KAPROS-E: Modular Program System for Nuclear Reactor Analysis, Status and Results of Selected Applications.

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1. Introduction

The modular program system KAPROS [1] has been developed in the research centre Karlsruhe for nuclear reactor investigations for more than 30 years. Although in the beginning it also was a main objective to include codes for thermal hydraulic calculations, for safety analysis, for transient analysis, etc., up to few years ago mainly modules for neutron physics calculations were included. After the successful implementation of KAPROS on UNIX/LINUX workstations, new efforts started to couple KAPROS with existing stand-alone codes for reactor system analysis. At present several stand-alone codes for a wide variety of applications are linked together to the extended version KAPROS-E. In this paper the capabilities of the powerful modular code system KAPROS-E are summarized, including some results of selected applications.

2. The modular concept of KAPROS

After a first phase of code development at FZK for nuclear reactor calculations with standard FORTRAN methods like “OVERLAY” techniques, it was recognized in the early seventies that a totally modular system with independent modules and common databases with standardized data transfer options would be very advantageous. Considerable efforts over several decades were spent for the realization of this **KA**rlsruhe **PRO**gram **S**ystem KAPROS. The system was utilized for most of the neutron physics research projects at FZK in the past. However, the first versions of KAPROS were strongly relying on capabilities of the computer centre at FZK with IBM mainframe computers and portability to other computer environments proved to be nearly impossible. The move from IBM mainframe computers to UNIX workstations required a major re-design of the system. This task was started in the late eighties and in the mid-nineties a UNIX version was operable on IBM RS6000 workstations. A further major modification (simplification) was implemented at the end of the nineties to run KAPROS on personal computers and workstations with LINUX operating system. The main characteristics of the current KAPROS LINUX version 2.02 are:

- The programming language for system programs and application modules is standard FORTRAN-77, with a few exceptions in the language C for dynamically loading of executables and memory management.
- Application modules may call each other (recursively) up to a level depth of 20
- Standardized data exchange between modules is available on several levels:
  - Pointer techniques and data blocks in fast memory.
  - Data blocks on disk storage.
  - Standardized archive blocks on disk storage or tape
- For the data exchange in fast memory inter-process communication techniques (IPC) are applied.

- On line documentation is provided for a large number of the current about 80 modules.
- Flexible free format input processing is supported, including checks of the data.
- For the most important intermediate results like cross sections, spectra, fluxes, etc. well-defined data block structures are applied.

3. Static reactor design with KAPROS

In reference [2] and its citations a comprehensive description of the KAPROS capabilities for static reactor design may be found. Some important characteristics are:

3.1. Cross section preparation and nuclear data libraries

KAPROS preserves the extensive developments in this area of the former Institut für Neutronenphysik und Reaktortechnik (INR) of FZK. Procedures and library systems developed in INR are available for a broad area of applications. The development has started for fast reactor applications and has been extended for epithermal and thermal reactors [2] and for ADS applications [3]. Data libraries with 26, 69, 75, 78 and 334 groups with upper energies varying from 10.5 to 150 MeV are available at present. A new procedure COLLIB [4] has been developed and validated for collapsing of a general master library to system dependant libraries with an arbitrarily number of coarse groups and with the same library structures as the master library. COLLIB enables to create easily few-group libraries for specific reactor classes, e.g. for dynamic simulations of fast reactor systems. Recently, the 69 group cross section libraries were extended with scattering data for hydrogen bound in zirconium hydride fuel [5] to be used in calculations of TRIGA type reactors.

3.2. Flux calculations and evaluations

KAPROS contains various modules for zero- to three-dimensional multi-group flux calculations in diffusion and transport approximations, with and without up-scattering treatment. Both finite differences and nodal methods for nearly all geometries of interest are available. Some of these modules are strongly coupled with KAPROS, other ones more weakly. A number of international codes is loosely coupled with the help of international standard interface files, e.g. MCNP(X), DANTSYS, DIF3D, CITATION. Powerful evaluation modules are available for the determination of the reactor parameters of interest.

