

**KAUST-TUM Special Partnership**  
proudly presents  
**Profiling & Performance Analysis of  
Parallel Applications**

**Hans-Joachim Bungartz**

TUM, Department of Informatics, Chair of Scientific Computing



Compact Course “Profiling & Performance Analysis of Parallel Applications”

KAUST, October 31 – November 1, 2010

# KAUST-TUM Special Partnership

**Memorandum of Understanding** (signed Munich, January 2008)

**Partnership Contract** (signed Munich, December 2008)

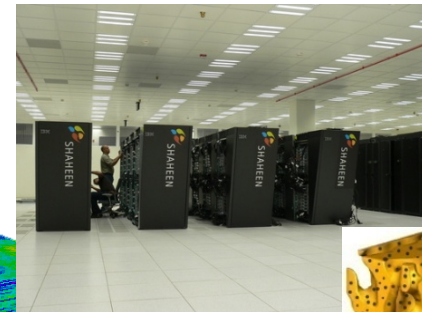
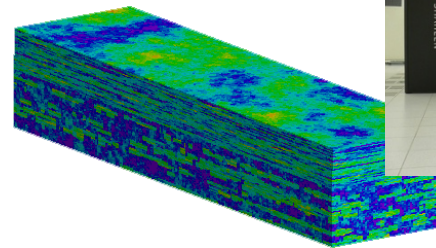
**Initial project phase: 2009–2013**

**Initial research projects:**

- **P1: Simulating CO<sub>2</sub> Sequestration**
- **P2: Virtual Arabia**
- P3: CO<sub>2</sub> Fixation

