Studying the facilities of scientific codes for automatization and optimization in grid workflows

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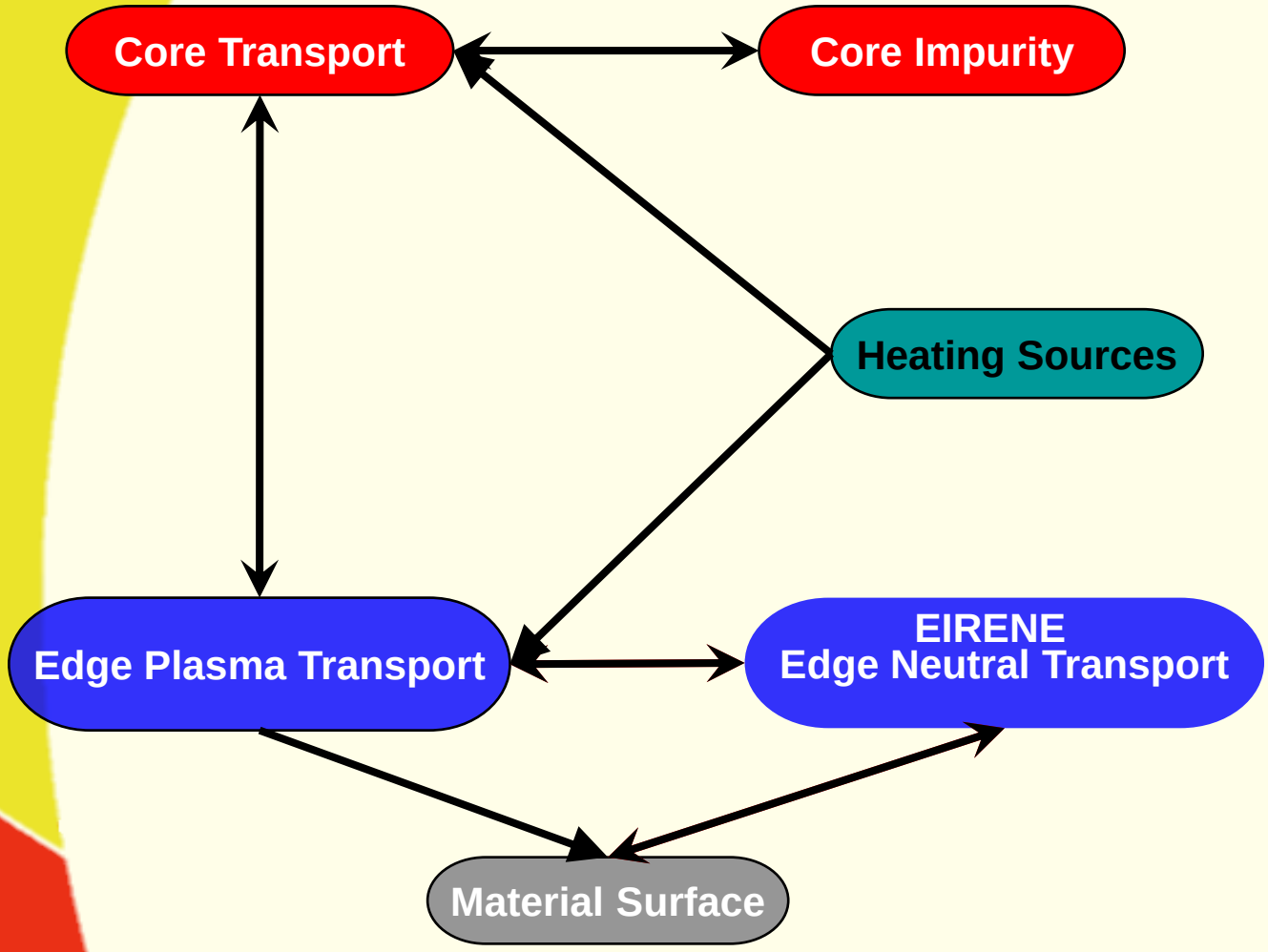
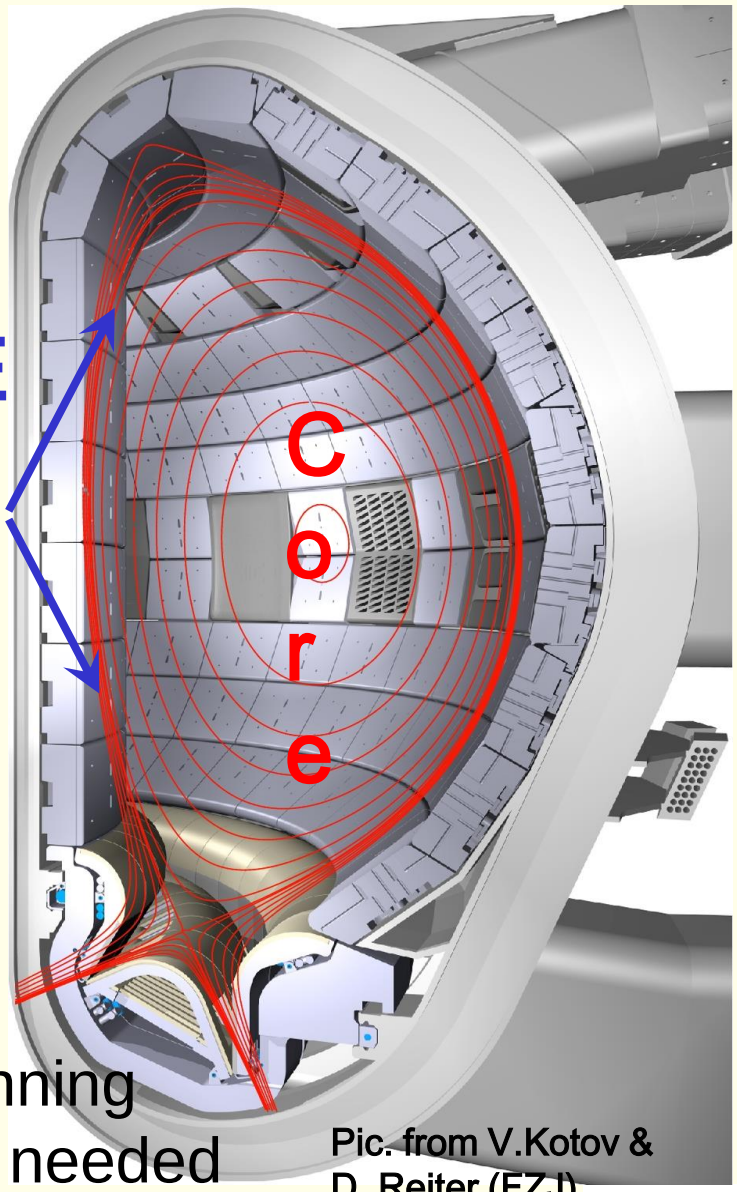
- -Scientific analyses of code and mechanisms — calculation
- -Code exploitation
  - -Identification of input and output — types, forms, size
- -Optimization and automatization
  - -Used/produced data
  - -Compilation/running
- - Visualization

