Gesellschaft für Anlagen-
und Reaktorsicherheit
(GRS) gGmbH

AC^2 2025

AC^2 User Manual

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1 Introduction

This manual provides an overview over topics that are common to all AC^2 codes. In addition, it provides guidance on setting up coupled AC^2 calculations, which complements guidance in the separate ATHLET and COCOSYS manuals and code documentation.

2 Overview on AC²

2.1 AC²

AC² firstly and fundamentally is the collection of the GRS system codes ATHLET, ATHLET-CD and COCOSYS for the simulation of normal operation, transients, accidents up to severe accidents with radioactive release at the site boundary. Its constituent codes have been developed by GRS for more than 40 years, and continue to be under development. These are

1. ATHLET: see section 2.2
2. ATHLET-CD: see section 2.3
3. COCOSYS: see section 2.4

The roles and interactions of AC² codes as well as the visualisation and interactive control tool ATLAS is illustrated in Fig. 2.1.

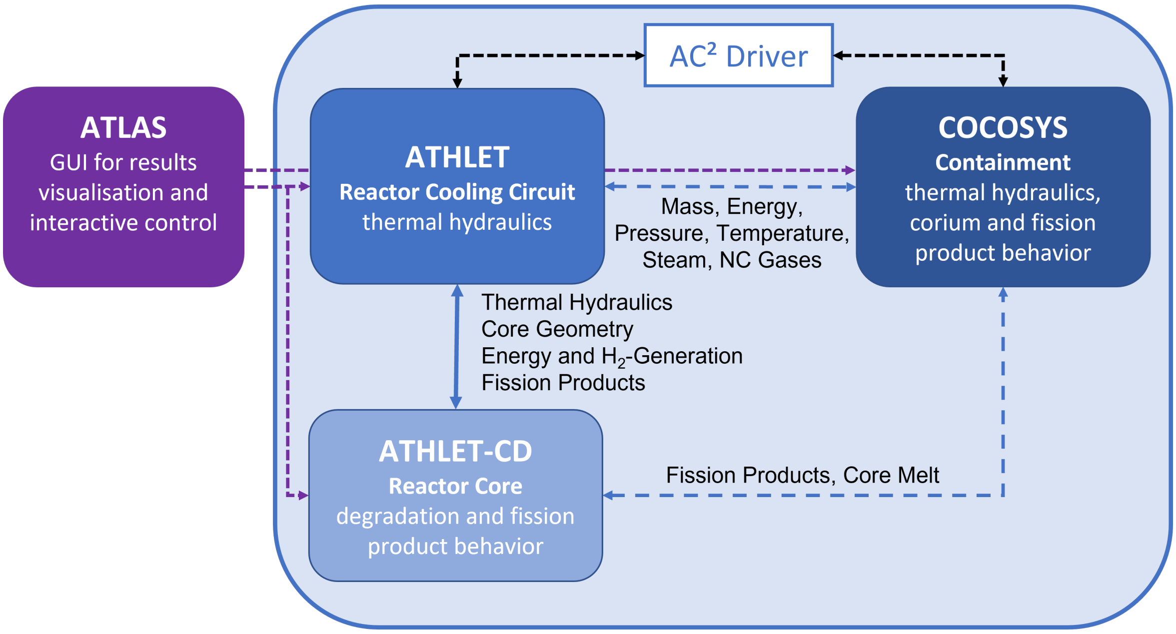

Fig. 2.1 Components of AC².

Secondly, AC² is a distribution of GRS codes containing above system codes as well as GRS codes used in or coupled to AC² or its constituent codes, coupling interfaces and productivity tools provided by GRS. These include:

1. NuT: A toolkit that serves as an interface to dedicated numerical libraries in order to support AC²-internal calculations, see also section 2.6.

2. AC^2 GUI: The user interface for starting calculations of AC^2 or its constituent codes and for accessing the code documentation.

3. AIG-II/GIG: Visualisation of ATHLET nodalisation and GCSM models. In addition, there are some further ATHLET tools.

4. ATHLET plug-in interfaces for accessing user-provided models for certain elements of a simulation.

5. ATHLET CFD/CSM interface: For coupling to CFD codes, particularly OpenFoam, and for coupling to CSM codes with the preCICE library.

