Kursnamn Best-practices in computational materials science

Omfattning (högskolepoäng) 3
ECTS credits

Tidsperiod 2-3 weeks
Course period

Antal platser 40
Maximum number of participants

Undervisningsspråk English
Language of instruction

Kursens syfte samt motivering till varför den bör vara fakultetsgemensam (max 150 ord)
Aim of course and motivation as to why it should be considered “multidisciplinary” to the extent that the faculty should allocate extra financing.
The course targets PhD students who are performing electronic structure calculations or numerical simulations as part of their research. The targeted areas are not only computational physics and chemistry, but also extend to applied mathematics, engineering, and computational biology.

The teachers of this course, Diana Iusan and Pavlin Mitev are working as researchers in the Departments of Physics and Chemistry, respectively. They are therefore aware of research problems occurring in current research. At the same time they are also working as application experts at SNIC-UPPMAX, focusing especially on compiling and optimizing numerical codes for different supercomputing architectures. Their mixed expertise is what makes them suitable for giving this course.

Kursinnehåll, kursens uppläggnings samt examinationsform (max 150 ord)
Contents, study format and form of examination

The content of the course is:

1. Best-practices in planning numerical simulations
2. Best-practices in the Vienna Ab-initio Simulation Package (VASP)
3. Best-practices in the RSPt code
4. Best-practices in the Gaussian code
5. Performance analysis, profiling, and debugging of codes
6. Tailored optimization of selected softwares at the Swedish National Infrastructure for Computing (SNIC)

The study format will consist of lecture notes and numerical exercises to be performed at different SNIC supercomputers.

The examination form will be in the form of individual written reports on projects taken from the current research of the PhD students. The results will be also discussed in a joint seminar involving all PhD students taking the course.

Målgrupp(er) (specifiera ämnen/inriktningar) samt rekommenderade förkunskaper
Target group(s) (specify, if possible, subject/specialization) and recommended background
This course is highly recommended for PhD students in physics, chemistry, computational biology, engineering and applied mathematics who are performing numerical simulations.

Background knowledge in Quantum Mechanics is recommended but not mandatory.

Huvudansvarig institution Department of Physics and Astronomy
Department with main responsibility

Andra inblandade institutioner (specifiera hur).
Other departments involved (specify how).
Department of Chemistry, where the co-teacher, Pavlin Mitev, is working as a researcher (50%).
SNIC-UPPMAX, where both teachers are employed as application experts (50%) and that is providing the computational resources to be used during the simulation labs and examination projects.

Kontaktperson/er (namn, e-postadress)
Contact person (name, e-mail address)
Diana Iusan, diana.iusan@physics.uu.se
Pavlin Mitev, pavlin.mitev@kemi.uu.se

Anmälan om kursdeltagande till
Application from course participants should be sent to
diana.iusan@physics.uu.se

Senast December 1st
Not later than

Kursen har tidigare givits (ange när) - med - deltagare (ange antal)
The course has previously been given (specify when and number of participants)