Calculation mechanisms
EUFORIA Workflow Infrastructure

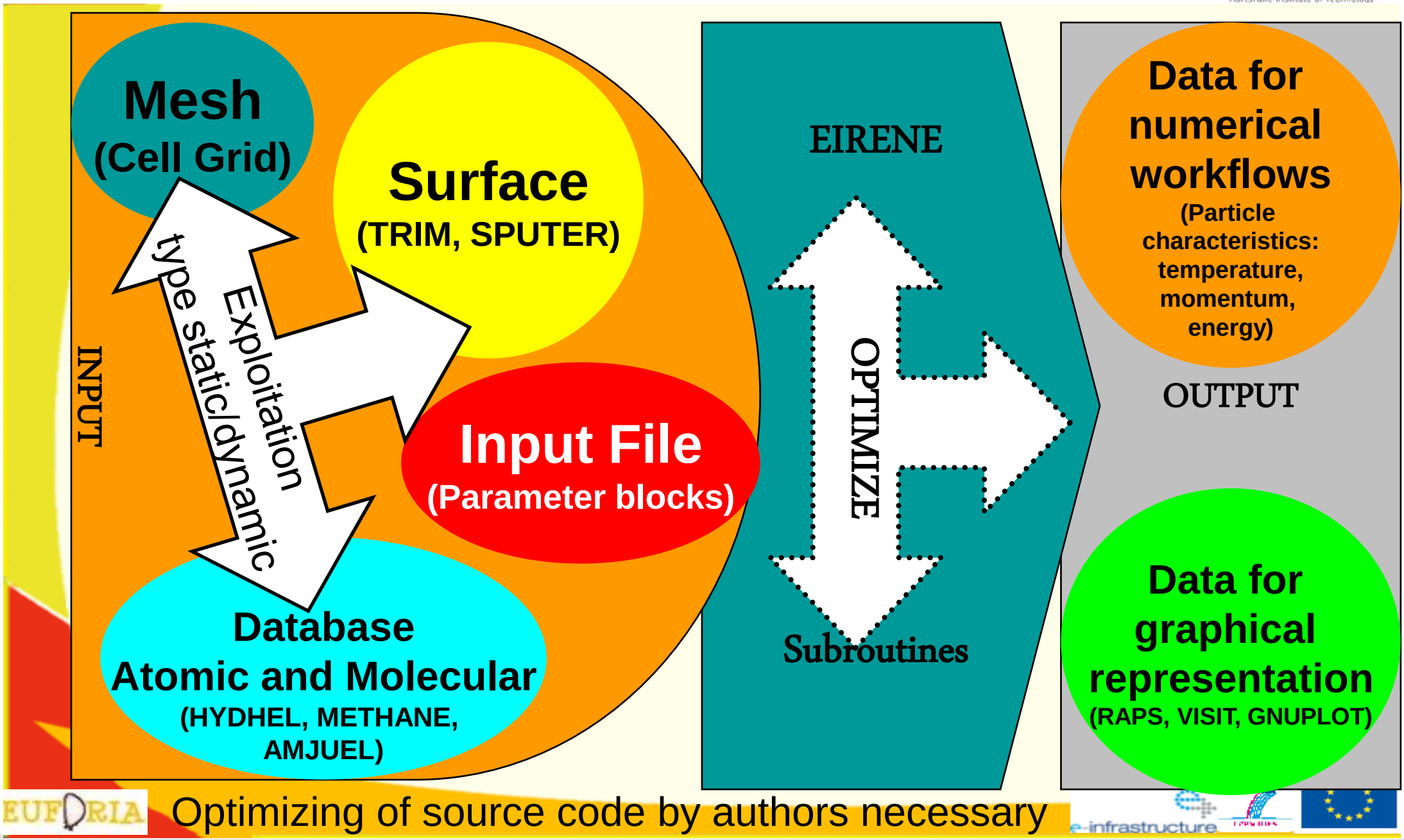




Pic. from V.Kotov & D. Reiter (FZJ)

