Karlsruher Institut für Technologie

SimLabs at KIT, meeting a Challenge

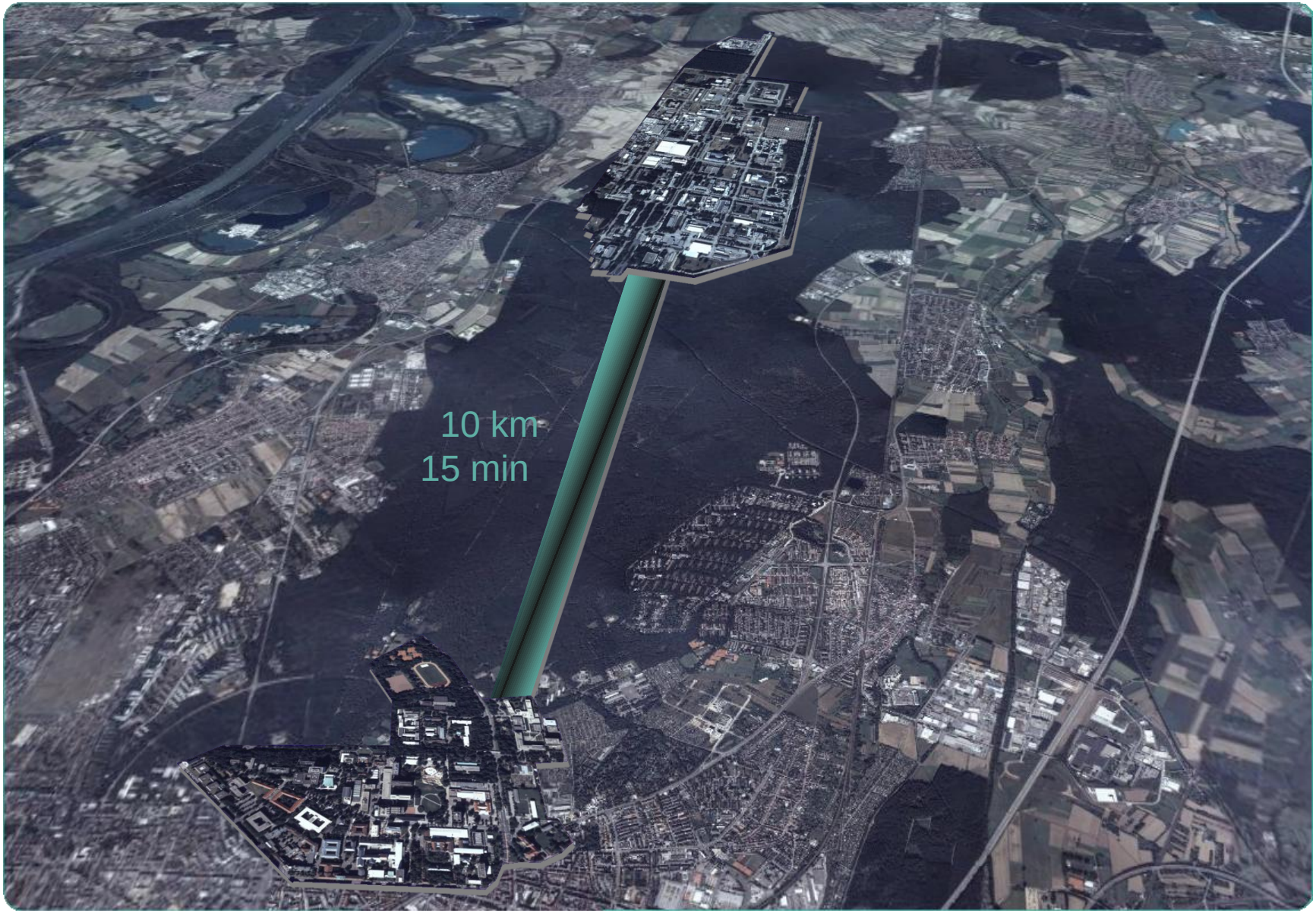
Frank.Schmitz@kit.edu

STEINBUCH CENTRE FOR COMPUTING - SCC

Agenda

- KIT, a large institution
- definition of SimLabs at KIT
- SimLab Climate and Environment
- SimLab Energie
- SimLab Elementary Particle & Astroparticle Physics
- SimLab NanoMikro
- a cross-section team between the SimLabs
- Conclusion

