A large-scale study of Hyperbranched Star-like polymers in high-performance computing systems

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Molecular architecture

**Core:** functionality, Molecular information about shape, size

**Surface:** reactive/non-reactive terminal groups influence chemical properties of molecules

**Branching dendrons:** interior, functionality and stiffness gives the shape

**Dendrimer:** well defined tree-like structure with high degree of molecular uniformity
Molecular architecture

G – generation
S – branch length

G: 0-7
S: 2-128
56 systems
Molecular architecture: dense melt
Molecular architecture: dense melt

<table>
<thead>
<tr>
<th>Molecules type</th>
<th>Mass of a molecule</th>
<th>Nr of molecules</th>
<th>Total nr of particles</th>
<th>Box size</th>
</tr>
</thead>
<tbody>
<tr>
<td>S2G7</td>
<td>1531</td>
<td>343</td>
<td>525133</td>
<td>85.1694</td>
</tr>
<tr>
<td>S4G7</td>
<td>3061</td>
<td>216</td>
<td>661176</td>
<td>91.967</td>
</tr>
<tr>
<td>S8G7</td>
<td>6121</td>
<td>216</td>
<td>1322136</td>
<td>115.865</td>
</tr>
<tr>
<td>S16G7</td>
<td>12241</td>
<td>125</td>
<td>1530125</td>
<td>121.6474</td>
</tr>
<tr>
<td>S32G7</td>
<td>24481</td>
<td>27</td>
<td>660987</td>
<td>91.9584</td>
</tr>
<tr>
<td>S64G7</td>
<td>48961</td>
<td>27</td>
<td>1321947</td>
<td>115.8595</td>
</tr>
<tr>
<td>S128G7</td>
<td>97921</td>
<td>27</td>
<td>6266944</td>
<td>194.6311</td>
</tr>
</tbody>
</table>
Computational challenges

- Large mass of molecules
- Large number of molecules
- Equilibration
- Slow dynamic (large arms)
Molecular Dynamics Approach

- Start configuration
  - Spatial
  - Thermodynamical
  - Geometrical

- Bonds, angles, rotations
  - van der Waals forces
  - Coulomb potential

- Taylor expansion of positions:
  - Verlet algorithm

- Newton’s equations

CHARMM, NAMD, LAMMPS, HOOMD-blue…
## Approach

<table>
<thead>
<tr>
<th></th>
<th>LAMMPS</th>
<th>HOOMD-blue</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Name</strong></td>
<td>Large-scale Atomic/Molecular Massively Parallel Simulator</td>
<td>Highly Optimized Object-oriented Many-particle Dynamics -- Blue Edition</td>
</tr>
<tr>
<td><strong>Institution</strong></td>
<td>Sandia National Laboratories</td>
<td>University of Michigan</td>
</tr>
<tr>
<td><strong>Programming languages</strong></td>
<td>C++, modularity</td>
<td>Python and C++ for CUDA code</td>
</tr>
<tr>
<td><strong>Parallelization</strong></td>
<td>Runs on single or multiple processors</td>
<td>Runs on GPUs (optimized for 1GPU)</td>
</tr>
<tr>
<td><strong>MPI</strong></td>
<td></td>
<td>OpenMP/SIMD</td>
</tr>
<tr>
<td><strong>Spatial-decomposition</strong></td>
<td>Spatial-decomposition of simulation domain</td>
<td>Shared memory computers</td>
</tr>
<tr>
<td><strong>License</strong></td>
<td>Open-source licence</td>
<td>Open-source licence</td>
</tr>
<tr>
<td><strong>Code changes</strong></td>
<td>No need to change the code (scripts)</td>
<td>No need to change the code (scripts)</td>
</tr>
</tbody>
</table>
## Approach

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<td>Sandia National Laboratories</td>
<td>University of Michigan</td>
</tr>
<tr>
<td>2D and 3D systems</td>
<td>2D and 3D systems</td>
</tr>
<tr>
<td>NVE, NVT, NPT, NPH, Parinello/Rahman integrators</td>
<td>NVT, NPT, NVE, NVT</td>
</tr>
<tr>
<td>Many force fields</td>
<td>Few force fields</td>
</tr>
<tr>
<td>Analysis on the fly (compute methods)</td>
<td>Script in Python, can be adapted to needs</td>
</tr>
<tr>
<td>More mature code</td>
<td>Code in development</td>
</tr>
</tbody>
</table>

- **Large systems**
- **Medium systems**, equilibration of large systems
LAMMPS

Large-scale Atomic/Molecular Massively Parallel Simulator

Scaled-size Polymer Chain Melt

scaled-size efficiency for runs with 32K atoms/proc

one processor timings are shown in parenthesis
Loop time of 49103.8 on 16 procs for 1000000 steps with 644544 atoms

<table>
<thead>
<tr>
<th>Time Type</th>
<th>Time (%)</th>
<th>Percentage</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pair</td>
<td>12668.6</td>
<td>25.7997</td>
</tr>
<tr>
<td>Bond</td>
<td>5395.71</td>
<td>10.9884</td>
</tr>
<tr>
<td>Neigh</td>
<td>9385.48</td>
<td>19.1135</td>
</tr>
<tr>
<td>Comm</td>
<td>6457.9</td>
<td>13.1515</td>
</tr>
<tr>
<td>Outpt</td>
<td>777.161</td>
<td>1.58269</td>
</tr>
<tr>
<td>Other</td>
<td>14418.9</td>
<td>29.3642</td>
</tr>
</tbody>
</table>

Force field ≈ 36%

Communication time ≈ 13%

Other > 50%
Different architecture comparison
HOOMD-blue

Highly Optimized Object-oriented Many-particle Dynamics -- Blue Edition

MPI + GPU benchmark
HOOMD vs. LAMMPS

Simulation Speed HOOMD vs. LAMMPS

BlueGene/L vs. 1 Desktop

Nanoseconds of simulated time per day

Processors

icms.cst.temple.edu/cyberchem.html
Remote visualization at HPC UdS

HPC Computer

2D VNC Desktop with already-computed images

Small desktop computer

Data stays here!

(3D Graphics)
Two granted access modes:
- high-priority one
- low-priority one
Molecular architecture

G: 0-7

S: 2-128

56 systems

G – generation
S – branch length
Radius of gyration

$R_g$ grows linearly with branch length ($S \times G$). Branch length and generation determines molecules grow.

No direct scaling with mass is possible (dendrimers are not fractals). Mass grow regime is determined.
The radially resolved density measurements show a hollow density profile. Stretched central arms prepare more space for conformational variations for arms away from the center.
Contact number:
Number of molecules that touch a given one. Maximum contact number for a hard sphere is 12.

Both intermolecular penetration and backfolding of terminal groups are present.

Two different regimes are present: loosely packed systems and compact colloidal-like molecules.
Summary

Scientific results:
Hollow center of the molecules.
Molecules getting more compact with growing generation.

On the computing side:
One has to be open to new computational possibilities to explore more realistic systems and to have a better understanding of the mechanisms at the mesoscopic level.
Complexity of the system demands usage of high performance computing systems, but heterogenity in ressources and complexity in parallelization ask for adaptibility of the scientific software.
Thank you for your attention!