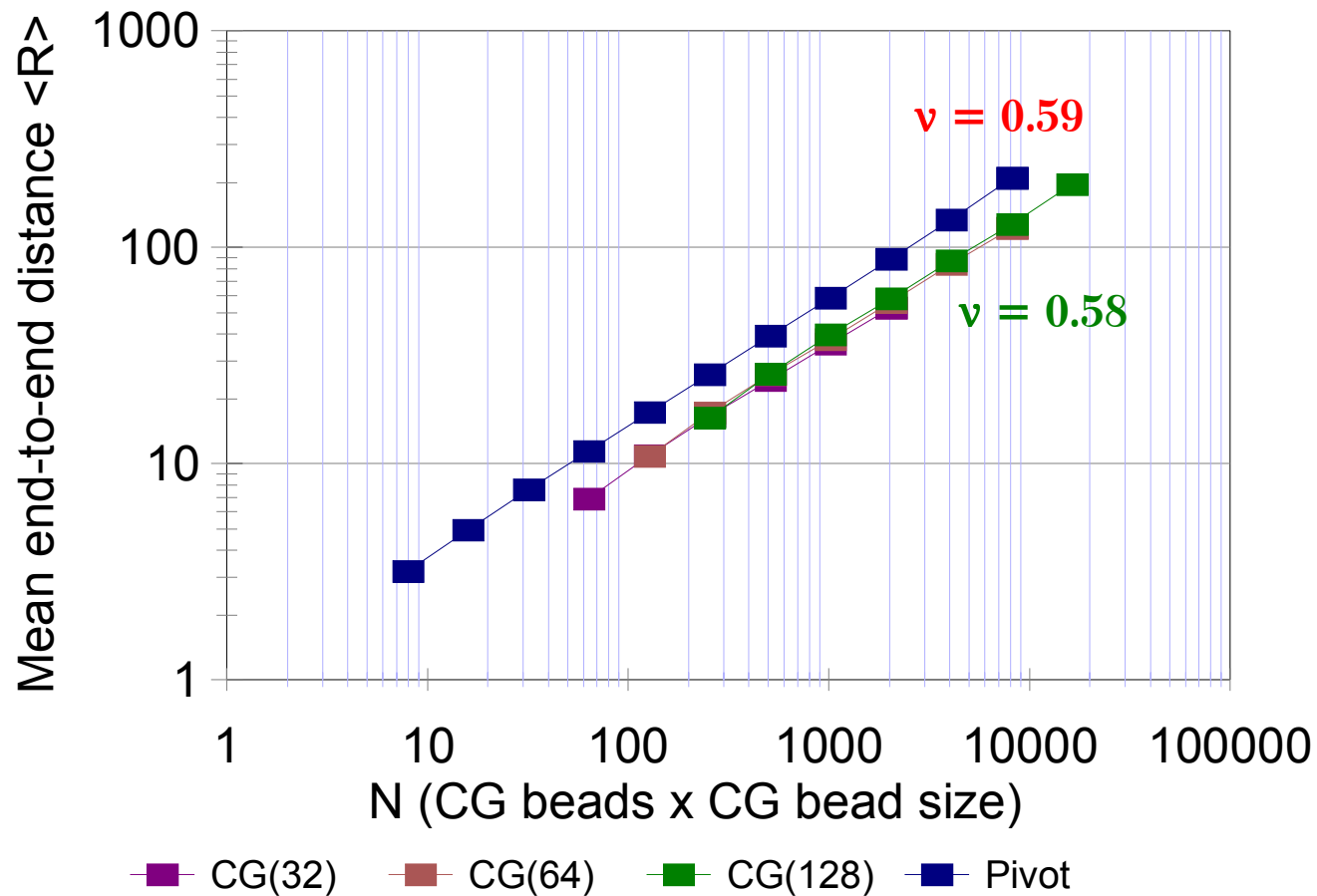
Generalized reptation-like moves

- Select a bond and generate new bond length and angle
- Drag one side of chain correspondingly
- Check for self-avoidance of new configuration
- Accept or reject state according to Boltzmann weights
- $O(N)$ between independent configurations (DDDA)



