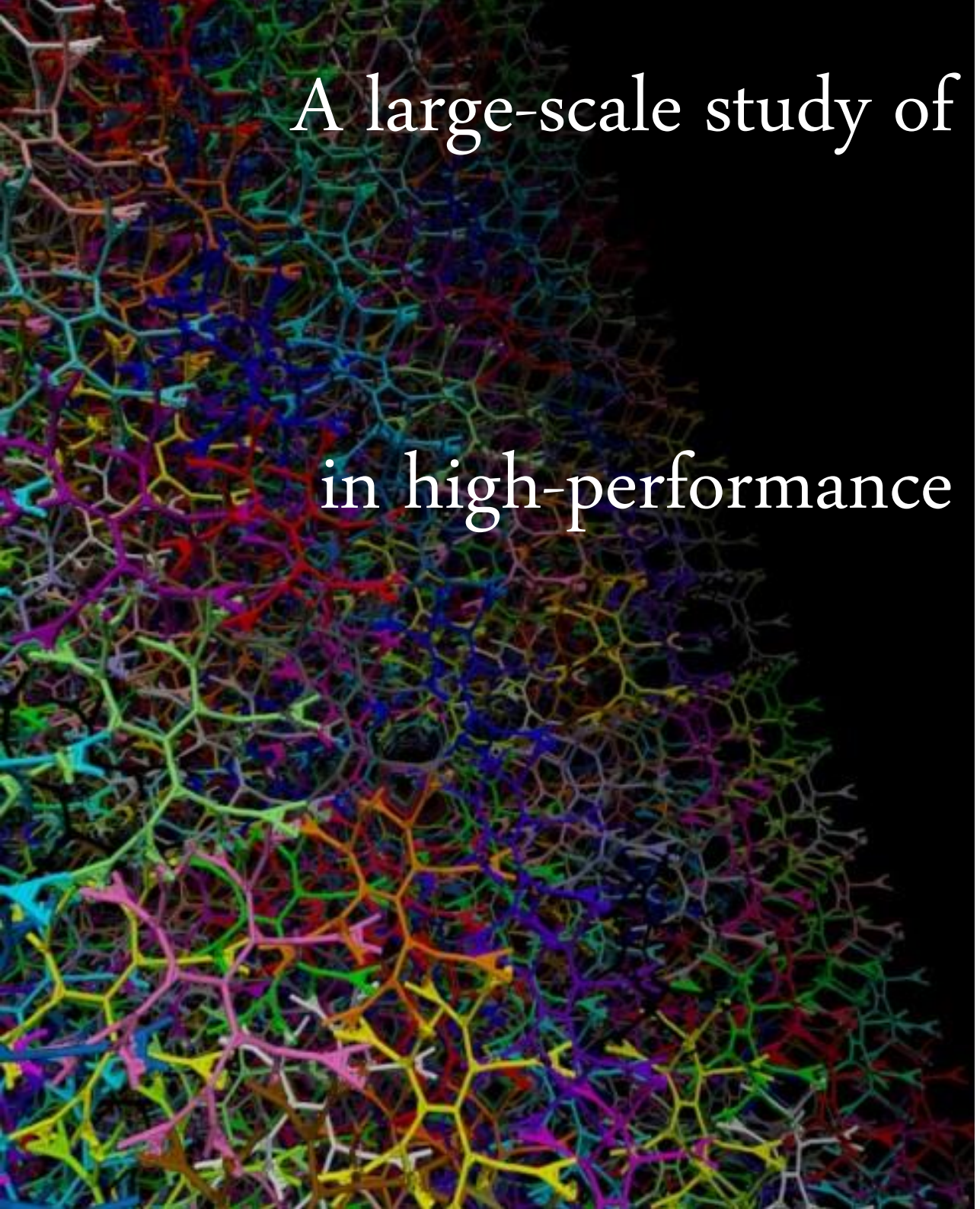

A large-scale study of Hyperbranched Star-like polymers in high-performance computing systems

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Institut Charles Sadron

Université de Strasboug, CNRS

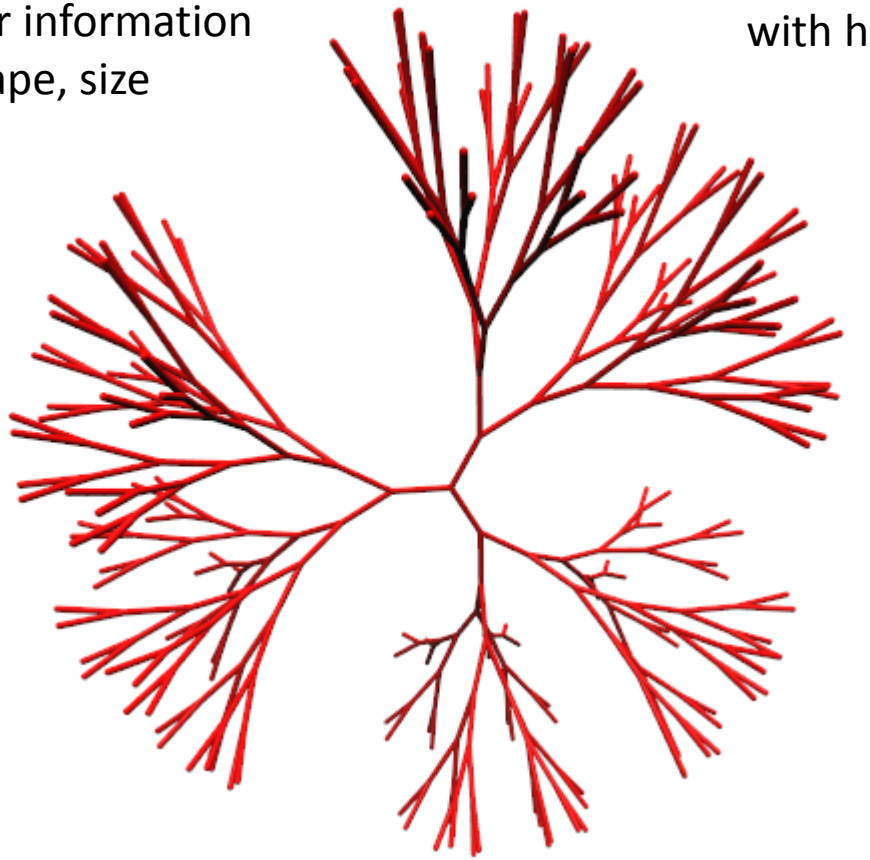
[Journées SUCCES 2013]

