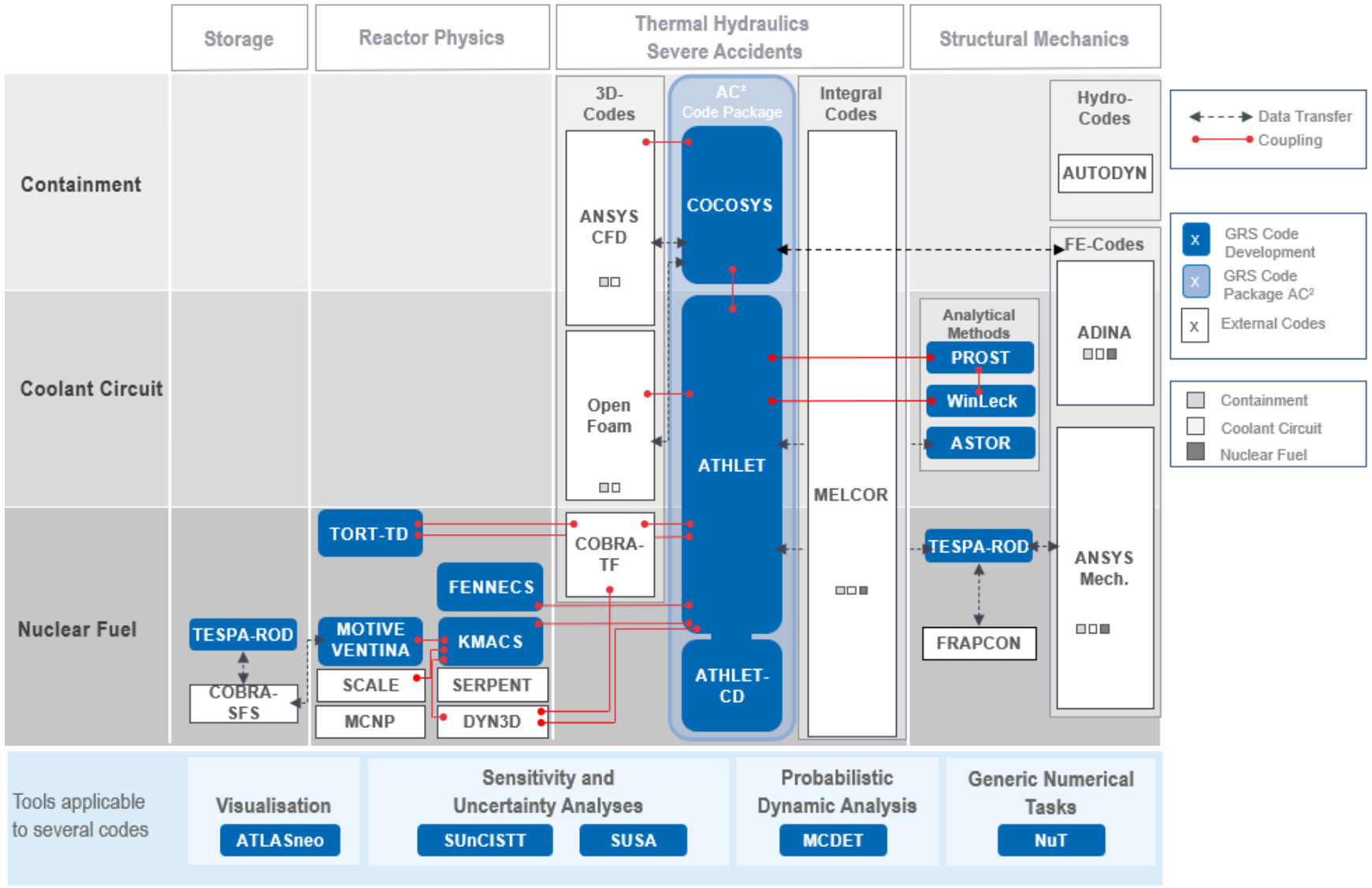
The Program Package AC² 2023

Fabian Weyermann, GRS

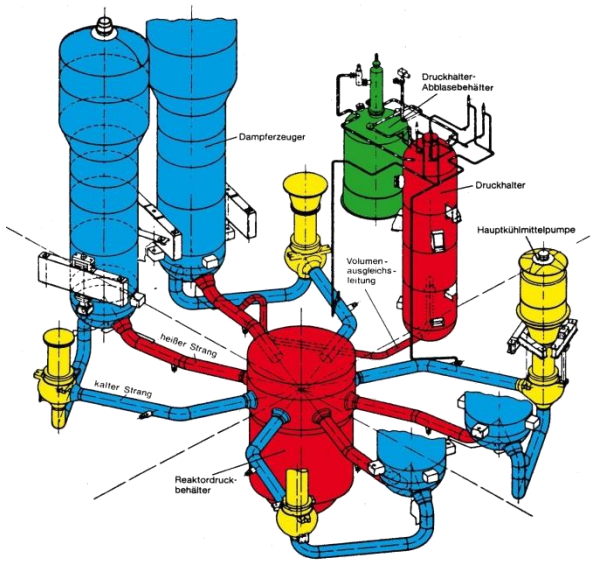
27.11.2023

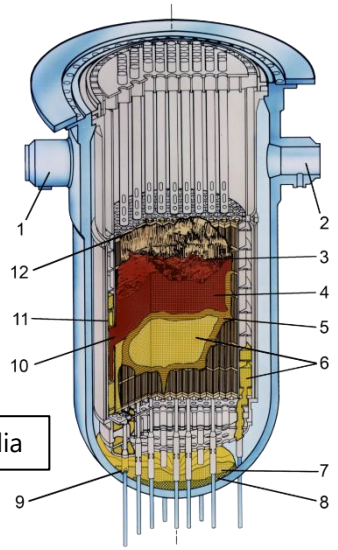
AC² User Meeting 2023

AC² within the GRS Simulation Chain



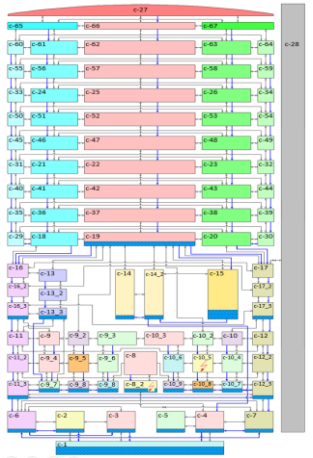
What is AC²?





From: 11), Wikipedia

AC²= ATHLET + ATHLET-CD + COCOSYS



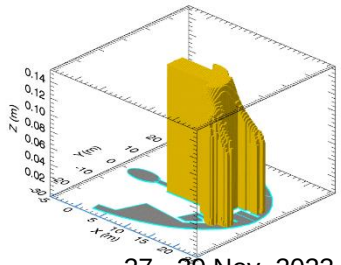
ATHLET
Cooling System
- Thermohydraulics
- Neutron kinetics
- I&C