6. 3D neutronics interface: For coupling to 3D neutronics nodal codes, such as DYN3D by HZDR, PARCS by the U.S. NRC, and FENNECS by GRS.

7. FENNECS: Finite element neutron diffusion equations solver, see section 2.5

8. PEMTY: Input mesh generation and visualisation tool for FENNECS.

9. COCPLOT: Plotting tools for COCOSYS and AC^2 output data.

10. ATLAS/ATLASneo: see section 2.7

11. ADM: Provide a grafical interface to build GCSM models and ATHLET thermalhydraulics models.

An overview of the distribution is given in Fig. 2.2.

The AC^2 distribution contains a substantial part of the nuclear calculation chain, which is maintained by GRS and used for the safety analysis of nuclear reactors, research reactors and other nuclear facilities as applicable. This calculation chain also includes several codes not or not yet part of the AC^2 distribution as well as several third-party codes used by GRS. An overview of the current nuclear calculation chain is shown in Fig. 2.3. Importantly, the GRS codes are available without a license fee for non-commercial research and development subject to a licence agreement and export control authorization, as their development and validation has been and continues to be largely funded by the German Federal Government based on decisions by the German Bundestag.

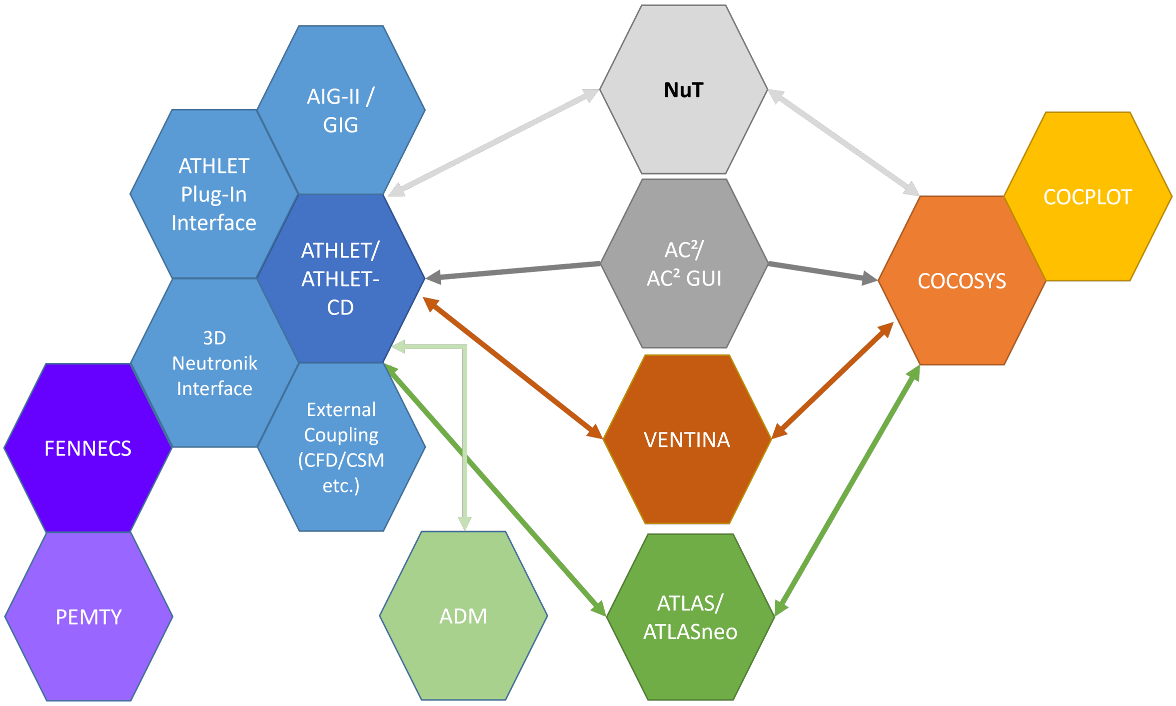

Fig. 2.2 Scope of AC² Distribution.