14 November 2013, Paris

Molecular architecture

Core: functionality,
Molecular information
about shape, size

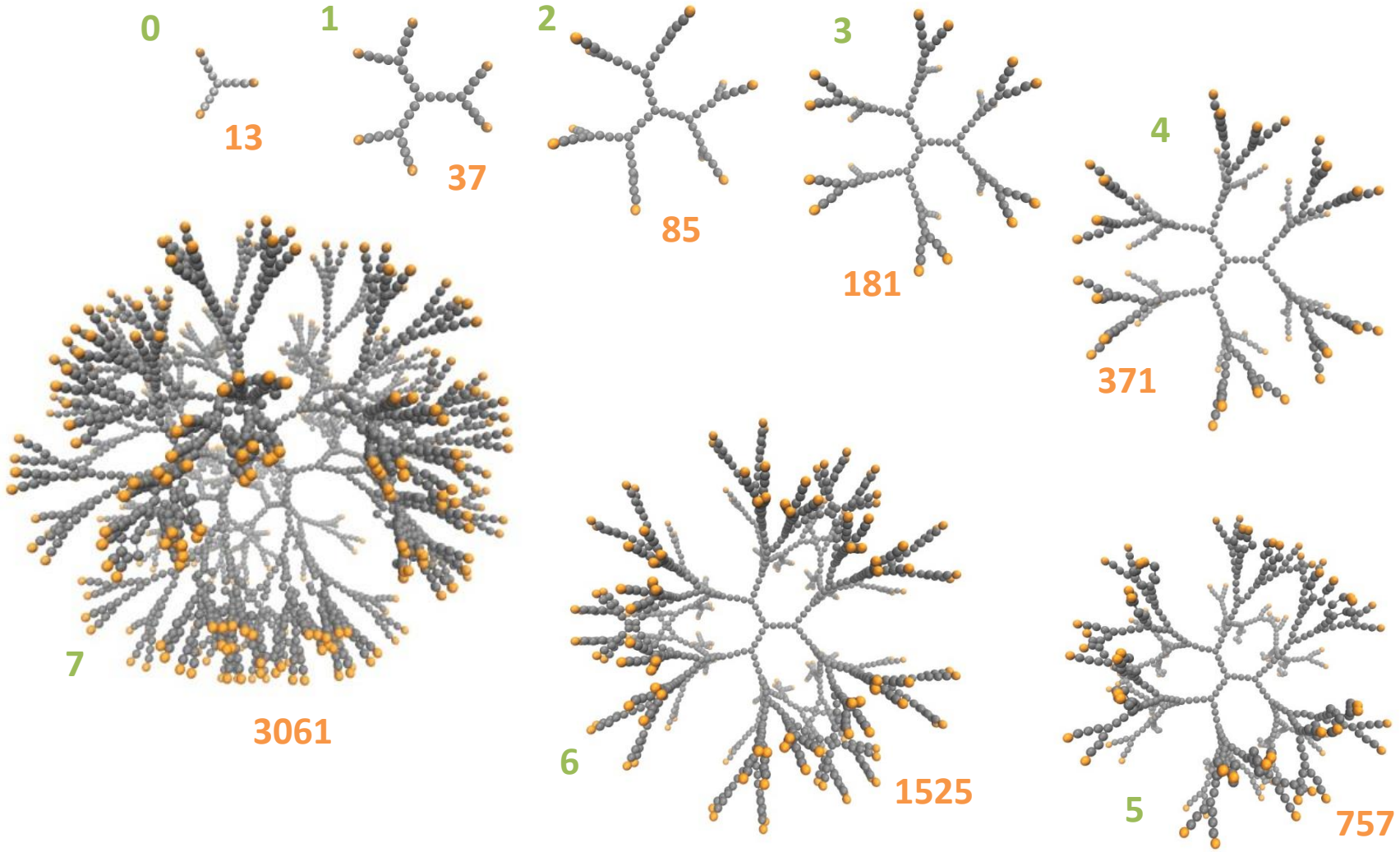
Dendrimer:
well defined tree-like structure
with high degree of molecular uniformity



