Nuclear Reactor Modelling and Simulation Toolkit (NuReMoST) – Numerical Reactor Model Configuration System with Interface to Simulation Codes

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Abstract. Nuclear Reactor Modeling and Simulation Toolkit (NuReMoST) is a new generation system for numerical simulation of the nuclear reactor. The system integrates typical simulation tasks, such as preparation of the design and geometry data, setup of the initial and boundary conditions, meshing tools, visualization functions, as well as several other related utilities and services. The core point of the system is to provide a standard interface for coupling of numerous simulation codes. The reactor data storage system collects simulation-related data in a consistent database with all possible and necessary details. NuReMoST provide an access to the stored reactor data and a standard interface for coupling with reactor simulation codes. The key feature of the system is to provide easy and effective tools for preparation of the reactor simulation model. Easy design with instant visualization provide quick and effective tool for the model preparation and quick update thanks to the instant visual user interface. NuReMoST is designed to provide easy coupling capabilities. The coupling tools with several popular reactor simulation codes are already included in NuReMoST, many others will be included in the near future. In addition, several simplified simulation tasks including steady-state thermal hydraulic and power distribution calculations are natively integrated into the system. Thus, even standalone NuReMoST version can be used for a quick evaluation and for educational purposes. At the moment, a conceptual prototype of the NuReMoST system is available. The samples of coupling interface with simple thermal hydraulics and neutronics models are presented and discussed.

Key Words: Numerical Reactor, data visualization, coupled codes

1. Introduction

Nuclear Reactor Modelling and Simulation Toolkit (NuReMoST) is reactor data storage and simulation system that is designed to simplify coupling of different reactor analysis codes and is also able to perform basic reactor simulations. Coupling with various neutronics, thermal hydraulics, structural mechanics, fuel behaviour codes etc. could be done with the help of NuReMoST. Once the geometry, initial and boundary conditions, as well as system elements are introduced in the toolkit storage, they can be used recurrently. The visualization provided is effective in understanding the proper geometry of the core and could also be used for educational purposes as basic calculations could be easily performed.

Figure 1 shows a sketch of coupling capabilities of NuReMoST. The coupling could be done easily and in an intuitive manner with system codes like TRACE [1], subchannel analysis codes like SAS4A [2], general purpose CFD codes like OpenFOAM [3], neutronic codes like MCNP [4], PARCS [5] and SERPENT [6], core disruptive accident analysis code for FBR ASTERIA-FBR [7] etc. It could also be coupled to existing platforms like SALOME [8], NURESAFE [9] and NURESIM [10]. Once the input is prepared in the required format through the help of easy to use graphical interface for date insertion, the toolkit can be used to couple various simulation codes as shown in *Figure 1*. Mesh size and density could be adjusted according to the requirement. Thermal expansion of nuclear as well as structural materials could also be calculated natively.



Figure 1 NuReMoST: Coupling different reactor analysis code via a central reactor data storage system.

2. Data storage of reactor geometry and parameters

2.1. Data storage format

All reactor data are stored in the Hierarchical Data Format (HDF), in the case of NuReMoST it uses the format HDF5 [11]. HDF could be used to store and organize a large amount of numerical data, which is the requirement of this toolkit as well. Originally developed at the National Center for Supercomputing Applications, HDF is supported by the non-profit HDF Group, whose mission is to ensure continued development of HDF5 technologies, and the continued accessibility of data stored in HDF. Other than its extensive capabilities to store and process huge amount of data, HDF5 format was chosen for its compatibility with several other programming languages like Fortran, C++, Java etc. If a new data storage format was to be developed then it would require considerable efforts in ensuring its compatibility with other major programming languages. HDF5 also removes the requirement to develop the compatibility for both Windows and Linux separately. The speed and efficiency of the format is also high as compared to other known storage formats available owing to its hierarchical structure in which data could be stored similar to the folder/file systems with different attributed to different set of data. It is also gaining significant popularity in the scientific community because of the above mentioned advantages. It is a community developed open source file format that could be used to organize, store, discover, access, analyze, share, and preserve data ranging from tiny datasets to mega datasets.

2.2. Storing data using the control center and its representation

The User Control Center (UCC) available in the toolkit provides the graphical user interface and could be called upon to create a new core setup, starting from the single pin to the subassembly level and, finally, to whole core and the reactor vessel. For example, defining the geometry of the reactor in the toolkit, it takes a very systematic approach starting from assemblies to insert data for the structure and material to the pin level and then eventually leading to making of the whole core. The idea is to store date in a very systematic format that could be extracted as per the requirement along with its proper representation to aid analysis. Figure 2 shows how each assembly in the core could be constructed separately. Any assembly from the radial representation of the core could be seen separately and axially. Then the cross-section at the desired axial level could also be represented. Depending upon the assembly, if it contains fuel, and the axial level, various fuel pins could be seen. *Figure 2* also shows the representation of wrapper wire used in sodium cooled fast reactors around the fuel pin.



Figure 2 Visualization capabilities of NuReMoST – from pin to complete core.

Similarly, *Figure 3* shows the radial and axial views of the reactor core after storing data through the user control center.



Figure 3 Radial and Axial Views of reactor core using NuReMoST.

2.2.1. Service utilities

The visualization shown in *Figure 2* and *Figure 3* requires setting up of the initial core data through the user control center. Visualization is only to aid user to understand the reactor

structure properly, the main power of the system lies in its capability to store large amount of data and ease of access with which it could be used for different purposes. The data stored is also not limited to the geometrical data but also initial and boundary conditions could be defined. The meshing tool available inside the toolkit could be used to create a uniform mesh to define the calculation nodes.