Mass and Energy Transfer

COCOSYS
Containment
- Fission products
- Hydrogen
- Core Melt

ATHLET-CD
Core Degradation
- Hydrogen
- PV failure

Hydrogen, Fission Products



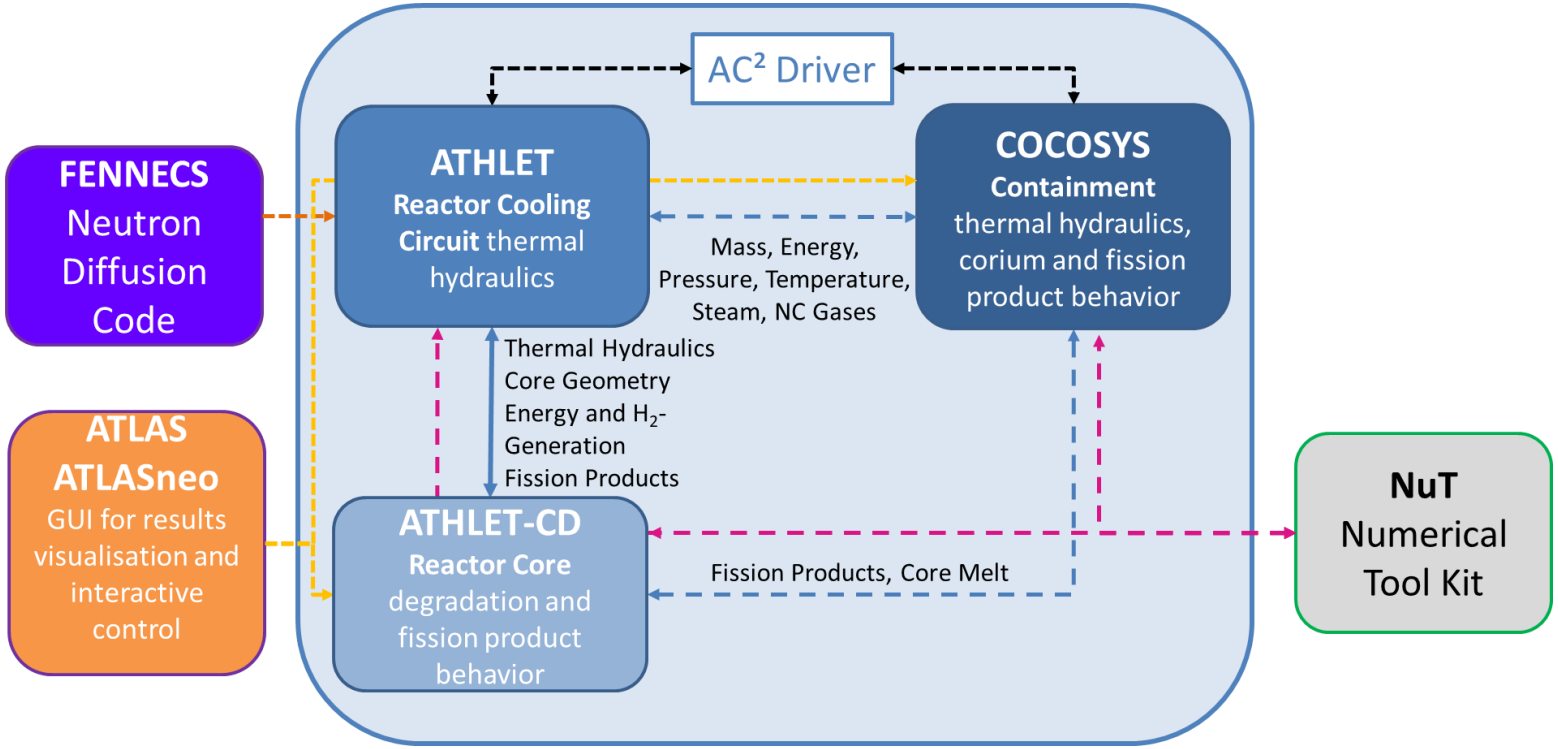
AC²: Overview and Components

AC² : System code package of GRS

- simulation of normal operation, design-basis accidents
- design extension conditions up to severe accidents including fission product release
- nuclear power plants, research reactors, advanced reactor designs and FE storage pools

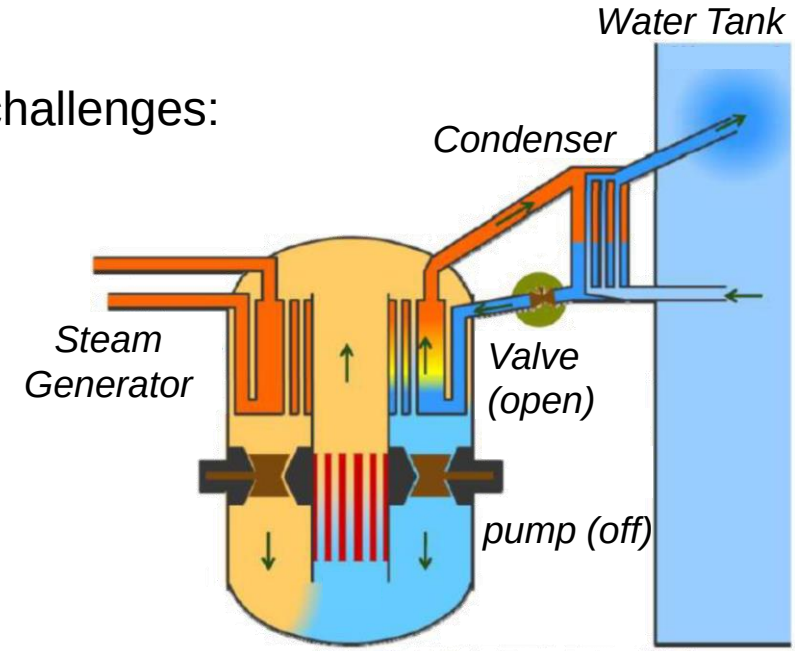
AC² features:

- **integral simulation of design basis and design extension conditions**

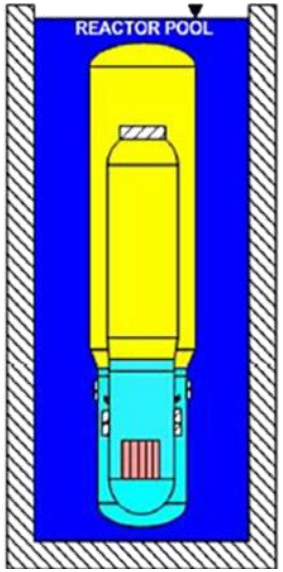


Motivation for the Development of AC² (1)

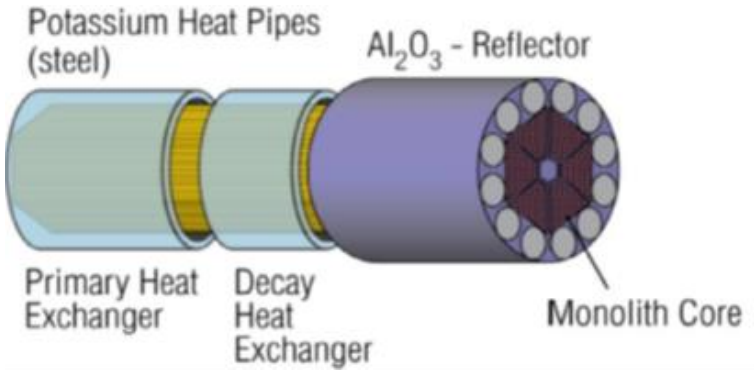
- New reactor concepts (Gen III,III+, SMRs, MMRs,…) impose special challenges:
  - Passive safety systems
  - Innovative components (e.g. compact heat exchanger, heat pipes)
  - New working fluids (e.g. Molten Salt, He, sodium, potassium, …..)
  - New containment concepts
  - Large water pools



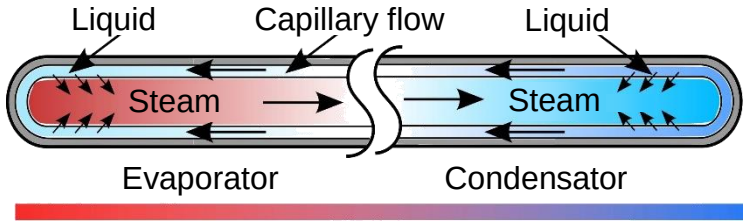
From: 2) J. Chénais, 2018



Adapted from: 6) M. Niemi 2017



From: 4) W. Sterbentz 2017



From: 3) techpowerup.com

Motivation for the Development of AC² (2)