Branching dendrons:
interior, functionality and
stiffness gives the shape

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

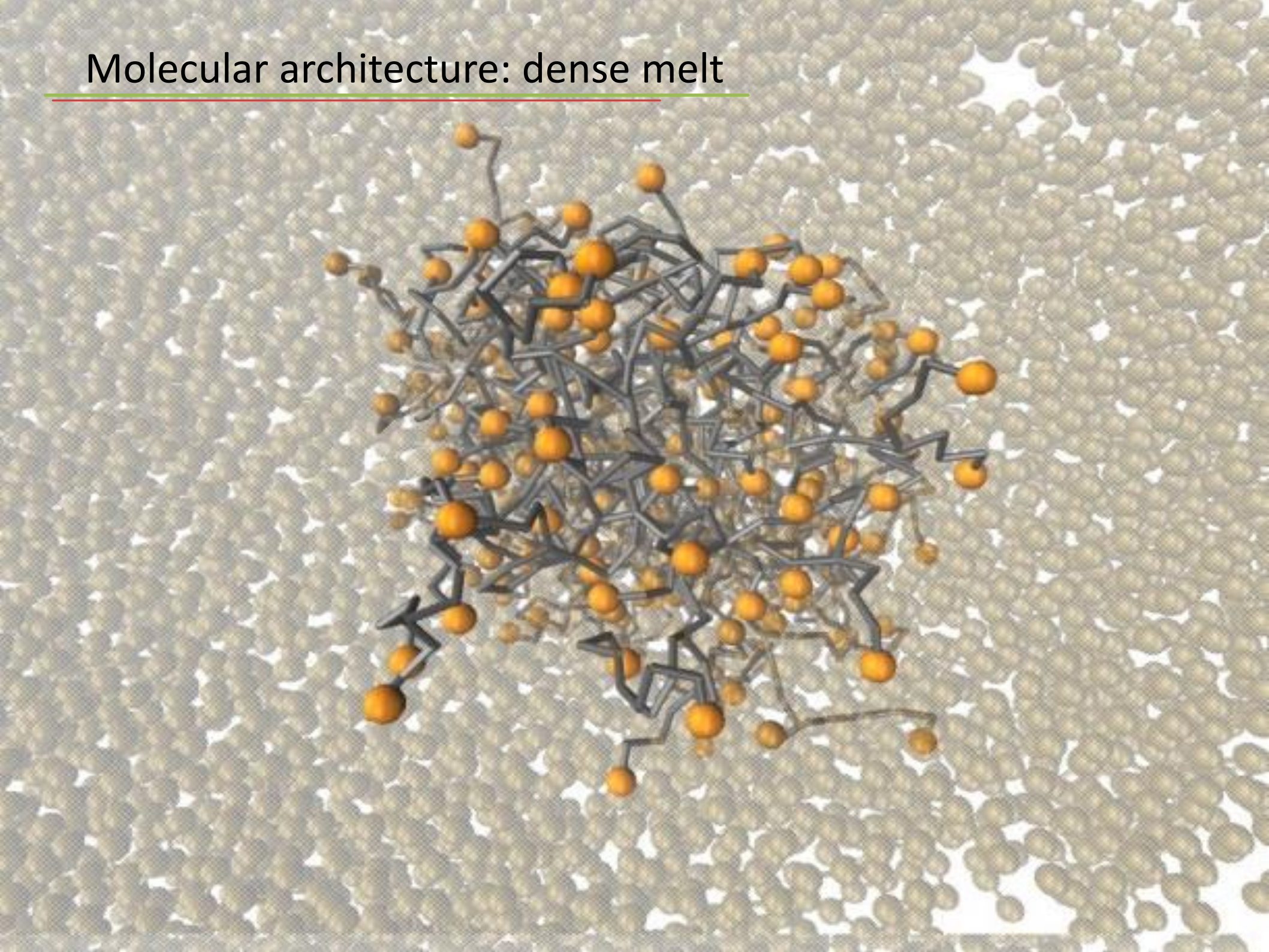
Molecular architecture



G: 0-7 × S: 2-128 = 56 systems

G – generation
S – branch length

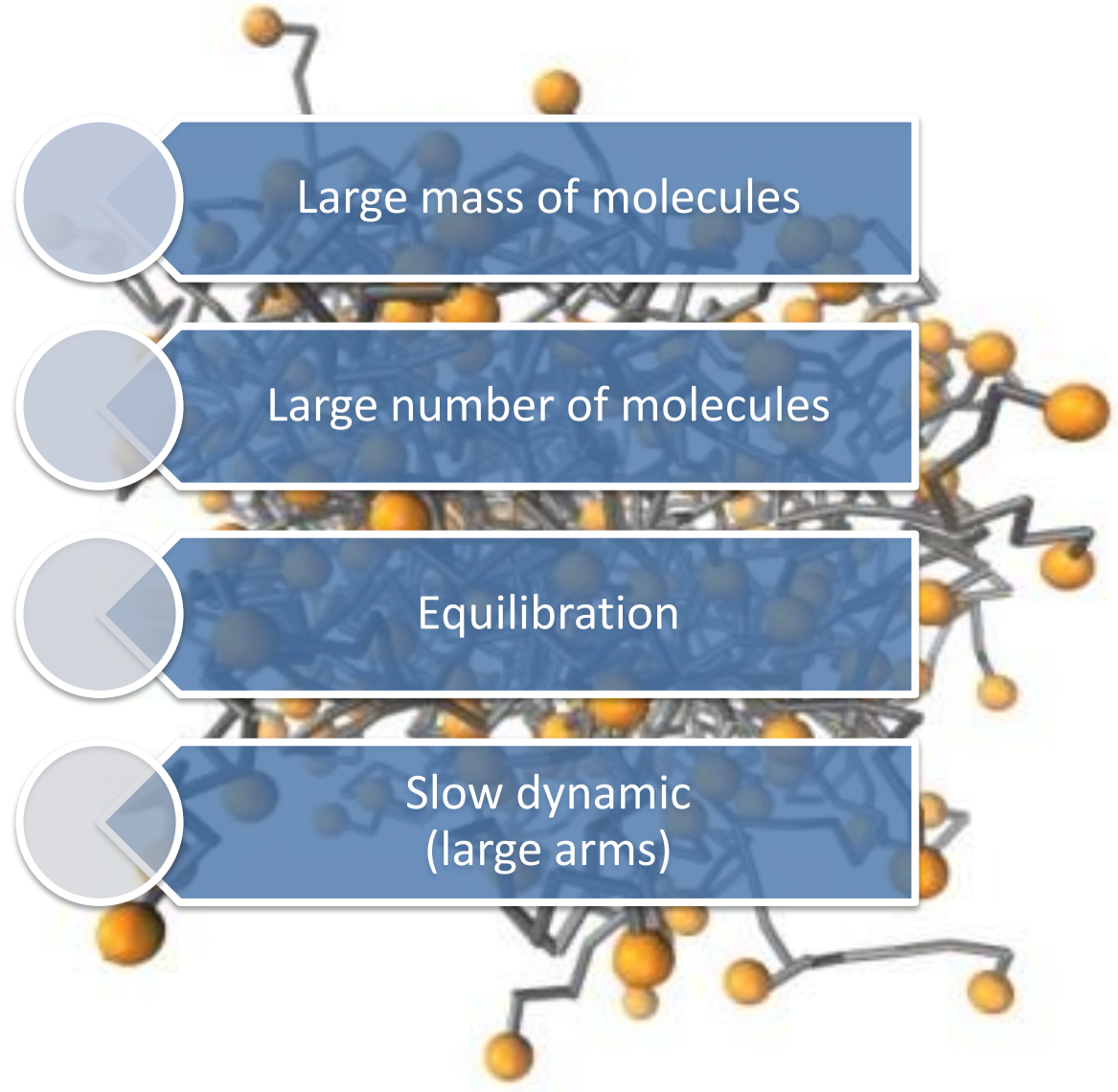
Molecular architecture: dense melt



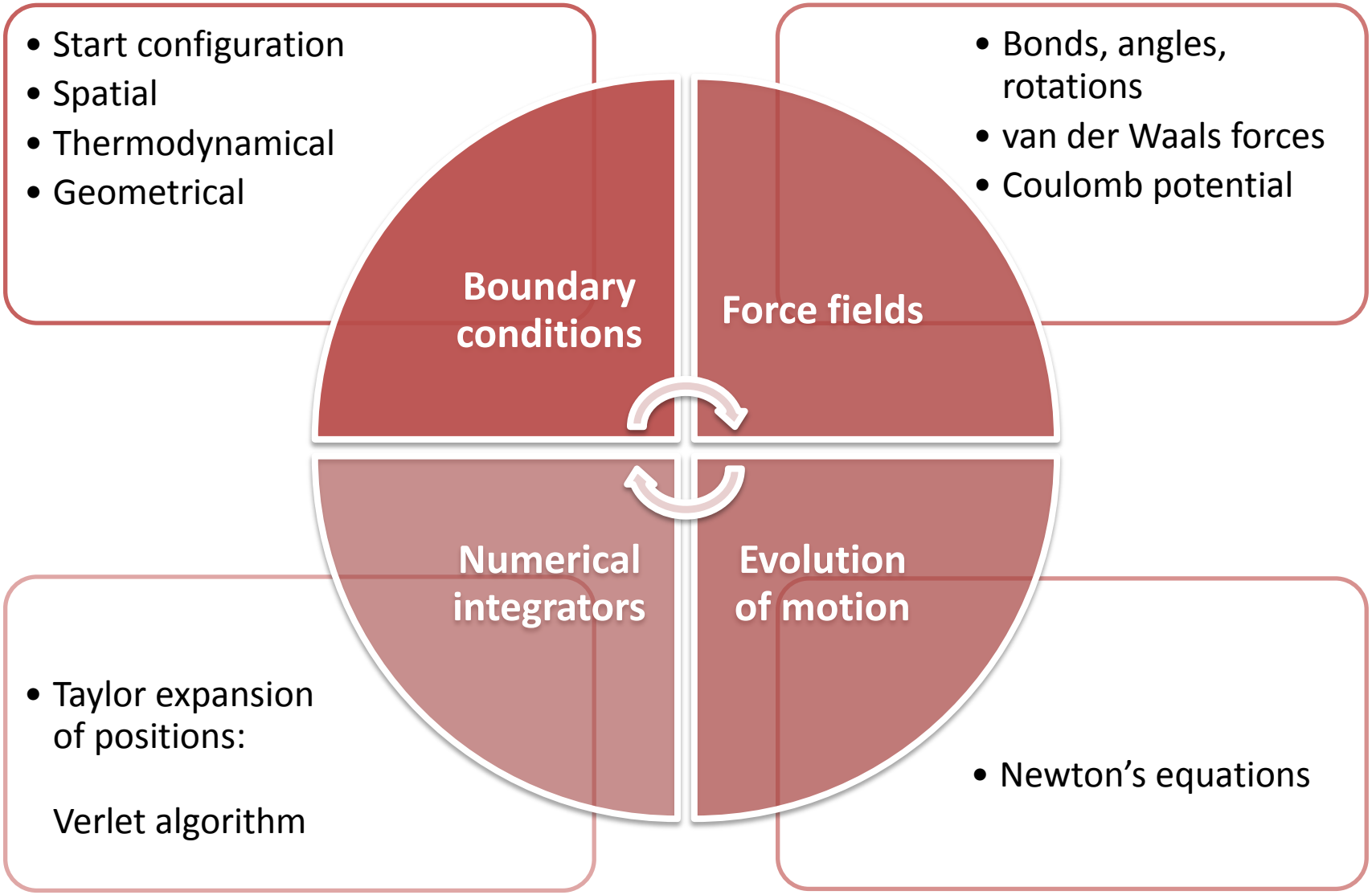
Molecular architecture: dense melt

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

Computational challenges



Molecular Dynamics Approach



CHARMM, NAMD, LAMMPS, HOOMD-blue…

Approach

LAMMPS **Large-scale Atomic/Molecular Massively Parallel Simulator** Sandia National Laboratories	**HOOMD-blue** **Highly Optimized Object-oriented Many-particle Dynamics -- Blue Edition** University of Michigan
C++, modularity	Python and C++ for CUDA code
Runs on single or multiple processors	Runs on GPUs (optimized for 1GPU)
MPI	OpenMP/SIMD
Spatial-decomposition of simulation domain	Shared memory computers
Open-source licence	Open-source licence
No need to change the code (scripts)	No need to change the code (scripts)

