Molecular Dynamics Simulations

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Groups

Contents presented here in :

- **MD Group, Prof. I. Samios. Chem. Dept. UoA.**
- **Dept. de Física i Enginyeria Nuclear, Prof. E. Guardia, UPC.**
- **HPC-Europa.**
- **IASA.**

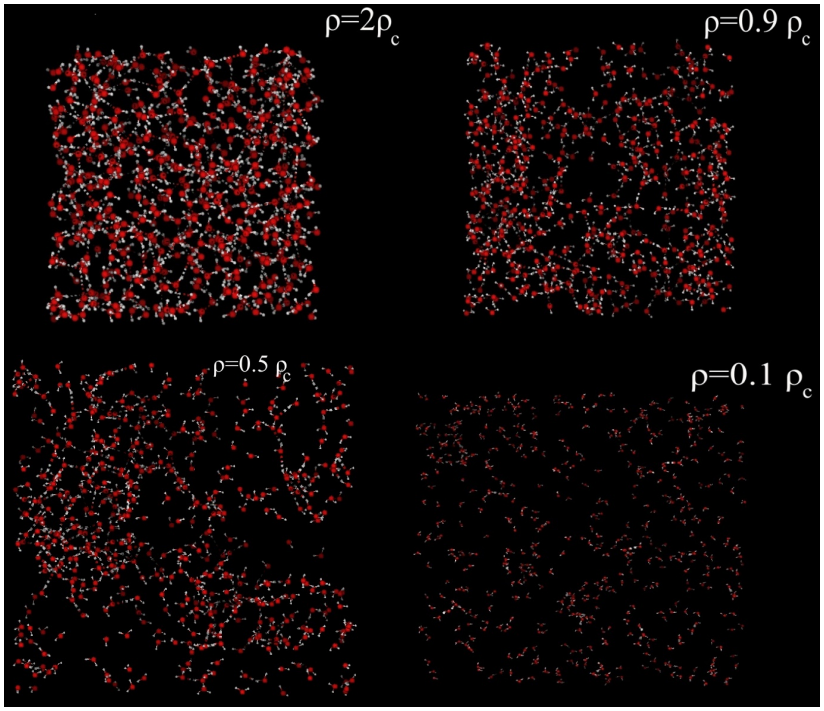
Research areas.

- **Supercritical fluids**
- **Room Temperature Ionic liquids**
- **Study of biologic interest molecules.**
- **Force field development.**

Computation Resources

- **Groups Clusters, cc.uoa.gr, Grid, FZJ, BSC.**

Supercritical Fluids



Small changes in conditions (P and/or T) => large changes in properties.

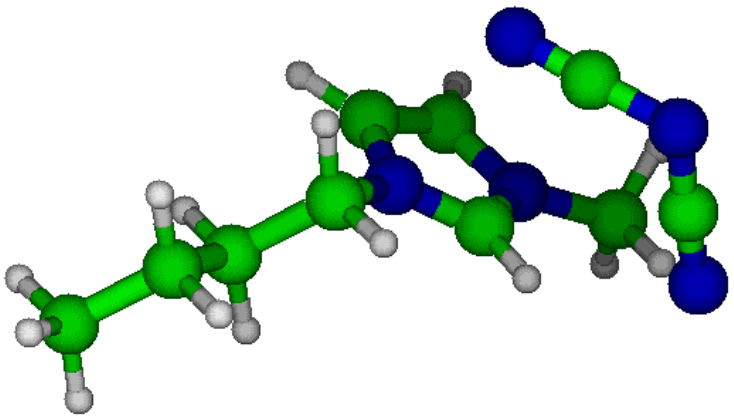
Most greenhouse gases are supercritical at normal temperatures.

Use in industrial applications as "common" solvents.