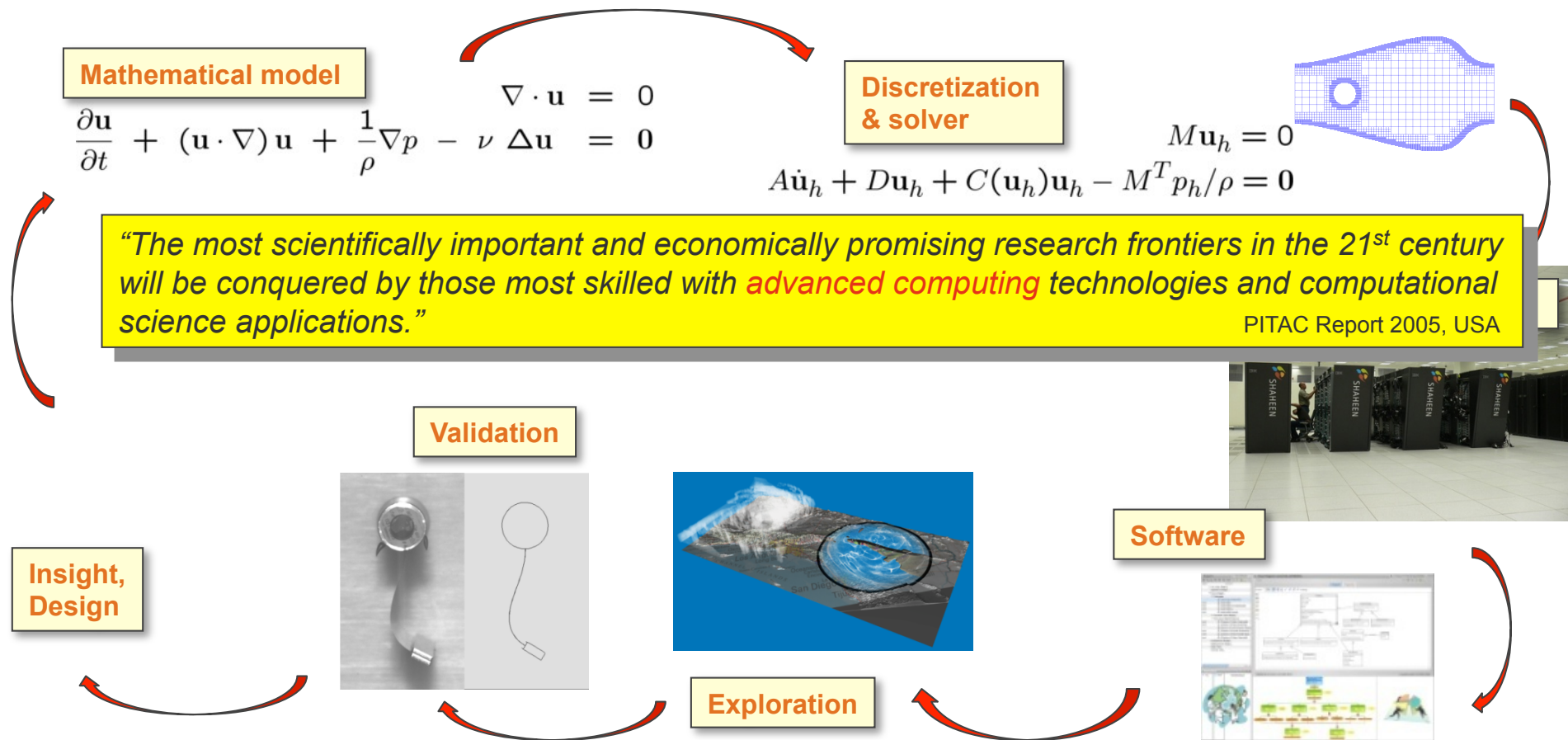
**Various consulting activities**

- Recruiting
- **This course**

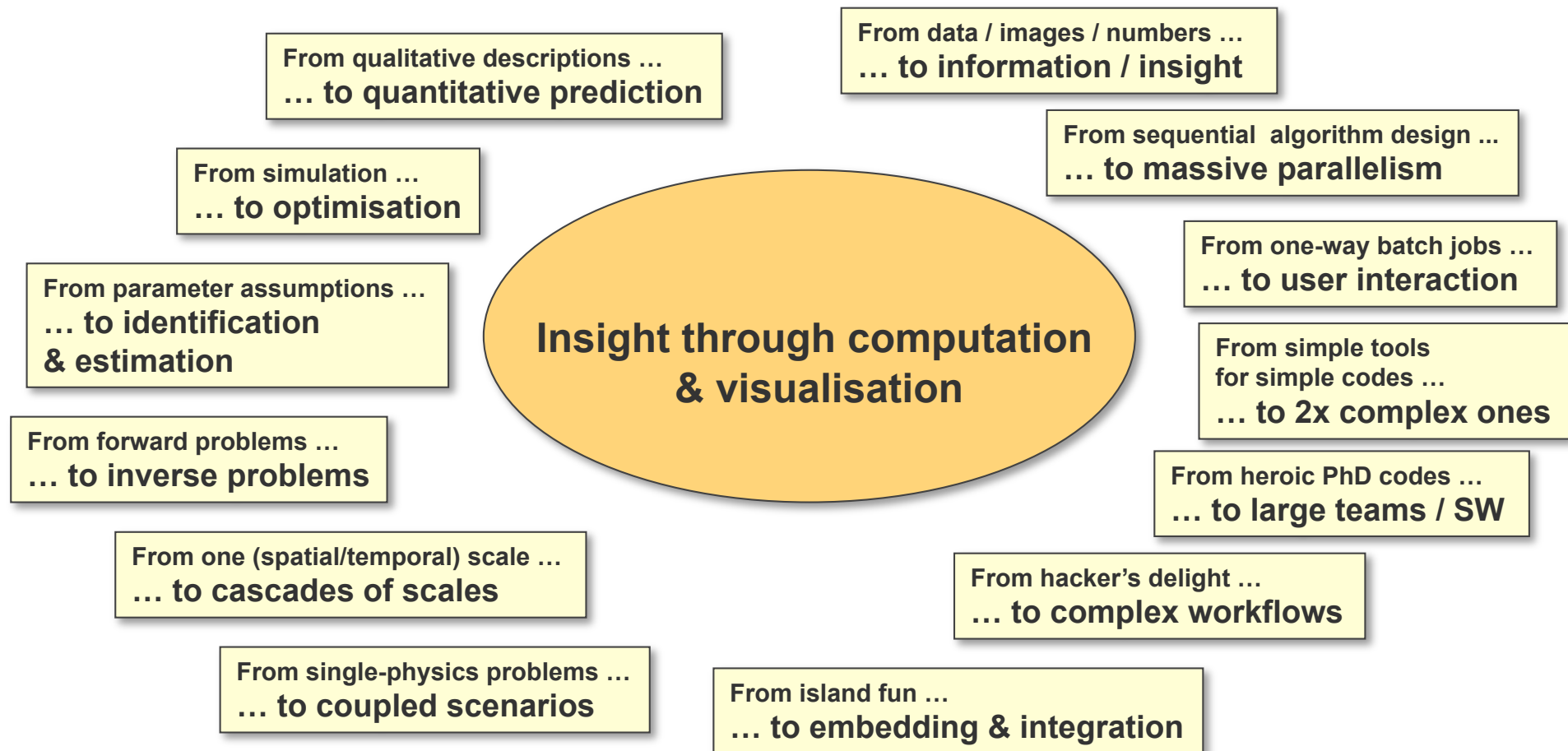


# Computational Science & Engineering

## Key technology for science & industry



## Computational Challenges: Trends & Requirements





# Anchoring @ TUM: MAC – Munich Centre of Advanced Computing

## Participating institutions:



## Involved disciplines:

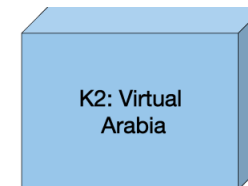
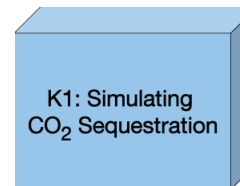
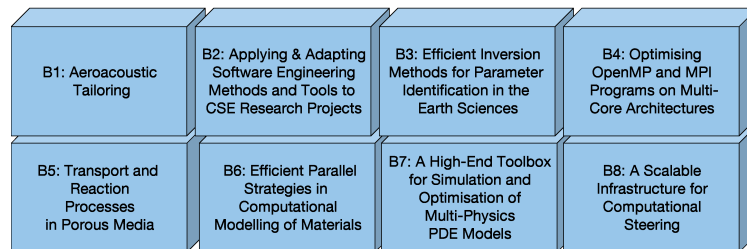
- Mathematics, informatics, and the sciences
- Mechanical, electrical, and civil & environmental engineering