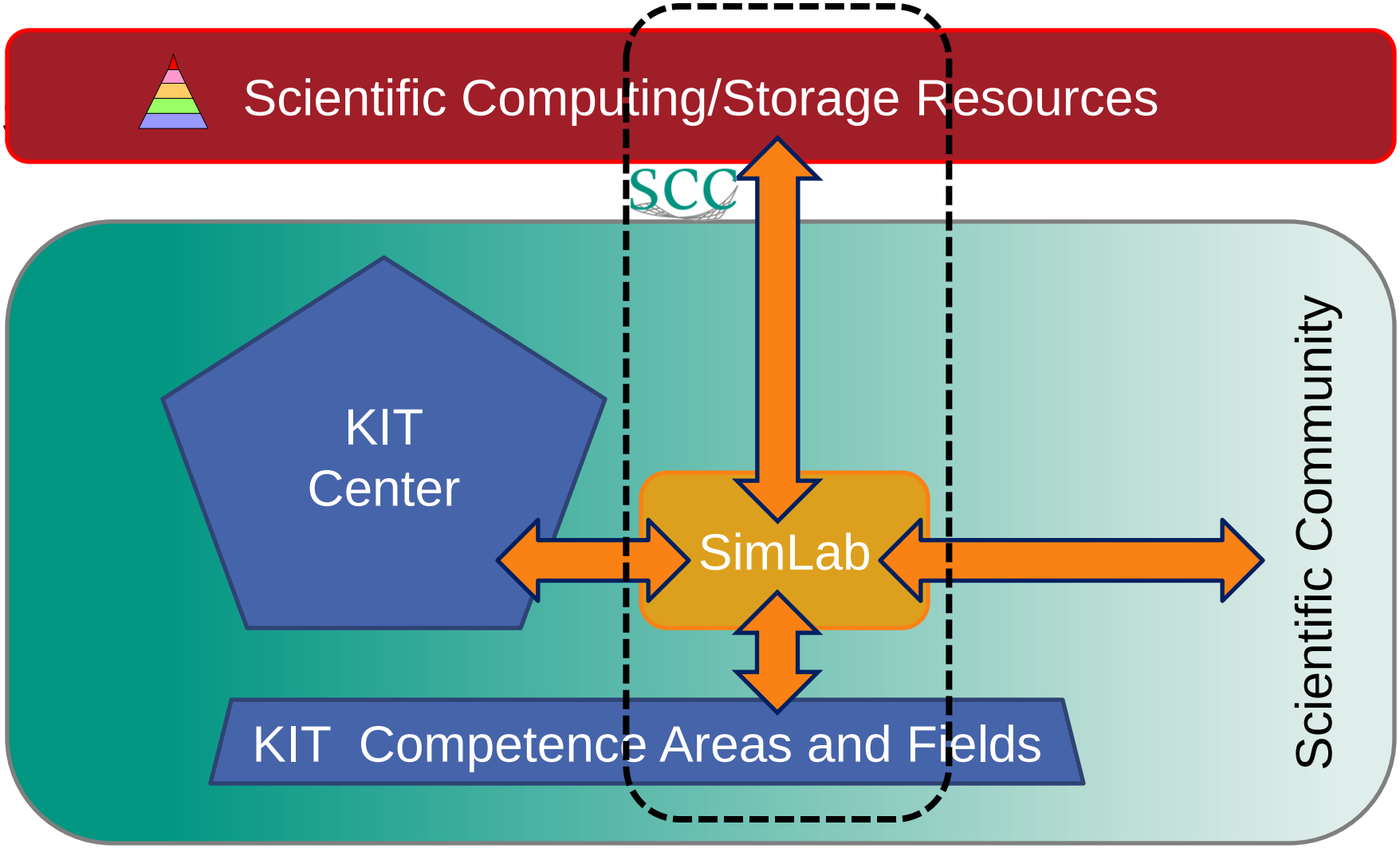
Video at www.kit.edu/english/kit_video.php



Simulation Laboratory (SimLab) Definition

- community-oriented research and specific scientific support
- integral part of the community → KIT Centers
- assistance in performing simulations on HPC systems
- core group located at SCC and associated scientists outside, but working strongly together → publications
- home of young scientist groups working in the area of scientific computing as an agreement between institutes and SCC
- support structure for software related problems on HPC systems
- knowledge of mathematical methods and algorithms, parallel performance
- advice users in finding infrastructure resources best fit to their scientific problem tools, parallel data I/O and optimal structures for data processing and people fit better to an asked question → LSDF and DIC

