Uni.lu HPC School 2018

PS7: Multi-Physics workflows: test cases on CFD / MD / Chemistry applications

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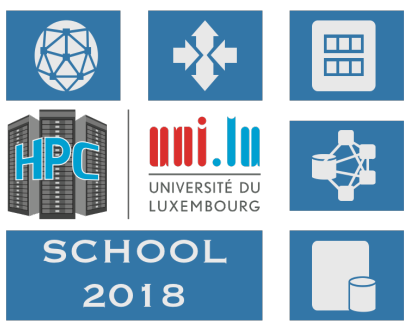
http://hpc.uni.lu

Latest versions available on Github:

UL HPC tutorials: https://github.com/ULHPC/tutorials

UL HPC School: http://hpc.uni.lu/hpc-school/

PS7 tutorial sources: ulhpc-tutorials.rtfd.io/en/latest/multiphysics/



Summary

Session Objectives

Practice utilization of parallel codes on UL HPC clusters

- Computational Fluid Dynamics
- Molecular Dynamics
- Chemistry software

Application	Description
NAMD	**Parallel molecular dynamics** code designed for high-performance simulation of large biomolecular systems
Quantum Espresso	Integrated suite of tools for **electronic-structure calculations and materials modeling at the nanoscale**
ABINIT	**Materials science package** implementing DFT, DFPT, MBPT and TDDFT
ASE	**Atomistic Simulation Environment** (Python-based) with the aim of setting up, steering, and analyzing atomistic simulations
NWChem	**Computational chemistry tools** scalable both in their ability to treat large scientific computational chemistry problems efficiently, and in their use of available parallel computing resources
OpenFOAM	**CFD package** for solving complex fluid flows involving chemical reactions, turbulence and heat transfer

Summary

Material Science HPC software env.

Software on UL HPC	In 2017 software set	In 2018 software set
ABINIT	8.2.3	8.6.3
ASE	3.13.0	3.16.0
CRYSTAL	17.v1.0.1	17.v1.0.1
ESPResSo	3.3.1	3.3.1
GROMACS	2016.3	2016.5
Meep	1.3	1.4.3
NAMD	2.12	2.12
NWChem	6.6.rev27746	6.8
OpenFOAM	4.1 (Gaia cluster)	v1712
QuantumESPRESSO	6.1	6.2.1
VASP	5.4.4.18Apr17	5.4.4.18Apr17
Yambo	4.1.4	4.2.1

Not exhaustive! A more complete list at `https://hpc.uni.lu/users/software/`

Quick Q&A

1. What particular software are you using?
2. Do you use it from the HPC global software sets?
3. Do you compile/install it yourself?
4. Would you like to have something added to the global set?
5. What computational patterns does it exhibit?
6. Is it scalable? What's the largest test that you've done?
7. Can we help you optimize your executions?

Questions?

http://hpc.uni.lu

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1. **Practical Session Objectives**
2. **Materials science HPC software environment**