3.3. Burn-up and depletion calculations

KAPROS contains several options to perform burn-up investigations. The main module BURNUP is based on the formalisms of the KORIGEN code [6]. The required one-group data for the evolution calculations can be provided within KAPROS with the help of best estimate weighting spectra, applied to the macroscopic multi-group zone dependant cross sections. The current 69 group master data library contains multi-group cross sections for activation analyses for about 800 isotopes, including more than 160 isotopes with data for full multi group transport calculations. Most of these group constants are derived from the JEF2.2 evaluated data library, using the standard processing program NJOY and local auxiliary codes for the preparation of the libraries in the Karlsruhe GRUBA format (see e.g. also [2]). Also, versions of this library with the replacement of 160 isotopes from JEFF3.0 and ENDF/B6 were created. For detailed core simulations, burn-up dependant parameterized macroscopic multi group cross sections of fuel assemblies on special data libraries may be generated in KAPROS and applied in the module ARCOSI [2].

4. Dynamic reactor calculations with KAPROS-E

The implementation of KAPROS in the UNIX workstation environment facilitates the coupling with large stand-alone codes. In the following sections three recent examples of code coupling in the extended KAPROS-E system are discussed.

4.1. SAS4ADS; coupling of KAPROS with SAS4A

The dynamics simulation of accelerator driven sub-critical systems (ADS) is very challenging because the underlying core physics differs significantly from the well-known procedures for critical systems [7,8]. For the simulation of transients in liquid metal cooled ADS the code SAS4A has been loosely coupled to KAPROS in the procedure SAS4ADS [9]. First results, e.g. for power profiles for beam on/off situations in a sodium cooled system have been presented in [9]. Recent investigations for a lead bismuth cooled ADS design in the PDS-XADS project of the 5. European Community Framework Program analyses the influence of beam trips on the stability of the sub-criticality level [10]. The fuel cracking mechanisms in the fresh fuel lead to reactivity changes in the order of 5 up to 10 cents due to beam trips of some seconds of duration.

4.2. R5PROC; coupling of KAPROS with RELAP5

For the investigation of a High Performance LWR, cooled and moderated by water at supercritical conditions, in the HPLWR project of the 5. European Community Framework Program, the RELAP5 code was loosely coupled to KAPROS in order to study the feedback between the thermal hydraulic and the neutron physics calculations [11,12]. The neutron physics calculations are performed on sub-assembly level. For the very complicated fuel assembly, a deterministic super-cell model, based on the moderator rod and its surroundings, could be validated by more detailed Monte Carlo calculations with MCNP4C. As a first step for coupled neutron physics and thermal-hydraulic investigations, the super-cell model is coupled with the thermal-hydraulic system code RELAP5, being improved for HPLWR applications, see reference [13]. The RELAP5 input model describes the whole reactor system, including a one-channel representation for the core. In this case the applied fuel assembly model for the neutron physics calculations seems to be adequate. The coupled calculations start with a cosine shape estimate for the power distribution in 20 axial zones in the RELAP5 core model. The resulting axial distributions of the densities of the fuel and coolant and of the temperatures of the fuel, clad and coolant in these 20 zones of the model are extracted from the RELAP5 output and processed as an input for KAPROS / KARBUS cross section generation. These cross sections are used for the calculation of an axial power distribution in the super-cell fuel assembly model with the TWODANT [13] code. The feedback of this new axial power distribution to the RELAP5 calculation may be repeated as many times as desired by input. The coupling of these codes RELAP5, KARBUS and TWODANT is organised within the KAPROS system in the procedure R5PROC.

4.3. Coupling of KAPROS with ATHENA and TRACE for gas coolants

Since gas coolant is becoming of more interest in nuclear reactors, investigations have been initiated to couple the KAPROS capabilities for nuclear calculations with an appropriate code for thermal hydraulic and transient calculations for gas cooled systems. At present first coupling investigations are in progress with an older version of the code ATHENA [14]. The preliminary results of these investiga-

tions are very promising [15] and it is intended to continue these efforts with the newest version of the ATHENA code or alternatively with the TRACE code [16].