## People:

- 22 professors with their groups
- 44 additional researchers (assistants, Ph.D. Students)



## Projects:



## MAC – Recent Developments

### Leibniz Supercomputing Centre

- Partner in the **Gauss Centre**, member of **PRACE**
- New buildings for Petaflop system **SuperMUC**

### Munich Computational Sciences Centre

- New research group on “HPC algorithmics and software”
- W2 professorship “HPC algorithmics and software”
- Joint professorship of IPP & TUM: Numerics for plasma physics



Photo: Ernst A. Graf



### Education in CSE – in Bavaria and @ TUM:



- Second funding period of the elite programme BGCE
- MAC implemented as a fifth pillar in TUM's Graduate School IGSSE



### New projects in the Advanced Computing context

- DFG (SFB/TR 89), BMBF (HPC software calls 1 & 2)
- G8 Exascale Initiative (4 projects from MAC among 25 finalists world-wide)
- TUM-IAS: Focus Group on HPC
- DEISA and KONWIHR projects

## Current Anchoring @ KAUST

### Divisions:

- CLSE (Chemical and Life Sciences & Engineering)
- **MCSE (Mathematical and Computer Science & Engineering)**
- PSE (Physical Sciences & Engineering)



### Research Centres:

- Catalysis
- Clean Combustion
- Computational Bioscience
- **Geometric Modeling & Scientific Visualization**
- Advanced Membranes & Porous Materials
- Plant Stress Genomics
- Red Sea
- Solar and Photovoltaics Engineering
- Water Desalination & Reuse

### Core Labs and Facilities:

- Catalysis
- **Advanced Computation & Visualization Facility**
- Analytical Chemistry
- Biosciences & Bioengineering
- Coastal & Marine
- Imaging & Characterization
- **Supercomputing**

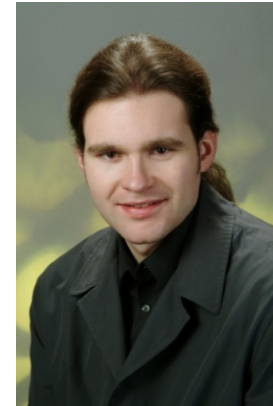
## P1 & P2 – Interactions with KAUST

### Consulting:

- Recruiting of 2 PostDocs  
(Jens Schneider, Thomas Amler)

### Projects:

- VR equipment for “Virtual Arabia”  
(now @ITüpferl, later @LRZ)
- Several guest researchers  
(1-day to 1-week stays)
- Virtual Arabia Coding Days  
(one week @ KAUST, scheduled  
for end of November)



### Education:

- KAUST Summer Internships: 2 current and 2 future KAUST students @ TUM
- Project-related courses at Ferienakademie 2009 & 2010

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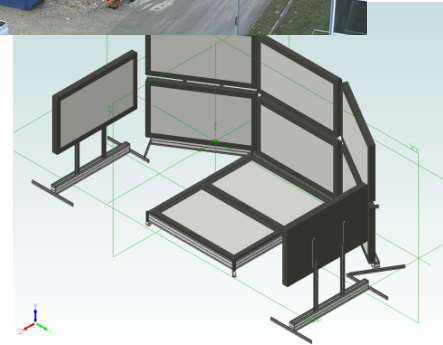
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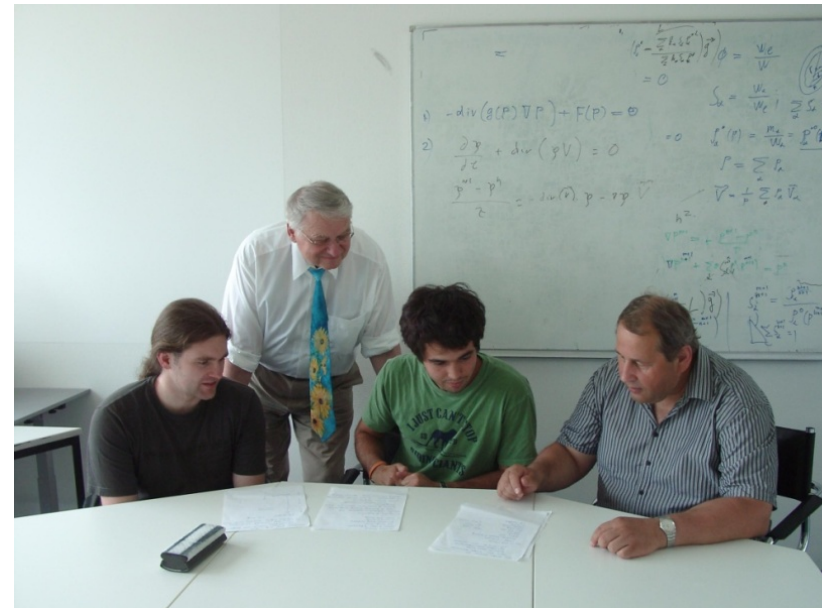
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Arturo Mora (MEX), Mohammed El Sayed (EGY), Shouhing Du (CHN), Luiz Faria (PAN)
- Project-related courses at Ferienakademie 2009 & 2010



## P1 & P2 – Interactions with KAUST

### Participation in KAUST events:

- WEP 2010:  
short course (Hoffmann, Witterstein) &  
lecture series (Bungartz, Weinzierl)
- Study group in industrial mathematics  
by OCCAM (Simon, Witterstein)