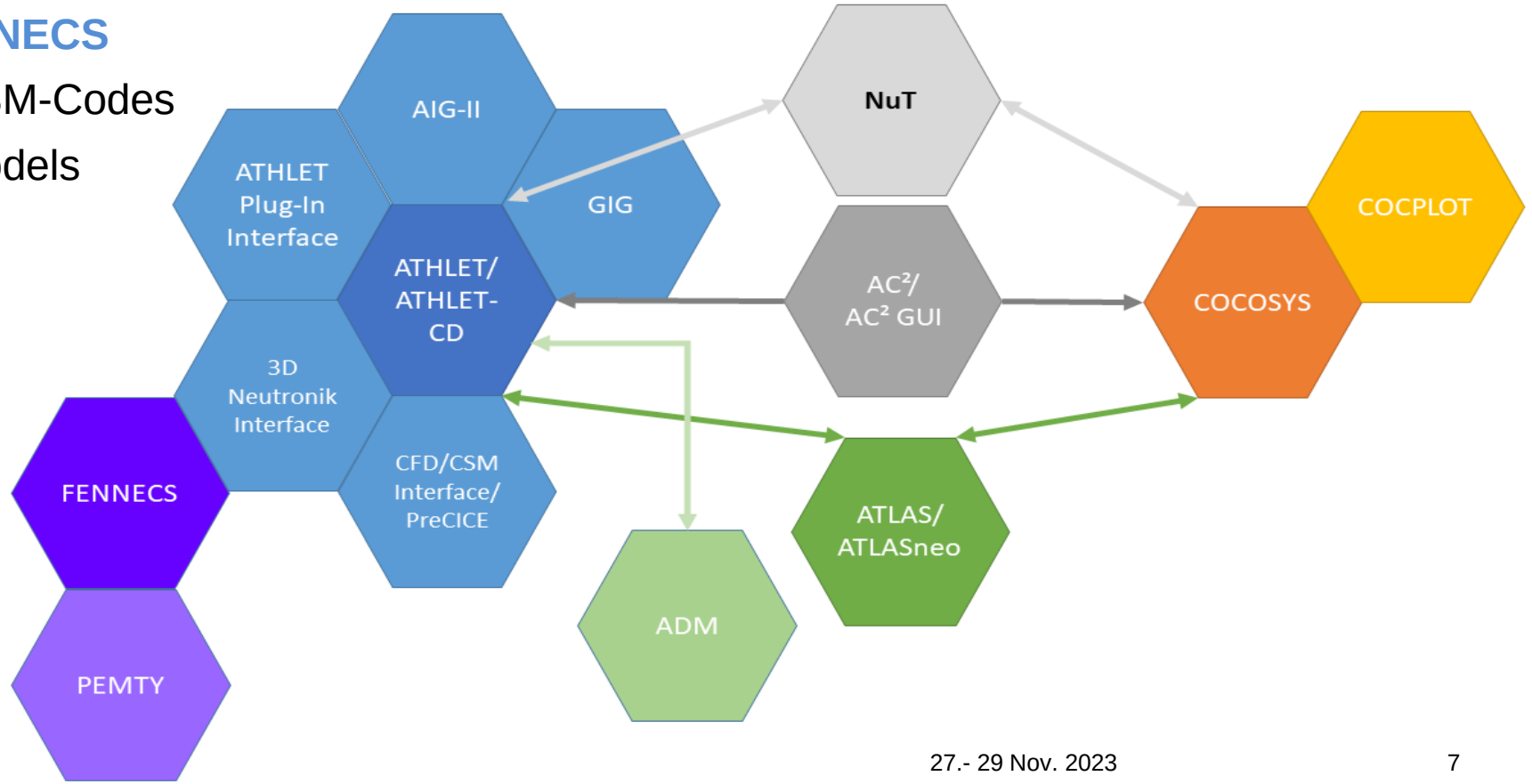
- **Advanced reactor concepts** require partially coupled (**multi-physics**) simulations of phenomena in the core, cooling circuit, containment and fuel pool

- **AC²** approaches this challenge by:
  - Further development of the specific models for **passive safety systems** and **innovative components**
  - **Coupling** ATHLET/ATHLET-CD und COCOSYS for the simulation of flow phenomena in cooling circuit and containment
  - Coupling thermo-hydraulics and neutron kinetics with **ATHLET and FENNECS**
  - **Simplifying input creation** for integral analysis
  - Improved compatibility of the **phenomenological models**
  - Extension to **new working media** and **homogenization** of material values
  - **Integral validation** of the overall system
  - Uniform programming standards and **QA requirements**

AC² 2023: Content of the Distribution

In addition to the AC² (**ATHLET**, **ATHLET-CD**, **COCOSYS**) code, **AC² 2023** package will also contain:

- **ATLASneo/ATLAS** for the visualisation of the simulation results and interactive control of plant simulators
- **ADM** (ATHLET Input Modeller) for graphical generation of thermo-hydraulic- und BOP models for **ATHLET/CD**
- **FENNECS**: 3D-Neutronic-Diffusion Code for compact cores
- **PEMTY**: Grid generator for **FENNECS**
- **Coupling Interfaces** to CFD/CSM-Codes
- **Plug-Ins templates** for User-models
- Tools für **ATHLET** und **COCOSYS**
- Documentation
- Sample inputs

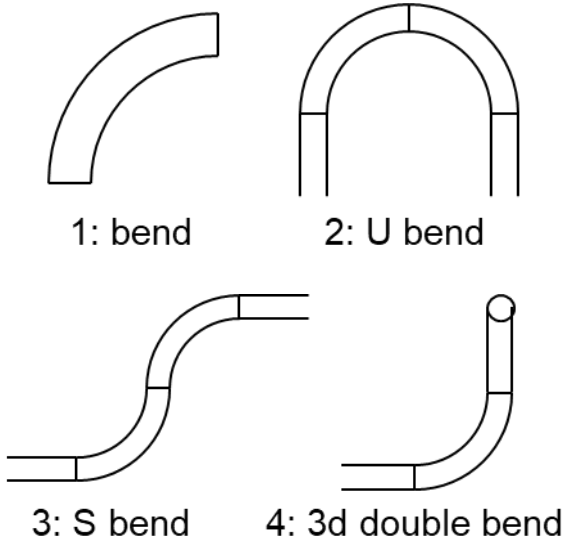


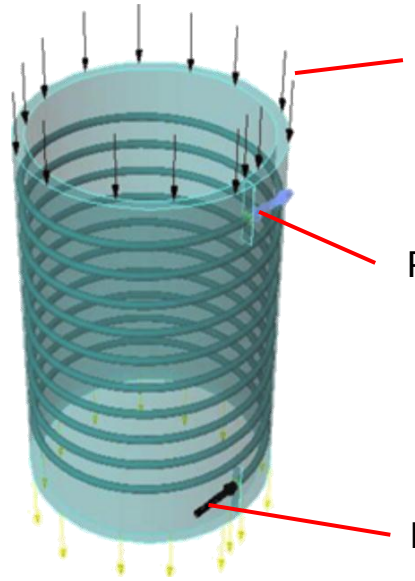
ATHLET 3.4

AC² ATHLET

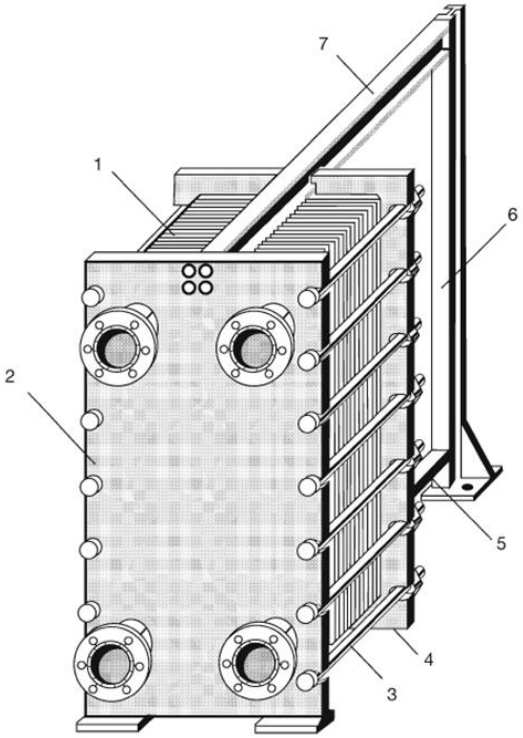
- **Numerous new and improved models**
  - Heat transfer and pressure loss correlations for **compact heat exchangers** in SMRs
  - Improved consideration of **form losses**
  - Widely updated **fuel rod model** for DBA analyses
  - **New two-phase working fluids** and NC gas components
  - Divers model updates, e.g. T-junction model, oxidation model

