# GPU - Accelerated Free Energy Estimation

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# Motivation

Fluid in nano scale confinement

Decreasing the distance

Increasing the distance

Liquid – Solid Transition?

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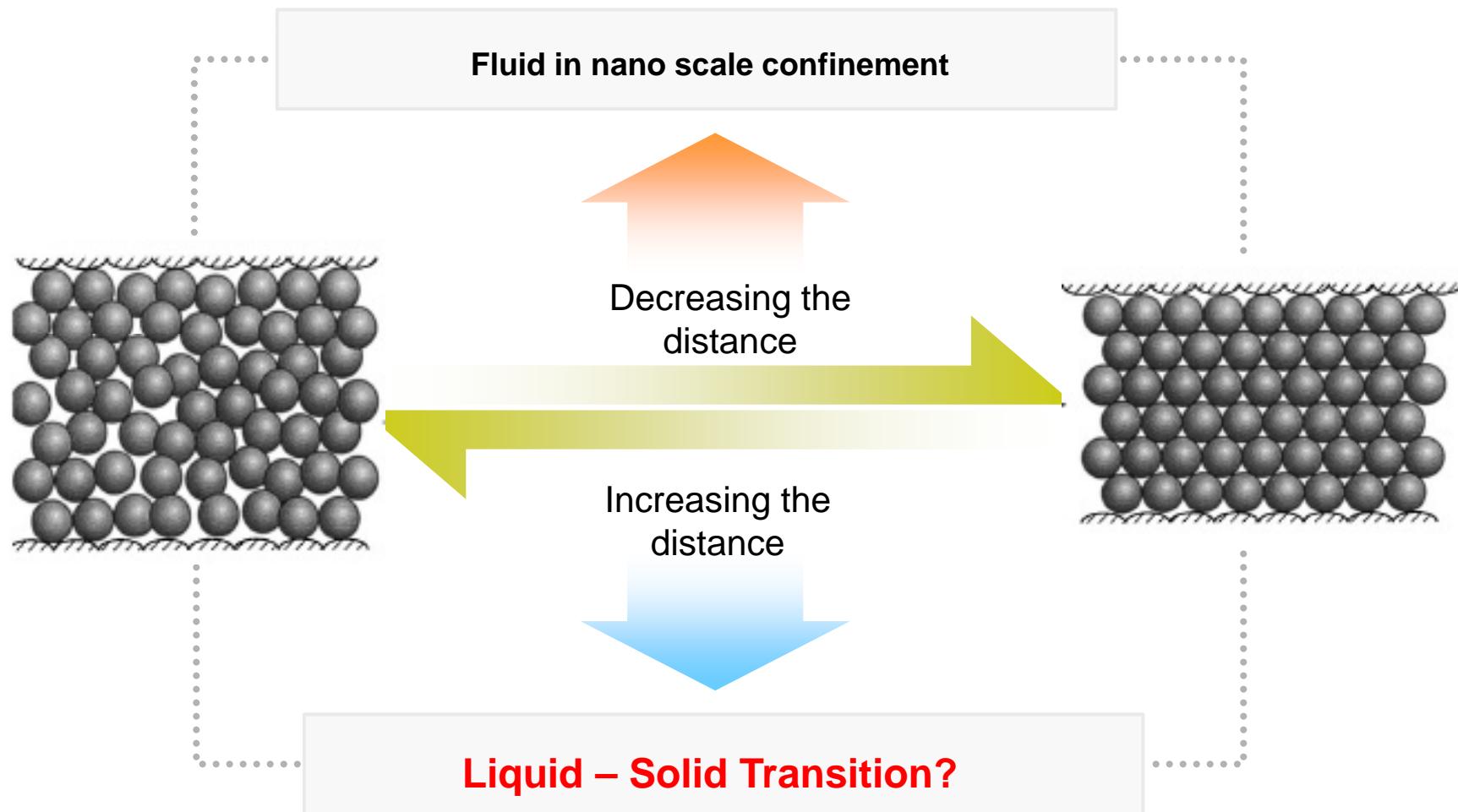
"Liquid-Solid Transition?"
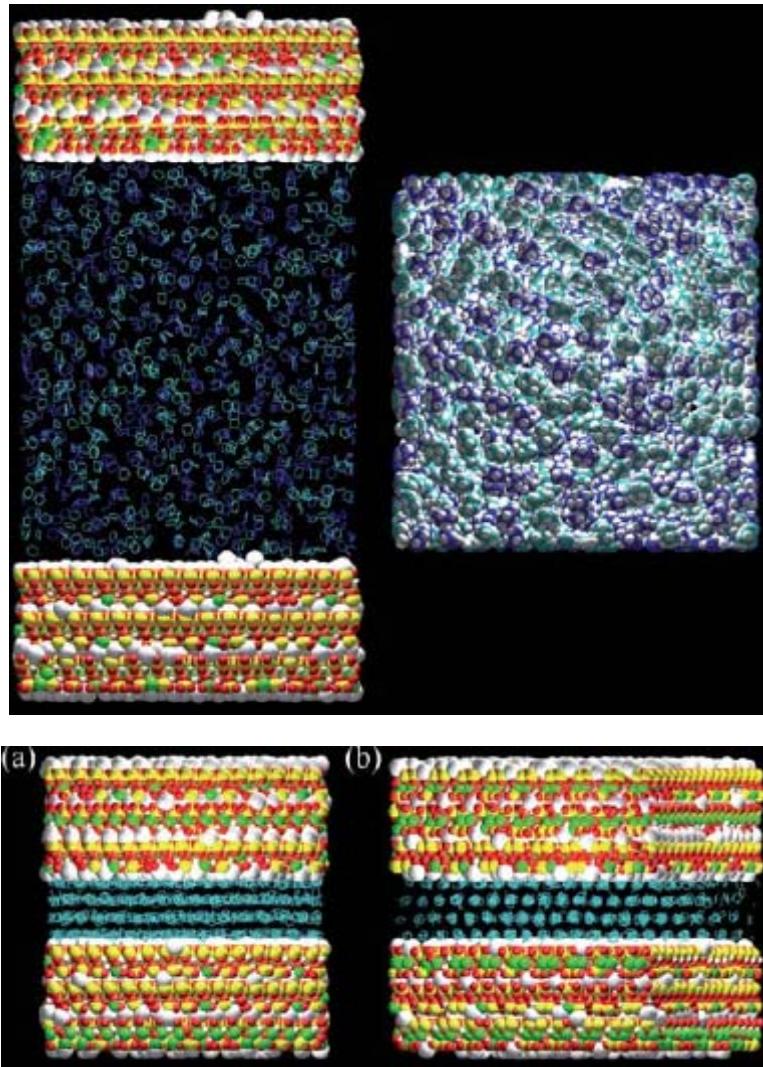
As the separation of two molecularly smooth wall is lower than a critical value, disordered state turns into an ordered state suddenly.