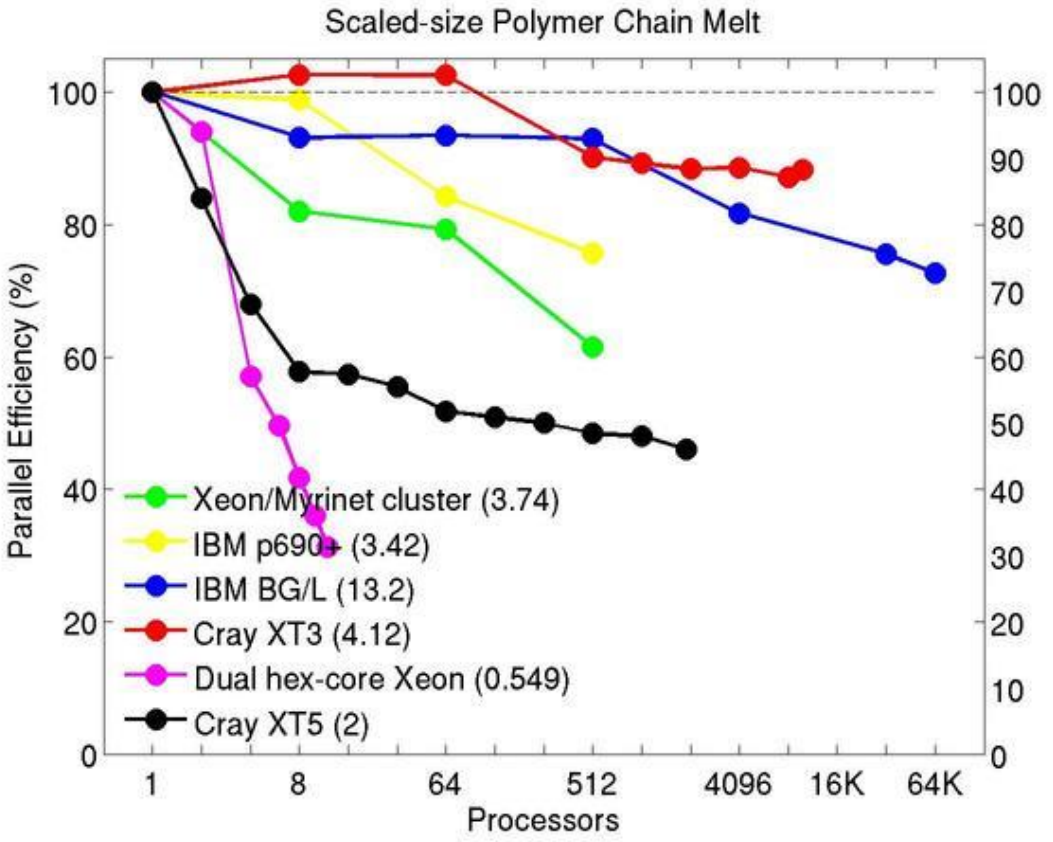
Approach

LAMMPS **Large-scale Atomic/Molecular Massively Parallel Simulator** Sandia National Laboratories	**HOOMD-blue** **Highly Optimized Object-oriented Many-particle Dynamics -- Blue Edition** University of Michigan
2D and 3D systems	2D and 3D systems
NVE, NVT, NPT, NPH, Parinello/Rahman integrators	NVT, NPT, NVE, NVT
Many force fields	Few force fields
Analysis on the fly (compute methods)	Script in Python, can be adapted to needs
More mature code	Code in development

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

LAMMPS

Large-scale Atomic/Molecular Massively Parallel Simulator



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

one processor timings are shown in parenthesis

lammps.sandia.gov

LAMMPS

Large-scale Atomic/Molecular Massively Parallel Simulator

```
Loop time of 49103.8 on 16 procs for 1000000 steps with 644544 atoms

Pair  time (%) = 12668.6 (25.7997)
Bond  time (%) = 5395.71 (10.9884)
Neigh time (%) = 9385.48 (19.1135)
Comm  time (%) = 6457.9 (13.1515)
Outpt time (%) = 777.161 (1.58269)
Other time (%) = 14418.9 (29.3642)
```