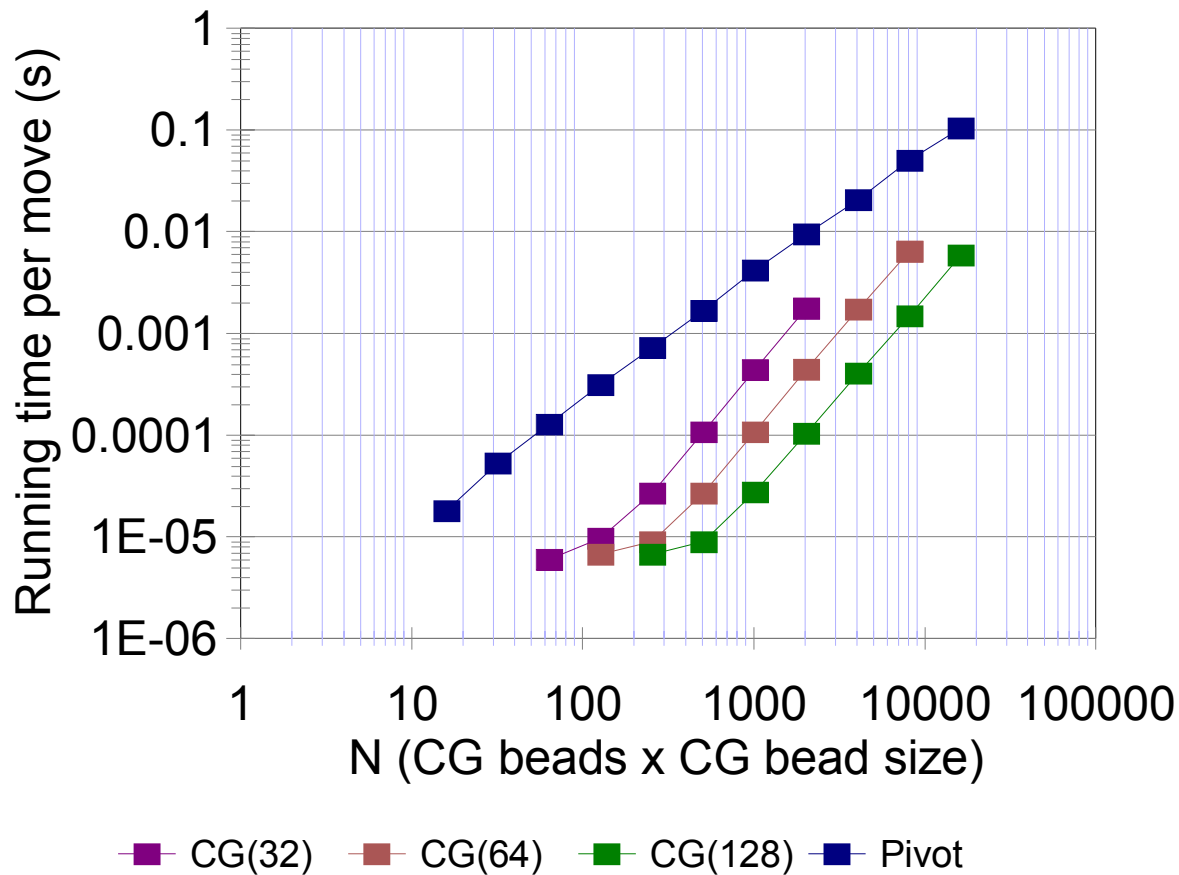
Coarse-graining v. atomistic model

Scaling preserved across CG scales



Coarse-graining v. atomistic model

Performance of CG model orders of magnitude faster



Pivot algorithm: $O(N)$.
CG algorithm: $O(N^2)$,
unoptimized.

But $N_{cg} \ll N_p$, so CG
algorithm is still
much faster.

Also, CG running
time is independent
of resolution scale.

