Karlsruher Institut für Technologie

SimLabs at KIT, a Strategy for the Future

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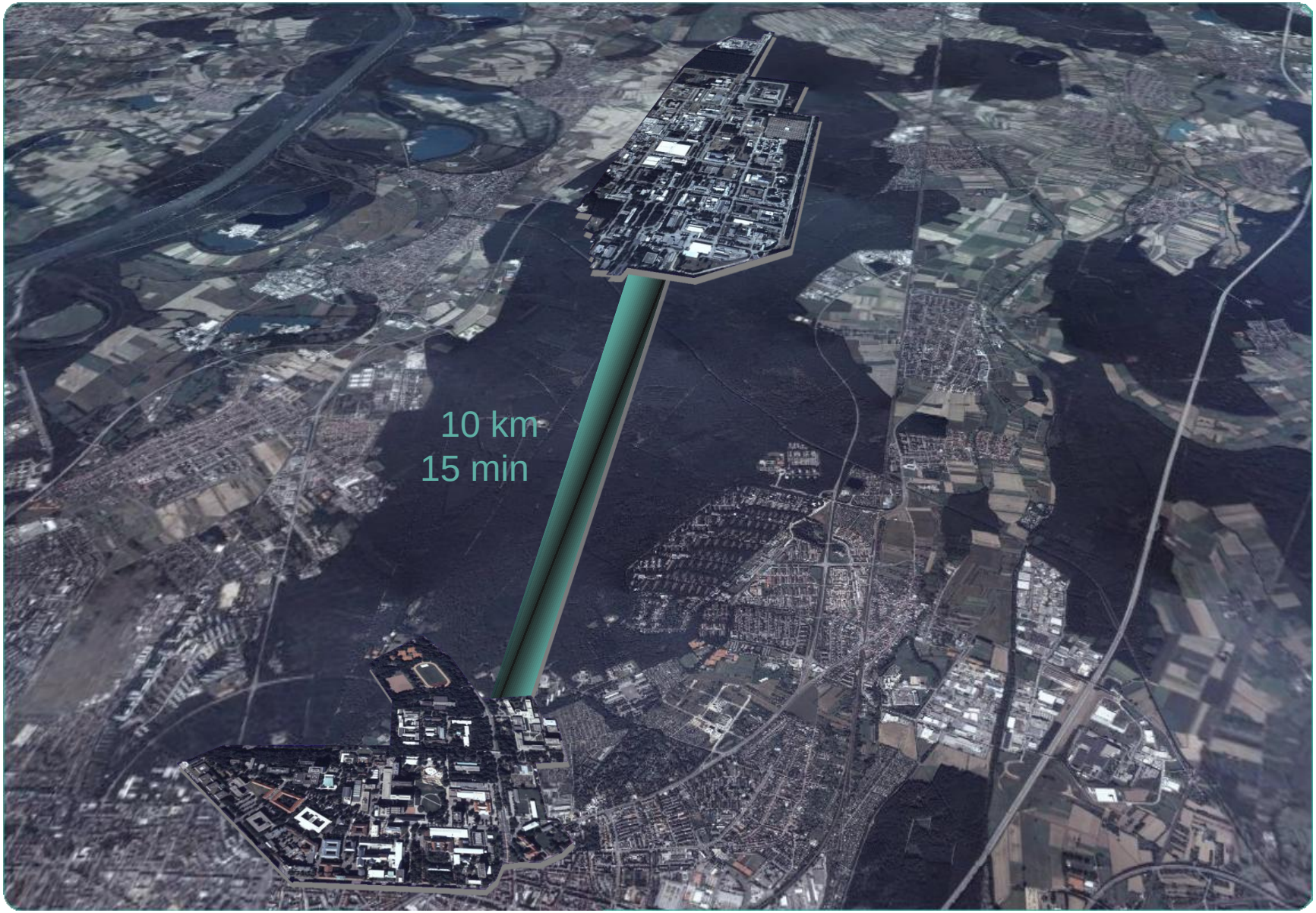
STEINBUCH CENTRE FOR COMPUTING - SCC

Agenda

- KIT, a large institution
- work to be done at SCC
- 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



