S.P.O.R.A.-dic changes of scientific simulation codes for high performance distributed computing

Gevorg Poghosyan

Steinbuch Centre for Computing (SCC)

Karlsruhe Institute of Technology (KIT)

Employees

8.000

Students

18.500

300
Professors

700
annual budget in Million Euros

The cooperation of

Forschungszentrum Karlsruhe GmbH
Universität Karlsruhe (TH)

KIT Research Centers:

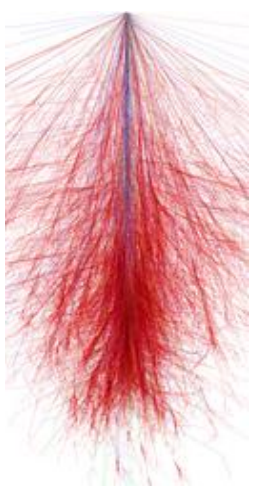- Energy
- Nano & Micro Science and Technology
- ***Elementary Particle and Astroparticle Physics***
- Climate and Environment

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Scientific Computing Lab (SCL)

SimLab Elementary Particle & Astroparticle Physics

■**Developing software for KCETA** (KIT Center Elementary Particle and Astroparticle Physics)
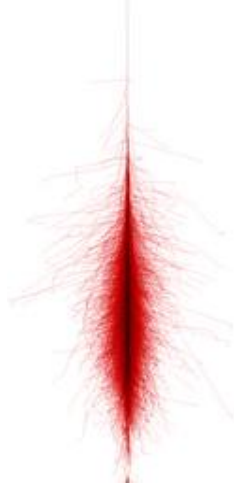
- ■ *Cosmic Rays (Augger, Kascade-grande)*
- ■ *Extended and intensified search for Dark Matter (EDELWEISS)*
- ■ *Flavour Physics - Quantum Field Theory: Quark Matter Physics*
- ■ *Neutrino Physics (KATRIN)*
- ■ *Experimental and Theoretical Collider Physics (LHC)*

■ *Support as S.P.O.R.A.*-dic changes for present and developable codes

- ■ **S**tandardization – code re-engineering: object oriented, I/O data format standardization
- ■ **P**arallelization – exploitation of code to find parallelization strategies
- ■ **O**ptimization – performance-analysis: infrastructure dependant
- ■ **R**elease – user friendly, easy to use, publicly available libraries of code and results
- ■ **A**daptation – to up-to-date HPC, Grid and Cloud computing EU infrastructures*

*PRACE – Partnership for Advanced Computing in Europe (DEISA+EGI+EGEE)