Force field ≈ 36%

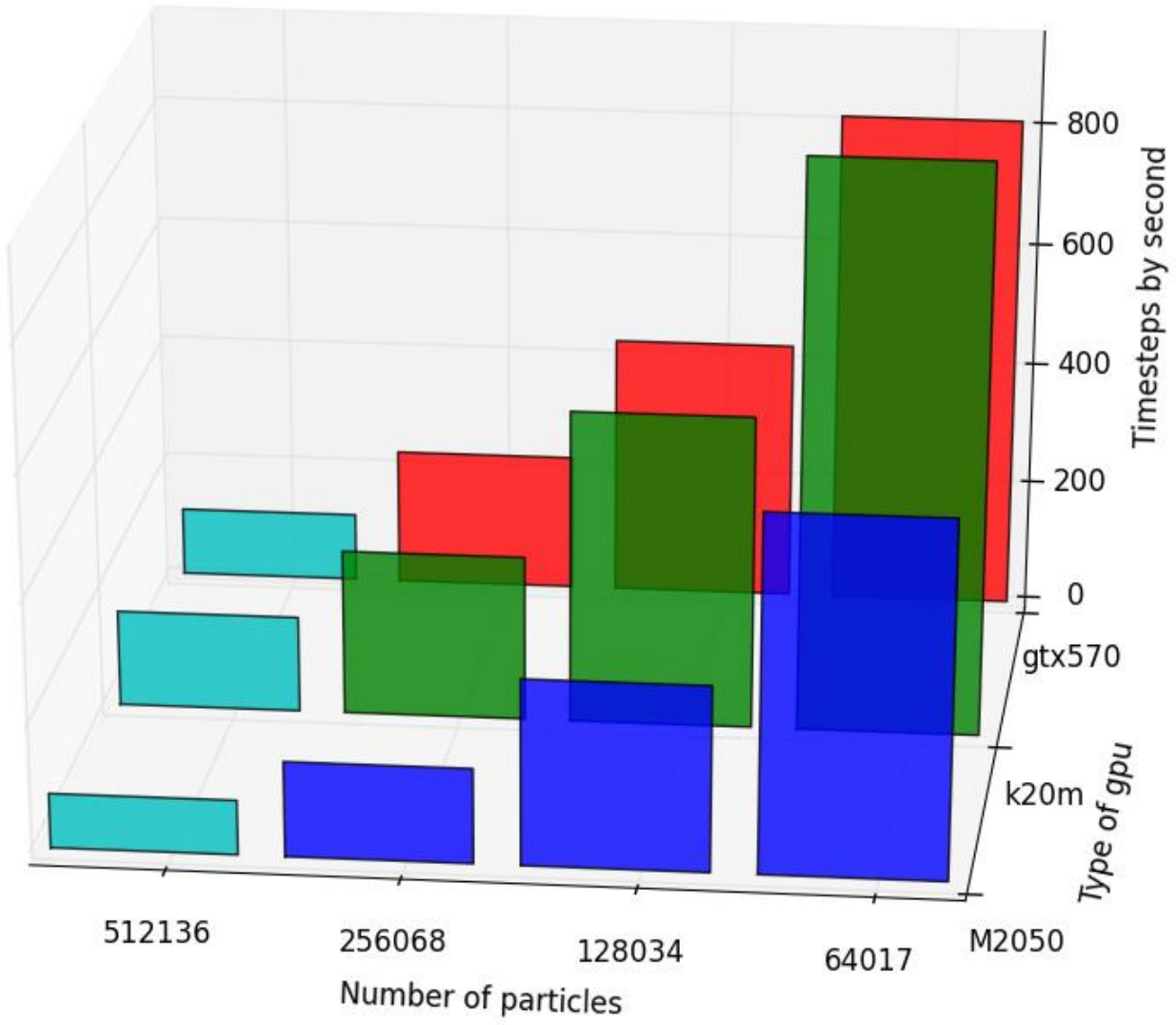
Communication time ≈ 13%

Other > 50%

HOOMD-blue

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

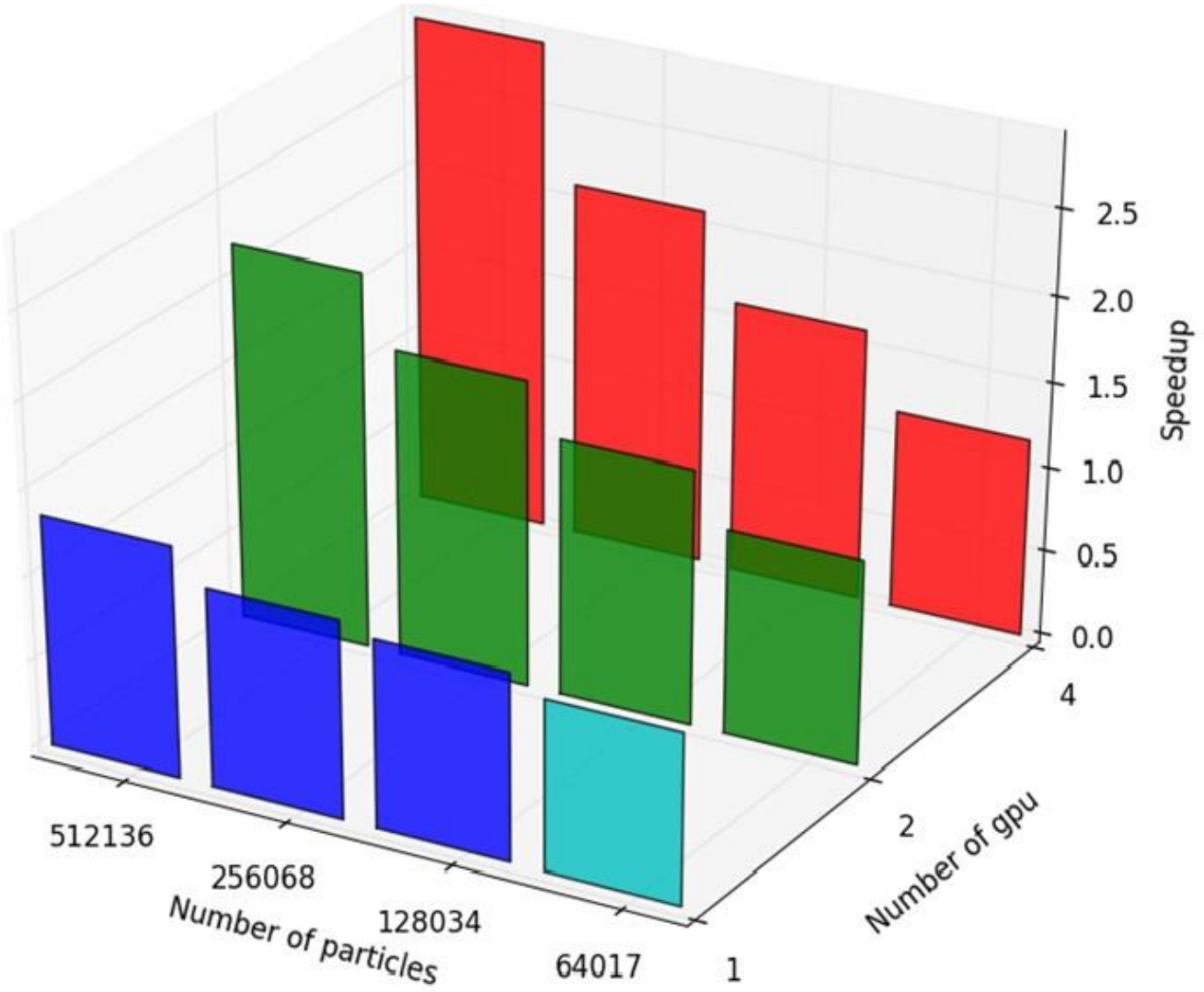
Different architecture comparison



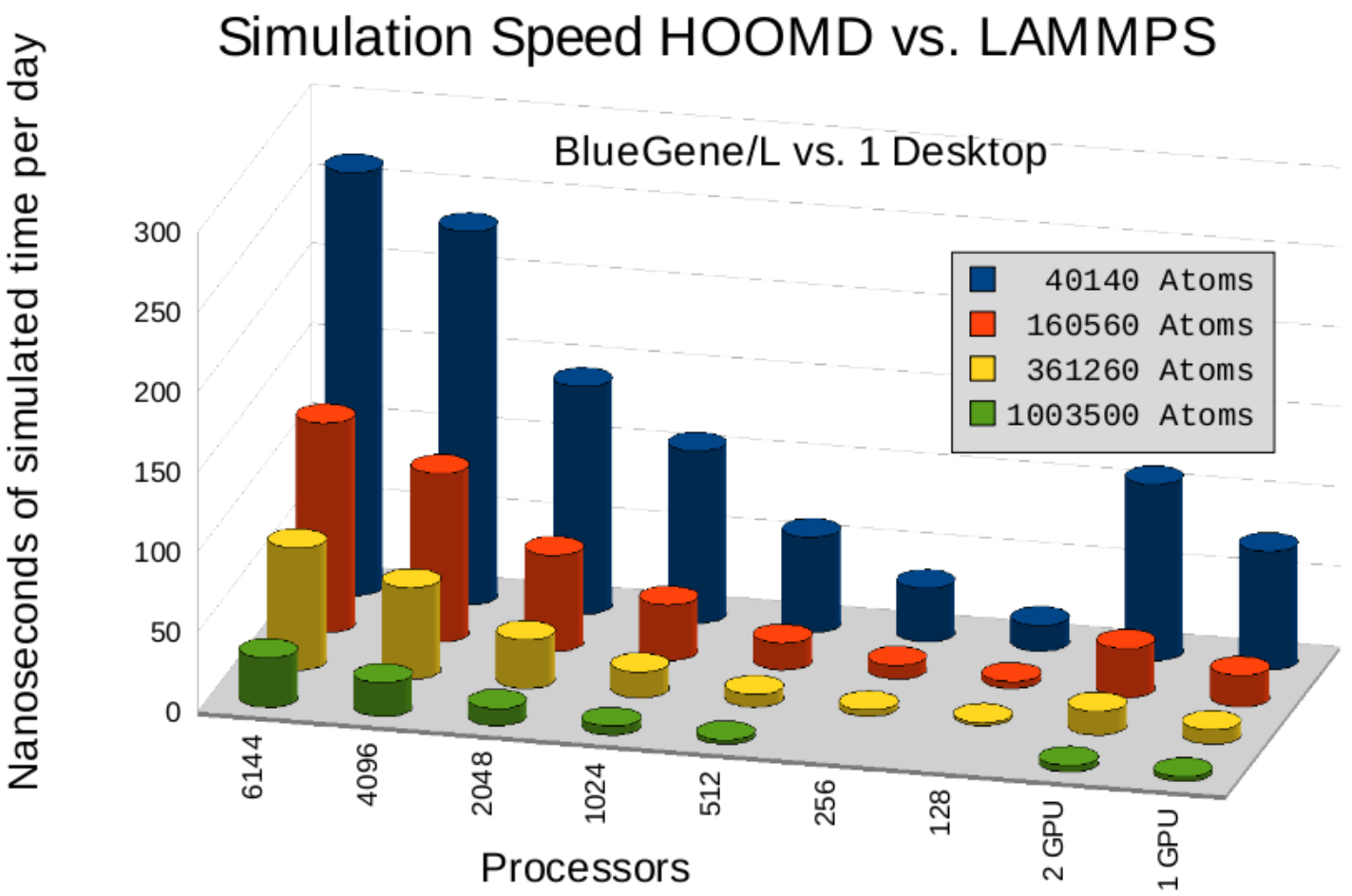
HOOMD-blue

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

MPI + GPU benchmark



HOOMD vs. LAMMPS



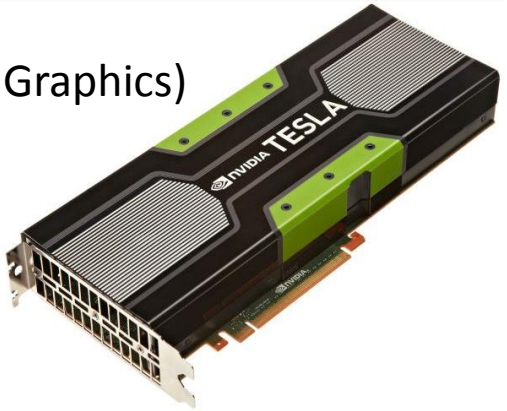