Simulation Laboratory (SimLab) Definition



SimLab Climate and Environment

Team leader: Dr. Oliver Kirner

- Research areas:
  Analysis of chemistry-climate interactions with help of long term simulations performed by the global model ECHAM5/MESSy (EMAC)

  Simulations with the regional model COSMO to examine the potential of wind energy in Chile and Thailand

  Development of a coupling tool for EMAC/COSMO to bridge the scales between regional and global atmospheric modelling
- Model development and applications:

  Optimization of EMAC through redesign of the advection kernel and implementation of new numerical algorithm for multi-core and many-core architectures.
- Working together with institutes at KIT and other national and international partners. HPC, DIC and LSDF knowledge is required!

SimLab Climate and Environment (2)

Wind Energy in Norte Chico in Chile

Objective

Evaluation of the wind energy potential in the heterogeneous area of Norte Chico in Chile (IV. and V. Region: Coquimbo and Atacama) in order to determine the location of wind power plants.

Method

Statistical-dynamic downscaling:
Classification of the large scale atmospheric conditions with cluster analysis.
Highly resolved numerical simulations for each cluster.
Usage of HPC infrastructure at KIT/SCC for simulation.

Collaborations

CEAZA (Centre of Advanced Studies in Arid Zones, Universidad de La Serena, Chile)
IMK (Institute of Meteorology and Climate Research, KIT)

SimLab Energy

Team leader: Dr. Olaf Schneider

Selected Challenges:

- security prediction for nuclear waste repositories
- simulation of
  - biofuel synthesis and other processes in chemical engineering
  - geothermal reservoirs
  - material behavior in nuclear facilities
  - radiation transport
  - hydrogen combustion
- model based design of fuel cells
- optimizations for
  - power plant operation planning
  - power trading

SimLab Energy (2)

Current activities:

- plasma modeling for the ITER fusion facility
  - using EIRENE, as part of EUFORIA FP7 project
- material simulations (Beryllium)
  - using VASP
- neutral gas transport simulations
  - using GASFLOW,
- establishing co-operations with industries
  - EnSoC: EnBW, SAP, Siemens, T-Systems, HP …

Projected activities:

- numerical simulation for the fuel synthesis
  - using TURBIT-VoF, DETCHEM, code coupling!
- monte-carlo simulation of radiation transport coupled with flow
  - using MCNP5 in a world-wide project

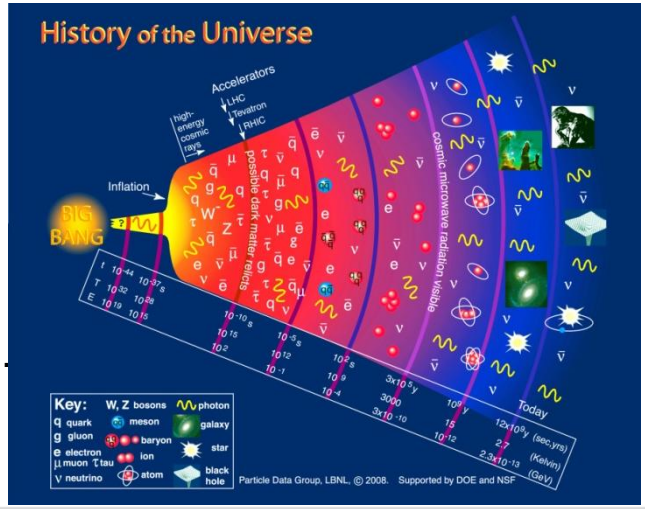
SimLab Elementary Particle & Astroparticle Physics

Team leader: Dr. Gevorg Poghosyan

- *Working together with KCETA* *(KIT Center Elementary Particle and Astroparticle Physics)*
  - Cosmic Rays (Auger)
  - Extended and intensified search for Dark Matter (EDELWEISS)
  - Flavour Physics - Quantum Field Theory: Quark Matter Physics
  - Neutrino Physics (KATRIN)
  - Experimental and Theoretical Collider Physics
  - Computational Physics - implementation of effective algorithms
- *Support as S.P.O.R.* -adic changes re-engineering of existing codes and algorithms
  - **S**tandardization – code re-structuring
  - **P**arallelization
  - **O**ptimization – performance-analysis (HPC, Grids and Clouds)
  - **R**elease – user friendly

