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GALAMOST: GPU-accelerated large-scale molecular simulation toolkit

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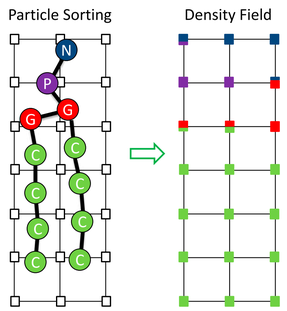
1. Abstract

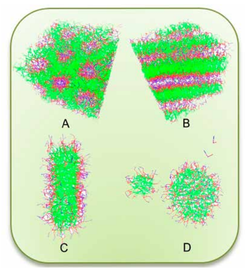
GALAMOST is a versatile molecular simulation package which is designed to utilize computational power of graphics processing units (GPUs) as much as possible. In addition to common features of molecular dynamics programs, it is developed specially for coarse-graining simulation of polymeric systems by encompassing some latest techniques, such as hybrid particle-field molecular dynamics, iterative Boltzmann inversion numerical potential method, soft anisotropic particle model, and chain-growth polymerization model. By continuously optimizing the algorithms, each method implemented on a single GPU by GALAMOST with the first released version 0.0.1 has gained a good performance.

2. Force fields

1. Alternative intermolecular force field

A hybrid particle-field molecular dynamics technique which can be regarded as an alternative analytical force field for intermolecular interactions has been ported from parallel CPU code OCCAM to GALAMOST. It replaces the pair interactions by the interactions on particles from the density field via coupling particle model to density field description to speed up some slowly evolving collective processes in MD simulations, such as micro-phase separation and self-assembly of polymeric systems. This method where self-consistent field theory and MD simulation are combined (MD-SCF) was proposed by Milano et al. (J. Phys. Chem.,2009, **130**, 214106).

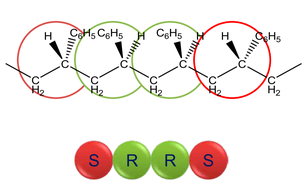


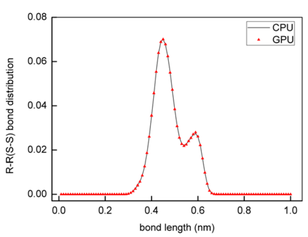


De Nicola et al. Theor. Chem. Acc. 2012, **131**, 1167

2. Numerical potential method

A numerical potential method has been incorporated in GALAMOST with the potentials derived from iterative Boltzmann inversion (IBI) method developed by Müller-Plathe and his coworkers or other structure-based coarse-graining methods. With the derived coarse-grained non-bonded, bond, angle, and torsion numerical potentials, the dynamic properties and thermodynamic properties of polymers can be studied.





Within each interval between the grid points, potentials are fitted to a cubic spline function. More specifically, for each $x_i < x < x_{i+1}$, let $\delta = x - x_i$, $V(x)$ is represented by:

$$V(x) = c_0 + c_1\delta + c_2\delta^2 + c_3\delta^3,$$

where x corresponds to particle-particle distance square, bending angle, and torsion interaction, respectively. i is the index of grid point and c_0 is the starting potential value of each grid point. Other parameters c_1, c_2, and c_3 are chosen to make the values of the first derivative and the second derivative at both ends of interval x_i and x_{i+1} equal to the correct value of function V. In this way, the potential is continuous up to second order through the whole interaction range.

3. Characteristic models

1. Soft anisotropic particle model

To simulate hierarchically self-assembled superstructures of anisotropic particles, an anisotropic particle model was proposed by Li et al. In this model, a kind of soft anisotropic particles is described by a soft anisotropic potential. With the implementation on GPU by GALAMOST, now we can efficiently simulate disk-like, rod-like, Janus, and triblock Janus particles with different anisotropic potentials.

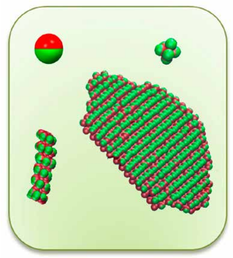
(1) disk-like (2) rod-like (3) Janus (4) triblock Janus

For example, the Janus particle potential (in reduced units):

$$U_{ij} = \frac{\alpha_{ij}^R}{2}(1 - r_{ij})^2 - f^\nu \frac{\alpha_{ij}^A}{2}(r_{ij} - r_{ij}^2)$$

$$f = \begin{cases} \cos\frac{\pi\theta_i}{2\beta}\cos\frac{\pi\theta_j}{2\beta} & \text{if } \cos\theta_i \geq \cos\beta \text{ and } \cos\theta_i \geq \cos\beta \\ 0 & \text{otherwise.} \end{cases}$$

where the magnitude of α^R_{ij} controls the strength of repulsion, α^A_{ij} controls the strength of attraction, and ν controls the angular width of attraction. θ is the angle between the vector assigned to particle and the interparticle vector.