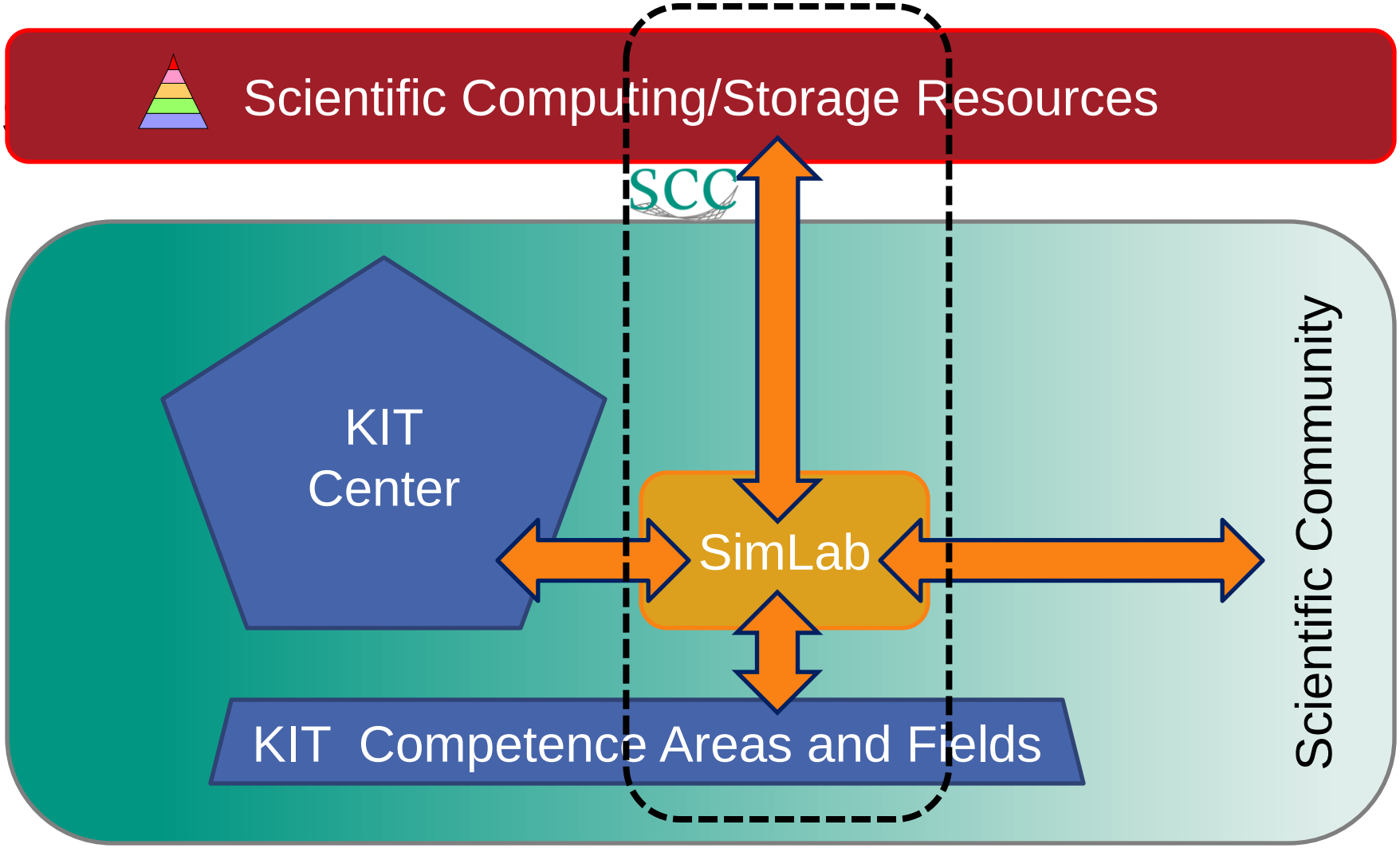
work to be done at SCC

- concentration on the Large Scale Data Facility (LSDF) for the long term storage of scientific data → >20 PB in 2010 → LHC, ANKA, BioQuant, ITG → facility in Germany and Europe
- SimLabs
- Cloud as an R&I project
- Grid, because SCC is delivering a service for the high energy physics community and D-Grid
- HPC for local and BW needs

