Progress in parallelization of ECMC in 2D hard-sphere system

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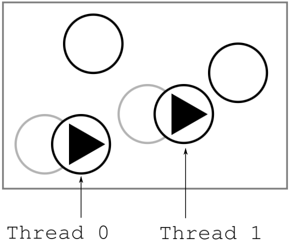
ECMC with multiple active spheres

A multiple-active-sphere straight event-chain (SEC) algorithm

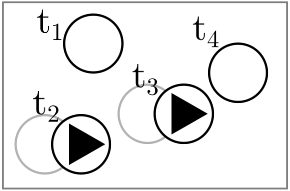
- Conceptual: all active spheres moves at same velocity at the same time (no interaction between active)
- Real: same direction and chain length, active spheres out-of-sync during the run, synchronized at the beginning and the end of the run



Pressure calculation $\beta P = \rho + \beta \frac{1}{l} \sum_{\text{lifting moves } i \to j} (x_j - x_i)$ (Michel, Kapfer, Krauth, J. Chem. Phys. 2013)
becomes $\beta P = \rho + \beta \frac{1}{kl} \frac{N-1}{N-k} \sum_{\text{lifting moves } i \to j} (x_j - x_i)$

Correctness of multithreaded ECMC

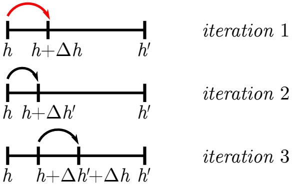
Local time t_i: time when sphere i reaches its current position



Horizon violation:

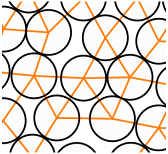
$$t_{active} < t_{target}$$

No horizon violation means correct final configuration. Restart if there is any horizon violation.



Implementation

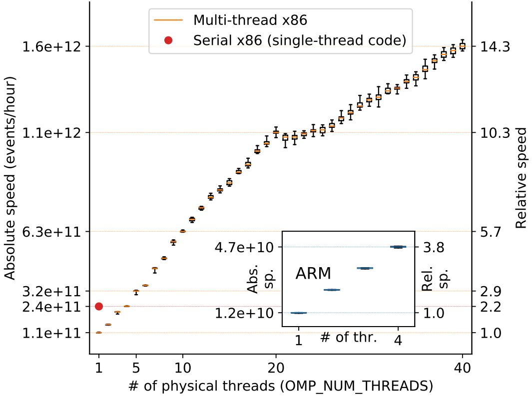
- Algorithm: multithreaded SEC algorithm in 2D hard-sphere system with constraint graph



  Constraint graph (Kapfer, Krauth, JPCS 2013): a neighbour list that lasts forever (single direction)
- Program written in C++ with OpenMP (shared memory)
- Use minimal amount of atomic variables
- Run on Intel Xeon 6230, 20(40) cores @ 2.10(3.90)GHz

Performance

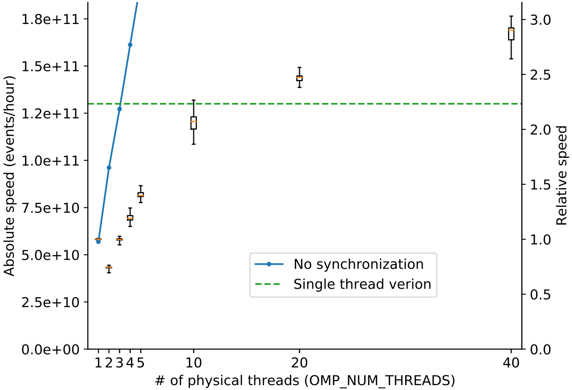
estimated # of events/hour when # of spheres $= 256^2$, no synchronization (Li, Todo, Maggs, Krauth, J. Comput. Phys. 2020)



Runs 100% in parallel, outputs wrong configuration, 100 times faster than in Bernard, Krauth, PRL 2011

Performance

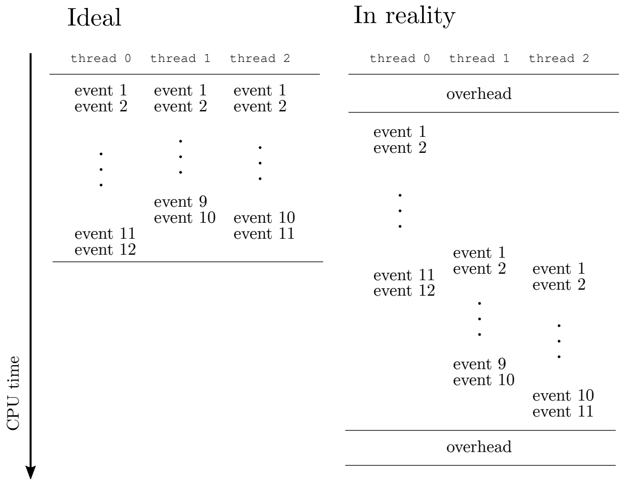
estimated # of events/hour when # of spheres $= 1024^2$ with synchronization (to be optimized)



10 times faster than in Bernard, Krauth, PRL 2011 (1.8×10^{10})
Constraint graph calculated on GPU (takes 1.5ms every 7ms)

Existing problems

- Parallel overhead



- Other optimization needed?

Conclusion

We

- found a parallelization scheme for ECMC
- obtained speedup in SEC algorithm
- believe that parallelization has potential

Future works

- State-of-the-art performance in 2D hard-sphere
- Generalizing the parallelization scheme and implement it in other systems/ECMC algorithms?

Collaborators: Synge Todo, A. C. Maggs, Werner Krauth, Yoshihiko Nishikawa

Based on Li, Todo, Maggs, Krauth, J. Comput. Phys. 2020 and manuscript in preparation