icms.cst.temle.edu/cyberchem.html

Remote visualization at HPC UdS

HPC Computer

VirtualGL
3D Without Boundaries

(3D Graphics)

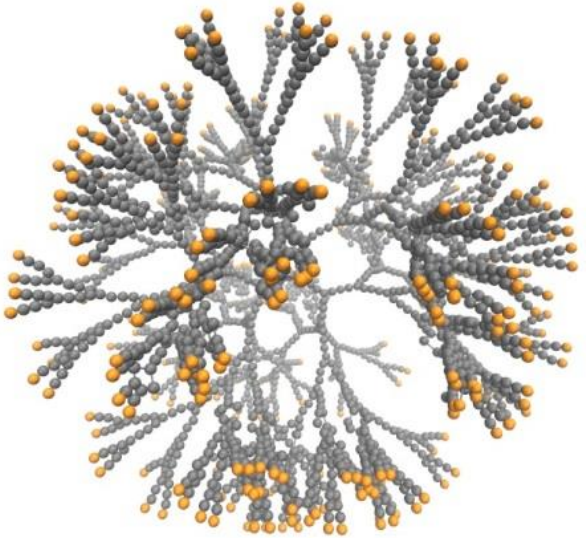


Data stays here !

2D VNC Destktop with
already-computed images

REAL VNC

Small desktop computer



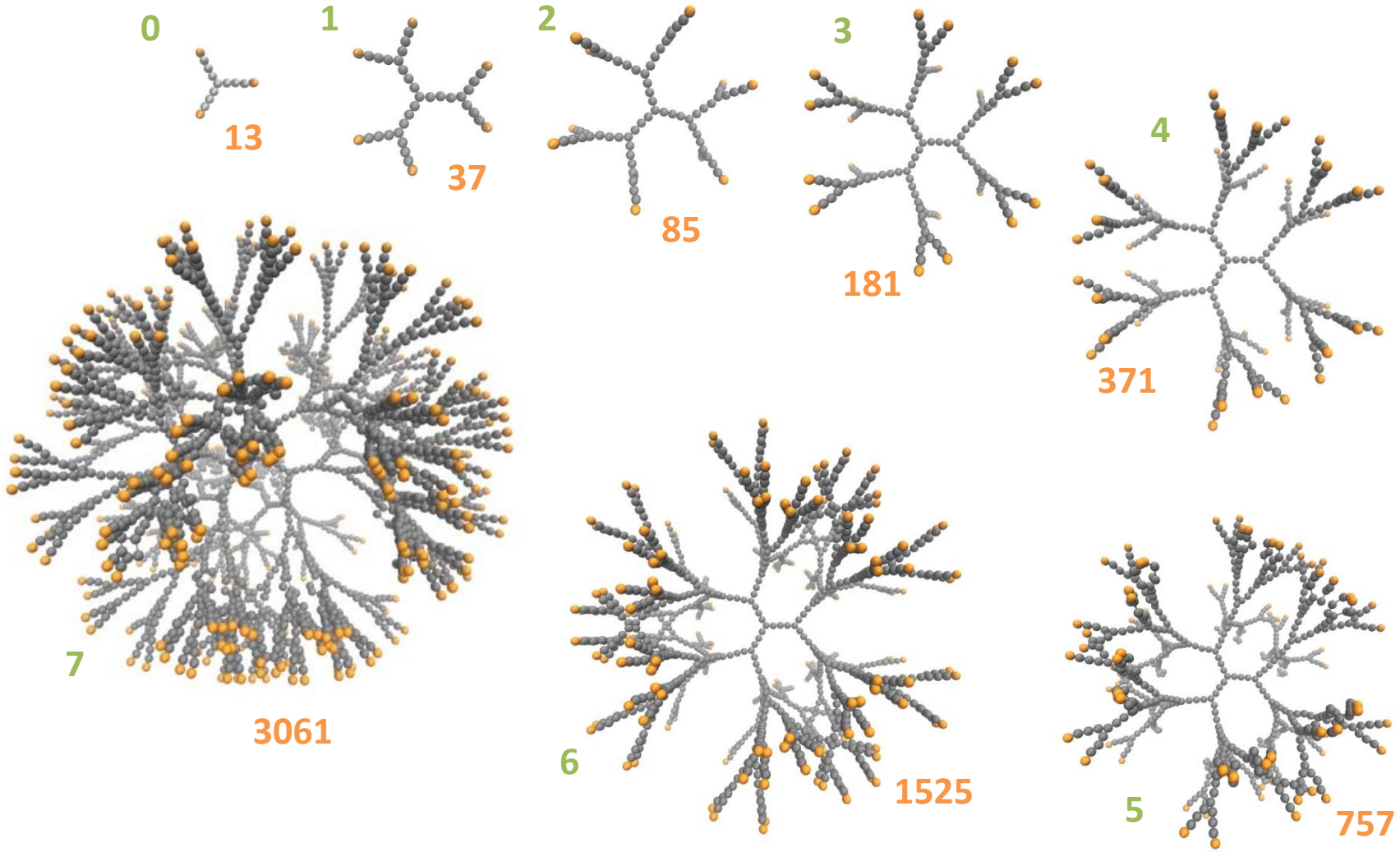
Two granted access modes:

- high-priority one
- low-priority one

Le pôle HPC
(High-performance computing)