### Workshops with KAUST participation / relation:

- 2 MAC Summer Workshops  
(2009: Shih & Keyes; 2010: Hoteit & Alsayyed)
- 3 project-related workshops at IGSSE annual  
gatherings 2009 & 2010
- ASIM SimTech Workshop 2011 @ TUM  
(Schneider)





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## P1 & P2 – Special Highlight: HPC & Shaheen

### Projects:

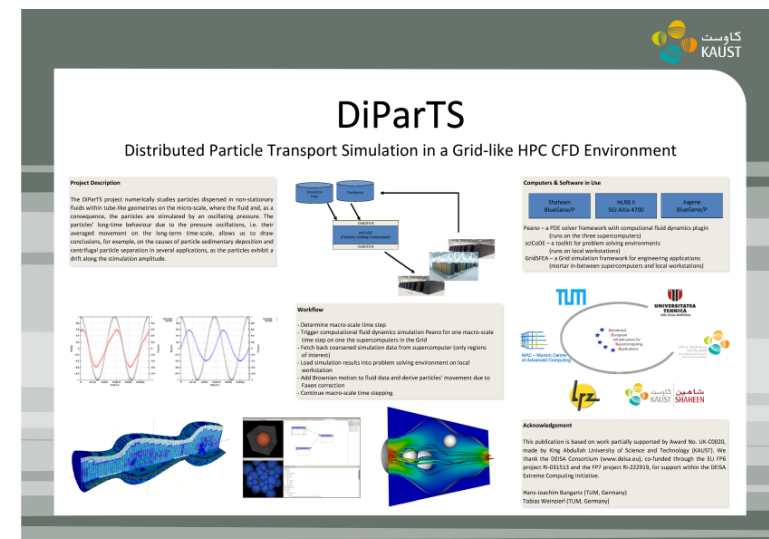
- Joint DEISA research project  
TUM – LRZ – KAUST – TU Cluj-Napoca
- Joint HLRB2 proposal TUM – KAUST  
pending

### Consulting:

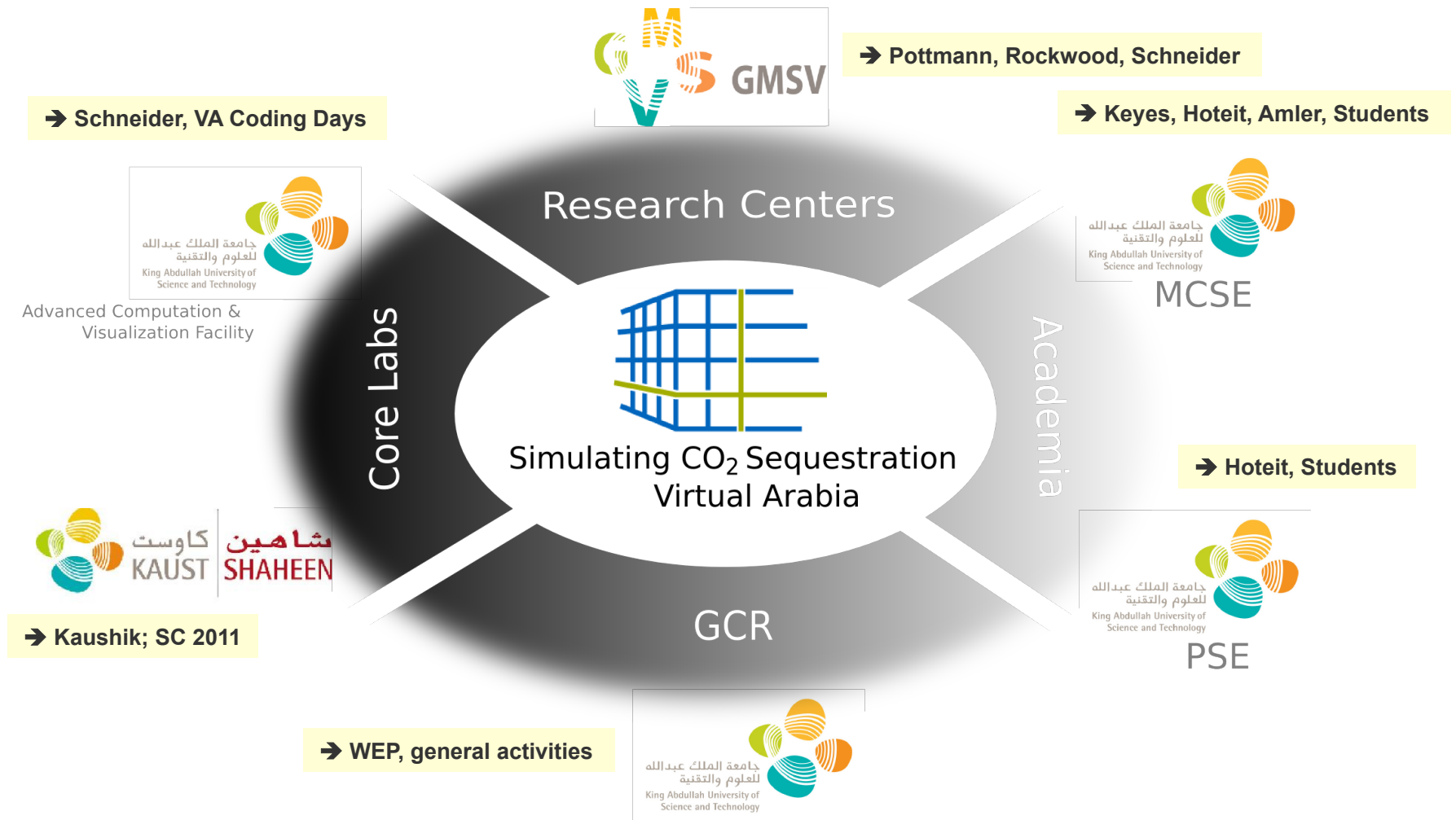
- Performance Analysis Course @ KSL /  
Shaheen: Oct 31 – Nov 1  
(7 researchers from TUM, Jülich  
Supercomputing Centre, and Dresden  
Computing Centre)