5. Summary and perspectives

The comprehensive, fully modular, code system KAPROS, developed at FZK for reactor physics calculations with large efforts during several decades, has been successfully re-designed for UNIX/LINUX operating system environments. On these systems loosely coupling of KAPROS with other stand-alone codes is convenient and couplings could be implemented for a number of neutron physics, thermal hydraulic and transient codes. The extended version KAPROS-E is running very stable on LINUX workstation PCs. The characteristics of KAPROS, its realization and the experience gained at FZK with implementation and applications, can be a valuable input to the activities in Europe to come to unified calculation tools for nuclear simulations.

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6. References

[1] H. Bachmann, G. Buckel, W. Hoebel, S. Kleinheins*, "The modular System KAPROS for Efficient Management of Complex Reactor Calculations",* Proc. Computational Methods in Nuclear Energy, Charleston CONF-750413 (1975)

[2] C.H.M. Broeders*, „Entwicklungsarbeiten für die neutronenphysikalische Auslegung von Fortschrittlichen Druckwasserreaktoren (FDWR) mit kompakten Dreiecksgittern in hexagonalen Brennelementen",* KfK 5072 (1992)

[3] C.H.M. Broeders, I. Broeders *„Development and validation of calculation procedures for the neutron physics investigations of ADS ",* IAEA TCM Argonne (2000)

[4] C.H.M. Broeders, R. Dagan*,"Generation of coarse group libraries with the KAPROS procedure COLLIB",* FZKA 6741, P397 (2002)

[5] M. Badea, C.H.M. Broeders, R. Dagan, A. Travleev, *„Neutron Physics Investigation Related to TRIGA Fuel"*, Eingereichter Beitrag Jahrestagung Kerntechnik Düsseldorf, 2004.

[6] H.-W. Wiese, B. Krieg*,* "*Erweiterung der KORIGEN-Datenbibliotheken und Berücksichtigung der Spaltprodukte aus Spontanspaltungen",* Internal report FZK, PSF3253 (1996)

[7 R. Dagan, C.H.M. Broeders*, D. Struwe, "Modifications of the Code SAS4A for Simulation of ADS Designs",* FZKA 6334, 2000.

[8] D.G. Cacuci, "*On perturbation theory and reactor kinetics: from Wigner's pile period to accelerator driven systems",* PHYSOR 2002, Seoul (2002)

[9] R. Dagan, C.H.M. Broeders, D.Struwe, W. Pfrang*, "SAS4ADS- 3D Space Time Dynamic Code System for ADS",* Reaktortagung Stuttgart, 2002

[10] R. Dagan, C.H.M. Broeders, D.Struwe, W. Pfrang*, "Source trips effects on operational and safety ADS modes",* AccApp03, San Diego (2003)

[11] C.H.M. Broeders, V. Sanchez, A. Travleev, E. Stein, *"Validation of coupled neutron physics and thermal-hydraulics analysis for HPLWR",* FZKA 6741, P290 (2002)

[12] C.H.M. Broeders, V. Sanchez, E. Stein, A. Travleev, *"Validation of coupled neutron physics and thermal-hydraulics analysis for HPLWR",* ICAPP'03, Cordoba (2003)

[13] V. Sanchez-Espinoza, W. Hering*, "Investigations of the Appropriateness of RELAP5/MOD3 for the Safety Evaluation of an Innovative Reactor Operated at Thermodynamically Supercritical Conditions",* FZKA 6947 (2002)

[14] E. Carlson, P. A. Roth, V., H. Ransom*; "ATHENA Code Manual".* September 1986. Idaho Falls, Inc. EGG-RTH-7397. Volume 2.

[15] R. Dagan, V. Sanchez, C.H.M. Broeders*;" ATHENADS - A Model for Gas-ADS simulation",*. Jahrestagung Kerntechnik, Berlin Mai 2003

[16] F. Odar, C. Murray, R. Shumway, M. Bolander, D. Barber, J. Mahaffy*; "TRAC/RELAP Advanced Computational Engine (TRACE) V4.0 User's Manual*", US NRC May. 2003