Fuel swelling and relocation





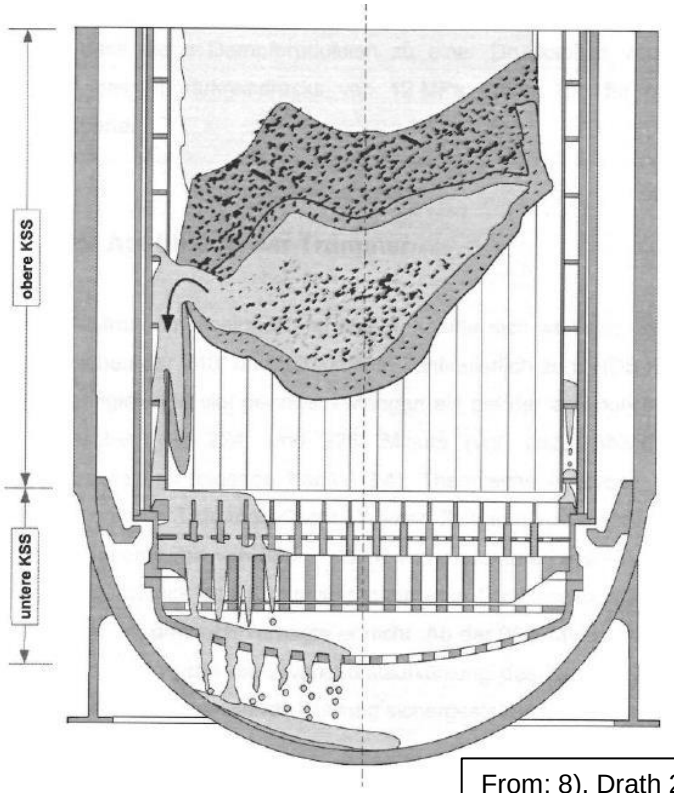
From: 6), Niemi 2017



From: 5) VDI 2013

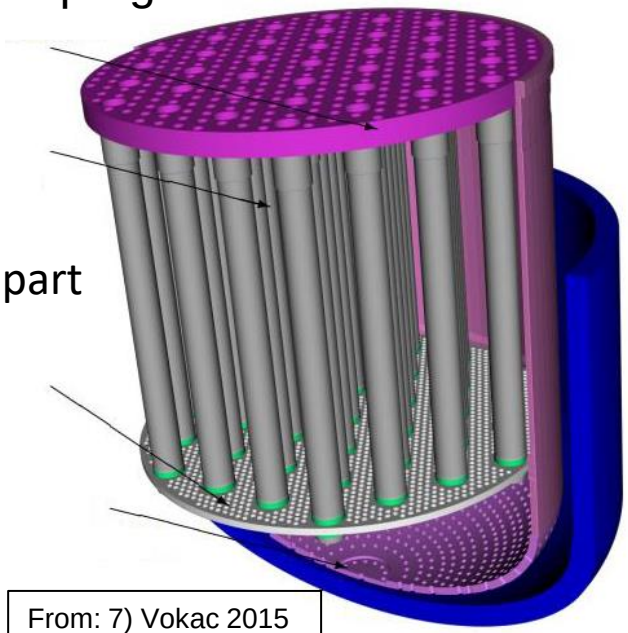
ATHLET-CD 3.4

- Melt **relocation** through the core bypass channel
- **VVER-440** specific model capabilities
  - Axial configurable core composition
- **Harmonization** between ATHLET-CD and ATHLET
  - Heat transfer correlations
  - ATHLET water properties used in AIDA
  - Further harmonization under progress



From: 8), Drath 2004

VVER-440 lower core part

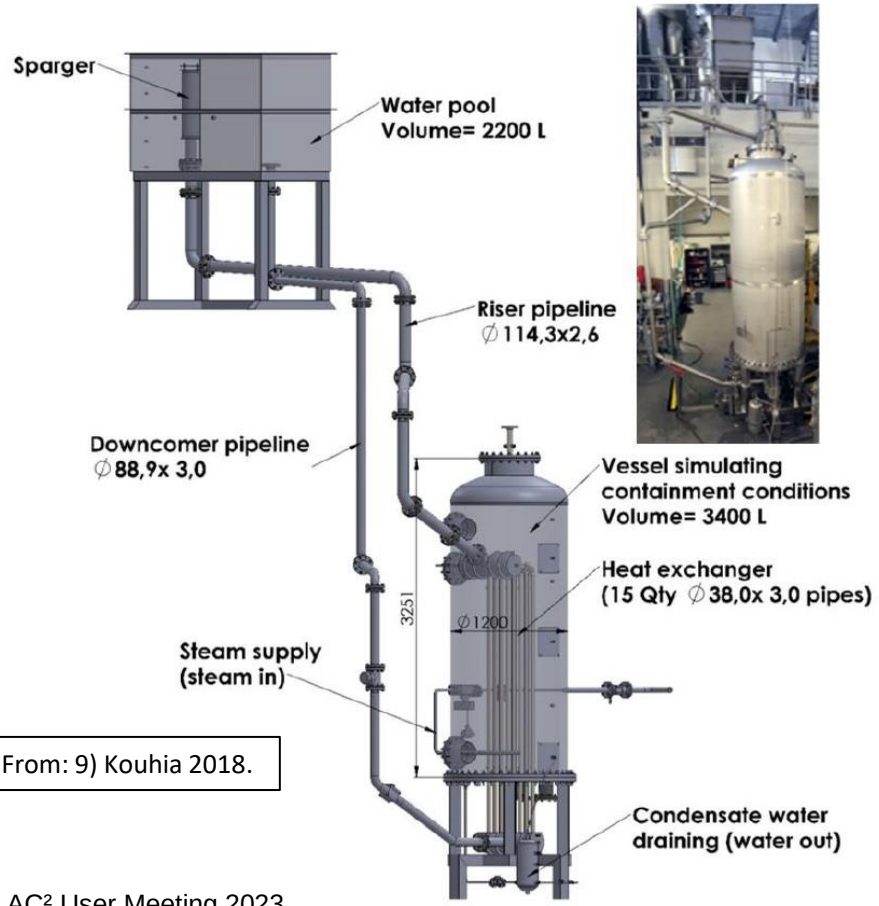


From: 7) Vokac 2015

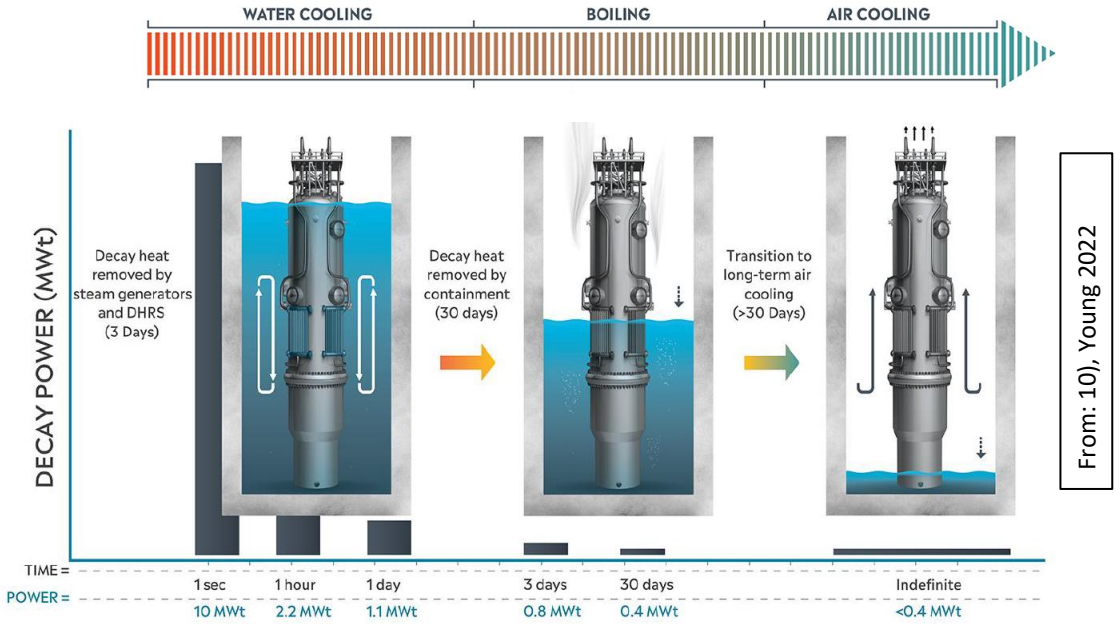
AC² ATHLET-CD

COCOSYS 3.2

- Improved **pool simulation** (heat transfer, boiling, level)
- Improved **building condenser** model (stability two-phase flow, non-condensable gases, pressure loss)



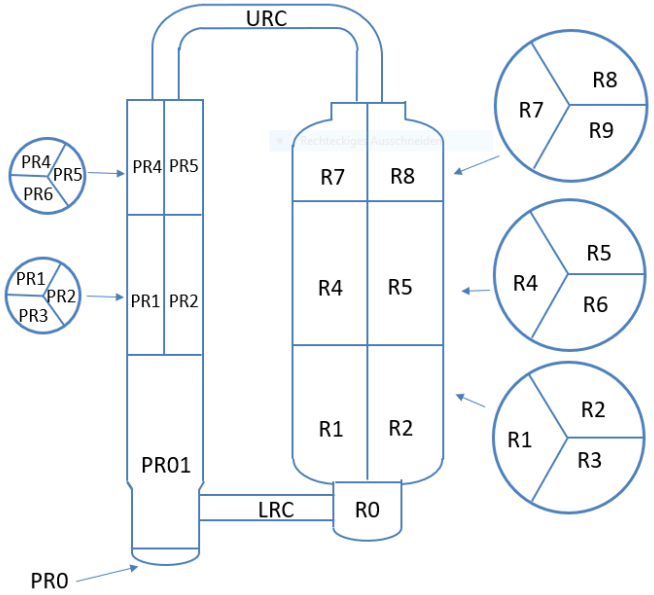
From: 9) Kouhia 2018.