Inhomogeinities

- **Local structure at near gas densities.**

Ionic liquids

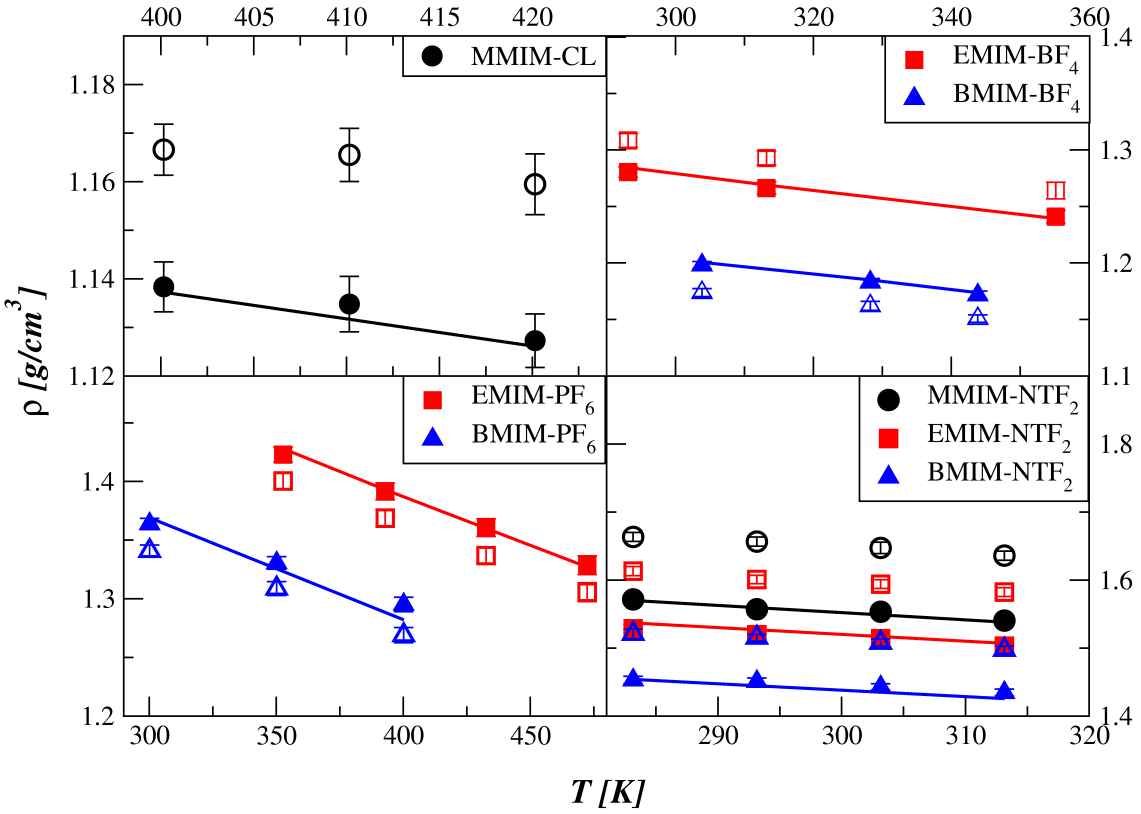


Room temperature Ionic liquids.

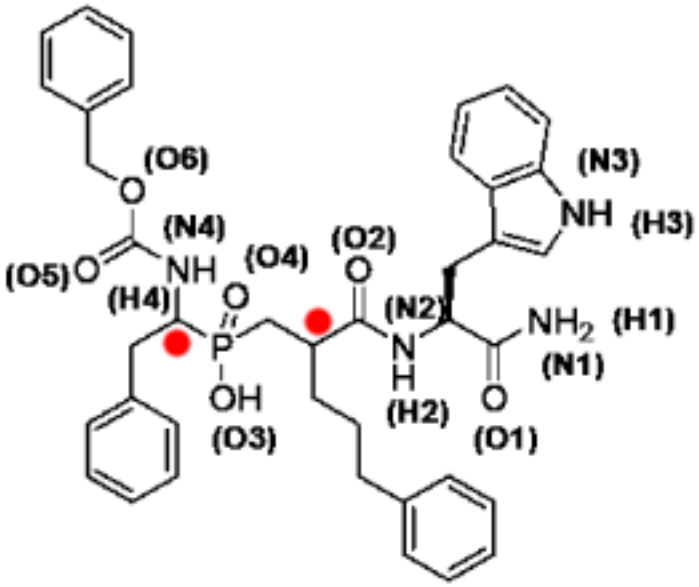
- Almost zero vapor pressure, inflammable, high thermal conductivity, thermal stability, ... => green solvents candidates.
- Tunable dissolving properties using mixtures of ions.