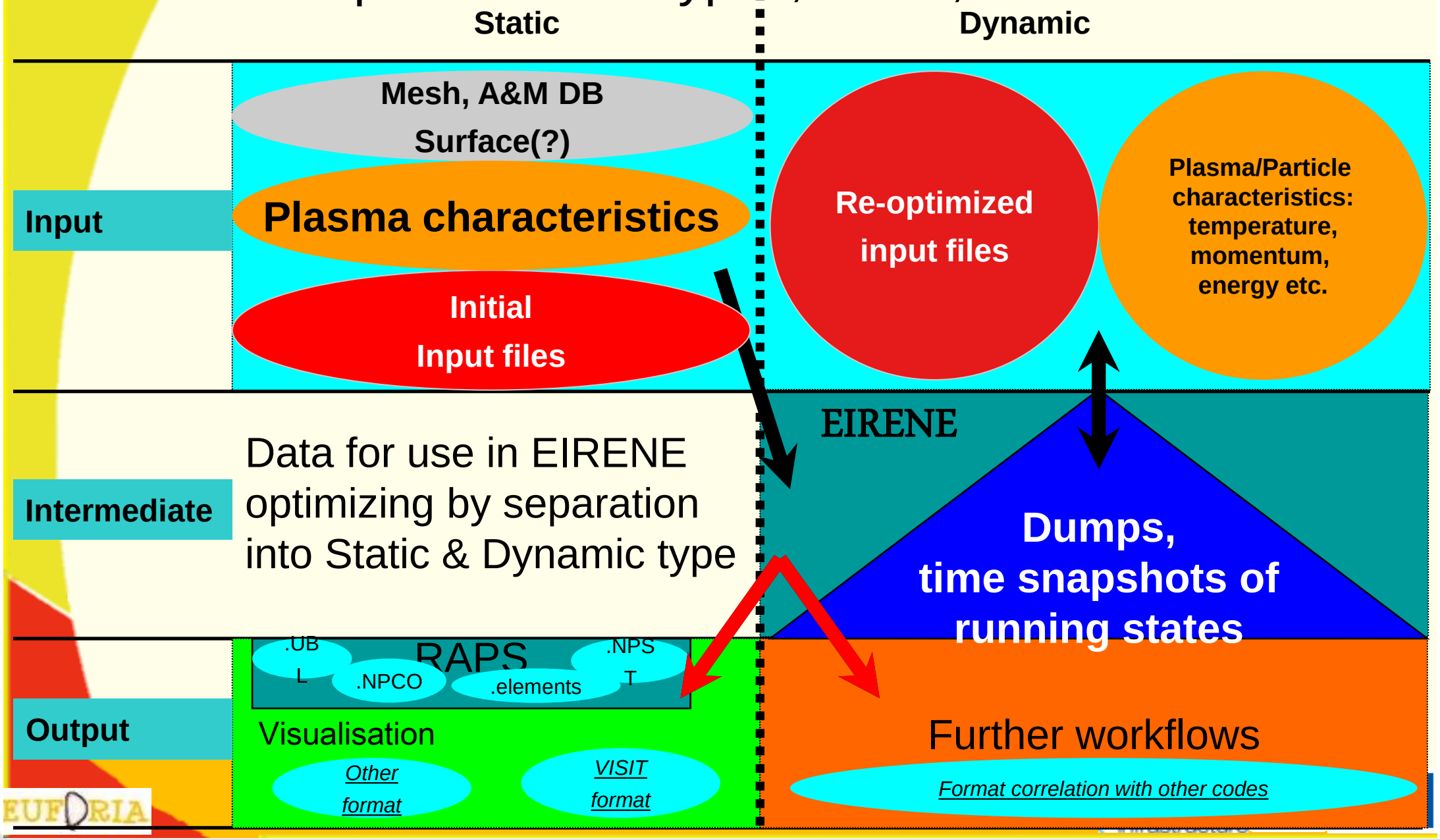
Porting onto grid an analyze and optimizing of running procedure of codes – communication in workflow needed