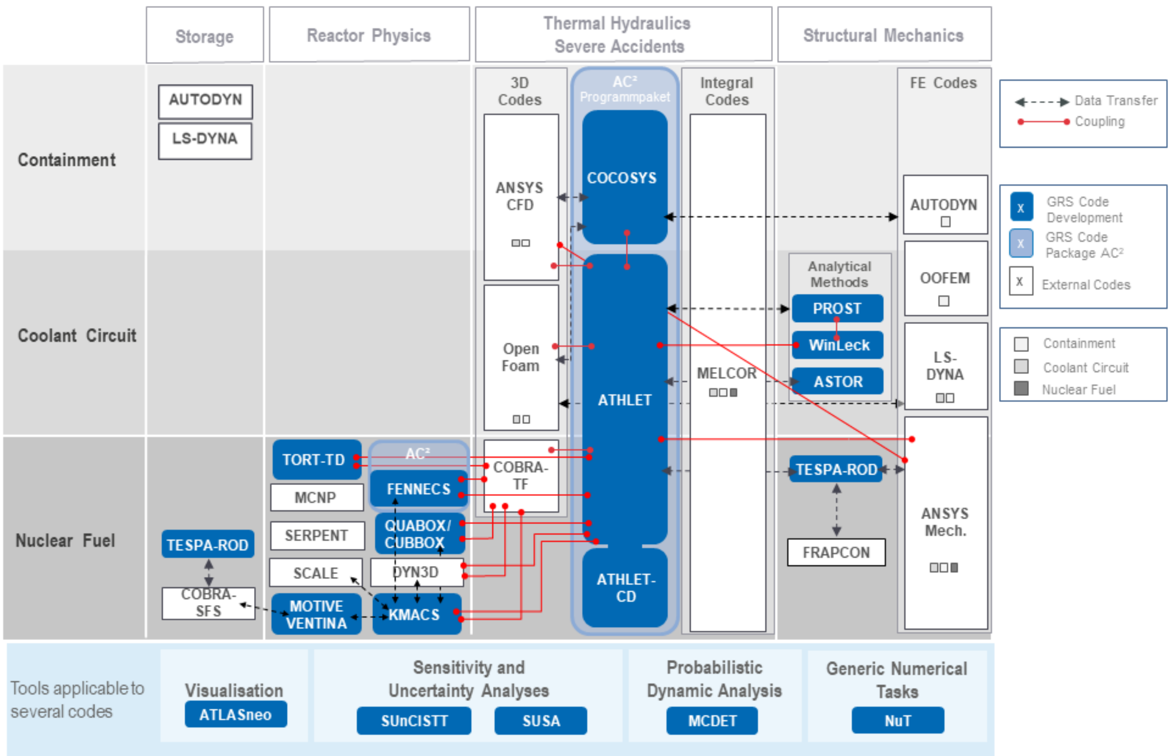

Fig. 2.3 AC² as part of the GRS nuclear calculation chain.

2.2 ATHLET

The thermal-hydraulic computer code ATHLET (Analysis of THermal-hydraulics of LEaks and Transients) is being developed for the analysis of operational conditions, transients and all kinds of leaks and breaks in nuclear power plants. The aim of the code development is to cover the whole spectrum of design basis and beyond design basis accidents (without core degradation) for PWRs, BWRs, SMRs and future Gen IV reactors with one single code.

The main code features are:

- advanced thermal-hydraulic models featuring compressible fluids as well as mechanical and thermal non-equilibrium of vapor and liquid phase
- availability of diverse working fluids: light or heavy water, helium, sodium, potassium, lead, lead-bismuth eutectic (LBE), supercritical carbon dioxide, molten salts as well as user-provided single-phase (non-boiling) working fluids
- heat generation, heat conduction and heat transfer to single- or two-phase fluid considering structures of different geometry, e.g., rod bundle or pebble bed
- interfaces to specialized numerical models such as 3D neutron kinetic codes or 3D CFD codes for coupled multiphysical and multiscale simulations
- control of ATHLET calculation by programming language independent user code enabling the coupling of external models
- plug-in technique for user provided code extensions
- modular code architecture
- separation between physical models and numerical methods
- OpenMP parallelization
- numerous pre- and post-processing tools
- continuous and comprehensive code validation

Detailed information on ATHLET can be found in the ATHLET User Manual, see /SCH 25/.