Force field development

Generic force fields are not accurate enough in description of properties of any system at any conditions. Development of systematic method to optimize force fields, at any conditions.



Solvation



Studies on solvation of biologic interest systems.

Separation of diastereoisomers. 4 isomers exhibit different solubility in ether and ethanol, making possible the large scale synthesis and separation.

Studies on catalytic systems.

Molecular Dynamics

System of N particles, in a usually cubic box, with periodic boundary conditions.

Solve a system of N differential equations of motion with time step of ~1 fs.

$$m_i \frac{\partial^2 r_i}{\partial t^2} = -\frac{\partial V\left(r_1, r_2, \ldots, r_N\right)}{\partial r_i}$$

Each particle's motion depends on the positions of, at least a subset, all particles positions at each time step.

Heavy use of 1/sqrt(r) calculation.

Performance limit ~N^2, various improvements ~N for large N.

Improvements using lookup tables for 1/sqrt(r).

Production of trajectory and mainly thermodynamic results.

Trajectory analysis, Calculation of properties.

Common MD codes

Classic MD codes	Classic and/or AB MD codes
DL_POLY	Cp2k
Gromacs	Quantum Espresso
NAMD	Gromacs-QM/MM
Lammps	CPMD
Mdynamix	Siesta
Amber	nwchem
Charmm	Gamess

Performance Comparison

Gromacs vs NAMD vs DL_POLY2

For a real simulated system of ~10k particles with the same run parameters (and results).

Relative performance

DLPOLY 2 : 1

NAMD : 6.3

Gromacs : 18 (sp) / 11.3(dp) – same results=> use sp in most cases.

Why this performance difference for the same (in theory) work?

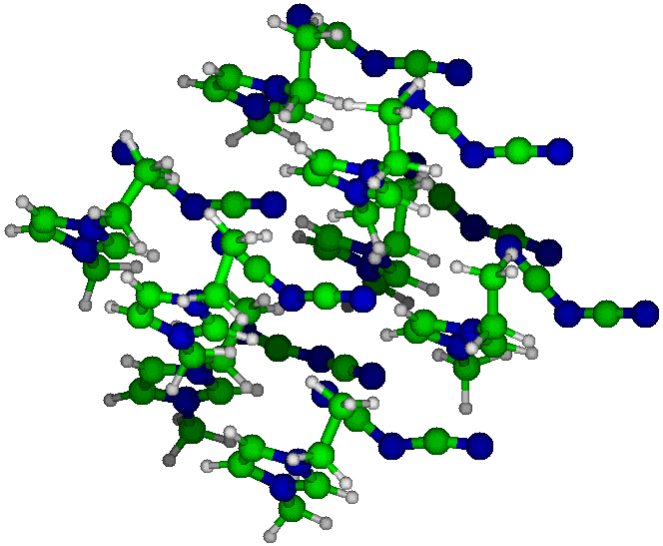
Performance Comparison

1. Gromacs and NAMD use domain decomposition, while DLPOLY2 particle decomposition => high volume of communication data=> sync issues. DLPOLY3 use domain decomposition.
2. Gromacs has the cpu intensive parts in assembly for common architectures, use lookup tables for 1/sqrt(r).
4. Gromacs has an internal topology builder and the freedom for user to specify (3D grid) topology.

Performance Comparison

Classic vs AB MD.

System : 8 emim-n(cn)$_2$



- For structural properties 50 ps with 8-32 pairs are adequate,
- For dynamic properties 10 ns with > 200 pairs minimum run.
- Typical run 256 pairs (~10000 atoms) for 10 ns.