### Outreach:

- Contributing to KAUST's booth at Supercomputing 2010 with a project poster



# Current Collaborations with KAUST – Overview



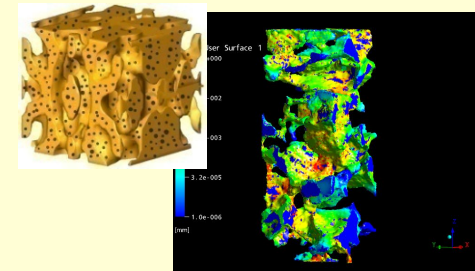
# P1: Simulating CO<sub>2</sub> Sequestration – Overview

## Goals

- design and investigate novel approaches to modelling and simulation of CO<sub>2</sub> sequestration
- in particular in the context of enhanced oil recovery
- involve both fine-grain simulations & and homogenisation approaches

## Research Plan

- modelling of CO<sub>2</sub> sequestration including parameter identification and numerical simulations
- hysteretic aspects of CO<sub>2</sub> sequestration modelling
- PDE-constrained optimisation in CO<sub>2</sub> sequestration
- multi-phase flow simulations on the pore scale
- numerical algorithms and interfaces for CO<sub>2</sub> sequestration
- implementation and optimisation of CO<sub>2</sub> sequestration on HPC systems
- data pre- and postprocessing



## Participants @ TUM (Coordination: T. Weinzierl)

- Mathematics @ TUM: Modelling & Numerical Analysis (Brokate, Hoffmann), Optimisation (Ulbrich)
- Informatics @ TUM: Scientific Computing (Bungartz)
- Engineering @ TUM: Fluid Mechanics (Manhart)
- Leibniz Supercomputing Centre (Bode)



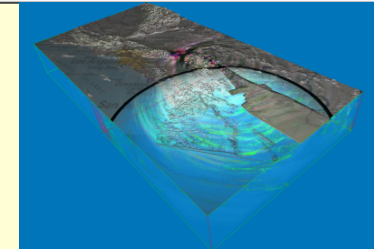
## P2: Virtual Arabia – Overview

### Goals

- develop a virtual environment for the interactive visual exploration of Saudi Arabia
- allow the user to look both above and underneath the earth surface in an integrated way
- provide a generic infrastructure for visual computing

### Research Plan

- hardware and system software platform
- efficient hierarchical interfaces of computation and visualisation
- innovative methods of VR and AR for a visual computing infrastructure
- GIS2BIM: multi-resolution models of constructions and built infrastructure
- realtime visual computing: core visualisation methodology
- data handling and data fusion

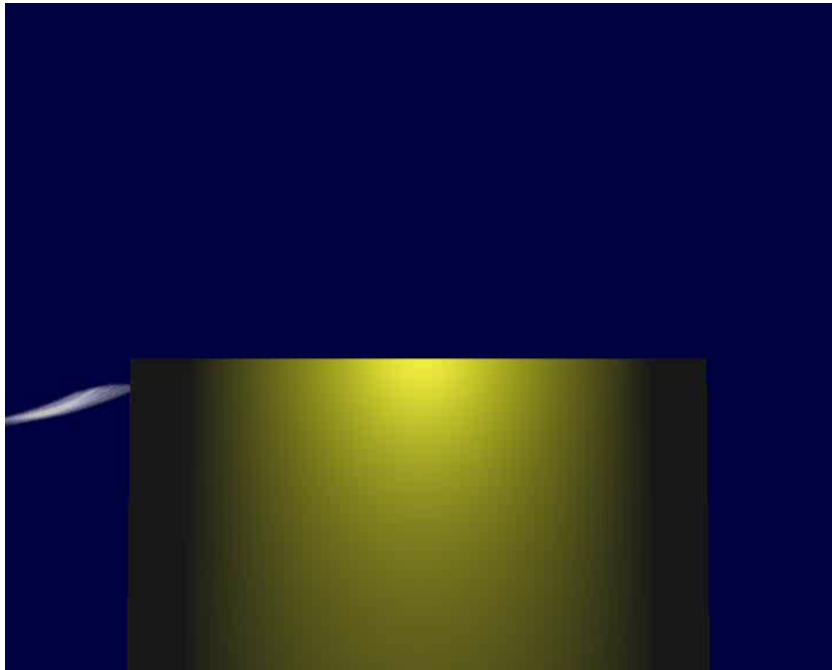


### Participants @ TUM (Coordination: T. Weinzierl)

- Informatics @ TUM: Visualisation (Westermann), AR (Klinker), Scientific Computing (Bungartz)
- Engineering @ TUM: Computation in Engineering (Rank)
- Leibniz Supercomputing Centre (Bode)