Simulation Laboratory (SimLab) Definition

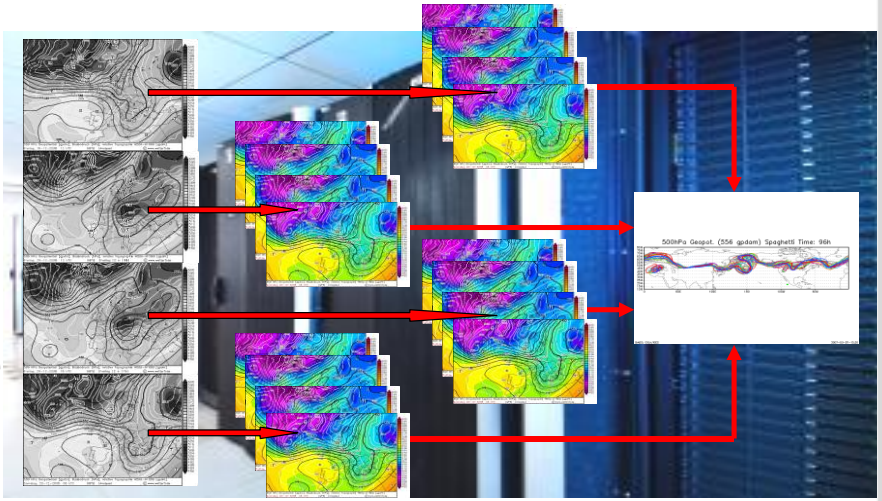
- community-oriented research and specific scientific support
- integral part of the community → KIT Centers
- assistance in performing simulations on HPC systems
- core group located at SCC and associated scientists outside, but working strongly together → publications
- home of young scientist groups working in the area of scientific computing as an co-operation between institutes and SCC
- support structure for software related problems on HPC systems
- knowledge of mathematical methods algorithms and parallel performance
- advice users in finding infrastructure resources best fit to their scientific problem
- SimLabs are part of the PoF “Supercomputing” from HGF (FZJ and KIT)

Simulation Laboratory (SimLab) Definition



SimLab Climate and Environment

focus on RESyM: Regional Earth System Modelling



- Research Areas are:
  Aerosol and climate processes
  Air quality
  Atmospheric and terrestrial water cycle
  Biogeochemical cycles
  High impact weather
  Bridging the scales between regional and global atmospheric modelling
- Working together with institutes at KIT and other national and international partners. HPC, DIC and LSDF knowledge is required!
- Model development and application:

  Atmospheric Model Systems and biosphere simulation environment:

  COSMO (Consortium for Small Scale Modelling)

  WRF (Weather Research and Forecast)

  MOBILE (Modular Biosphere Simulation Environment)

SimLab Climate and Environment

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

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

Current activities:

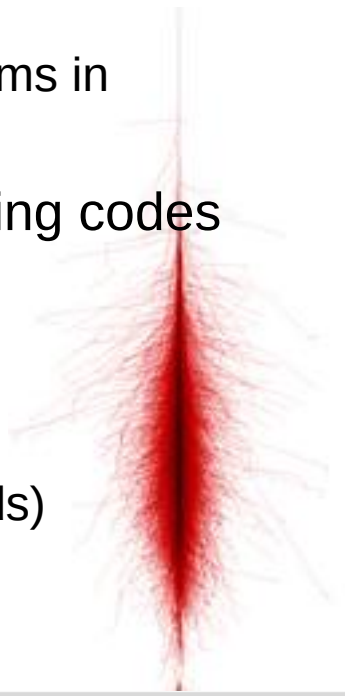
- plasma modeling for the ITER fusion facility
  - using EIRENE, as part of EUFORIA FP7 project
- material simulations (Beryllium)
  - using VASP, in cooperation with IMF
- neutral gas transport simulations
  - using GASFLOW, in cooperation with IKET
- simulation of rarefied gas dynamics in cryogenic pumps
  - in cooperation with ITP
- establishing co-operations with industries
  - EnSoC: EnBW, SAP, Siemens, …

Projected activities:

- numerical simulation for the fuel synthesis
  - using TURBIT-VoF, DETCHEM, in cooperation with ITCP and IKET
- monte-carlo simulation of radiation transport coupled with flow
  - using MCNP5, in cooperation with INR

