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AN INITIATIVE FOR THE DEVELOPMENT AND APPLICATION OF OPEN-SOURCE MULTI-PHYSICS SIMULATION IN SUPPORT OF R&D AND E&T IN NUCLEAR SCIENCE AND TECHNOLOGY

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ABSTRACT

Modelling and simulation (M&S) have gradually become irreplaceable tools in the field of Nuclear Science and Technology (NS&T), including nuclear energy systems. This is partly due to growing computational resources and advances in computational science and partly to the difficulties to finance, build and license new experimental facilities. However, the utilization of M&S for research and development (R&D) and education and training (E&T) applications is somewhat hampered by limited accessibility to controlled and sensitive nuclear M&S tools as well as by the desires of the developers of these tools to retain their intellectual property (IP). Open-source software and open-access data are growingly perceived as means to accelerate innovation by promoting synergistic collaborative developments while lowering the barriers associated to code distribution, modification, and sharing. Open-source software development is ideal for R&D and E&T purposes because it permits the enhancement of understanding, the use of advanced computational methods and it promotes the cooperation among researchers and scientists, without rigorous constraints on quality assurance or reliance on proprietary data for technology-specific validation. As a fundamental research tool, this helps to mitigate constraints related to dual use of such technology. It is in this context that an initiative is being launched under the aegis of the International Atomic Energy Agency (IAEA) to promote the development and application of open-source multi-physics simulation in support of R&D and E&T in NS&T. This paper presents scope and objectives of this initiative.

KEYWORDS: modelling and simulation, open-source software, open-access data, E&T initiative, collaborative research development, IAEA

1. INTRODUCTION

For decades, modelling and simulation (M&S) have represented irreplaceable means to support reactor design and licensing, as well as central tools for research activities. Exponential growth of the available computational resources and relentless progress in the field of computational science, have empowered M&S to the point that design-by-simulation is gradually becoming a dominant paradigm in engineering, and in particular in the nuclear field. This trend is also favored by the growing difficulties of funding and licensing new complex and costly experimental facilities. The recent flourishing of activities dedicated to the design of advanced nuclear reactors and fuels, as well as to the life extension of operating nuclear power plants, have further nurtured M&S with the need of novel, more flexible and more accurate simulation codes. Concurrently, open-source and collaborative software development is increasingly perceived as an effective way to stimulate synergies, avoid duplication of work, involve a broader community, enhance verification, and, ultimately, accelerate innovation. Recognizing the increasing interest in these developments worldwide and the work already carried out in some institutions on open-source software and open-access data, in 2019 the International Atomic Energy Agency has designated EPFL as a Collaborating Centre in the area of "high-fidelity multi-physics nuclear simulation techniques for open-source code development and verification" [1,2]. This new IAEA collaborating center represents the basis of a broader multilateral initiative [3] presented in this paper.

2. BACKGROUND INFORMATION

Despite several impressive developments, the utilization of M&S for research and development (R&D) and education and training (E&T) is still challenged by the need to reconcile conflicting objectives that tend to slow down developments and inhibit collaborative work. Management and protection of intellectual property (IP) are typical examples of such conflicting objectives. Often, software licenses forbid source-code distribution or modification to protect the intellectual property rights of the developers, which de facto limits collaboration to those with access and tends to fragment the community based on the tools available to them, resulting in what we refer to as closed codes (CCs). Code licensing procedures also tend to significantly slow down collaborations, where many users, notably in developing countries, are effectively excluded from using several codes due to the high cost of licenses and/or the cost of the administrative procedures associated with licensing. IP management is a necessary means to protect industrial interests and guarantee a competitive market. It has promoted the independent development of several code systems for reactor analysis, which represent today an invaluable asset for reactor design and licensing; additionally, it has provided regulatory authorities independent means to verify and validate the performance of M&S tools required in a heavily regulated industry. A strict IP management system is then still required for protecting proprietary data and technology-specific models. However, separation of proprietary information from basic models and simulation tools for reactor analysis is often possible, allowing both academic and industrial entities to benefit from open developments of these models and tools. Several research and industrial activities have shown that modern numerical libraries and programming languages allow for the development of high-quality simulation codes from scratch in months. In some applications, these codes may surpass legacy codes in terms of code implementation and computational performance. Hence, a balance should be established between the closed source development of M&S tools and the need to utilize open-source codes to facilitate capability development and knowledge enhancement.