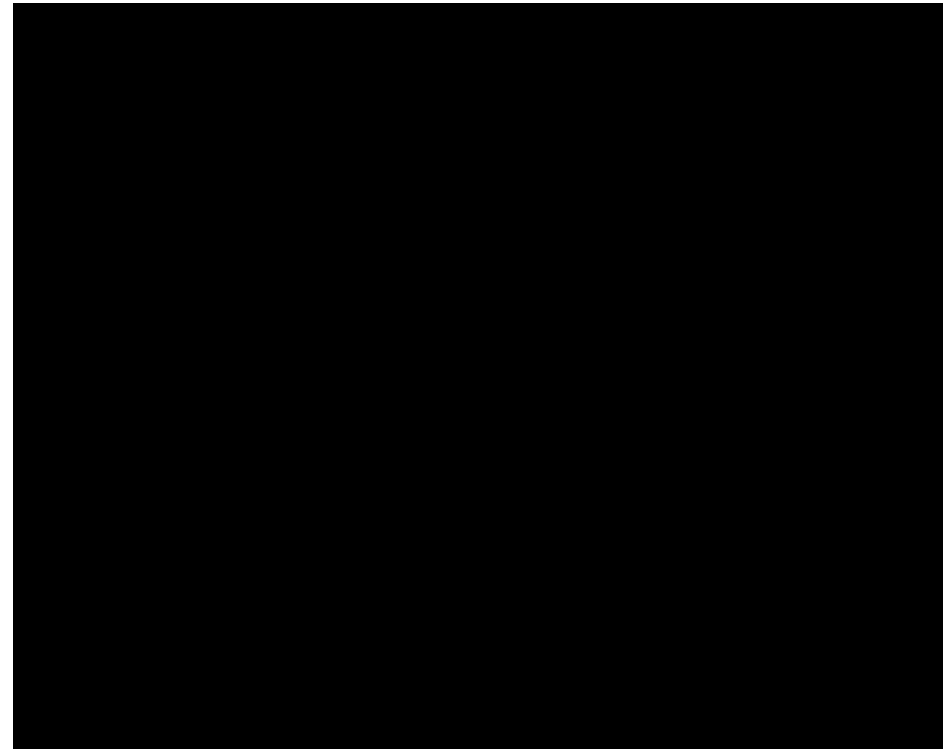


## Subproject Core Visualization (R. Westermann)



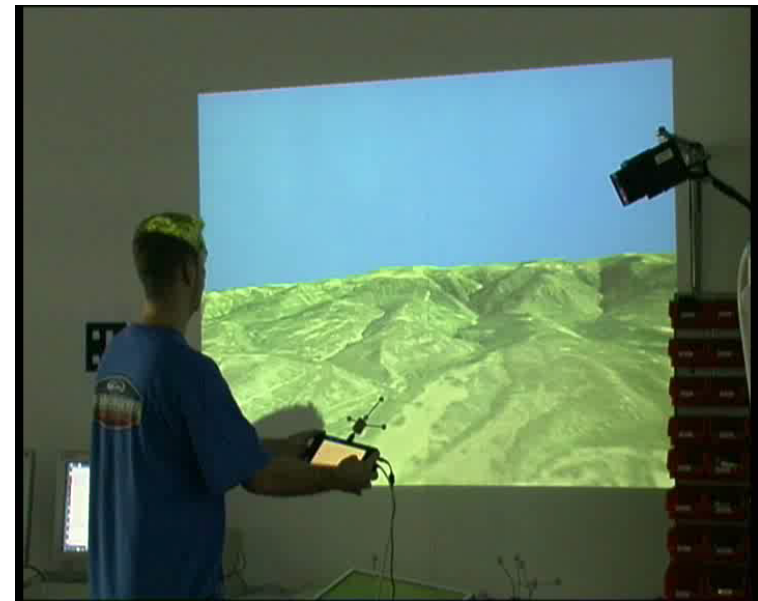
LES fluid simulation (128x128x256).  
Particle-based fluid visualisation. Dye injection and  
visualisation as in real wind tunnel.  
[Single desktop system (Intel dual core/nvidia GPU);  
video directly captured from screen.]

Visual exploration of the Terashake 2.1 earthquake simulation.  
Particle tracing was used to classify interesting wave types as they  
typically occur in earthquakes. Particle traces show typical flow  
patterns caused by compressional, shear, and Love waves.  
[Single desktop system (Intel dual core/nvidia GPU);  
video directly captured from screen.]