Docherty, H. and P.T. Cummings Soft Matter, 2010. 6(8): p. 1640-1643.

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Einstein Crystal Method

A

Total Free Energy
A0 + A1 + A2

10 or 20 MDs

A1

Turn on Intermolecular Interaction

A2

Turn off Spring Bond Interaction
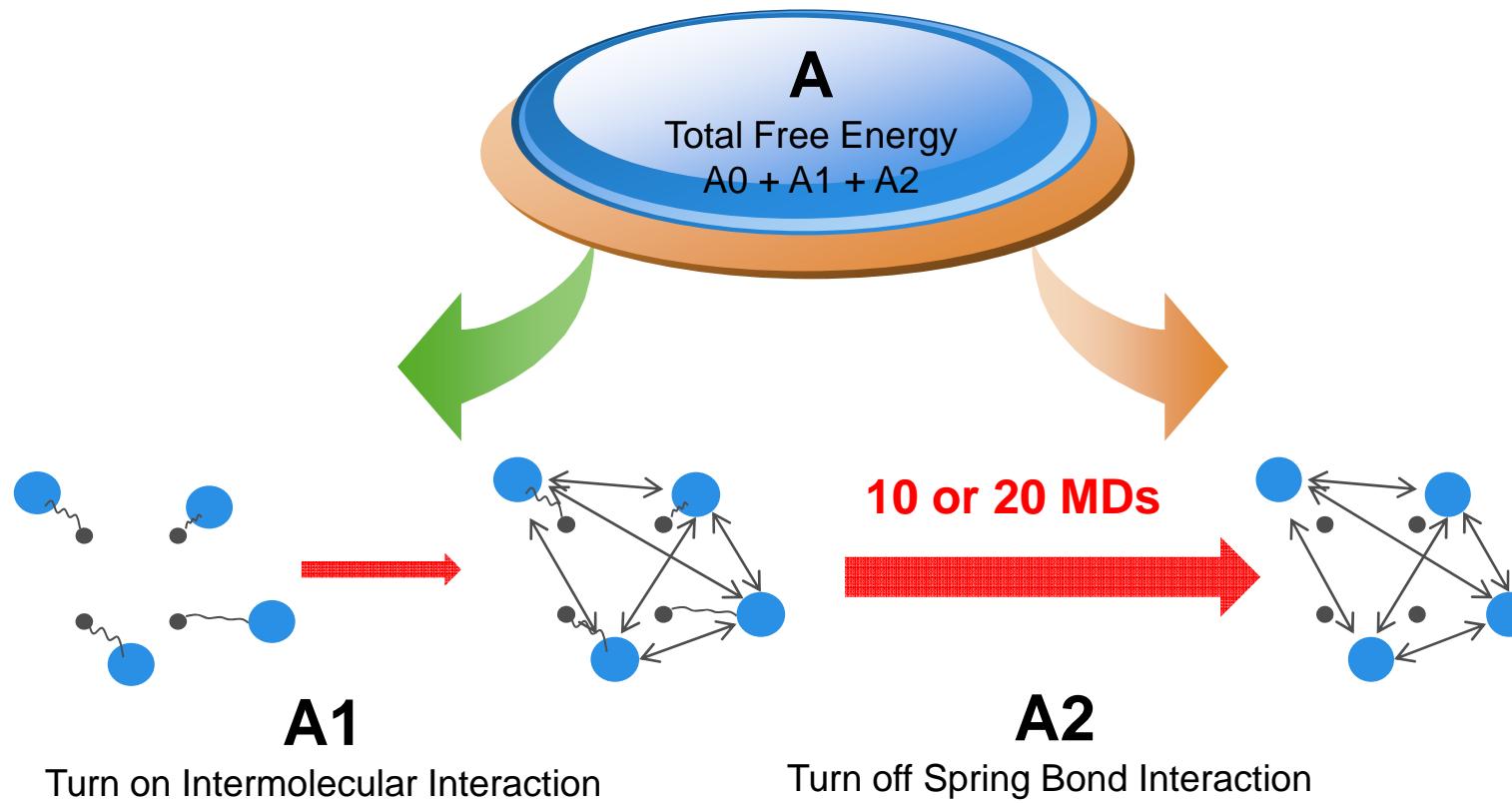
$$A_2 = A_{sol}^{CM} - A_{Ein-sol}^{CM} = -\int_{\ln(c)}^{\ln(\Lambda_E+c)} \frac{\left\langle U_{Ein-id} \right\rangle_{N,V,T,\lambda} (\lambda\Lambda_E + c)}{\Lambda_E} d(\ln(\lambda\Lambda_E + c))$$

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Potentials in MDs

Spring Interaction(between atom and its lattice site):

$$U_{Ein-id,i} = \Lambda_E (r_i - r_{i0})^2$$

Lennard-Jones potential:

$$U_{LJ,ij} = 4\varepsilon_{ij}\left[(\frac{\sigma_{ij}}{r_{ij}})^{12} - (\frac{\sigma_{ij}}{r_{ij}})^6 \right]$$