CCs and open-source codes target different spheres of influence and application in terms of maturity of methods and implementation. Open-source codes often feature a lower technology readiness level, making them suitable for R&D and E&T, while CCs target commercial applications of already mature ideas. Increased open source development permits one to readily adopt modern programming languages and benefit from continuous evolutions in software management and control; acquired know-how may be then incorporated into the development of industry- and licensing-oriented M&S tools. Many of the industry standard nuclear simulation codes are several decades old and have been typically developed by nuclear scientists and engineers, often with a limited interaction with other scientific communities. Until recently, only some of these codes have incorporated modern best coding practices in their development. Many legacy codes have been subsequently used, validated, refined and extended for several decades, but their modernization from a programming viewpoint required considerable resources and time. Moreover, in the case of industrial codes, these changes could also impact the associated safety study methodologies and licensing. The development of an open-source platform for nuclear science and technology analyses will permit the adoption, demonstration and utilization of modern programming languages as well as software development best practices that hereto before have not been widely implemented in the nuclear community. Furthermore, it allows for an E&T model that better integrates code application and development, thus discouraging black box application and improving understanding.

Another significant issue that arises in the development and use of advanced M&S tools is their dual use nature. Many countries often restrict access to such codes through export control regulations to minimize the risk of non-peaceful applications. On the other hand, many countries share a mutual concern for the safe operation of nuclear facilities throughout the world, as the consequences of a nuclear accident can have wide-ranging impacts. This conflicting need to limit proliferation while enhancing safety can be aided through the common development and deployment of open source codes for R&D and E&T. Open-source code development provides the opportunity to enhance knowledge of the fundamental, coupled physics associated with the complex phenomena in any nuclear facility, without delving into specific reactor technologies that may represent an export control concern.

3. OPEN-SOURCE CODE DEVELOPMENT

Collaborative open-source software development is unburdened by many of the obstacles and inefficiencies CCs face, outlined in the section above, and can help stimulate R&D by providing a broad range of knowledge and high bandwidth for productivity from a large community of contributors. The potential benefits of open-source developments are well demonstrated by the tremendous progress made today in the field of machine learning, whose community is traditionally linked to an open-source development model [4]. Similar practices are being adopted in the nuclear field as well. An example of this is the development of OpenMC [5] which in just a few years has widely been accepted as a valid alternative to CCs to accelerate research objectives in national labs and academic institutions. Another example is the development of several OpenFOAM®[1]-based solvers [6,7,8,9,10], which in the last few years have allowed researchers to quickly develop tools for the analysis of advanced reactor systems.

Incidentally, many modern libraries for scientific computing are open source, which stimulates, and sometimes enforces by license terms (viz. GNU GPL license), the release of resulting codes as open source. This so-called copy-left then limits the use of several libraries in CCs. In this sense, the choice of a specific licence for open-source code development can have an impact on the transferability of results to the CC community. Simulation codes based on scientific computing libraries feature cutting-edge numerical algorithms, typically allowing for optimal scaling on high-performance computing systems. Open-source libraries also benefit from continuous development and integration of progress from several fields of science and engineering. Codes that are developed using these libraries can automatically incorporate state-of-the-art numerical features with little or no maintenance by the code developers. Finally, modern numerical libraries are often written according to modern programming paradigms. A typical example is object-oriented programming (OOP). OOP allows clearly associating parts of code (called "classes") to specific variables and functionalities. This promotes transparency in functionalities and interactions, and strongly facilitates code modification, maintenance, and sharing. OOP also allows creating several layers of programming by exposing different levels of complexity to users with different expertise. For instance, in OpenFOAM, an engineer can program a solver by using high level functionalities for creating and solving equations, separate from concerns about model discretization, mesh management, and matrix operations and manipulations. At the same time, an expert on numerical methods can modify classes associated to discretization and matrix solution regardless of test models. Software organized into sets of building blocks/classes can also reduce the overhead associated with the computational infrastructure required for testing new ideas in the area of methods development. This – along with the possibility to have access, modify and redistribute the code - allows OpenFOAM and the other open-source software to benefit from contributions of the scientific community at large and facilitates contribution based on the developer's, often extensive, expertise in a specific area.

Traditional downsides of open-source collaborative development are limited quality control, fragmented developments, and lack of documentation. However, progress in the IT field helps nowadays mitigating them. Tools like Wiki pages, web-forums and Git repositories are made free-accessible by several web services. These tools help minimizing the need for documentation and of an organized user support; they promote a collective contribution to documentation, tutorials and Verification & Validation (V&V); furthermore, they favor large-scale interactions among users and developers. Distributed version control

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[1] *https://www.openfoam.com/legal/trademark-policy.php*

tools like Git, along with code sharing and collaboration platforms, facilitate practices like code review, issue tracking, and continuous integration testing that are critical to quality control of open source software projects. Operating-system-level virtualization in the form of containers facilitates distribution of applications and, in turn, their use by third party organizations. This is an important new asset in a field that has been historically plagued by non-trivial installation procedures. Finally, cloud computing allows an immediate deployment of software with various features and computational requirements. These tools can expedite collaboration and aid in quality assurance; however, in the end, the overall success of projects may still be limited by the community's ability to foster a culture around the project which is respectful and welcoming to new contributors, while being diligent in maintaining project's high standards.

