What Graduate Students Should Learn about
Scalability, Efficiency, and Performance
in the Multicore Era

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in collaboration with many more

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Universität Erlangen-Nürnberg
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SIAM Parallel Processing
Where is Erlangen?
Overview

- CS&E vs. CS and Math
- What should a CS&E curriculum include
- Erlangen CS&E Programs
  - (Graduate) courses for CS&E students
    - with emphasis on HPC
  - (Master) Thesis topics
- Conclusions
The Two Principles of Science

Theory
- Mathematical Models, Differential Equations, Newton

Experiments
- Observation and prototypes
- empirical Sciences

Computational Science
- Simulation, Optimization
- (quantitative) virtual Reality
Current main stream programs do not educate students in CS&E

- CS&E is not (a specialization within) Computer Science
- CS&E is not (a specialization within) (applied) Mathematics
- CS&E is not part of or specialization within any other Science or Engineering Discipline

CS&E is the science of methods using computation for understanding and solving problems in science and engineering

CS&E uses computation to
- understand
- predict
- and optimize objects of scientific study

Any CS&E program must be interdisciplinary

CS&E education requires more than just offering its constitutive components
- It is not enough to offer only a mix of existing courses from CS, Math, and a „target discipline“. This does not grow together by itself!
- Synergistic Courses in Scientific Computing, CS&E projects, ...
CS&E education must include

- methods and techniques coming from
  - mathematics
  - computer science
  - one (or more) target discipline
- examples how CS&E methods are applied
- project experience
- practical experience with the full CS&E pipeline (not just parts of it)
- communication skills with colleagues from other disciplines

CS&E applications require lots of compute power:

- CS&E students must learn (to use) parallel computers
Computational Engineering at Erlangen

- started as International Master program in 1997 (with sponsoring from DAAD)
- taught in English
- undergraduate program (taught in German) since 1999
- organized from within Computer Science
- offers specializations in
  - Computational Mechatronics
  - Information Technology
  - Automatic Control
  - Material Sciences
  - Fluid Dynamics
  - Mechanics
- Students must choose an „application field“ (and then stay with it)
Computing Equipment

LSS Cluster
- 8x4 (+ 9x2) Nodes
- CPU: AMD Opteron 848
- RAM: 8x16 Gbyte
- High-Speed Network InfiniBand

Erlangen Computing Center (RRZE) Cluster
- 217 compute nodes
- Each with two Xeon 5160 "Woodcrest" chips (4 cores)
- High-Speed Network InfiniBand

Bavarian Academy of Sciences (LRZ) HLRB-II
- SGI Altix 4700
- 9728 Itanium Cores, 62 TFlops
- 40 Tbyte memory

Various „Toys“, such as
- Cell Processor (Play stations)
- GPUs (ATI and Nvidia)
- GPU-cluster

Access to German and European Supercomputing Infrastructure
- Large NEC vector processor at Stuttgart
- 72 racks of Blue Gene at Jülich
- QPACE (Cell Cluster)
## CE Graduate (Master) Program

### CE Master Degree

<table>
<thead>
<tr>
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<th>Details</th>
</tr>
</thead>
<tbody>
<tr>
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<td></td>
</tr>
<tr>
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<td>(with TU Munich)</td>
</tr>
<tr>
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International CE Students 1997-2009

Männer: 256 + 29*)
Frauen: 96 + 11*)

Nordamerika:
• Kanada 1
• USA 4

Lateinamerika:
• Bolivien 1 +1
• Brasilien 4
• Costa Rica 1
• Ecuador 1
• Kolumbien 4
• Kuba 1
• Mexiko 3
• Nicaragua 1
• Peru 1
• Venezuela 1
• Chile +1

Westeuropa:
• Deutschland 40 + 12
• Frankreich 1
• Griechenland 2
• Irland 1
• Österreich 1
• Spanien 2 +1
• Italien +1

Afrika:
• Ägypten 4
• Algerien 1
• Eritrea 1
• Gambia 1
• Kenia 1
• Kamerun 4
• Mauritius 1
• Senegal 1
• Sudan 1
• Tunesien 2
• Zimbabwe 1
• Uganda 1

Nahe Osten:
• Iran 2 + 2
• Israel 1
• Jordanien 2
• Libanon 5 +1
• Syrien 7 + 1
• Türkei 15 + 1