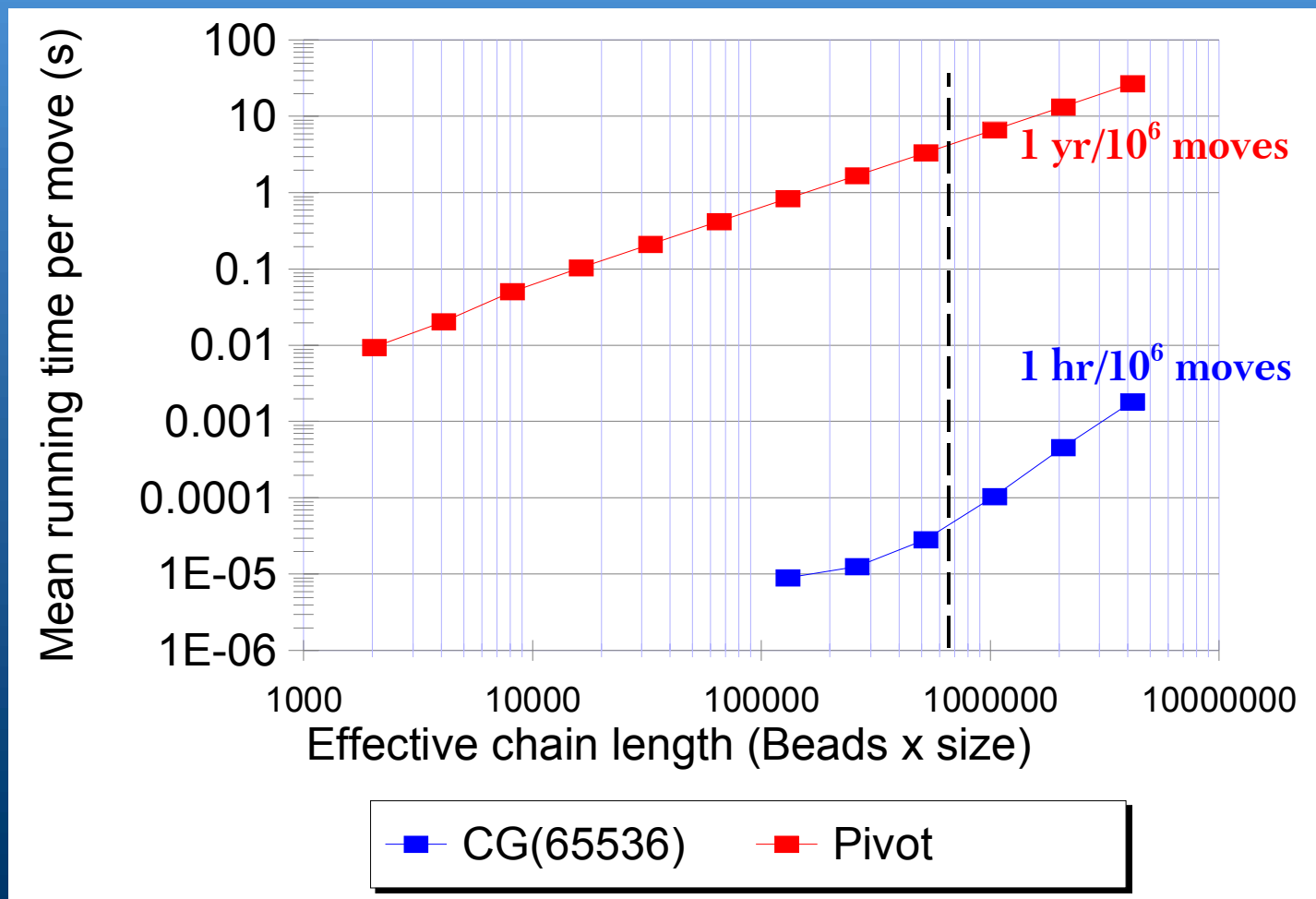
Extending the model

Making the model truly “multiresolution”

- Our coarse-grained algorithm *doesn't care where its inputs come from*:
 - ▶ Experimental data
 - ▶ Detailed atomistic simulation
 - ▶ Another coarse-grained simulation at a finer scale.
- We can perform simulations at one scale, and feed the resulting data into the simulation at a coarser scale.

Hierarchical model results

Four-stage model performance comparison



Conclusions

A highly-efficient coarse-graining method

- Without correcting potentials or other “fixes,” correct scaling results are obtained, even across multiple levels of simulation.
- *Unoptimized performance* is orders of magnitude faster than efficient atomistic simulations.
- Easily able to simulate system lengths currently unobtainable via direct atomistic simulations.

Applications

Extensions of the model

- Multiple chains and polymer melts
- Fitting of coarse-grained potential models
- Extensions to sample problems
 - ▶ Polymer-colloid interactions
 - ▶ Charged polymers
 - ▶ Phase diagrams
 - ▶ Polydisperse models

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Questions?