From: 10), Young 2022

AFT2:

- **NewAFT** becomes **AFT2**
- Consideration of **FP and aerosol transport in ATM_FULL**
- **pH model** is now available **in NewAFP**

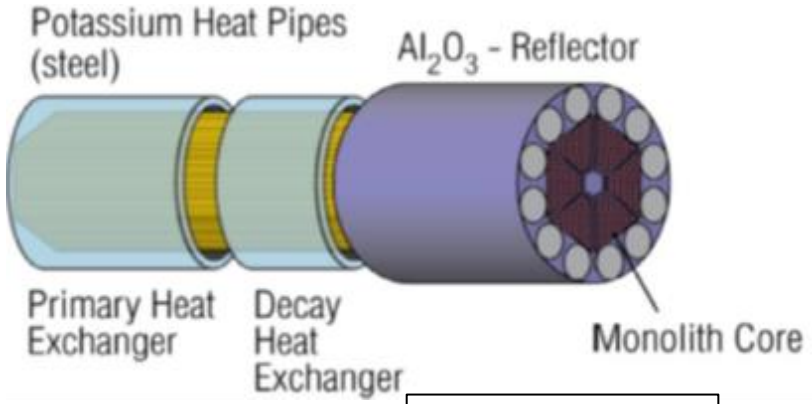


FENNECS – Deterministic Neutron Kinetics Code for Irregular Geometries

FENNECS

- **F**inite **E**leme**N**t **NE**utroni**CS**
  - Time-dependent 3-d few-group **finite element**-based **diffusion** and **SP_3 transport** (steady state) code
  - Geometrical flexibility to model **complex** and **irregular geometries** of **SMRs** and **MMRs**
  - Also applicable to **Generation IV** reactor concepts and **LWRs**

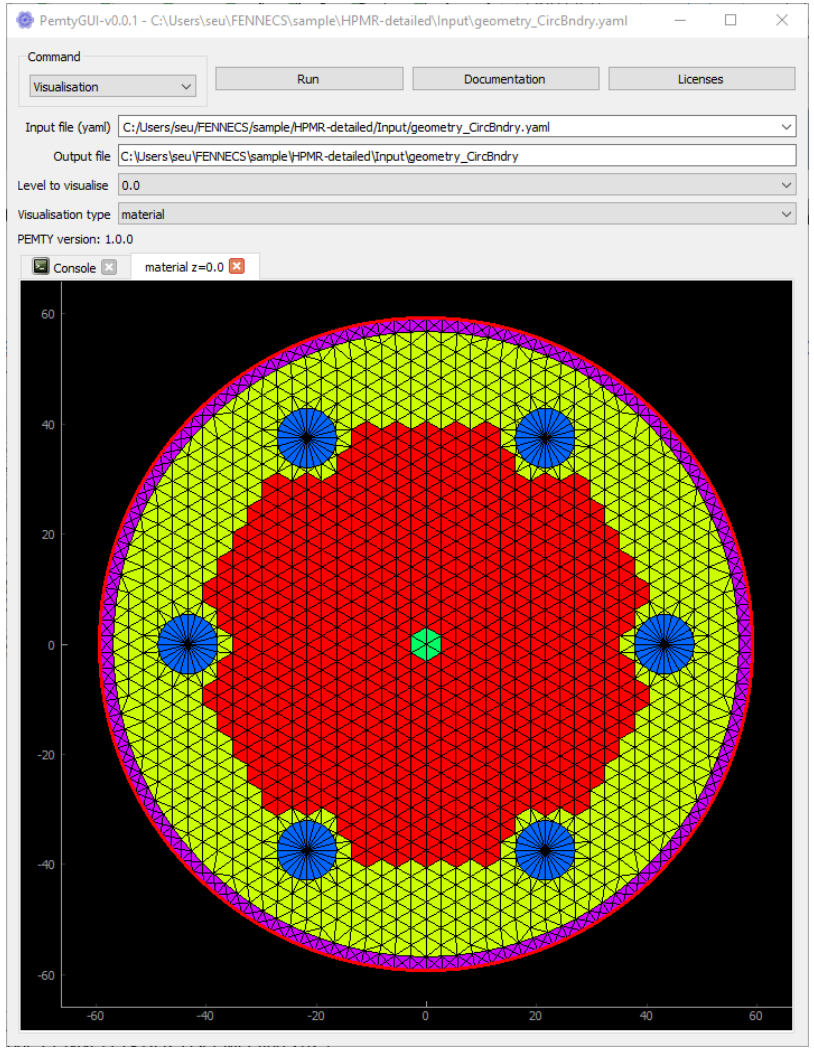
- **Features:**
  - **Coupled** with the GRS thermal-hydraulic system code **ATHLET**
  - **Coupling with CTF in progress**
  - **Core radial thermal expansion model** for SFR simulations
  - **Control rods:**
    - **Axial** movements, different axial material zones,
    - in-plane **rotation** of **control drums**.
  - Critical **boron search**.
  - **Iodine/Xenon** and **Promethium/Samarium** dynamics
  - **Visualization**: geometry, material, power density, neutron flux distribution, thermal-hydraulic parameters

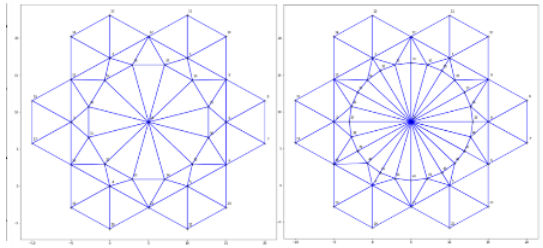


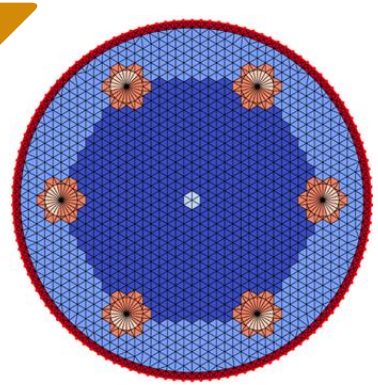
From: 4), Sterbentz 2017

PEMTY – Software for Meshing Irregular Geometries for FENNECS

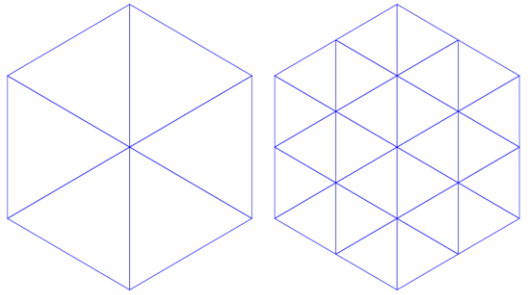
Python External Meshing Tool with Yaml input