Südasien:
• Bangladesh 1
• Indien 64 +7
• Nepal 1
• Pakistan 10 +3
• Sri Lanka 1

Südostasien:
• Indonesien 4
• Philippinen 1
• Thailand 1
• Vietnam 2

Südostasien:
• Vietnam 2

Osteuropa / Zentralasien:
• Bulgarien 14
• Estland 1
• Kasachstan 1
• Rumänien 4 +2
• Russland 8 +1
• Serbien 2
• Ukraine 10
• Ungarn 9
• Usbekistan 1

Ostasien:
• China 94 + 6
• Südkorea 1

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• Kuba 1
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• Nicaragua 1
• Peru 1
• Venezuela 1
• Chile +1

Frauen: 96 + 11*)
Männer: 256 + 29*)

∑ = 352 + 40*)
aus 56 Ländern

*) Started in 2009
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Joint program with TU Munich within the Elite Network of Bavaria: http://www.elitenetzwerk.de

Started in 2005 and recently been extended until 2015

For exceptionally talented and motivated students.

Motto: “Do more, get more!”

Awarded with degree “Master of Science with Honours”.

Regular CE master program plus additionally 30 ECTS:

- 10 ECTS for project work
- 10 ECTS for CE specific lectures
- 10 ECTS for soft skill courses.
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DAAD Double Master Degree

- Started in 2008 together with the Royal Institute of Technology in Stockholm.
- Idea:
  - 50% of the master studies are done in Erlangen,
  - 50% done in Stockholm (or vice versa).
  - The graduates get degrees from both universities
- international experience and intercultural exchange
- Generous stipends by DAAD
- Profit from existing expertise in CSE at both universities

This is more than the sum of two excellent programs.
Double Degree Program

- Students beginning at Erlangen
- Students beginning in Stockholm

1st year
- FAU Erlangen-Nürnberg
- KTH Stockholm

Core Courses (taught at both universities)
- 15 ECTS Numerical Analysis
- 15 ECTS Applied Mathematics
- 15 ECTS Scientific Computing

Joint Workshop – in depth advising of students to prepare the transfer
- 15 ECTS Preparatory Courses for Specialization (partly given by Guest Prof. from KTH)
- 15 ECTS Preparatory Courses for Specialization (partly given by Guest Prof. from FAU)

Transfer

2nd year
- Choice of Specialization in
  - 15 ECTS Visualization and Image Processing
  - 15 ECTS High Performance Computing
  - 15 ECTS Electives
- Choice of Specialization in
  - 15 ECTS Bio-Modelling
  - 15 ECTS Computational Fluid Dynamics
  - 15 ECTS Electives

30 ECTS Master Thesis
- Conducted at host university
- Co-supervised by instructor from home-university
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COSSE
Computer Simulation for Science and Engineering

Erasmus-Mundus: EU-Project
about 1 Billion Euro, mostly stipends
about 100 International Master Programs,

„Double mobility“ required:
Master studies must be done in two different countries, but not in the country where the Bachelor degree was achieved.

COSSE is a joint project between:
KTH Stockholm (Coordinator), TU Delft, TU Berlin, and FAU Erlangen
COSSE – Study Plan

1st and 2nd Sem.:

- Compulsory core courses
  - Numerical Analysis
  - Applied Mathematics
  - Scientific Computing
  - 15 ECTS

Joint Workshop:

- Preparatory courses for specializations
  - 15 ECTS

3rd and 4th Sem.:

- Bio Mod alt. Mat Sci: Electives
  - 15 ECTS
- Num Lin Alg alt. CFD: Electives
  - 15 ECTS
- Control alt. Optimization: Electives
  - 15 ECTS
- HPC alt. Visualization: Electives
  - 15 ECTS

Master Thesis Project
- 30 ECTS
- Joint home and host university
Parallel Computing Courses

- **Advanced Programming Techniques**
  - required for beginning CE graduate students (who did not have an undergraduate CS major)
  - covers C++ and a few parallel computing concepts

- **Simulation and Scientific Computing I+II**
  - required for students who did not have equivalent undergrad courses
  - includes a first introduction to
    - architecture aware programming (caches, SSE, ...)
    - OpenMP and MPI programming
  - includes lab sessions, programming exercises, student projects

- **Cluster Computing**
  - Using clusters with various programming paradigms (Java, C++, ...)