3. Using the toolkit

3.1. Setting up of the reactor data

Upon the start of the application the user control center could be launched as shown in *Figure* 4. As soon as the control center opens it shows a template for the reactor setup file. The new core setup could be created using the file menu in the UCC window. The core basic data is stored in HDF5 format as explained in section 2, and can be edited using the HDF5 editor available in the toolkit. The HDF5 structure file that opens first contains all the linked data set that needs to be filled in order to get the proper geometry of the reactor.



Figure 4 NuReMoST user control center (UCC).

The basic reactor template file that is created contains a simple subassembly of 5 types, viz. coolant, fissile, blanket, control rod and an example subassembly. More subassemblies could also be added depending upon the requirements of the core geometry. This can be done by simply copying and pasting one of the SA and SA_setup files, renaming them and then inserting the desired values. Here in *Figure 5* a new dummy assembly is created using the HDF5 editor. The HDF5 editor shown in *Figure 5* is used to enter the setup data for each type of subassembly defining the geometry. *Figure 6* shows how the geometry data such as number of pins, width of the subassembly, gap thickness etc. is inserted for the subassembly of type 'fertile'. Similarly data could be inserted for each type of subassembly.



Figure 5 HDF5 editor to input reactor data.

Once this is done, the data input could be done for pins through the pin core setup tab where pin data such as clad thickness, pellet diameter etc. could be entered for each type of subassembly defined in previous steps.



Figure 6 Inserting data for the fissile subassembly.

Once all the data is inserted, the core setup tab is used to arrange the assemblies at the desired locations in order to produce the core map. The core is arranged in a circular manner with the innermost assembly as ring one, the next six assemblies as ring two and then 6n+1 assemblies in each subsequent ring. The outer core could be arranged depending upon the number of blanket assemblies. There are few other features while establishing the core structure that could be easily followed through the use of manual.

3.2. Other features of the toolkit

There are several other features of the toolkit such as meshing tool, setting up of initial and boundary conditions. There are some internal native simulation tools available in the tool kit to do simple steady state flux/power distribution, steady state thermal hydraulics simulation, calculation of thermal expansion of the structure due to increase in the temperature etc. The fuel pellet properties could also be defined; the data required for coupling and post processing etc. could also be inserted. The 3D model could be converted to the two-dimensional model for faster calculations.

4. Conclusions

The basic structure of the nuclear reactor modeling and simulation toolkit NuReMoST is described in the paper with major emphasis on setting up the basic reactor core geometry. The advanced features of the toolkit have been summarized and explained. NuReMoST is under development and when fully developed the IAEA could use the toolkit to collect and store the data on different reactor designs and configurations. The reactor data then can be used for the benchmark exercises by the participating organizations to perform neutronics, thermalhydraulics, fuel behavior, as well as coupled multi-physics simulations. This toolkit

could also be used for various benchmarking and modeling and simulation exercises. For example, once the Coordinated Research Project (CRP) is finished the stored database could be used by other organizations of the IAEA Member States to perform their own calculations and code verification. The distribution of data would become very easy and the steady state calculations could easily be performed. The basic data stored for different reactors could also be used for education and training purposes.

REFERENCES

[1] Bajorek, S. (2008). TRACE V5. 0 Theory manual, field equations, solution methods and physical models. *United States Nuclear Regulatory Commission*.

[2] Cahalan, J. E., & Wei, T. Y. C. (1990). *Modeling developments for the SAS4A and SASSYS computer codes* (No. CONF-900804-10). Argonne National Lab., IL (USA).

[3] Fiorina, C., Clifford, I., Aufiero, M., & Mikityuk, K. (2015). GeN-Foam: a novel OpenFOAM® based multi-physics solver for 2D/3D transient analysis of nuclear reactors. *Nuclear Engineering and Design*, 294, 24-37.

[4] Shultis, J. K., & Faw, R. E. (2011). An MCNP primer. Kansas State University, Manhattan.

[5] Joo, H. G., Barber, D., Jiang, G., & Downar, T. (1998). PARCS: a multi-dimensional twogroup reactor kinetics code based on the nonlinear analytic nodal method. *PARCS Manual Version*, *2*.

[6] Leppänen, J., Pusa, M., Viitanen, T., Valtavirta, V., & Kaltiaisenaho, T. (2015). The Serpent Monte Carlo code: Status, development and applications in 2013. *Annals of Nuclear Energy*, *82*, 142-150.

[7] Ishizu, T., Endo, H., Tatewaki, I., Yamamoto, T., & Shirakawa, N. (2012). *Development of integrated core disruptive accident analysis code for FBR-ASTERIA-FBR*. American Nuclear Society, 555 North Kensington Avenue, La Grange Park, IL 60526 (United States).

[8] Ribes, A., & Caremoli, C. (2007, July). Salome platform component model for numerical simulation. In *Computer Software and Applications Conference, 2007. COMPSAC 2007. 31st Annual International* (Vol. 2, pp. 553-564). IEEE.

[9] Chanaron, B., Ahnert, C., Crouzet, N., Sanchez, V., Kolev, N., Marchand, O. & Papukchiev, A. (2015). Advanced multi-physics simulation for reactor safety in the framework of the NURESAFE project. *Annals of Nuclear Energy*, *84*, 166-177.

[10] Chauliac, C., Aragonés, J. M., Bestion, D., Cacuci, D. G., Crouzet, N., Weiss, F. P., & Zimmermann, M. A. (2011). NURESIM–A European simulation platform for nuclear reactor safety: Multi-scale and multi-physics calculations, sensitivity and uncertainty analysis. *Nuclear Engineering and Design*, 241(9), 3416-3426.

[11] The HDF Group, HDF5 Home Page, https://support.hdfgroup.org/HDF5