Strasbourg

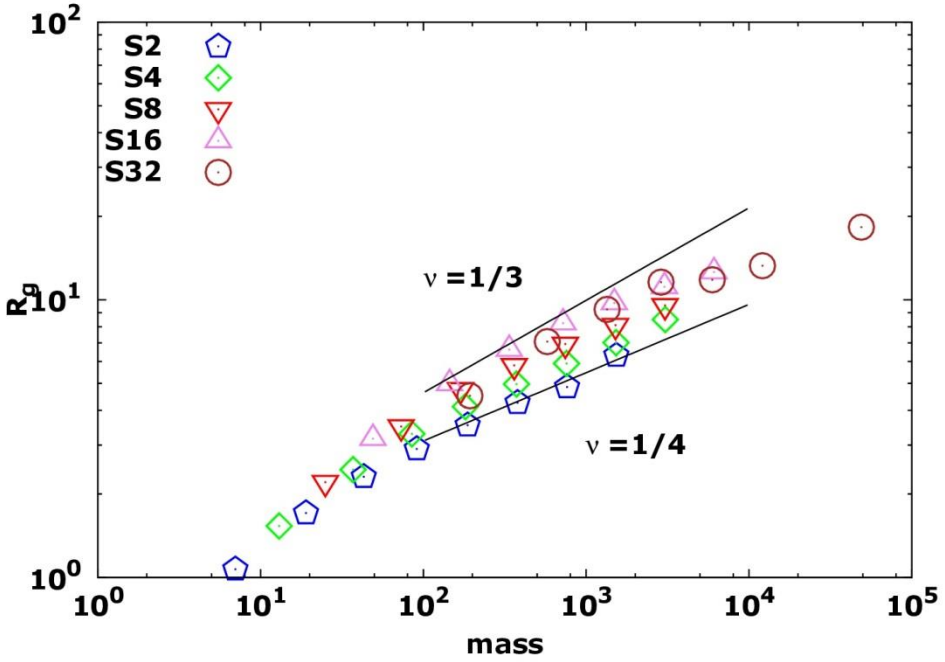
Molecular architecture



G: 0-7 × S: 2-128 = 56 systems

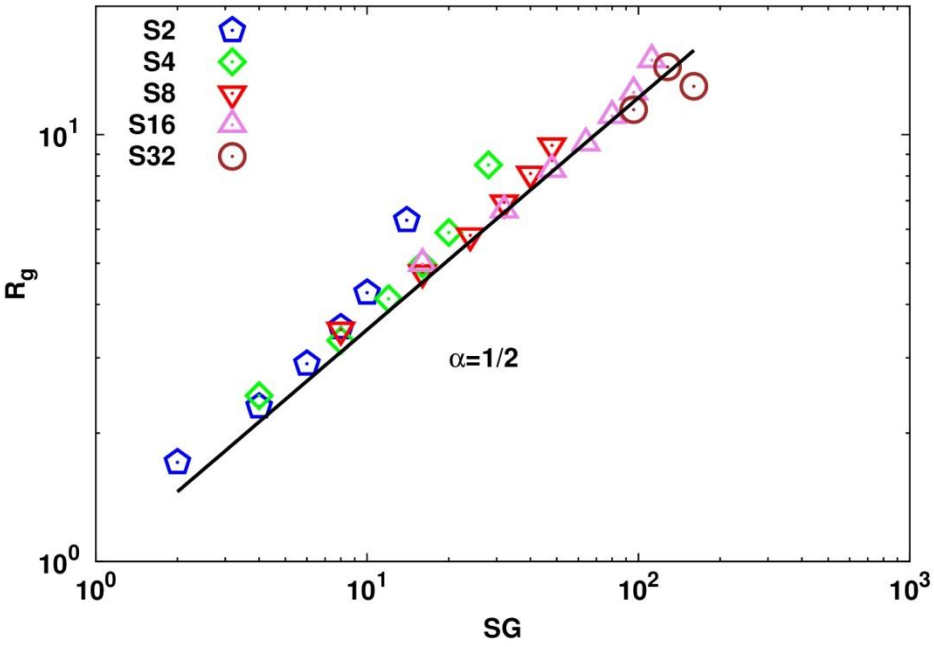
G – generation
S – branch length

Radius of gyration

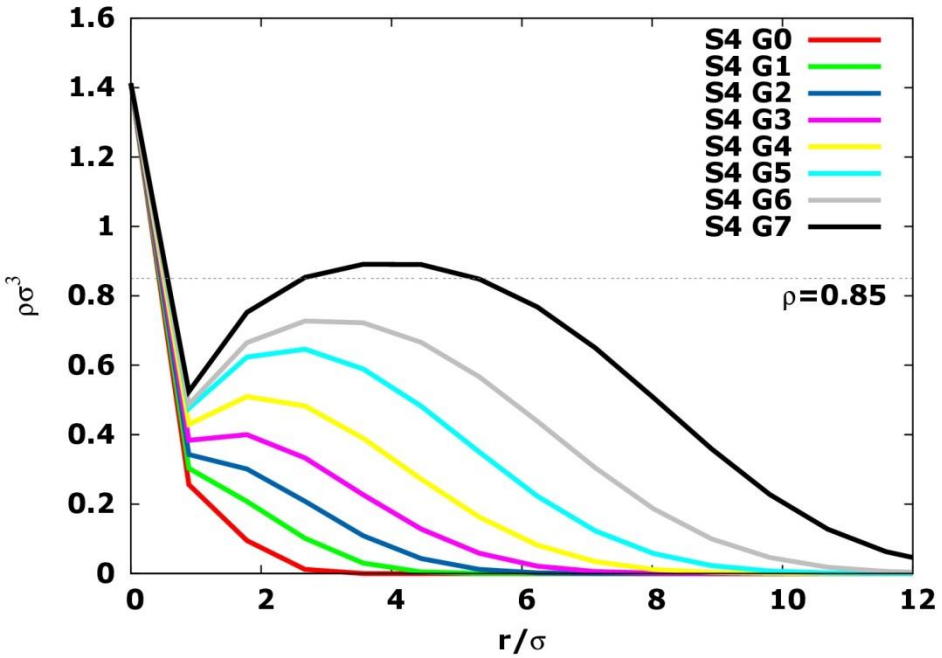


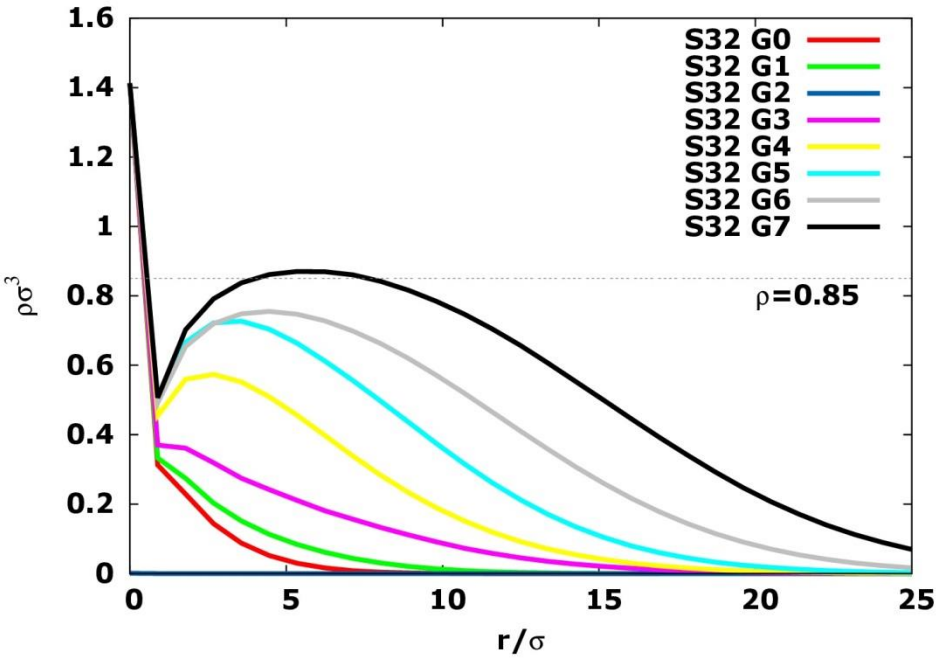
No direct scaling with mass is possible (dendrimers are not fractals).
Mass grow regime is determined.

