DE LA RECHERCHE À L'INDUSTRIE

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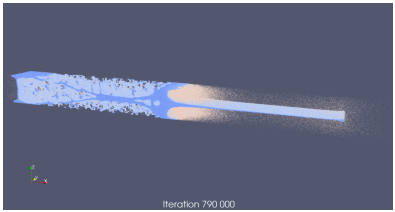
# IHPCSS poster session

## An Adaptative Mesh Refinement Fit for Large Scale Heterogeneous Molecular Dynamics Simulations




Raphaël PRAT

*Department of theoretical and applied physics*
*CEA*

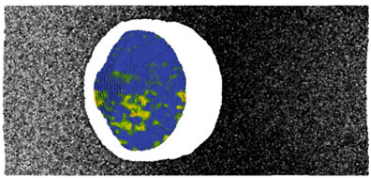
# 1. Molecular Dynamics

Molecular dynamics (MD) :

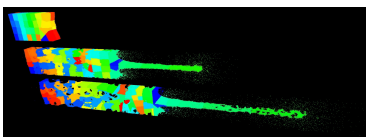
- Computational method used to study dynamical properties of a particles system
- Numerically integrating Newton's equations
- The force on particles is given by the gradient of a potential
- N-body simulation

Common potentials are :

- The Lennard-Jones potential (LJ)
- The Embedded Atom Model (EAM)



Copper embedded in Carbon (LCBOP2)



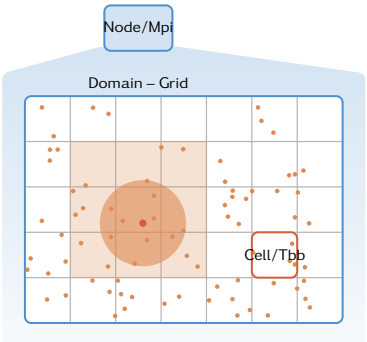
Micro-jetting of Copper

# 2. ExaSTAMP Project

ExaSTAMP is a MD code which has been recently developed at CEA.

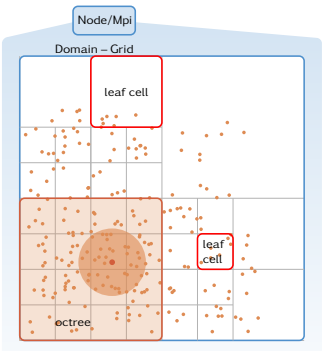
## ExaSTAMP's guidelines :

- Large scale MD simulations
- MPI & thread-based parallelization (OpenMP/Intel TBB)
- Effective vectorization
- Friendly for developers
- Optimized for Xeon Phi architecture (KNL)

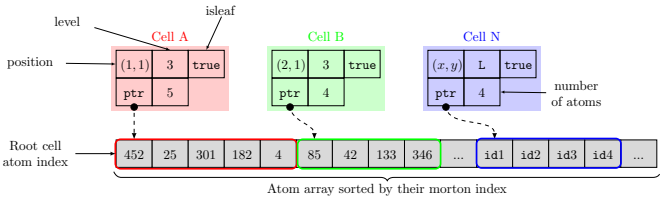



Other software : LAMMPS
Build Neighbors list : Cell-linked method, rverlet
Choc : $\Rightarrow$ Balance limited, lower vectorization efficient

# 3. Octree Structure for heterogeneous density

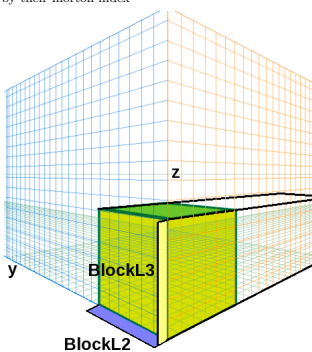



AMR divides the domain into root cells which are divided in 8 (4 in 2D) cells if there are too many atoms



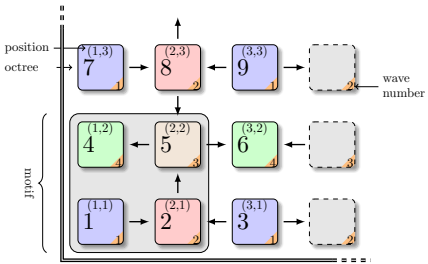

Natural Cache blocking :
⇒ Optimized cache L3

Cache oblivious with Z-curves
⇒ Optimized cache L2



# 4. Task Dependency Graph

Aim : Avoids thread concurrencies (Mutex)




Wave method combined with AMR :

- One octree = one task
- The tree depth must be at least one
- Each octree is classified toward 8 Waves (4 in 2D)
- Wave (n) unlocks Wave (n+1)

# 5. Results and Future Work

*Computation of 32M atoms of Copper on a Knight Landing (KNL) with 68 cores without hyper-threading*

Results :

- Comparison with ExaSTAMP code without AMR with OpenMP (one MPI process)
- Lennard Jones potential : 40% gain
- Sutton Chen potential (EAM) : 14 % gain

Future work :

- Task scheduler to improve affinity between threads and tasks
- Make comparisons with LAMMPS
- Test with several MPI processes and combine with Zoltan partitioning
- Find refinement criteria applied for molecular dynamics simulations