SimLab Elementary Particle & Astroparticle Physics (2)

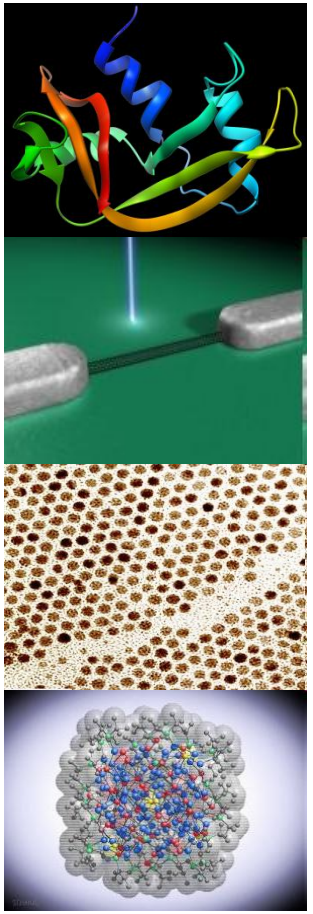
- Astrophysical objects – laboratories under extreme conditions
  - *CORSIKA* – simulation of extensive air showers
  - Interaction, propagation and decay of particles
  - 10^{16} eV → 3 PC-days; 10^{20} eV → 150 PC-years !
- Outreach
  - Users from 47 countries for 50 experiments
    - AUGER South – Argentina (soon also AUGER North in USA)
    - KASCADE Grande - Germany
    - AMANDA – Antarctica
  - Results
    - The simulation package Corsika is using the KIT infrastructure
    - The definition of the coarse grain parallelism and the first runs.
    - Internship students are working on this approach.



Simulation Laboratory NanoMikro

Team leader: Dr. Ivan Kondov

- Multiscale modeling and simulation
  - Nanoelectronics – electron transport through molecular nanostructures, impact of lattice defects
  - Nanophotonics – multiscale modeling employing hybrid quantum-classical approaches
  - Highly accurate calculation of weak interactions in metal nanoclusters
  - Phonons and electron-phonon coupling in high-temperature semiconductors and carbon nanotubes
  - Protein structure prediction via stochastic optimization
  - Interaction of actinide ions with metal surfaces (nuclear waste disposal)
  - Development of advanced materials for nuclear fusion and fission facilities – multiscale modeling and atomic scale simulation



Simulation Laboratory NanoMikro (2)

- Activities and Cooperations
  - Simulations of protein tertiary structure prediction
  - Calculation of phonons and electron-phonon interactions with MBPP and PERT (lattice dynamics)
  - Simulation of electron transport through single molecular and atomic contacts (nanoelectronics)
  - DFG Center for Functional Nanostructures (CFN)
  - Cooperation's at KIT
  - “Baden-Württemberg Stiftung” project hpc5 for 2009 until 2012
  - HGF Young Investigator’s Group, proposed for 2011 until 2015
  - Intended participation: European FP7 Calls 6 & 7
- Existing codes
  - Turbomole, MBPP PERT, POEM, FlexScreen, CASINO

Cross-section team

- very close and integrated into the SimLab structure
- helping if there are problems in the area of
  - numerics
  - software
  - languages
  - access to HPC, DIC-systems and to the LSDF
  - GPGPU
- and other stuff!

Conclusion

- SimLabs are the glue between:
  - scientific computing
  - optimal usage of infrastructure resources
  - Science
- SimLabs are interfaces between communities and local experts and support teams
- The functionality of SimLabs can not described as the traditional user support of a Computer Centre
- SimLabs are one of the keys for R&I at SCC

Thank you for your attention!

Questions?

- I'll also be around after the talk.
- People responsible for the SimLabs:
  - Climate and Environment: Oliver.Kirner@kit.edu
  - NanoMikro: Ivan.Kondov@kit.edu
  - Elementary Particle & Astroparticle Physics: Gevorg.Poghosyan@kit.edu
  - Energy: Olaf.Schneider@kit.edu
- Email: Frank.Schmitz@kit.edu
- Web: www.scc.kit.edu/forschung/5960.php