TCCM course «Advanced Computational Techniques»
Aspet, France, 18 – 22 November 2024

Lecturers : Peter Reinhardt (Paris), Anthony Scemama (Toulouse), Élisa Rebolini (Grenoble)

Schedule :

	Monday	Tuesday	Wednesday	Thursday	Friday
9:00 – 10:30	Introduction	HPC	Profiling + ex.	Good practice	Networks
10:45 – 12:15	Compilation	C (2) + application	Memory / Disk	QC problems	Parallel
15:00 – 16:30	Linux / Hands-on / bash	Precision / Stability / Fortran	MP2 / 4-index	Project	Project
16:45 – 18:15	C (1) + application	Complexity / matrices	Sorting Algo	Project	Project

- two online courses introducing Linux (P. Reinhardt)
  - Wednesday, 13 November 9 – 11 a.m. Installing Linux
  - Thursday, 14 November, 9 – 11 a.m. Starting to work with Linux, basic commands
- five days of lectures and practical work
- exam on 9 December
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home work to be completed by 10 January 2025
Available ressources :

- Local WiFi
- Connection to CINECA
- Local parallel machine (40 procs) with queueing system (SLURM)

Bring your own Laptop with you – with an operational Linux on it !!

<u>Monday :</u>
General introduction to programming and computing, overview of the schedule (P. Reinhardt)
Compiled code versus interpreted code (A. Scemama)

Practical session to be locally operational, bash scripts and Linux syntax (P. Reinhardt, A. Scemama)
Introduction to C as basic programming language, translation to machine code, with simple applications (addressing, branchings, loops, documentation, hierarchy) (A. Scemama, P. Reinhardt)

<u>Tuesday:</u>
Introduction to High-Performance Computing, local →regional → national → European etc organisation, communication, latency, Amdahl's law (A. Scemama)
2nd course on C with applications (A. Scemama, P. Reinhardt)

Internal representation of numbers, numerical precision, stability of calculations, introduction to FORTRAN (P. Reinhardt)
Complexity of algorithms, linear algebra problems as examples (É. Rebolini)

Wednesday:
Data storage and accessibility, latency,memory models, pipelines, programming on vector processors (É. Rebolini)
Möller-Plesset perturbation theory as recurrent problem in quantum chemistry, transformation from integrals over basis functions to integrals over molecular orbitals

Standard problems of computational science: sorting algorithms, linear algebra
Good practice when programming: strategies, documentation, tests, structuration, decomposition into independent pieces for different tasks

Thursday:
Models for parallel computing, OpenMP, MPI, farming, Amdahl's law, data organisation, Master-Worker scheme, parallel I/O
Typical problems in Quantum Chemistry: search for eigenvalues, iterative solutions of linear algebra problems, self-consistent methods, dressing techniques, fitting procedure, interpolation

Afternoon: selected items of the previous days, student project

Friday:
Types of networks, data handling, accessibility, addressing machines for parallel execution
Profiling a code, debugging, programming tools

Afternoon: selected items of the previous days, student project

The lecturers:

- Peter Reinhardt

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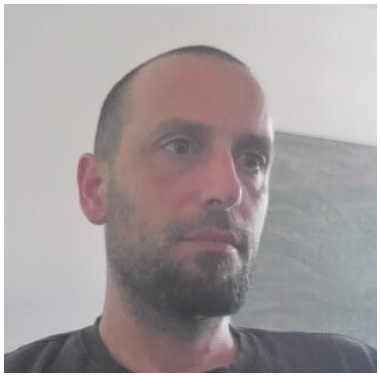
  - PhD thesis in 1995 in Bonn, Germany : ab-initio investigations of rutile surfacesPostDoc in Toulouse, Barcelona, Dresden, perturbation and CI methods applied to periodic structures in localized orbitals
  - since 1999 Maître de Conférences (Assistant Professor) in Paris, Laboratoire de Chimie Théorique, University Pierre-et-Marie Curie, now Sorbonne University
  - contributions to CRYSTAL, Molpro, Dalton, quantum package and experimental code for correlation in localized orbitals
  - Web site: https://www.lct.jussieu.fr/pagesperso/reinh/
  - Mail address: Peter.Reinhardt@sorbonne-universite.fr

- Anthony Scemama



  - PhD thesis in 2004 in Paris : reactivity in atmospheric environment and Monte-Carlo analysis of electron localization
  - PostDoc in Leiden, Netherlands, development of Monte-Carlo methods and wavefunction representations
  - since 2006 research engineer in the CNRS, development of highly parallel codes for ab-initio calculations, Toulouse, France
  - main developer of the “Quantum Package”, a versatile environment for ab-initio calculations
  - Web site: https://www.cnrs.fr/fr/personne/anthony-scemama
  - Mail address: Anthony.Scemama@irsamc.ups-tlse.fr

- Élisa Rebolini

  - PhD thesis in 2014 in Paris : Range-separated density-functional theory for molecular excitation energies
  - PostDoc in Oslo, Norway, excitation energies by range-separated DFT, algorithms for efficient calculation of correlation energies on parallel computers
  - since 2017 researcher at the Institute Laue-Langevin (ILL) in Grenoble
  - contributions to Molpro, Dalton, embarrassingly parallel research code for perturbation theory (Oslo), code RelaxSE pour calculs MRCI de haute précision (Grenoble)
  - Web site: https://www.ill.eu/users/support-labs-infrastructure/computing-for-science/people/elisa-rebolini
  - Mail address: Elisa.Rebolini@ill.fr