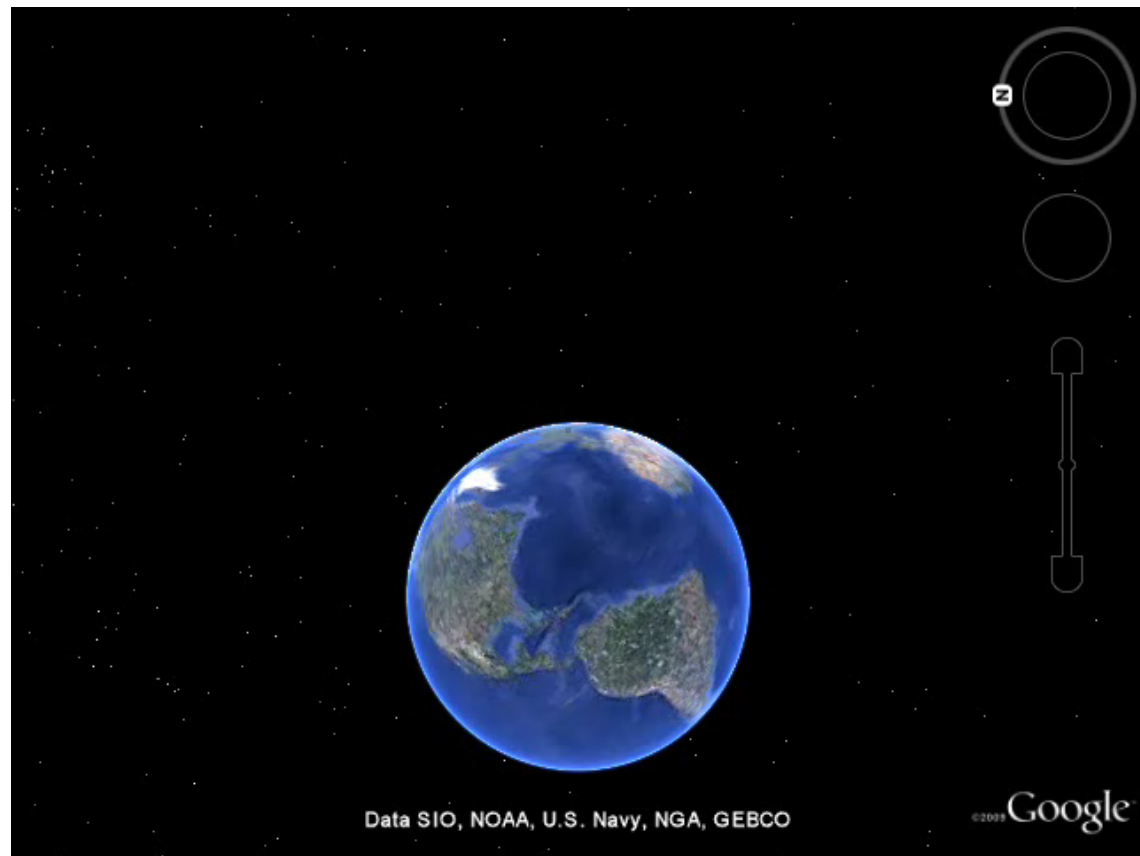
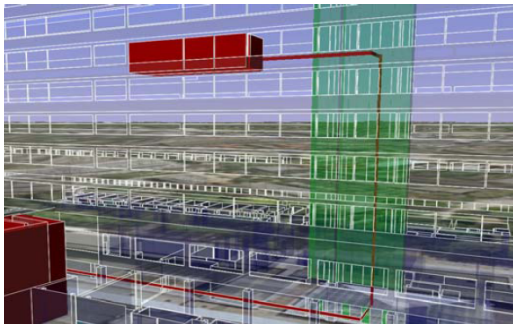
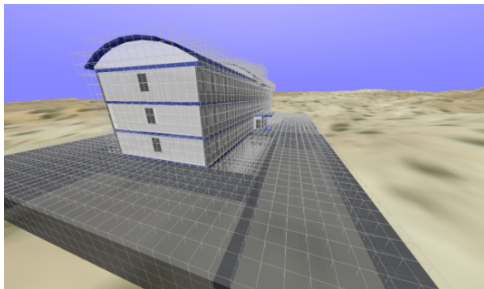


## Subproject Augmented Reality (G. Klinker)

- **Issue: How to travel through the immersive environment to explore:**
  - The effects of a simulation (SP Bungartz) or
  - Information access of a specific location (SP Rank).
- **Two control mechanisms have been found and realized in a first prototype to tackle both mentioned aspects:**
  - An airplane-like maneuvering mechanism
  - A car-like steering mechanism
- **How to combine into a controlling device with an intuitive and integrated control for the user's position and orientation?**
- **Guidance of users to points of interest**



## Subproject GIS2BIM: Multi-Resolution Models of Constructions and Built Infrastructure (E. Rank)



## Advertising: Next Events to Come

### “Virtual Arabia Coding Days”

- *Where?* KAUST campus
- *When?* December 4–6, 2010
- *Who?* All Ph.D. candidates and research assistants involved in “Virtual Arabia” – guests from KAUST very welcome!
- *Host?* Jens Schneider
- *Why?* Algorithmic developments ready for transfer to KAUST
- *What?* Implementation sessions