- **Programming Techniques for Supercomputers (elective)**
  - In-depth treatment of performance programming and
  - high performance computer architecture

- Regular seminars, such as „Cell Processor Programming“
- Parallel Computing as part of courses such as „Numerical CFD“
Programming Techniques for Supercomputers (1)

- Lecture
  - 2 hrs lecture + 2 hrs exercises (5 ECTS)
  - Regular module since summer term 2000

- Audience
  - Computational Engineering (Master)
  - PhD and diploma students from computer Science, Physics, Engineering, Materials Science,…
  - 15 – 25 students each summer term

- Developed and taught by HPC group of Erlangen Regional Computing Center based on experience from HPC user support

- Students should be able to write an efficient serial and parallel program for numerical kernels on modern architectures
Programming Techniques for Supercomputers (2)

Main topics

- Introduction to basic hardware concepts for sequential and parallel computers *Numerically efficient simulation requires a different view of hardware than that presented in computer architectures lectures...*
- Efficient sequential programming *This needs always to be the first step for efficient parallel computing*
- Potentials and Limitations of Parallelization
- Shared Memory Programming (OpenMP)
- Distributed Memory Programming (MPI)
- Basic Performance Modeling is used throughout the lecture and tutorial *What performance can I expect at best for a given problem on a given architecture*
- Tutorial: Students do their exercises on RRZE HPC production clusters *So they get used early to the HPC environments, e.g. batch systems*
Programming Techniques for Supercomputers (3)

- Summer term 2010
  - 4 hrs of lecture
  - Additional topics include e.g.
    - Hybrid programming
    - Programming GPUs
    - Multi-Core aware / specific programming approaches

- Some experiences
  - Students enjoy to work on (large) parallel machines
  - Performance Modeling needs to be done from day one
  - Sometimes it is hard to get them started soon
  - Some are already C programming experts others are bloody beginners…
Examples of CE (Master) Thesis

- B. Gmeiner: Extension of a Software Package for Hierarchical Hybrid Grids
- S. Strobl: GPU-Based Rigid Body Dynamics
- J. Halwai: Performance Analysis of Hybrid Parallelization Techniques for Large Scale Lattice Boltzmann Simulations on Multicore Platforms
- T. Heller: SSE Optimierung of the PE Physics Engine
- D. Ritter: A Fast Multigrid Solver for Molecular Dynamics on the Cell Broadband Engine
- L. Yi: Efficient GPU Implementation of an MIR PPA Reconstruction Algorithm
- D. Bartuschat: A parallel patch-based approach for the reduction of quantum noise in CT-images
- D. Brinkers: Algorithms for sparse matrices on the CBEA
- Y. Sun: Parallel Solution for Differential-Algebraic Equations in power plant simulation
- S. Geißelsöder: Shared memory parallelization of the pe physics engine
- J. Habich: Performance Evaluation of Numeric Compute Kernels on NVIDIA GPUs
- M. Kavasoglu: Simulating Transformer Noise
- Yuanjun Zhang: Numerical Methods for Simulating Transformer Noise
Conclusions
What else do we do?

- Parallel Multigrid Algorithms on 10,000 cores and beyond
  - Talk by UR this afternoon (5:00pm) in MS 16 „Challenges in Parallel Adaptive Mesh Refinement“
- Parallel Rigid Body Dynamics MS 54 Friday 1:20-3:30 pm
  - Talk by Klaus Iglberger on Friday 1:20 pm
  - Poster by Tobias Preclik „Parallel Rigid Body Dynamics“
- Talk by UR this morning in MS 4: „Multigrid for Multicore“
- Parallel Lattice Boltzmann Methods for Complex Flows
  - no talk
- Performance Analysis:
  - Talk by Georg Hager (Erlangen Computing Center) in MS 45, Friday 9:50-11:50 am „Analysis of Hybrid Applications on Modern Architectures“
Conclusions :-)  

Parallel Supercomputer Performance is Easy!

- If parallel efficiency is bad, choose a slower serial algorithm
  - it is probably easier to parallelize
  - and will make your speedups look much more impressive

- Introduce the “CrunchMe” variable for getting high Flops rates
  - advanced method: disguise CrunchMe by using an inefficient (but compute-intensive!) algorithm from the start

- Introduce the “HitMe” variable to get good cache hit rates
  - advanced version: Implement HitMe in the “Transgalactic Hash-Brown Lookaside Table of the Multi-Threatened Cash-Filling Spock-Tree“ Class
    - ... impressing yourself and others

- Never cite “time-to-solution”
  - who cares whether you solve a real-life problem anyway
  - it is the MachoFlops that interest the people who pay for your research

- Never waste your time by trying to use a complicated algorithm in parallel
  - Use Primitive Algorithm => Easy to Maximize your MachoFlops
  - A few million CPU hours can easily save you days of reading in boring math books
Thanks for your attention!

Questions?

Slides, reports, thesis, animations available for download at: www10.informatik.uni-erlangen.de