2.2.1 Code Structure

The code ATHLET features a modular code structure that allows an easy maintainability and expandability of the modelling basis to satisfy the demands of new applications and future reactor designs. As illustrated in Fig. 2.4 the code comprises five basic modules that focus on the calculation of phenomena relevant for safety analyses of a nuclear power reactor:

- Thermo-Fluid dynamics (TFD)
- Heat Conduction and Heat Transfer (HECU)
- Neutron Kinetics (NEUKIN)
- Control and Balance of Plant (GCSM)
- Fission Product Behaviour (FPB)

The TFD system of ordinary differential equations is solved fully implicitly with the inbuilt numerical integration method FEBE. Other independent modules can be coupled without structural changes in ATHLET by means of dedicated interfaces. Moreover, ATHLET can be extended by user provided feature implementations. The plug-in concept enables the users to apply ATHLET more individually by either requesting a specific extension from GRS or even by developing the needed feature on their own.

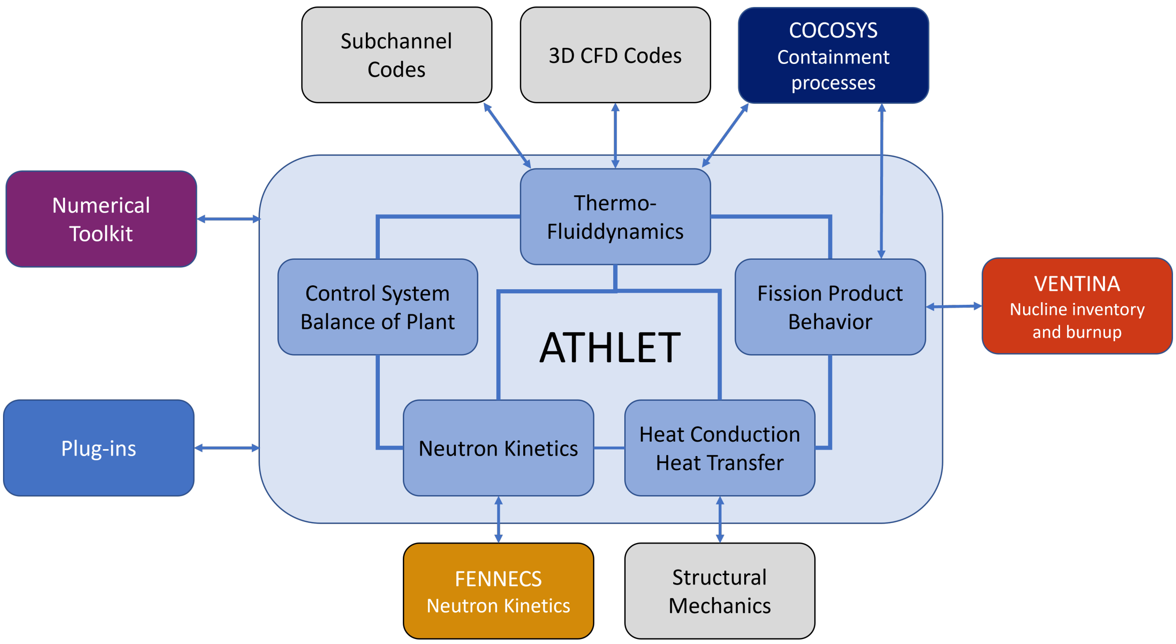

Fig. 2.4 ATHLET code structure

2.2.2 Validation

The development of ATHLET was and is accompanied by a systematic and comprehensive validation program. The validation is mainly based on pre- and post-test calculations of separate effects tests, integral system tests including the major International Standard Problems, as well as on actual plant transients. A well-balanced set of tests has been derived from the CSNI Code Validation Matrix. The tests cover phenomena which are expected to be relevant for all types of events of the envisaged ATHLET range of application for all common LWRs including advanced reactor designs with up-to-date passive safety systems, spent fuel pool applications as well as research reactors. The validation of ATHLET for SMR designs and future Gen IV reactors is underway. More information can be found in the ATHLET validation report /HOL 25a/

2.3 ATHLET-CD

The severe accident code ATHLET-CD /LOV 25/ covers the phenomena related to core degradation in a PWR, BWR or VVER type reactor. Similar to other relevant code systems, ATHLET-CD also divides the core region radially into concentric rings, axially into different nodes /LOV 25/.In each ring at a given height, all fuel rods behave identically, and they are represented by a so-called hypothetical representative fuel rod. This summarizes the extensive properties of all fuel rods within the given ring. This assumption is necessary because in a typical reactor there are many thousands of fuel pins. Simulating each of these fuel rods would make the calculation prohibitively expensive.