Code exploitation – Analyzing EIRENE flow chart



Optimizing of source code by authors necessary

Optimization and automatization
Grid optimal DATA types, forms, size



VISUALISATION

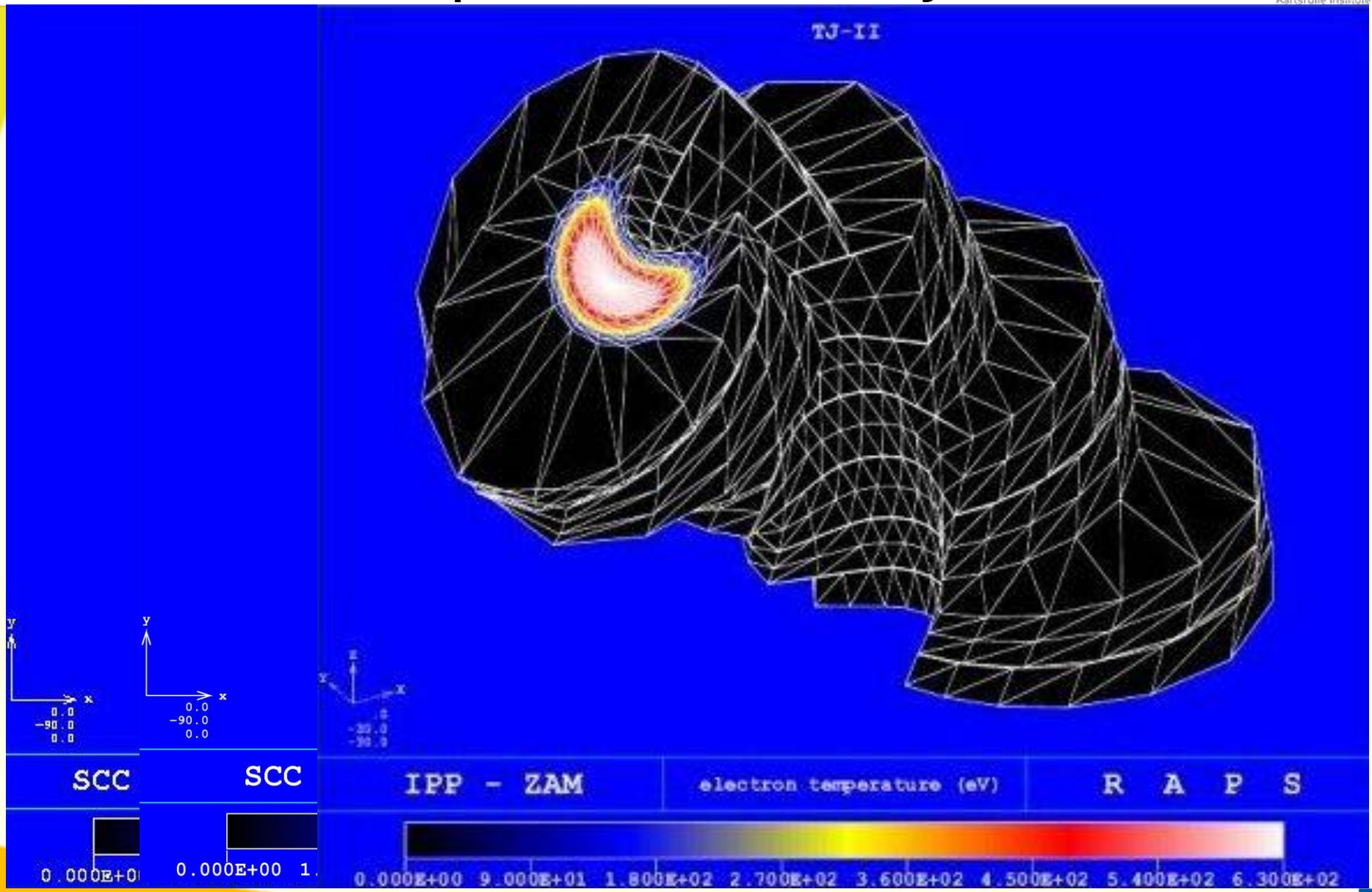
Critical - Definition of output file format to used in visualization/post-& pre-workflows

1. Change simulation code to natively write its data in format used in visualization/postworkflow tool
   - *RAPS* conform outputs delivers EIRENE since 2002
2. A conversion utility to post-process data files
   - *VISIT* (JRA4)
   – About 33 formats including rectilinear, curvilinear, unstructured or point meshes in 2D and 3D

Exception - ASCII text file format containing pairs or triples x, y, z floating point values for simple curves