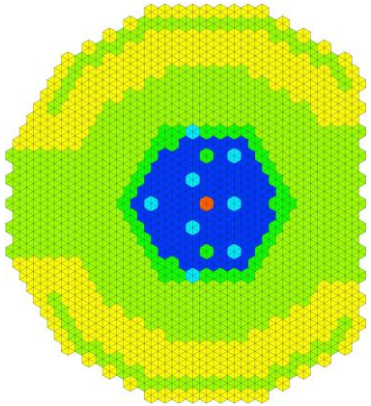




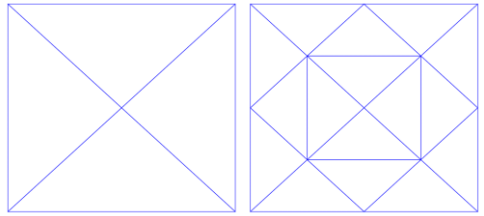


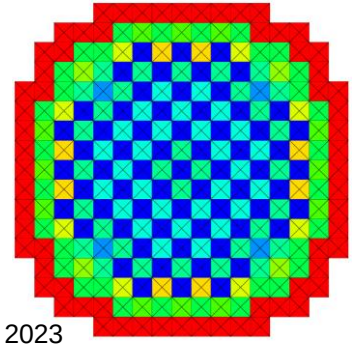
MMR





SFR

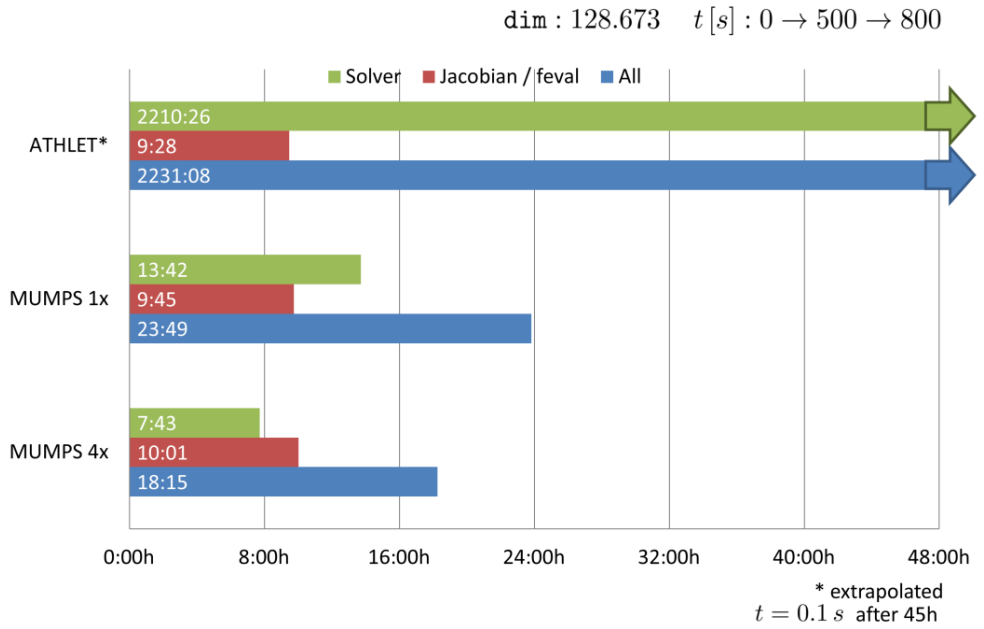




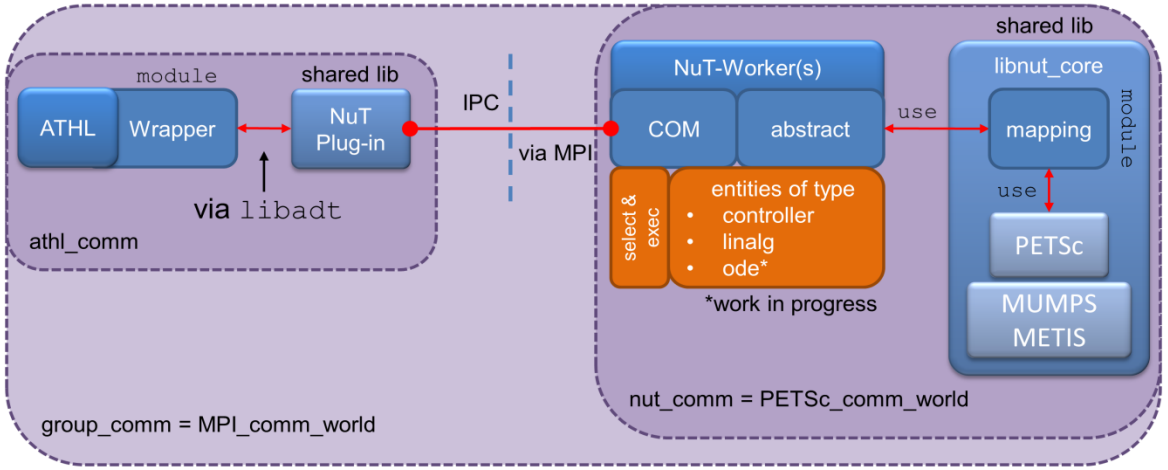
LWR

Numerical Toolkit (NuT) v2.0.2

- Numerical Toolkit (**NuT**)
  - Based on PETSc Library (open source)
  - Coupled via MPI-Interface
  - Multithreading
- Significant performance gain for **ATHLET**



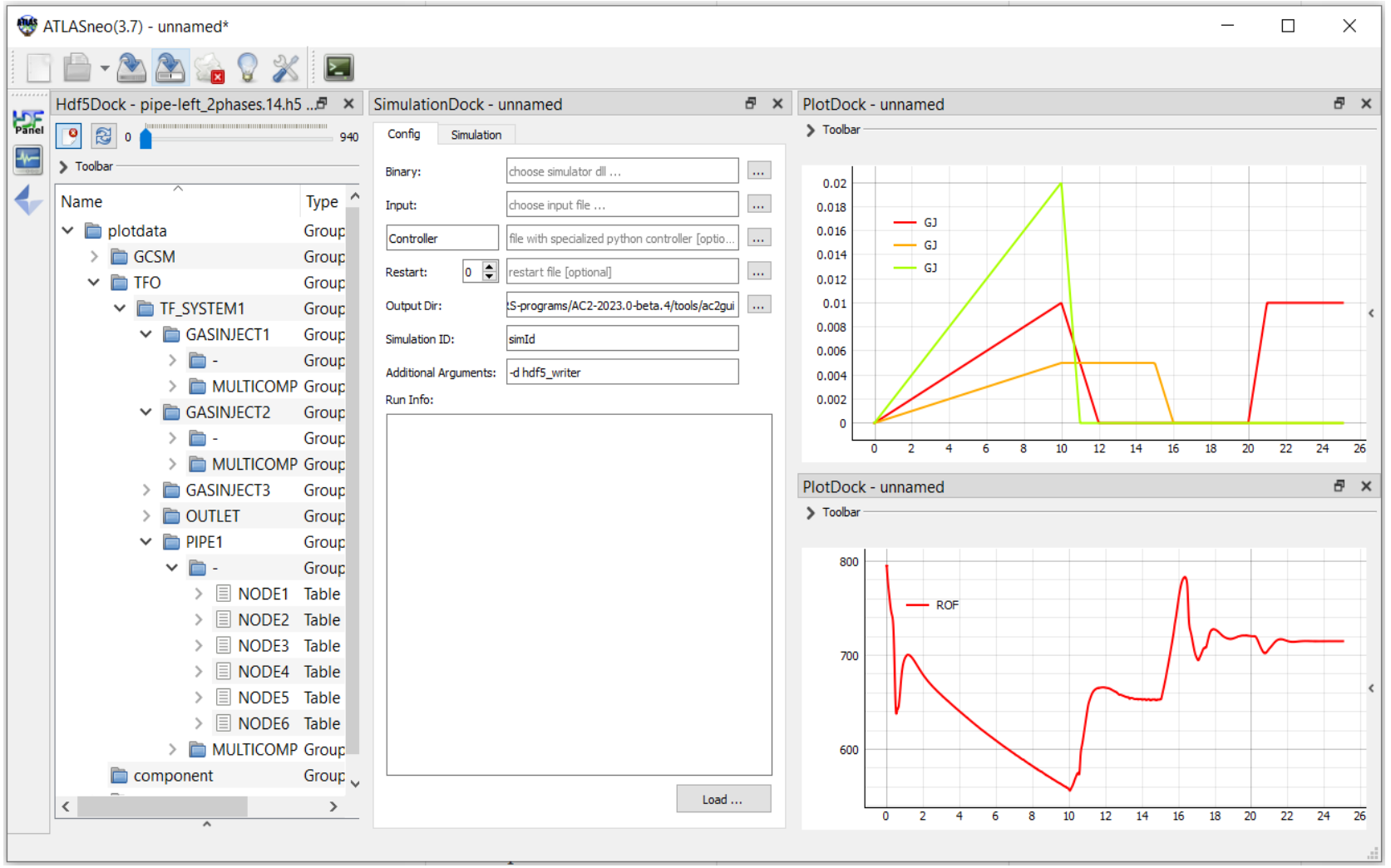
- New feature:
  - Support of **COCOSYS THY-module RAMAIN**
- Current development work:
  - Support **coupled calculations** of ATHLET/CD and COCOSYS with common equation system




```
mpiexec -n 1 ./athlet : -n 4 ./nut
```