ATHLET-CD consists of several modules, which are shown in Fig. 2.5. These interact with each other and with ATHLET /SCH 25/ during an ATHLET-CD simulation. In addition, full AC^2 simulations are possible by using the coupling interfaces to COCOSYS as shown below.
Information on the validation status of ATHLET-CD is given in its validation report /HOL 25b/.

2.4 COCOSYS

The containment of a nuclear power plant is the final of several barriers to retain radioactive substances. It consists of a gas-tight steel shell enclosing the reactor and a thick concrete shell designed to protect the steel shell from external hazards. In the event of an accident, coolant escaping from the cooling system, i.e., radioactively contaminated water and steam, is collected inside the containment. However, the

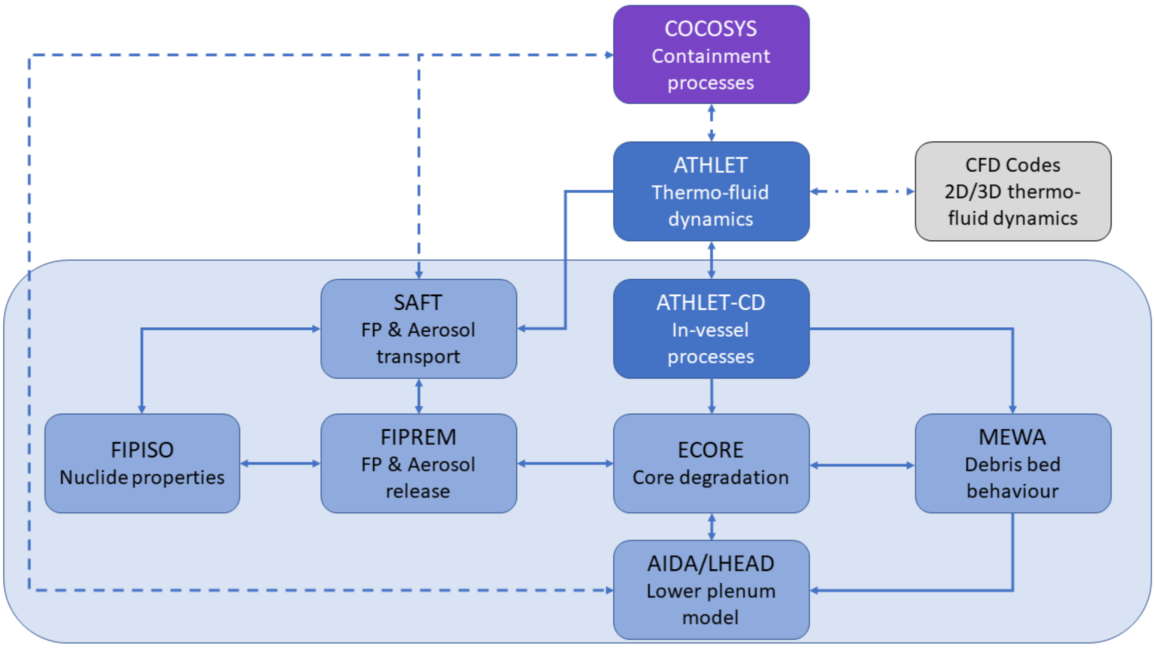

Fig. 2.5 ATHLET-CD code structure

retaining function of the containment may put be at risk by an accident. With its simulation code COCOSYS (COntainment COde SYStem), GRS is able to investigate the thermal hydraulic and chemical-physical processes inside the containment during incidents and accidents. In addition, COCOSYS can be used to determine the radioactive source term. This indicates the type and quantity of radioactive substances that may be released from a damaged containment into the environment. The determination of the source term including the time history of the release is important to be able to plan disaster control measures and to initiate them in case of an actual accident.

2.4.1 Code characteristics and structure

COCOSYS is a so-called 'lumped parameter code', i.e., a numerical simulation program in which the containment is divided into cells. For each of these cells, a defined thermodynamic state (temperature, pressure and gas composition) averaged over the cell is calculated (see image). Dynamic processes are represented by exchange processes between zones and between zones and structures (walls, floors, ceilings). This approach allows the simulation of events over several hours and days.