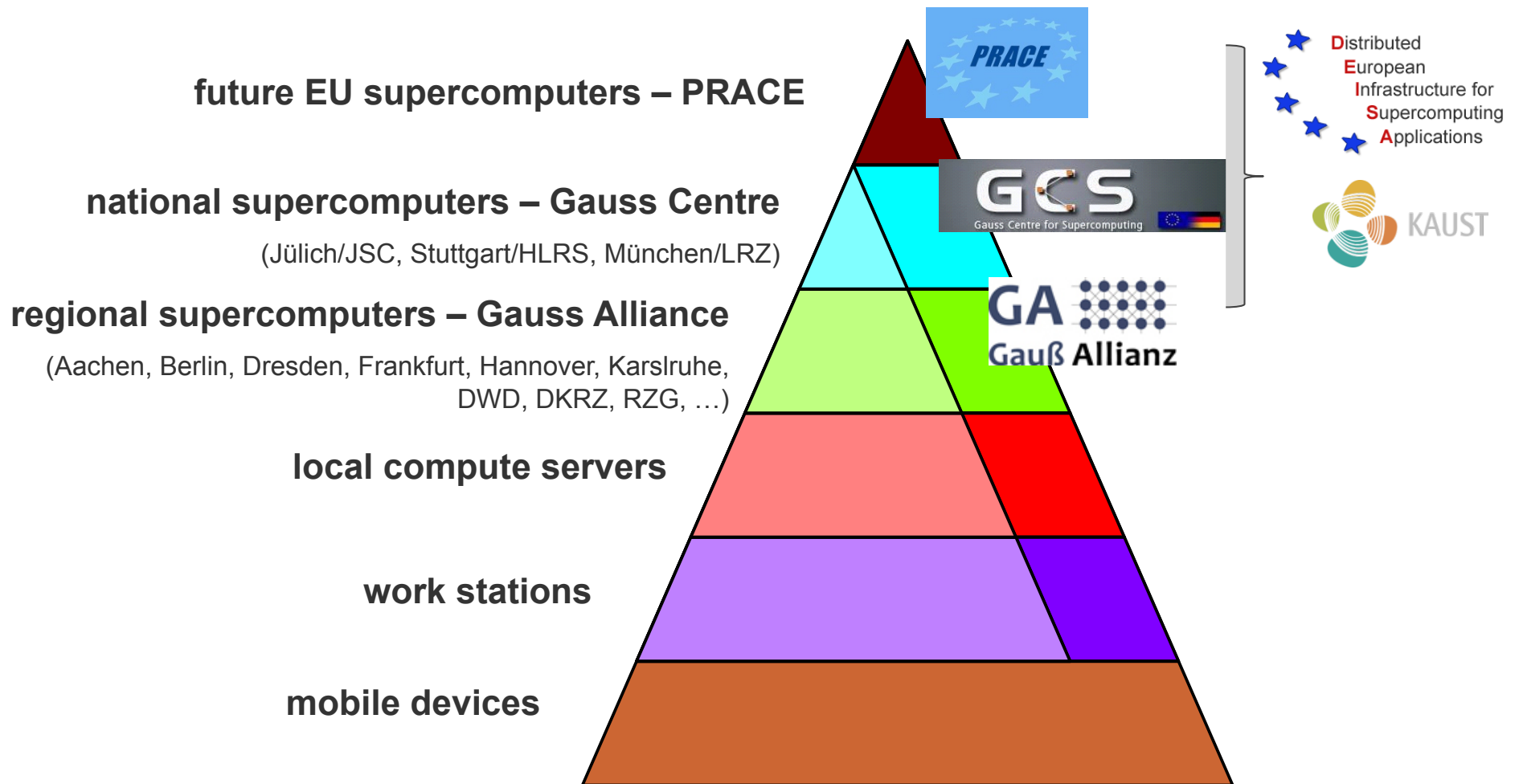
**ASIM Workshop, March 14–16, 2011, Munich** KAUST participation

**IGSSE Annual Meeting, June 7–9, 2011, Raitenhaslach** KAUST participation

**MAC Summer Workshop, July 2011, Munich** KAUST participation

**KAUST Summer Internships @ TUM, June–August, 2011** KAUST participation

# Organisation of HPC in Germany & Europe



## Virtual Institute – High-Productivity Supercomputing

The virtual institute in a...



- Partnership to develop **advanced programming tools** for **complex simulation codes**
- Goals
  - Improve code quality
  - Speed up development
- Activities
  - Tool development and integration
  - Training
  - Support
  - Academic workshops
- [www.vi-hps.org](http://www.vi-hps.org)





## VI-HPS – Partners



### Forschungszentrum Jülich

- Jülich Supercomputing Centre



### RWTH Aachen University

- Center for Computing and Communication



### Technical University of Dresden

- Center for Information Services and High Performance Computing



### University of Tennessee

- Innovative Computing Laboratory





## VI-HPS – Partners (cont'd)



### German Research School for Simulation Sciences

- Laboratory for Parallel Programming



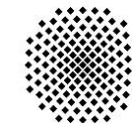
### Technische Universität München

- Chair for Computer Architecture



### University of Stuttgart

- High Performance Computing Centre



**Universität Stuttgart**

Funded by



## People

### Head, Planning, and Organisation:

Hans-Joachim Bungartz, TUM

Tobias Weinzierl, TUM

### Course Implementation

Nicholas Allsopp, KAUST

Michael Gerndt, TUM

Matthias Weber, Technical University of Dresden

Josef Weidendorfer, TUM

Felix Wolf, German Research School for Simulation Sciences

Brian Wylie, Jülich Supercomputing Centre



*And now: Enjoy the course!*