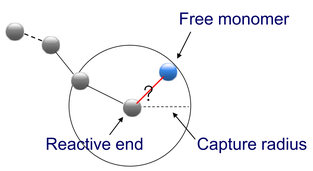
Li et al. Soft Matter, 2012, **8**, 6693-6697

2. Stochastic chain-growth polymerization model

To study some phenomena related to polymerization, a chain-growth polymerization model in MD was proposed by Liu et al. Now this model is efficiently and stably implemented on GPU by GALAMOST. The polymerization rate r_p is decided by the reaction probability P_r with the preset value $0 \leq P_r \leq 1$.

$$r_p = -\frac{d[M]}{dt} = \frac{[P^*]P_r}{\tau}$$

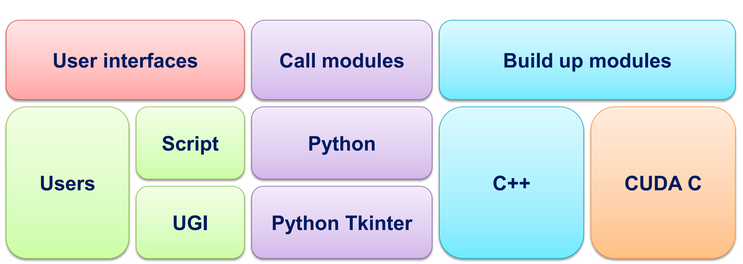
where $[M]$ is the free monomer concentration, $[P^*]$ is the concentration of growth centers in the system, and τ is the reaction time interval.

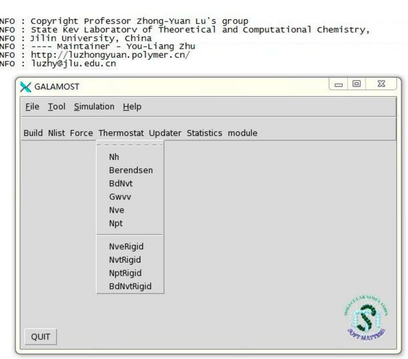


If $P < P_r$, connect;
Else if $P > P_r$, do not connect.

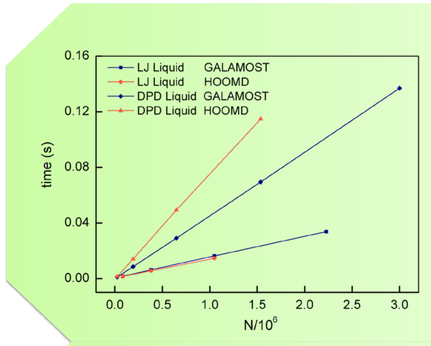
Liu et al. ACS Macro Lett. 2012, **1**, 1249−1253

4. Package structures



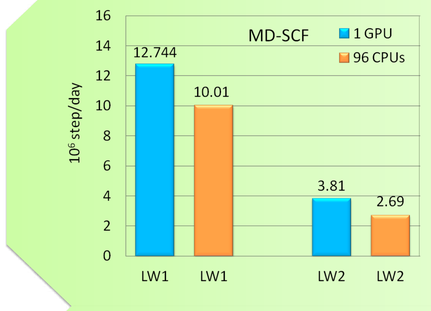


5. Performance



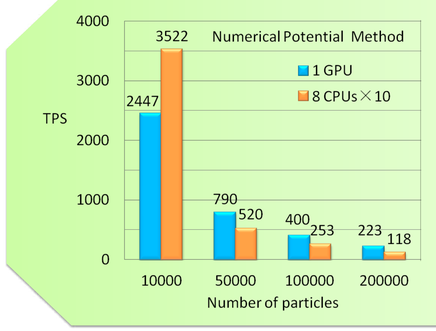
The average costing time per time step of GALAMOST and HOOMD[1] by simulating LJ liquid with a packing fraction of 0.2 and DPD liquid with a reduce number density of 3.0 systems with different system sizes both on GTX 580.

[1]J. Comput. Phys. 2008, **227**, 5342



The comparisons of the performances between parallel CPU code OCCAM[2] on Intel E7330, 2.4GHz and GALAMOST on GTX 580 as million of time steps/day have been plotted for lipid (DPPC) and water systems, LW1(307,200 particles) and LW2 (1,048,576 particles).

[2]J. Comput. Chem. 2012, **33**, 868.



The comparison of performances by simulating polystyrene systems with different number of particles between parallel CPU code IBIsCO[3] on Intel E5440, 2.83GHz and GALAMOST on GeForce GTX 680

[3]J. Comput. Chem. 2011, **32**, 1475.

Acknowledgment:
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