COCOSYS consists of three main modules:

- Thermal hydraulics: calculations of pressure and temperature, gas and steam flows, evaporation and condensation processes, and hydrogen and carbon monoxide combustion.

- Aerosol and fission products: calculations regarding chemical-physical processes, e.g., radioactive iodine in the atmosphere of the containment, deposition, aerosol leaching and filtering processes
- Melt-concrete interaction: calculation of, among other things, gas formation through thermochemical reaction of the melt with concrete.

There are specialised models running in the background of the modules in which the processes are largely simulated mechanistically.

One of the strengths of COCOSYS, apart from the diversity of the processes taken into account, is that the complex interactions - as far as they are known - are also simulated. For some time now, the individual codes COCOSYS and ATHLET or ATHLET-CD (thermal hydraulics in the cooling system and core destruction) have been joined under the umbrella of the GRS code package AC2 and are increasingly used in combination. Thus, interactions and feedback effects between the cooling system and the containment during accident sequences can be simulated in even more detail and the behaviour of the plant during the entire accident sequence can be simulated.
A detailed description of COCOSYS is given in the user manual /**lt:coco33**/.

2.4.2 Validation and application

Since the beginning of code development, COCOSYS has been extensively validated. This includes, in particular, successful pre- and post-calculations of experiments at test facilities in Germany and abroad. COCOSYS was also validated on the basis of the real core meltdown events at Fukushima. Furthermore, GRS regularly participates in national and international benchmark simulations (so-called code-to-code comparisons).

GRS has carried out numerous research activities with COCOSYS for different reactor designs. The results of this work have helped to widen the state of knowledge on accident sequences and to evaluate and improve concrete backfitting measures. One example is the arrangement of catalytic recombiners in the containment for the efficient recombination of hydrogen released during an accident. In addition, COCOSYS was used in international research projects to clarify and understand the accident sequence in Fukushima. Numerous organisations at home and abroad use COCOSYS for reactor safety research.

But COCOSYS can also be used to investigate interesting questions outside the field of nuclear technology. For example, GRS uses COCOSYS to analyse the spread of the naturally occurring radioactive noble gas radon in buildings in order to derive targeted measures and recommendations for action to reduce the radon activity concentration. During the coronavirus pandemic, GRS investigated the behaviour of aerosols containing SARS-CoV-2 viruses in an exemplary indoor scenario. In doing so, it demonstrated the high significance of airborne virus-containing aerosols and quantitatively confirmed the effectiveness of ventilation measures and FFP2 facemasks.

For more information on the validation of COCOSYS see the regression testing report /ARN 25/.

2.5 FENNECS

Researchers worldwide are working on small modular reactors (SMR) and micro reactors (very small modular reactor, vSMR). Many of these new reactor concepts are being developed for specific applications and have special core geometries. In order to be able to simulate the neutron-physical behaviour of these cores, GRS is developing the simulation code FENNECS (Finite ElemeNt NEutroniCS), see /SEU 25/.

SMRs place fewer demands on the site and can therefore be deployed more flexibly than conventional nuclear power plants. Thus, SMRs can be used to supply remote cities and industrial plants with electricity and heat. Some of these concepts are already being realized in some countries. Example projects are the floating Russian small power plant Akademik Lomonosov or the CAREM under construction in Argentina and the ACP-100 under construction in China. Others are in advanced planning stages, including the SMR concept of NuScale (USA), in which several reactor modules are arranged in a common water basin for emergency cooling.

With the smaller core geometries of SMRs, however, the neutron kinetics simulation codes developed and established for large reactor cores can reach their limits. It becomes even more obvious with micro reactors, which are e.g., intended in the military or as propulsion systems for ships and in space travel. Their reactor cores have completely new geometries and configurations and are cooled with alternative media (e.g., liquid potassium). One example of this is horizontal configurations cooled by heat pipes.

With the development of FENNECS, GRS creates the conditions for being able to assess the three-dimensional core behaviour of SMRs and vSMRs both in operation and in case of disturbances or under accident conditions in a safety-related and independent manner.

