

SPPEXA- Doctoral Retreat 2013

September 16-20 at TU Darmstadt

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Topic & Venue

The first Doctoral Retreat & Coding Week on "Application & Algorithm: Combination of Software Tools and Programming" takes place on September 16 - 20, 2013 at TU Darmstadt. All PhD students within SPPEXA are cordially invited to participate.

Fees & Residential

There will be no registration fee; free coffee breaks, lunch & welcome dinner are included.

SPPEXA provides free accommodation at an local Youth hostel: 2 or 4 bed rooms in Jugendherberge Darmstadt (<http://www.djh-hessen.de/jugendherbergen/darmstadt>). During the workshop week all hotels in the region are mostly occupied due to the IAA in Frankfurt and rooms are available only at an extra charge. If separate accommodation aside the Youth Hostel is required, please organize your own accommodation at your own costs.

Goal

This workshop aims to bridge the gap between various sciences to foster cross discipline understanding in context of the SPPEXA project and to provide a forum for exploring new ideas. Application & algorithm PhD students will have the opportunity learn about terms, definition, and impact of basic mathematical algorithms used in computational science. Furthermore, this workshop will provide background in the field of efficiency, performance modelling and memory consumption, and how these aspects should be respected in code design. Tools & computer science PhD students have the chance to learn about working style and daily problems of application scientists. This workshop will also provide all PhD students with an overview of the applications and methods used in various SPPEXA projects, and the restrictions emanated from physical or mathematical modelling.

Method

All PhD students are expected to provide a short presentation (max. 10 Minutes, 5 slides) of their project and their own research question. Besides user presentations, the workshop provides lectures supplemented by labs with the aim to facilitate cross-topic students collaboration.

Preparation

All participants are kindly asked to answer a brief questionnaire before the actual workshop, in order to prepare and adjust the workshop material according to the participants needs. This questionnaire will be available a month before the workshop.

Hardware

For the labs all participants are kindly asked to use their own Laptop (WLAN).

Thematic Program

Detailed time schedule (including breaks for coffee, tea & lunch) will be announced in September

Monday: Introduction

14:00 -14:15 Welcome

14:15 -18:00 Participant project presentation, goals and expectation of the workshop

19:00 Welcome Dinner

Tuesday: Solving the Physical Problem – methods and their behaviour in regard to accuracy and HPC (Bolten, Klimach, Schäfer, Sternel)

9:00 – 16:00

- Conservation equations
- Methods to solve PDE: Finite Elements, Finite Volume, Spectral Methods
- Discontinuous Galerkin Method.
- Meshes, Meshless, moving boundaries
- Multigrid (Geometric & Algebraic)

16:00 (Tuesday)

- Darmstadt sight seeing

Wednesday: Introduction to Parallel Computer Architectures and Programming with OpenMP (Wienke)

9:00-17:00

- Why Multicore Architectures?
 - SMP & ccNUMA
- Introduction to OpenMP
 - Core Concepts like Parallel Region, Worksharing, Tasks
 - Synchronization and Memory Model
 - Investigating Data Races & Deadlocks
- Lab: OpenMP Basics
 - Performance Tuning with OpenMP
 - Measuring OpenMP Performance with Tools
 - Load Balancing
 - Memory Placement and Thread Binding
 - False Sharing
 - Implementing I/O Pipelining, private vs. shared data
 - Avoiding Synchronization Overhead
 - Vectorization with OpenMP

Thursday: Basics of Node-Level Performance Modeling and Optimization (Hager, Wellein)

9:00-17:00

- A quick survey of modern processor architecture: Units, pipelines, SIMD, SMT, caches, memory
- Microarchitectural exploration via benchmarks
- Basic performance modeling: Roofline
- Model-guided optimization on the example of a Jacobi smoother
- Impact of SIMD, SMT and ccNUMA

Lab: Performance issues on the node

- Measuring divide latency
- The STREAM benchmarks as a starting point for Roofline modeling
- Modeling and improving the performance of a stencil smoother
- Performance vs. scalability vs. saturation
- Optional: Indirect memory access

17:00-18:00 **Learning outcome**

All participants prepare one slide about the learning outcome:

Looking at the „incoming“ questions: what is answered, what is new, has the personal perspective changed on the addressed topics?

Friday: Remarks & Outcome

9:00-10:00

Remarks to Scheduling, Partitioning, Placement & Compiler Options (N.N.)

10:00-13:00

Presentation and discussion of the outcome

Closing