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



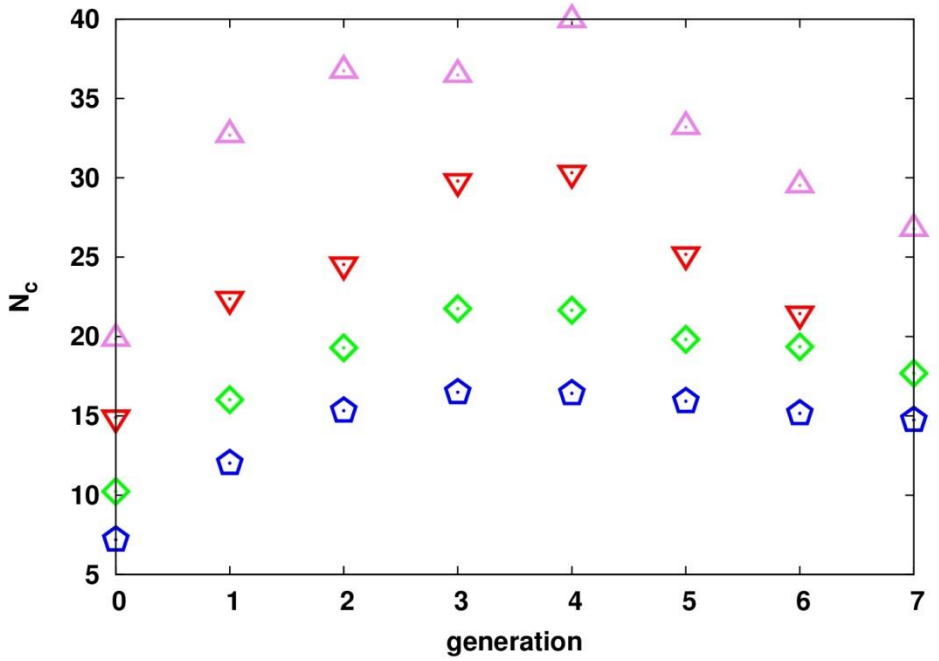
Density profile





The radially resolved density measurements shows a hollow density profile. Stretched central arms prepare more space for conformational variations for arms away from the center.

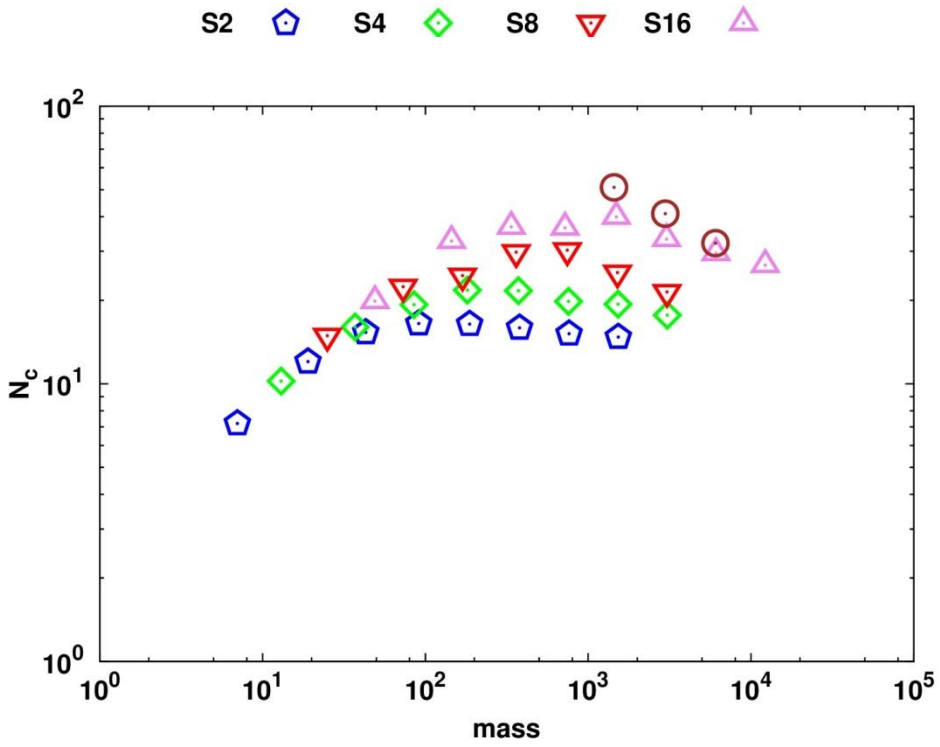
Contact number



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:

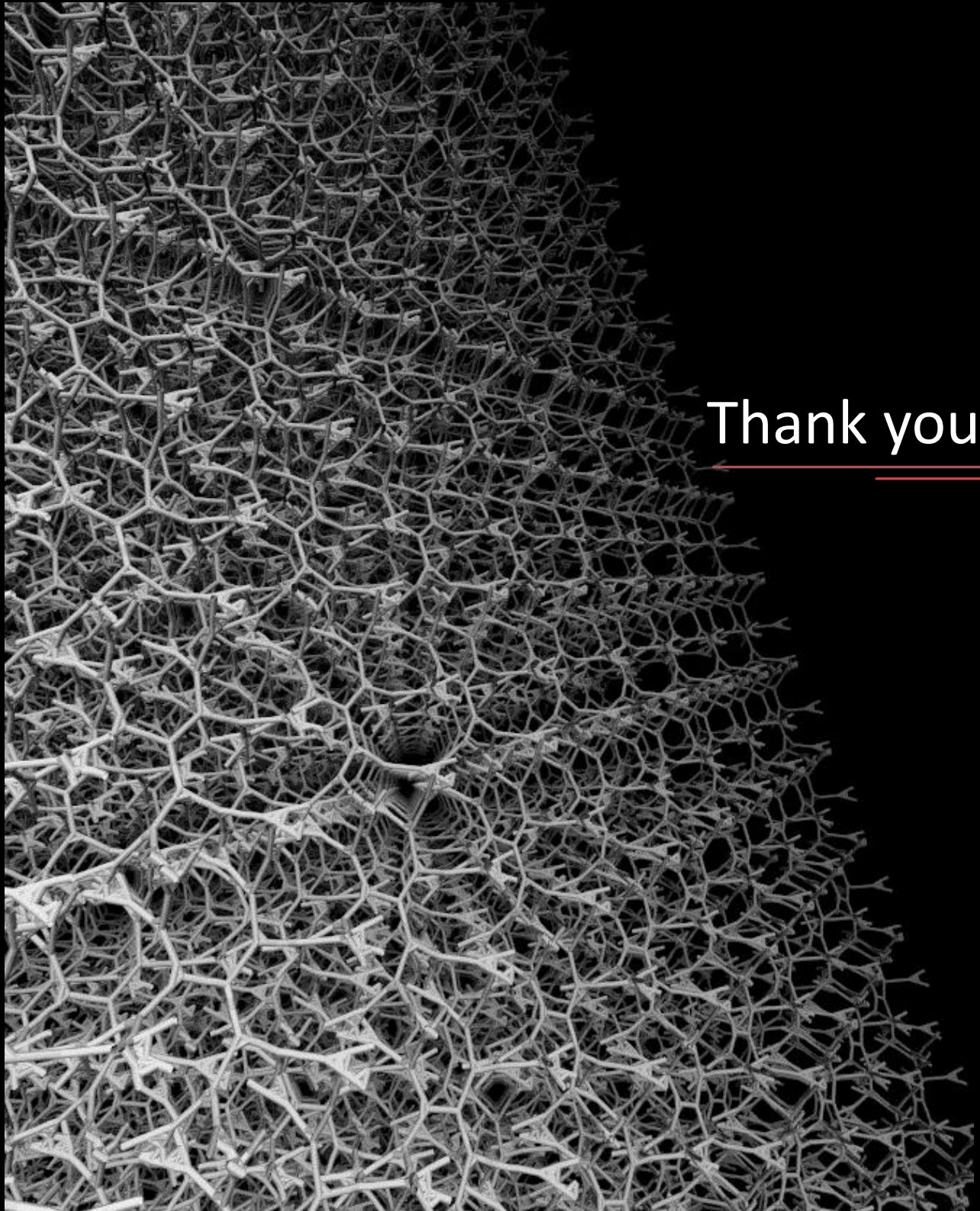
Hollow center of the molecules.

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!