In FENNECS, the finite element method (FEM) is used to solve the diffusion equations. Here, the core is divided into a finite number of elements ("spatially discretised") that can be well adapted to complex core geometries thanks to variable size and shape. The neutron-kinetic behaviour of each of these elements and the interactions of neighbouring elements are then calculated.
Innovative core geometries can also contain moving components, e.g., rotating control rod drums. In order to take these and other time-dependent effects into account, FENNECS has been extended accordingly. Furthermore, the code is coupled with the thermohydraulics code ATHLET (part of the GRS code system AC2), so that the retroactive effect of temperature effects on the neutron kinetics is also recorded. In addition, GRS is currently developing PEMTY (Python External Meshing Tool for Yaml input), a separate tool that handles the discretisation of an irregular core, which is required as input for FENNECS.

Early versions of FENNECS were successfully tested on two advanced reactor concepts with regular core geometries (based on a code-to-code comparison for the sodium-cooled concept ASTRID and in the OECD/NEA benchmark for the gas-cooled high-temperature reactor MHTGR). The current code version was convincing i.a. in a research project of the International Atomic Energy Agency (IAEA) on the China Experimental Fast Reactor (CEFR). In another research project, the simulation of a microreactor developed by Argonne National Laboratory (USA) was carried out. Current work focuses on the further development as well as on the verification and validation of FENNECS and PEMTY.

2.6 NuT

The Numerical Toolkit (NuT) can be utilized by ATHLET and COCOSYS's thermo-hydraulic module Ramain to support their internal numerical calculations during a simulation run. NuT's direct support of the time integration process is optional and can be activated for stand-alone as well as coupled computations. Further dedicated tasks exist in AC^2 that are always handle by NuT and that do not require any user interaction. Efficient and scalable linear algebra algorithms and data structures are made available via NuT. For further details see /STE 25/.

2.6.1 Supported configurations and intended users

NuT 2.1 requires AC^2 2025 in order to be available for the AC^2 codes ATHLET and ATHLET-CD as well as COCOSYS. Vice versa, ATHLET/CD and COCOSYS of AC^2 2025 do not support any version of the Numerical Toolkit lower than 2.1.

In principle the Numerical Toolkit can be used by any application written in C/C++ or Fortran, either by accessing NuT via its MPI-based IPC[1] interface or by direct linking. For further information on this topic contact GRS.

2.7 ATLAS/ATLASneo

Complex computer programs can now be used to simulate processes in nuclear power plants, from normal operation to serious accidents. An important tool in this area is the ATLAS analysis simulator developed by GRS. Key points of ATLAS. The fundamental goal of ATLAS development was to provide a uniform simulation environment in which the result data is clearly displayed graphically and the simulation process can be influenced interactively. The interactive control of the simulation can be carried out with similar intervention options as in a real power plant.

2.7.1 Simulation codes that can be visualized with ATLAS

A number of dynamic computing programs are currently available in ATLAS that cover a wide range of reactor safety analyses. These currently include:

- ATHLET/ATHLET-CD (GRS, reactor cooling circuit and systems)
- COCOSYS (GRS, reactor containment and building)
- ASTEC (GRS and IRSN, entire system)
- MELCOR (SNL, complete system)

These programs include models for the reactor cooling circuit with thermal hydraulics and heat transfer, for reactor systems and control technology, for neutron dynamics, for nuclear destruction processes and the pressure build-up and fission product behavior in containment.

[1] Inter-process communication

2.7.2 Further development of ATLAS to ATLASneo

The ATLAS calculation code is currently being completely revised and modernized. In addition to a new appearance, the new version ATLASneo offers intuitive operation. In addition to controlling various dynamic simulation programs, real data from power plants can also be evaluated. The controls can be flexibly adjusted and calculations can be compiled interactively and semi-automated. ATLASneo can be used on Microsoft® Windows, for the next release it is planned to support also Linux-based OS. For large simulation data, ATLASneo supports the HDF5 data format. In order to create meaningful visualizations of data, dynamic images can also be used in the future in addition to trends.

2.7.3 Use and benefits

ATLAS is currently used by research and regulatory organizations nationally and internationally for a wide range of applications. Worth mentioning are the detailed analysis simulators for German nuclear power plants created on behalf of the Federal Environment Ministry, the carrying out of so-called “human factor analyses”, the training of personnel in the area of serious accidents and the use as a visualization tool for various calculation codes.

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