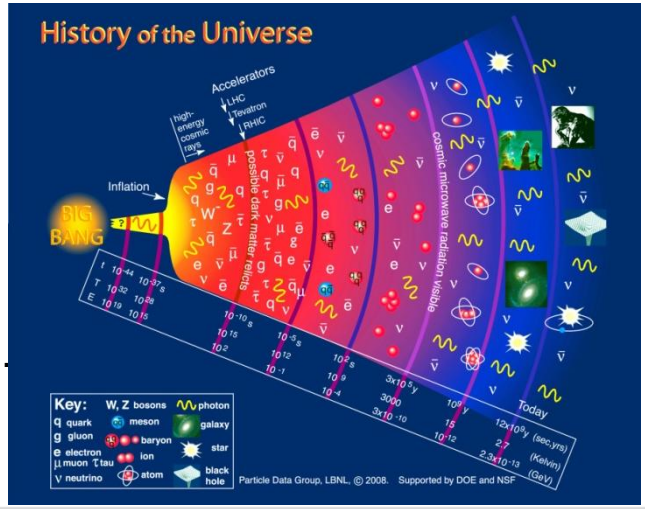
SimLab Elementary Particle & Astroparticle Physics

- *Developing software for 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 in specialized computer programs
- *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



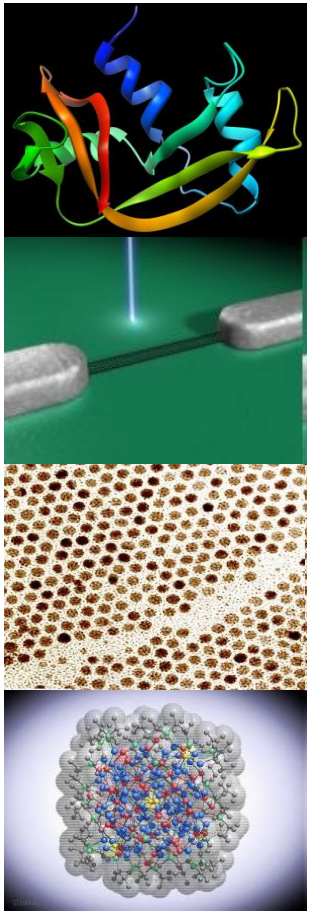
SimLab Elementary Particle & Astroparticle Physics

- 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

- 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

- 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 with other instituts at KIT
  - “Baden-Württemberg Stiftung” project hpc5 for 2009 until 2012
  - HGF Young Investigator’s Group, proposed for 2011 until 2015
  - European FP7 Call 7 → MMM@HPC
- Existing codes
  - Turbomole, MBPP PERT, POEM, FlexScreen, CASINO

Cross-section team

- works together with SimLabs
- helping if there are problems in the area of
  - numeric
  - software
  - languages
  - access to HPC, DIC-systems and to the LSDF
- and other stuff!

SimLab	third-party funded	co-operations
Energy	▶ Euforia ▶ bwGRiD	▶ IKET ▶ ITS ▶ IHM ▶ INR ▶ Geophysik
NanoMikro	▶ HPC-5 ▶ MMM@HPC ▶ GPUqCHEM	▶ INT ▶ TFP ▶ IFP ▶ CFN ▶ TURBOMOLE GmbH
Climate and Environment	▶ TaxES (Towards an Exascale Earth System Model)	▶ IMK ▶ DLR ▶ MPI Chemistry Mainz ▶ CEAZA ▶ Thailand
Elementary Particle & Astroparticle Physics	▶ KCETA Graduiertenschule (Exzellenz-Initiative)	▶ IK ▶ Uni Frankfurt ▶ Uni Wrocław, ▶ Yerevan, Armenia
Cross-section team	▶ GPGPU (STUP) ▶ Linsol-Turbit	▶ FSM (Department of Fluid Machinery at KIT)

Conclusion

- SimLabs are the glue between:
  - scientific computing
  - optimal usage of infrastructure resources
  - Science
- The functionality of SimLabs can not described as the:
  - traditional user support of a Computer Centre
  - work to be done in an institute
- SimLabs are new and innovative
- 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: Dr. Oliver Kirner
  - NanoMikro: Dr. Ivan Kondov
  - Elementary Particle & Astroparticle Physics: Dr. Gevorg Poghosyan
  - Energy: Dr. Olaf Schneider
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