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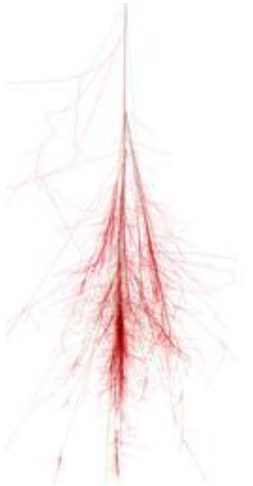Steinbuch Centre for Computing (SCC)
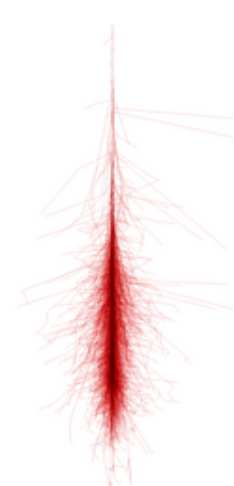
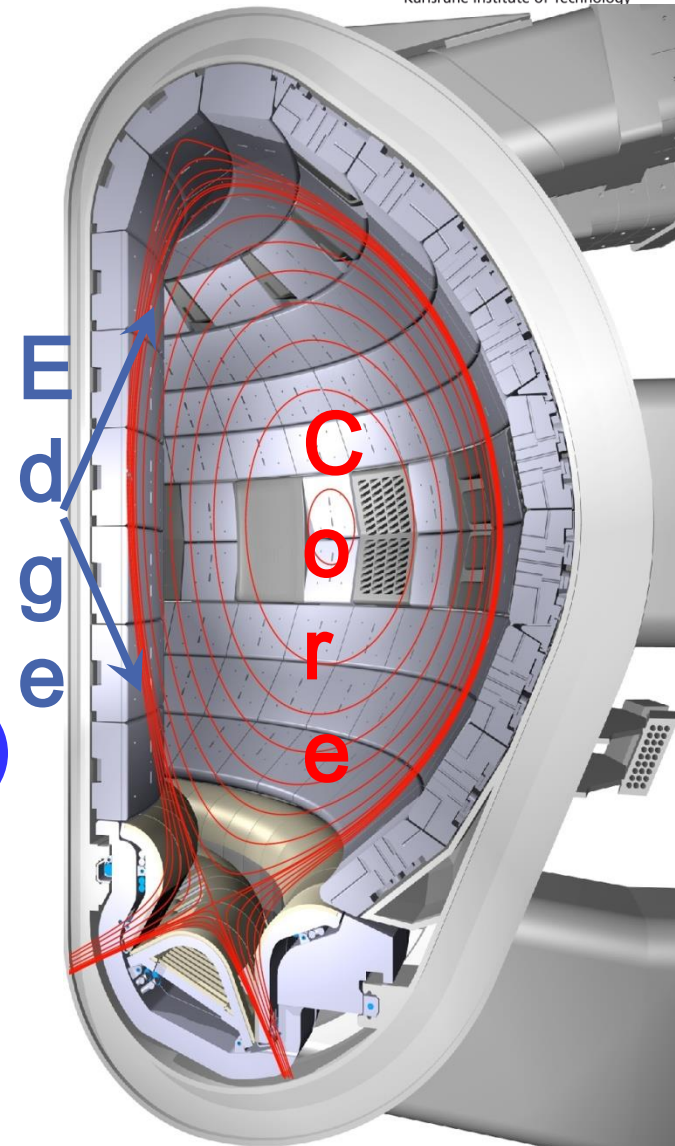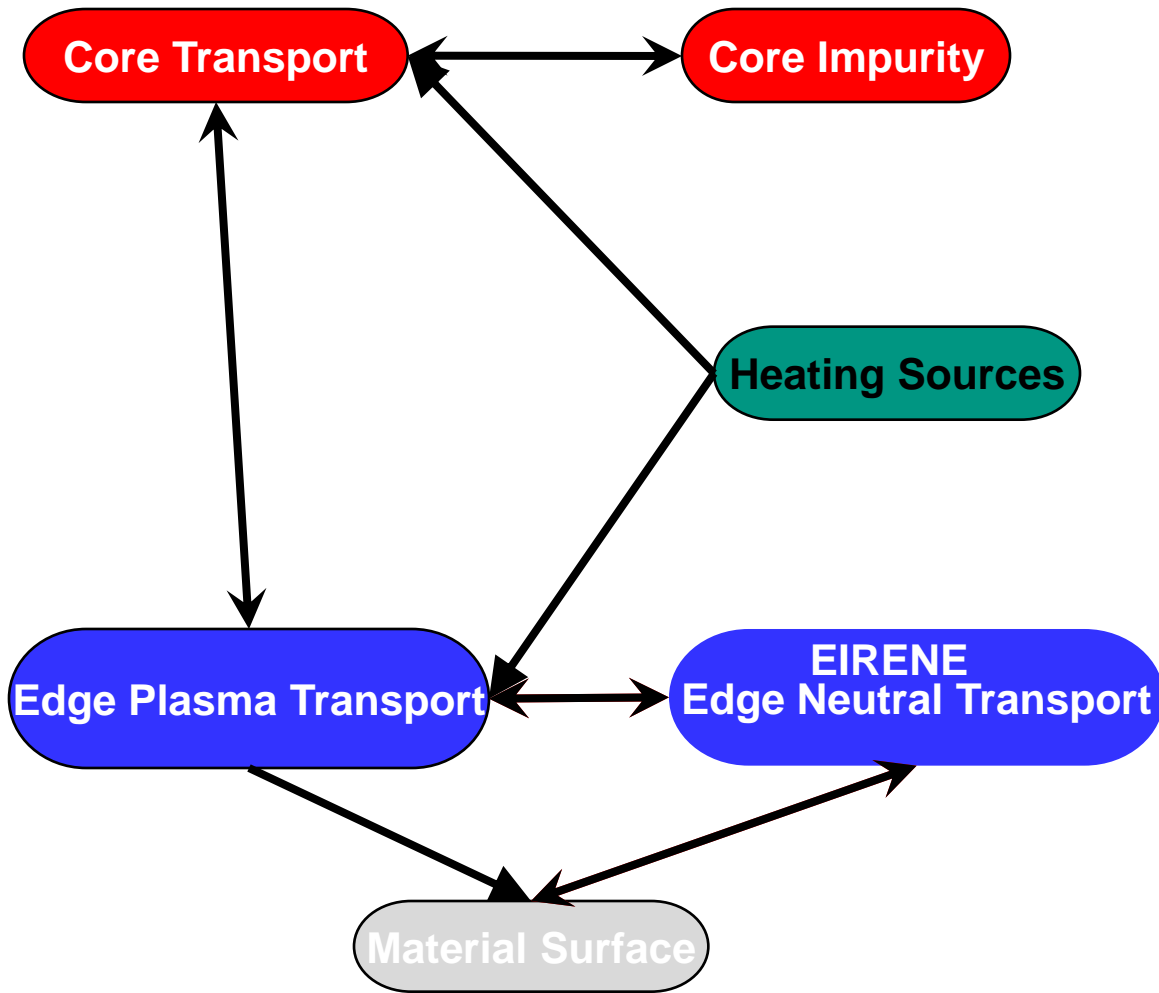Scientific Computing Lab (SCL)