– *Gnuplot, xmgrace, VISIT* or any simple 2D/3D vis.tool

RAPS conform outputs delivered by EIRENE



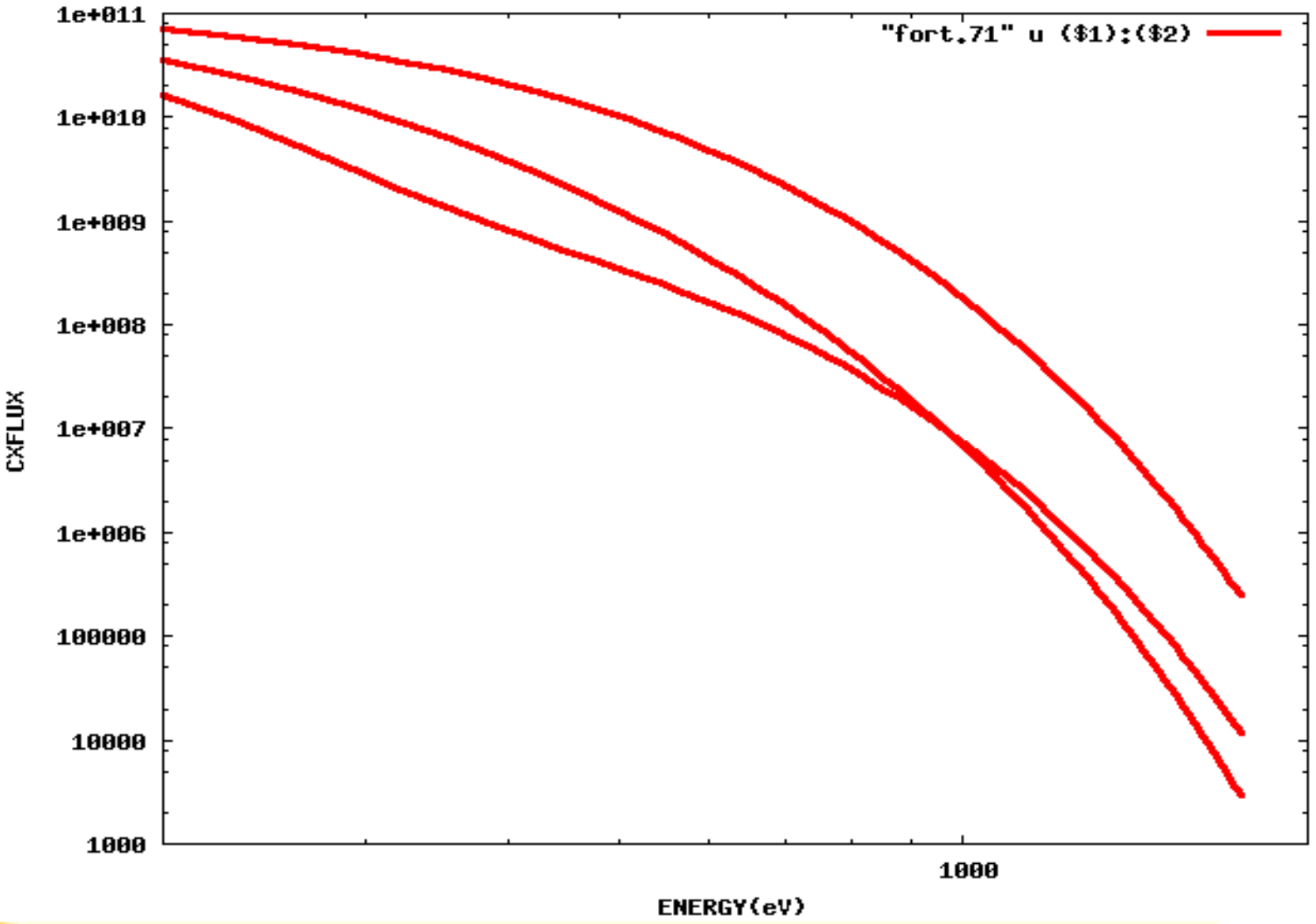
Simple 2D visualization from ASCII files