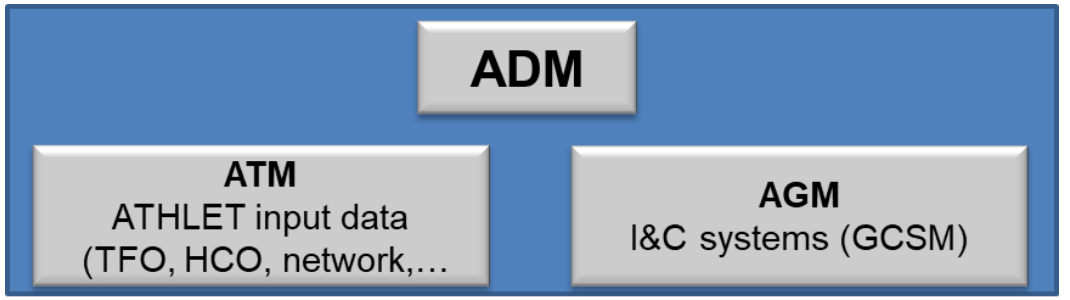
ATLASneo

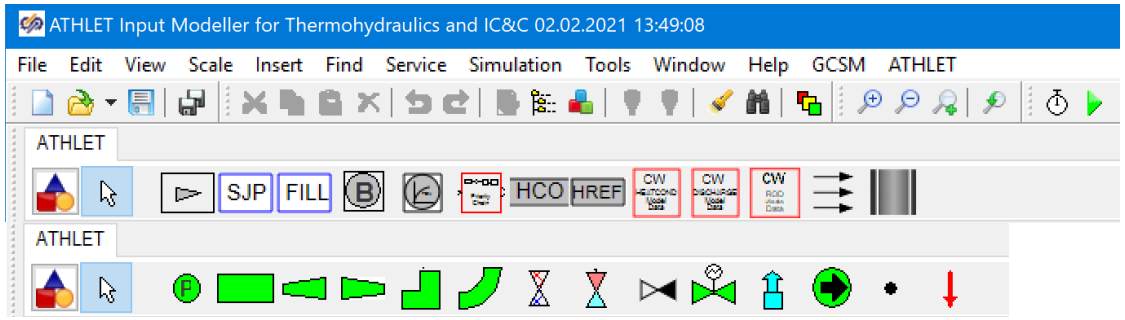
- Dynamic simulation control
- Postprozessing
- Runs under Windows and Linux
- Dataformat: **HDF5**
- pdf2HDF converter
- 2D-visualization in development

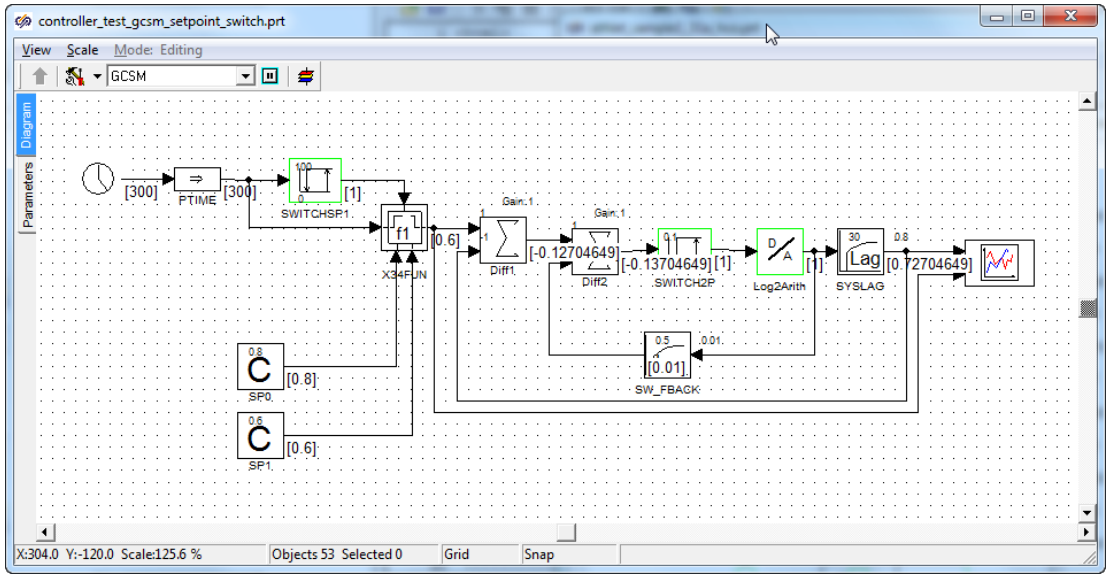


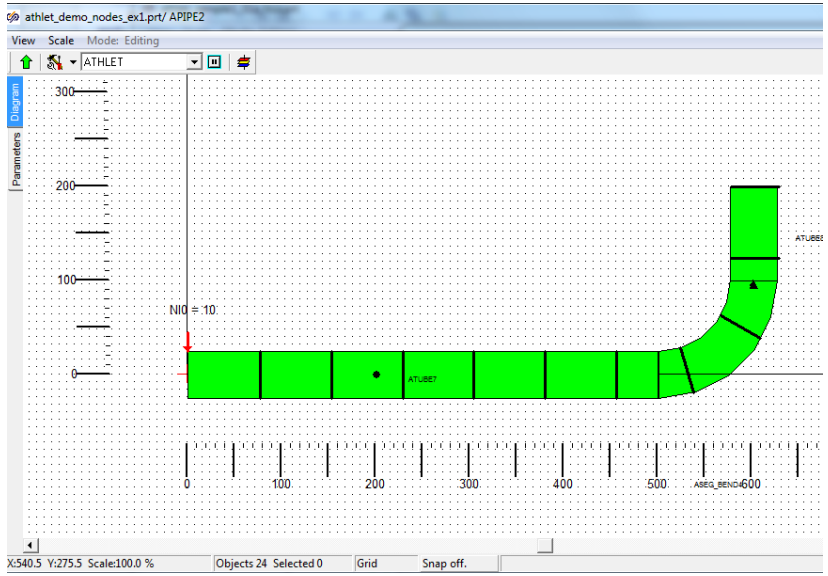
AC² Design Modeller (ADM)

- Interactive application for graphical modeling and input generation for ATHLET
  - ATHLET GCSM Modeller (AGM)
    - Used for system simulation in several plant simulators
  - ATHLET Thermohydraulic Modeller (ATM)
    - Supports many models (TFO, HCO, ROD,…)







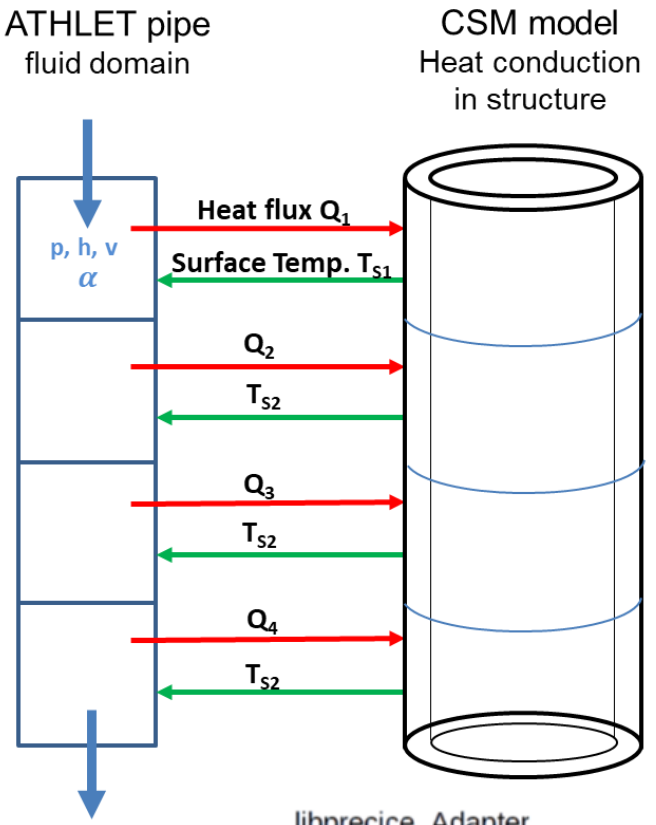


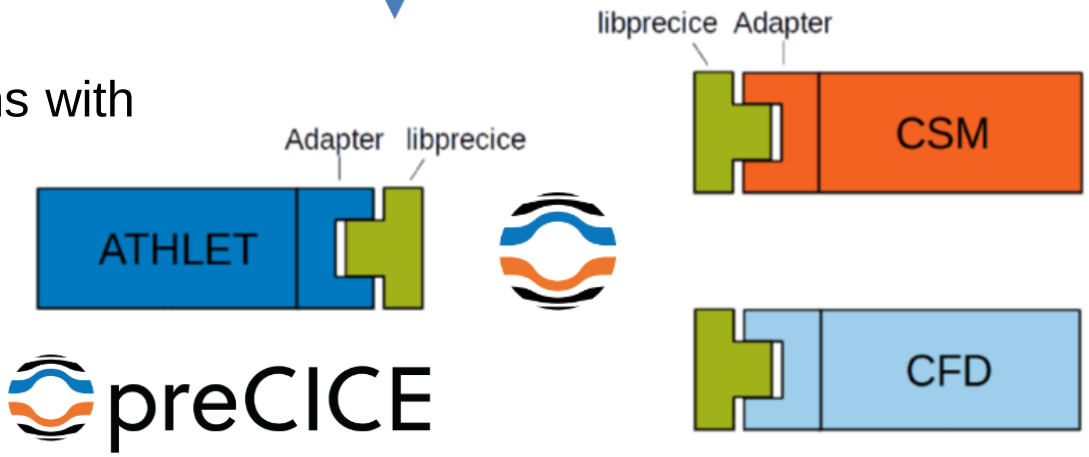
Coupling Capabilities of AC²

- Neutronic-Codes
  - **FENNECS,** QUABOX/CUBBOX, DYN3D (HZDR), PARCS
  - BIPR, KIKO3D (KFKI, HU), **TORT-TD, KMACS**
- Subchannel-Codes
  - COBRA-TF (NC State Univ., USA)
- CFD-Codes
  - ANSYS CFX, OpenFOAM
- Structure Mechanics Codes
  - ASTOR, WinLeck**, CalculiX**