Classic MD.

Gromacs.

0.58 Core Hours/ns

ABMD.

Cp2k.

43532 Core Hours/ns

Performance Comparison

Why to do ABMD with this speed ratio ?

Classic MD applies ***ONLY*** to non reacting systems => ABMD necessary for reacting systems.

Mixed Methods exist to efficiently handle reacting systems

(Gromacs-QMMM, Gamess)

Necessary to obtain results that are used in Classic MD.

Why to do Classic MD if all answers are in ABMD?

Obvious speed/accuracy reasons, depening on what we are looking for.T here are certain reaons to prefer ABMD.

What to select to study a system ?

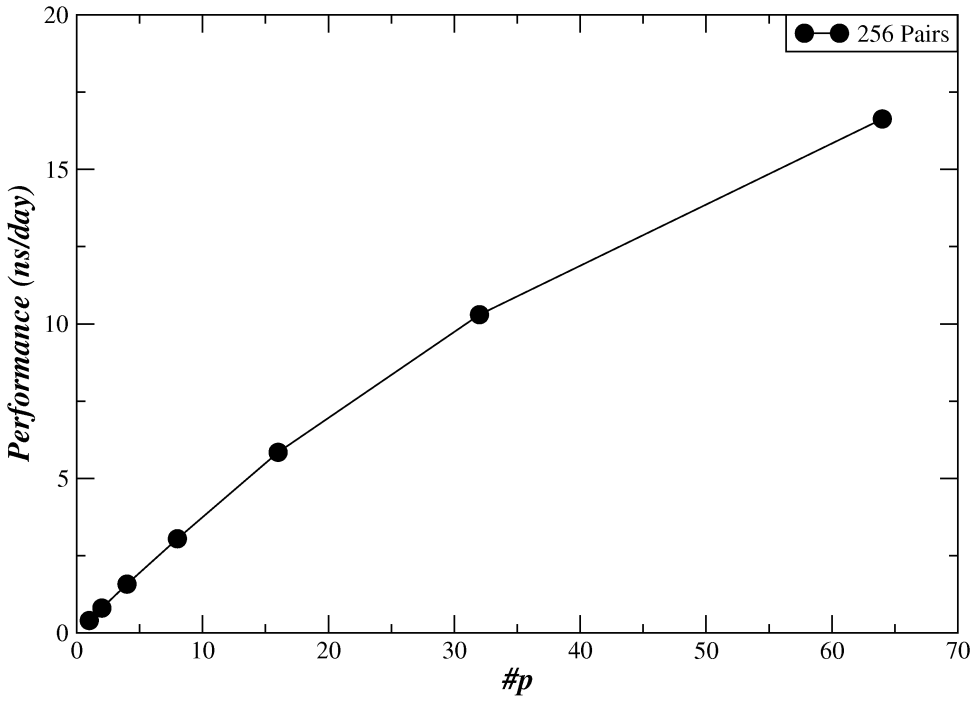
It depends on what you are looking for.

Gromacs on Marenostrum

- 10240 IBM PPC 970MP@2.3 Ghz
- 20 TB memory
- 480 TB storage
- Myrinet and Gigabit Interconnection
- Slurm Workload manager
- SuSe

Optimization-Evaluation

- **Compile all the required libraries and code with full compiler optimizations and PPC Altivec support.**
  - 38% speed up of serial and parallel code with respect the existing (same version) binaries. Results reproducible.
- **Evaluation of scalability and cost analysis (Allocated time fixed)**
  - Cost (CPU Hours/ns) minimum at 27 (grid 3x3x3) procs, with parallel efficiency > 100%.
- **Larger system sizes (1000 pairs) scale linearly up to 512 procs.**



Production

- 30000 Core Hours, most in 2 weeks.
- 3.5 TB data for post processing.
- More than 2 years runs required to obtain the same data using locally available resources.

References

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More coming soon...

Thank you.

Questions ?