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Algorithms in CPU Approach

MPI

Spatial Decomposition
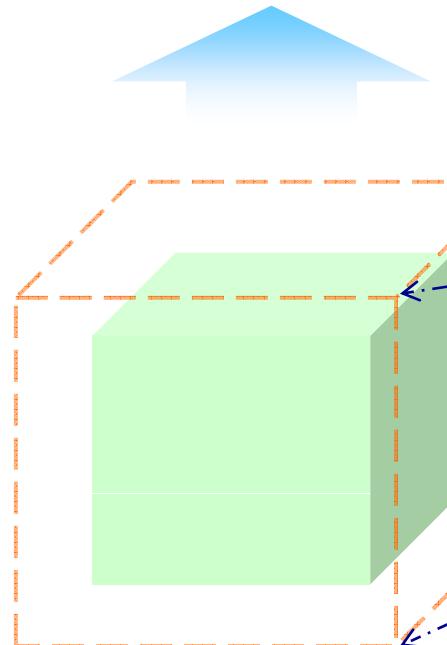
Verlet neighbor-list algorithm

http://www.intel.com
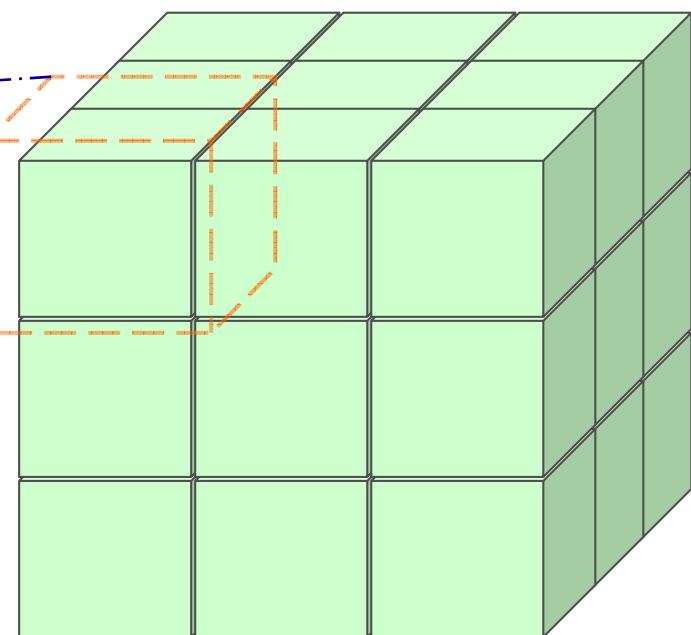
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Why GPUs?

http://codeblue.umich.edu/hoomd-blue/benchmarks.html
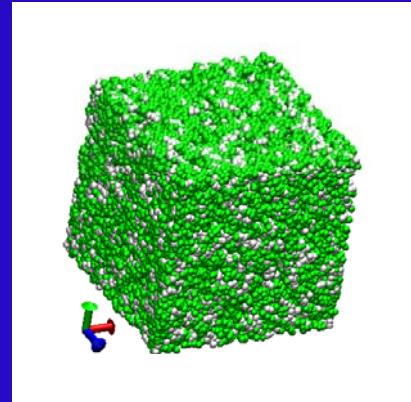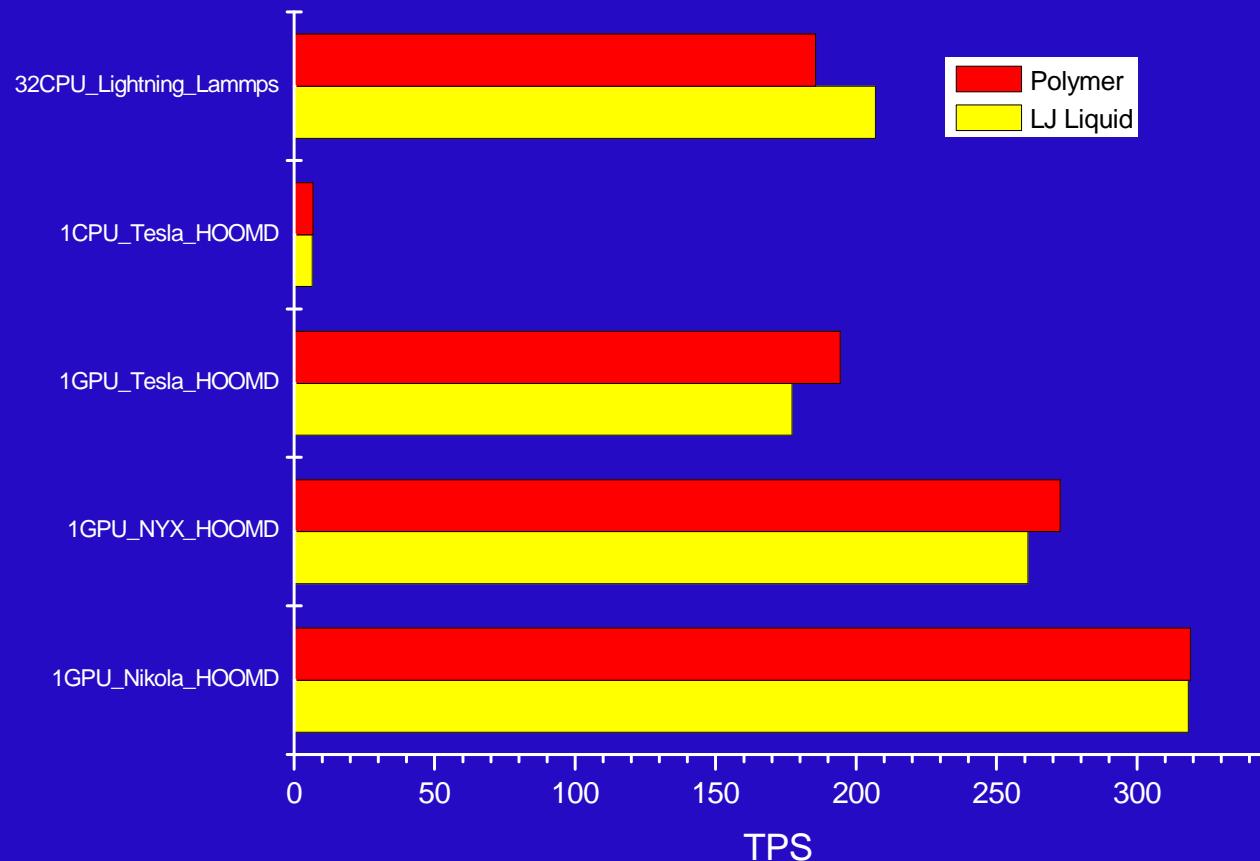
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Computing with GPU