Cosmic Rays

Fe

μ

p

γ

- Determine showers in Eath Atmosphere
  - mean values
  - fluctuations
  - correlations
- Deduce properties of primary particle:
  - particle type (proton ,iron, n, ...)
  - energy
  - direction (anisotropy, point source)
- CORSIKA COsmic Ray SImulation for KASCADE*
  - Under development since 1989
  - 700 Users (50 countries for 50 experiments)
    - AUGER South – Argentina (soon North in USA)
    - KAUGER ASCADE Grande - GermAUGER any
    - AMANDA – Antarctica
- *KASCADE = KArlsruhe Shower Core and Array Detector*

CORSIKA Code http://www-ik.fzk.de/corsika/

- Monte Carlo Simulation for elementary processes
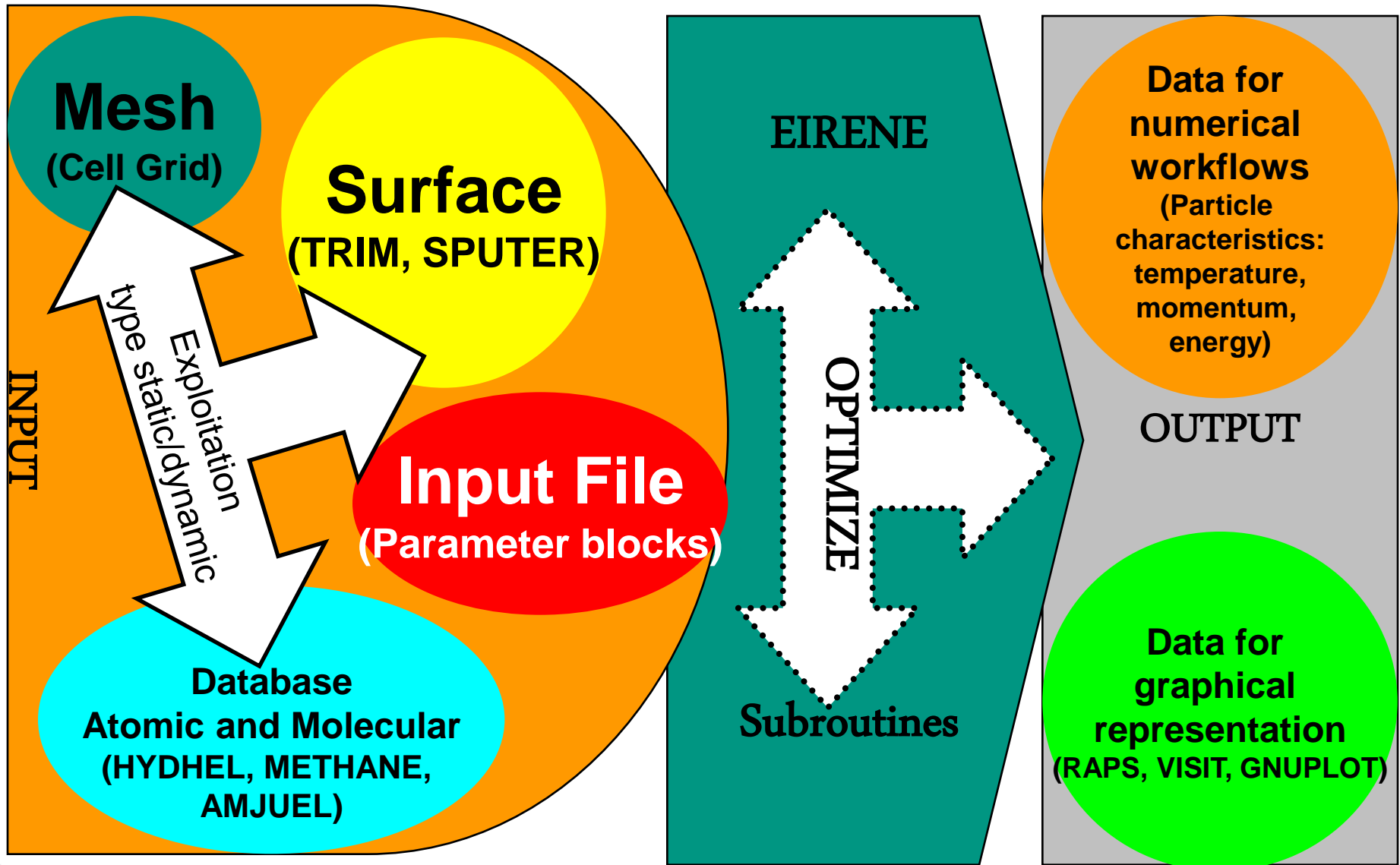 - Environment: atmosphere, Earth magnetic field
  - Particle: type, energy, position, direction, time
  - Range: cross section, life time
  - Transport: ionization energy loss, deflection in Earth magnetic field
  - Interaction / decay with production of secondaries – *source of systematic uncertainty*:
    - high-energy hadronic interaction model (QGSJET - *Pomeron phenomenology*)
    - low-energy hadronic interaction model (URQMD – *Quantum Molecular Dynamics*)
    - electromagnetic interaction (EGS4-electron gamma shower: Bremsstrahlung)
- 30+ models and tools tuned at collider energies extrapolated to 10^{20}eV
- Secondary particle storage on stack for future shower reconstruction

- 10^{16} eV $\rightarrow$ 3 PC-days; 10^{20} eV $\rightarrow$ 150 PC-years !

- The coarse grain parallelism for running the code without re-engineering brings only 5 time speedup

EU Fusion fOR ITER Application (EUFORIA) Workflow Infrastructure

Core Transport ↔ **Core Impurity**

Heating Sources

Edge Plasma Transport

EIRENE Edge Neutral Transport

Material Surface

Edge

Core

Analyzing EIRENE flow chart

Mesh
(Cell Grid)

Surface
(TRIM, SPUTER)

Exploitation
type static/dynamic

INPUT

Input File
(Parameter blocks)

Database
Atomic and Molecular
(HYDHEL, METHANE, AMJUEL)

EIRENE

OPTIMIZE

Subroutines

Data for numerical workflows
(Particle characteristics: temperature, momentum, energy)

OUTPUT

Data for graphical representation
(RAPS, VISIT, GNUPLOT)

Automatization of infrastructure implementations

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