

COMPUTE retreat

20-21 August, 2012

Melvyn B. Davies
Department of Astronomy
and Theoretical Physics

<http://cbbp.thep.lu.se/compute>

What is COMPUTE?

- COMPUTE is a research school within the Science Faculty at Lund University
- It brings together partners from many departments within Science Faculty
- Will provide PhD courses
- Seminar speakers
- Student travel to conferences
- Annual retreat
- Funded 2012-2016

COMPUTE partners

Partner	Abbreviation	Contact(s)
Astrophysics	AP	Melvyn B. Davies, Anders Johansen
Biochemistry and Structural Biology	BSB	Ingemar André
Centre for Mathematical Sciences	CMS	Eskil Hansen, Joachim Hein
Computational Biology and Biological Physics	CBBP	Anders Irbäck, Tobias Ambjörnsson
Experimental High Energy Physics	EHEP	Anders Oskarsson, Oxana Smirnova
Lunarc	LUNARC	Magnus Ullner
Mathematical Physics	MP	Claudio Verdozzi
Medical Radiation Physics	MRP	Michael Ljungberg
Microbial Ecology	ME	Dag Ahrén, Anders Tunlid
Physical Chemistry	PC	Per Linse
Physical Geography	PG	Ben Smith, Veiko Lehsten
Theoretical Chemistry	TC	Magnus Ullner, Per-Åke Malmqvist
Theoretical High Energy Physics	THEP	Torbjörn Sjöstrand, Leif Lönnblad

COMPUTE Steering Group

- Tobias Ambjörnsson (study director)
- Melvyn B. Davies
- Joachim Hein
- Anders Irbäck
- Anders Johansen (study director)
- Magnus Ullner

Today's programme

13:00-13:05	Welcome
13:05-13:20	COMPUTE news (travel grants, courses, seminars)
13:20-14:20	Sara Santesson (Department of Communication and Media, LU): “Science communication”
14:20-15:00	PhD student talks (1,2)
15:00-16:00	Coffee break, socialising in groups, poster viewing
16:00-17:20	PhD student talks (3,4,5,6)
17:20-18:20	Oxana Smirnova (Department of Physics, LU): “Principles of distributed computing in data-intensive science”
18:20-19:00	Check in
19:00-20:30	Dinner
20:30-21:30	Michael Green (Data Intelligence A/S, Copenhagen, LU alumnus): “Sales modeling and the art of quantifying medias effect on consumer behavior”

Tomorrow's programme

07:00-08:30	Breakfast
08:30-08:50	Check out
08:50-09:30	PhD student talks (7,8)
09:30-10:20	Coffee break, poster viewing
10:20-11:00	PhD student talks (9,10)
11:00-11:30	Sara Santesson: "Reflection on PhD student talks"
11:30-12:00	Closing words, with poster prize
12:00-13:00	Lunch
13:00-13:30	Take down posters
13:30	Bus leaves ÅhusStrand
15:00 (app)	Arrival Lund



Efficient programming of modern HPC architectures

Jonas Lindemann
Joachim Hein

Lunarc

Course Outline

- Introduction to the scripting language Python
- Introduction to Fortran
- Modularised software development
- Multilanguage development
- Parallel computing using distributed and shared memory
- Commonly used commands of the OpenMP API
- Commonly used commands of the MPI API
- Parallelisation techniques for scientific applications

Practicalities

Period: HT1 2012
Start: 4th September 2012
Credits: 7.5 hp

Lectures: Tuesdays and Fridays: 10 am
Tutorials: Tuesdays: 1 pm

Prerequisites: Basic programming knowledge

Assessment: Coursework (continuous assessment)

Monte Carlo and Molecular Dynamics Tools

- Fall 2012, 7.5 hp, starts ~5 November and ends in January
 - One-week introduction
 - 5 one-week projects
 - elementary particle physics (Torbjörn Sjöstrand)
 - medical radiation physics (Michael Ljungberg)
 - astronomy (Melvyn B. Davies)
 - biological physics (Anders Irbäck)
 - physical/theoretical chemistry (Magnus Ullner, Per Linse, Mikael Lund)
 - One-to-two-week extension of one of these projects
 - Registration opens soon
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COMPUTE Seminars

- ~2-4 seminars each semester, broadly focused on scientific results obtained using computational methods
- Accommodation + reasonable travel costs covered
- Speaker suggestions to Melvyn B. Davies or Anders Irbäck
- Info: cbbp.thep.lu.se/compute
- Next seminar: 25 October by Chris Lintott, Oxford

Travel Grants

For what?

- Workshops, conferences, and summer/winter schools
- Conference fee, air/train fare, and hotel

For whom?

- Registered COMPUTE students
- Active COMPUTE students have higher priority

How?

- Two rounds/year (first announcement soon)
- No retroactive applications