Fermi Architecture

neighbor-list

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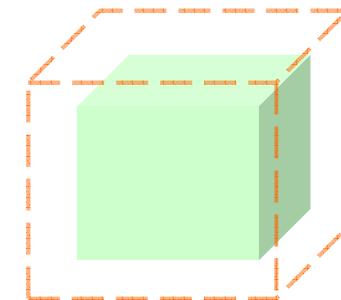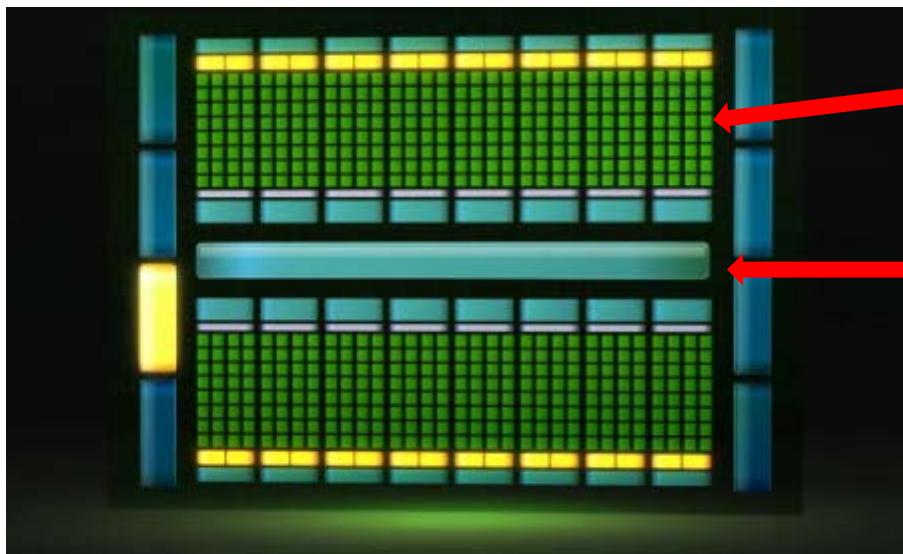
Thanks For Your Attention!