Outputfile

Fort.71

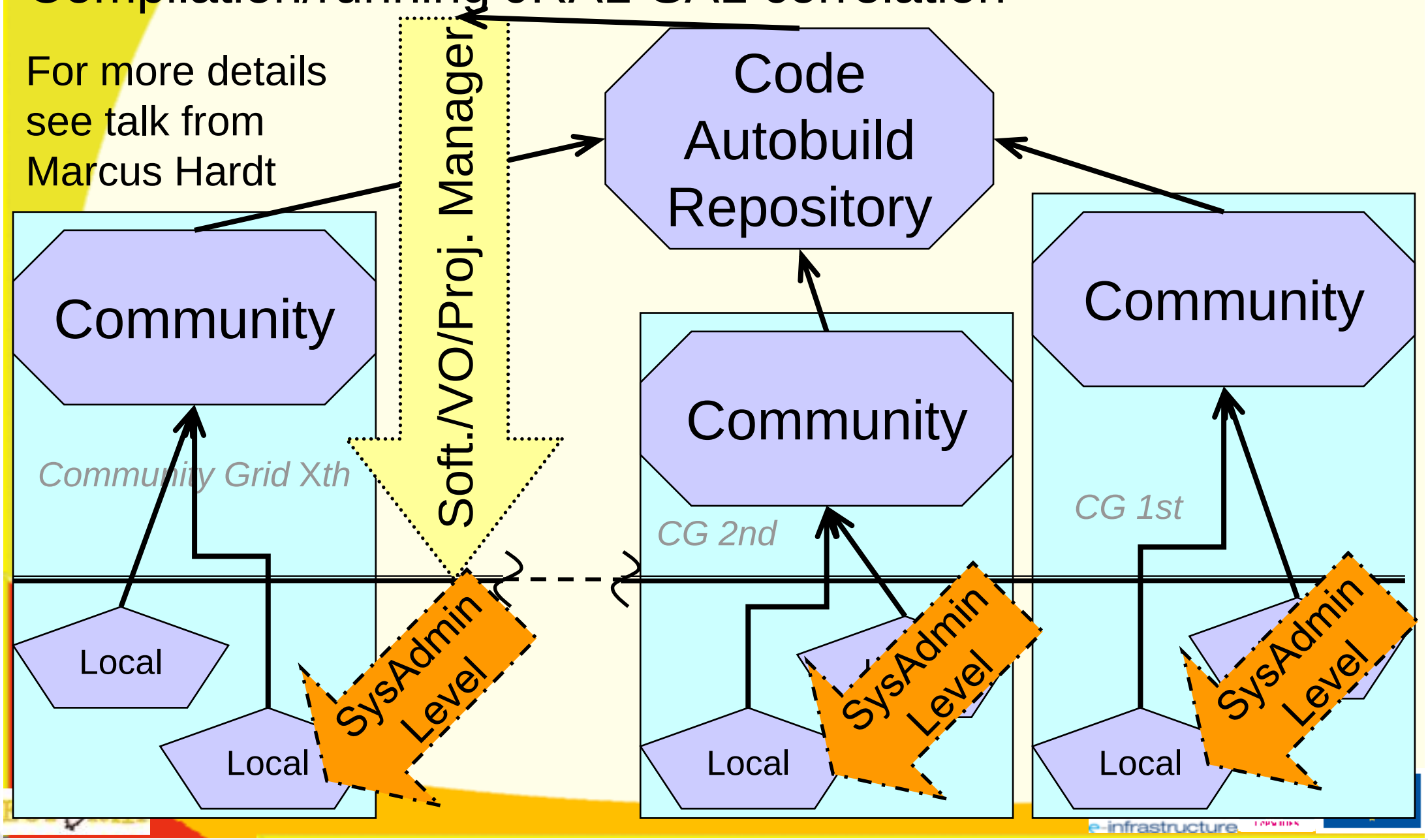
Energy spectrum for the CX fluxes

Visualization scripts to use grid jobs and workflows are simple for ACSII type files



Optimization and automatization Compilation/running JRA1-SA1 correlation

For more details see talk from Marcus Hardt



Outlook and Conclusions

- **Dynamic and static type** of input/output files have been identified and separated
- **Unified schemata and nomenclature** for definition of input/output files needed to be used
- **Integration into workflows** of EIRENE and other gird ported codes, needs I/O format optimization
- **Benchmarking and tests** using visualizations or extra grid optimized scripts, will minimize disruptions in workflows
- **Automated release/building infrastructure** would help to keep results relevant to last scientific progress