- **Plugin-Interface** to couple user-defined models/functions with **ATHLET/ATHLET-CD**

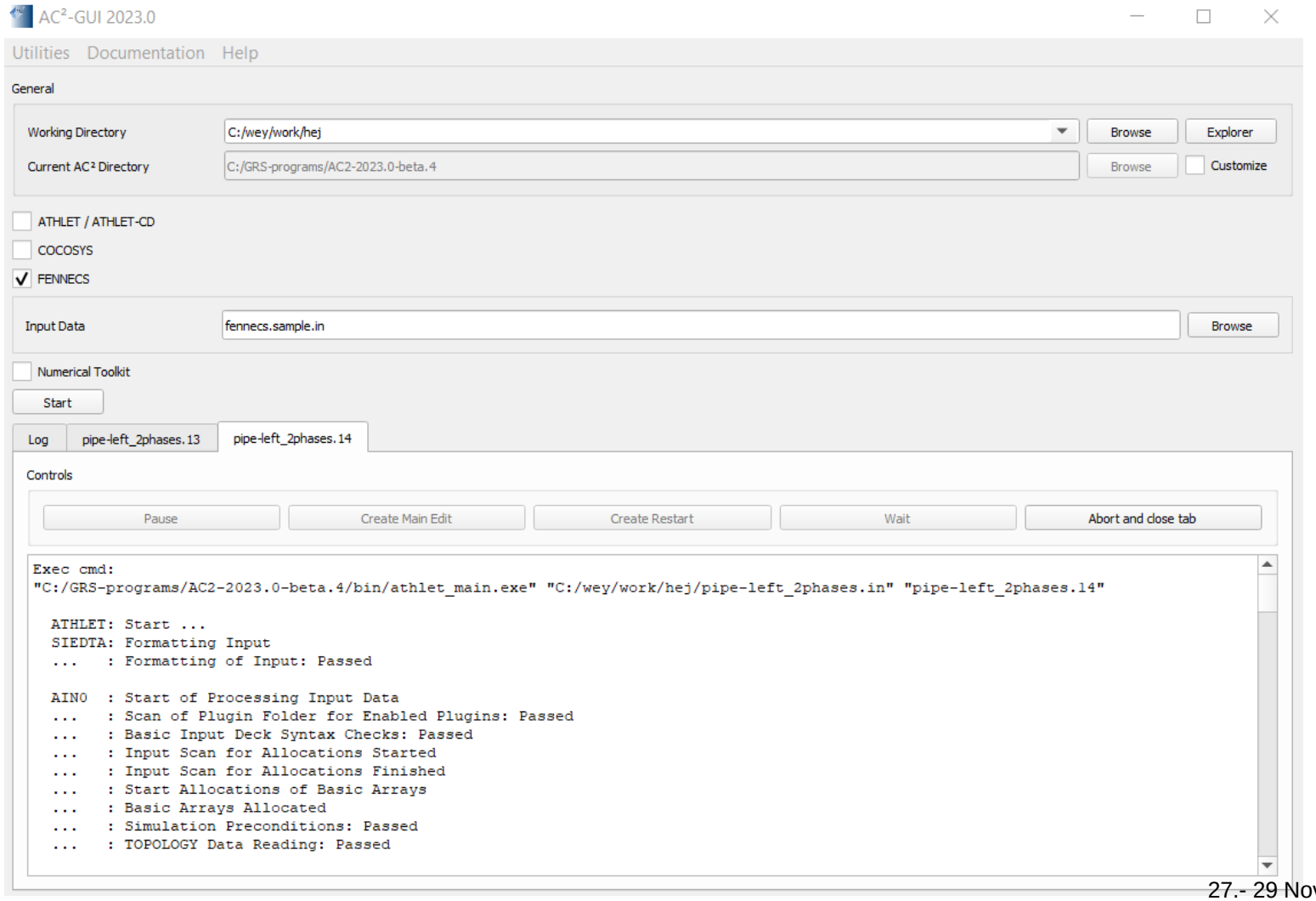
- **New**: Interface to coupling library **preCICE**





AC² - GUI

- AC² GUI to start ATHLET/CD, COCOSYS and FENNECS stand-alone and coupled calculations



AC² 2023: Development and Validation

- All AC² Codes are developed and validated under strong quality assurance.
- The goal is a program that is validated in accordance with **regulatory requirements** (**SiAnf, SSG-2**) and can be used in nuclear regulatory procedures. The continuous validation of the AC² programs for 46 years establishes their value for research, development and application
- In addition to **GRS**, **AC²** programs are validated and partly developed by **long-standing partners** of GRS. These are particularly **German research institutions**.

RUHR UNIVERSITÄT BOCHUM RUB

HZDR HELMHOLTZ ZENTRUM DRESDEN ROSSENDORF

RWTH AACHEN UNIVERSITY

KIT Karlsruher Institut für Technologie

TECHNISCHE UNIVERSITÄT DRESDEN

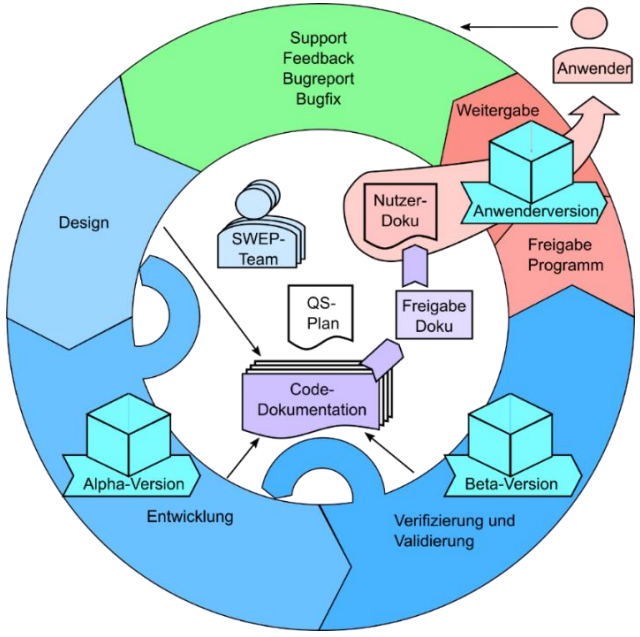
JÜLICH Forschungszentrum

Universität Stuttgart

Hochschule Zittau/Görlitz UNIVERSITY OF APPLIED SCIENCES

TECHNISCHE HOCHSCHULE DEGGENDORF

AC²-Development Process



CPU Affinity

- Intel CPUs processors (12th Gen and later) feature Performance-cores (p-core) and Efficient-cores (e-core)
  - p-core provide 2 logical high-performance processors
  - e-core provide 1 logical processor efficient, but not a fast
- .**Problem:** Windows 10 confines every background process to the slower e-cores

➡ **As soon as the AC²-GUI is in the background your simulation slows down (about 50%)**

Our Solution: Environment variable `AC2_CPU_AFFINITY`

- Specify CPUs to be used for AC²-Simulation: Set **`AC2_CPU_AFFINITY to`**
  - individual CPUs, e.g. **`AC2_CPU_AFFINITY =`** ‘0,2,3‘
  - CPU ranges, e.g. **`AC2_CPU_AFFINITY =`** ‘0-3,10-12‘

Detailed Instruction in the **AC²-User Manual** (determine CPU type, setting environmental variable)

Summary and Outlook

- New Release AC²-2023
  - New neutronic physics code **FENNECS** and Analysis tool **ATLASneo**
  - Lots of new features in **ATHLET, ATHLET-CD, COCOSYS, NuT** available

- Lots of interesting talks in the next three days
  - Presentations on the new versions of **ATHLET, ATHLET-CD, COCOSYS, NuT, FENNECS, ATLASneo**
  - Talks on **special new features**, e.g. new working fluids, AFP2-module,…
  - Information on **current projects**
  - Presentations of our **Users** on their **applications** of AC²

Literature:

1) F. Weyermann, D. Eschricht, A. Wielenberg, T. Steinhoff, Ph. Schöffel, C. Spengler, L. Lovasz: AC² User Manual, GRS gGmbH, 2023
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