4. OPEN-ACCESS DATA

The availability of open-access data is a necessary ingredient for a successful code development based on an open-source collaborative strategy. It allows for a basic quality control by allowing verification of developed codes. Open-access is a clear trend in the scientific domain, with several universities and public bodies openly supporting this strategy [11,12]. In the private sector, a frequent practice is that of releasing enough data to stimulate research in a specific field. This is, for instance, the case for machine learning, where large open-access databases have recently been made publicly available by companies like Amazon and Microsoft. This trend towards open-access data is not yet prevalent in the nuclear field due to proliferation concerns and the resulting export restrictions. However, the aforementioned open-access policy for publicly funded research also applies to the nuclear field. In addition, new data from past experiments are made available every year. A prominent example is the recent release from the Oak Ridge National Laboratory of a large fraction of the technical reports that were developed during the Molten Salt Reactor (MSR) project. These data have largely contributed to the flourishing of activities on MSR in the last 10 years [7,9,13,14,15], and are commonly employed for code validation and code-to-code benchmarks. Nuclear data libraries (JEFF, ENDF, JENDL, etc.) and data processing tools (NJOY, FRENDY, etc.) have started to be released openly. Los Alamos National Laboratory has also begun openly providing nuclear cross-section data sets, which were previously unavailable without a MCNP®[2] license.

5. SCOPE AND OBJECTIVES OF THE INITIATIVE

Open-source codes and open-access data hold promise for stimulating research and supporting education in the field of M&S. However, a successful development strategy requires a well-connected community and suitable tools for communication and collaborative development. It is in this context that an initiative is being launched under the IAEA aegis aimed at the development and application of open-source multi-physics simulation tools in support of research, education, and training in NS&T, and in particular for nuclear reactor analysis.

The initiative will foster an international collaborative effort in the nuclear community towards a common open-source simulation platform in support of research and education. This will also give to nuclear new-comer countries, and in general to developing countries, access to high-quality software and training, as

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well as immediate access to collaboration with well-recognized experts in the field. Specific objectives of this international initiative are to:

- Build and preserve knowledge in the field of open-source simulation codes and open-access data;
- Facilitate the exchange of information within the community;
- Conduct a survey on existing open-source simulation codes and open-access data and help making them accessible;
- Define best practices for collaborative open-source code development;
- Assess features, gaps and opportunities for integration of already developed open-source modules and codes;
- Facilitate sharing of reference solutions, standard benchmark problems, and input data for specific applications;
- Starting from the available mature and well-supported open-source codes, develop an open source platform, including verification through standard problems and code-to-code comparison, and documentation;
- Promote the individual tools and platform in education and research environments;
- Organize and participate in related E&T activities;
- Ensure sustainability of the effort;
- Ensure export control compliance.

A first expected outcome will be the creation of living catalogues of available codes, data and related training material. These lists will provide a valuable overview of available resources to interested users and developers. They will help to identify gaps and, in turn, establish development priorities, avoid duplications, and stimulate synergies and collaborations. Starting from the initial list of codes, it is expected that a consistent multiphysics platform will gradually be developed, including documentation and training material. To support these efforts, the initiative will make use of several tools, including a public Git repository and discussion forums organized, in particular but not exclusively, by the IAEA. In addition, sessions and workshops at topical meetings will be organized to foster communication, while summer schools supported by the IAEA will be organized to involve young researchers and professionals and promote sustainability of the effort.

6. PATH FORWARD

As a means to initiate collaboration, an expert group has been established that will monitor new developments; establish and update the above-mentioned lists of codes, data and gaps; and develop guidelines for collaborative code development and for R&D in the field. It will also advise the IAEA by recommending benchmarks, training courses, publications and Coordinated Research Projects (CRPs). Workshops and special sessions at conferences will also be fostered. Alongside this effort, educational material will be continually developed and curated to accompany the initiative.

Collaboration is being put in place with relevant stakeholders in the field of code and data distribution, and in particular with the OECD Nuclear Energy Agency Data Bank and with the Radiation Safety Information Computational Center at Oak Ridge National Laboratory. An active interaction will be pursued with national, regional and international educational networks to promote the use of open-source tools as a way to improve understanding and to motivate students and young professionals. Interested institutions are sought to support the creation of open-source code and open-access data, as well as to make use of available open-source codes for future developments. In particular, the involvement of nuclear newcomer countries is encouraged. Collaboration tools are also being put in place, including a devoted IAEA website, a Git repository, a discussion forum, and a Wiki.

Three concrete technical projects have been identified as first steps towards the development of a consistent multiphysics platform, as well as to prepare for new collaborations in the field. One such project regards the coupling of OpenFOAM and OpenMC. This combination will provide cutting-edge multiphysics capabilities by allowing for coupled simulations of Monte Carlo neutron transport with computational fluid dynamics, porous medium treatments, etc. A preliminary external coupling is being developed at the North Carolina State University, while a more advanced coupling is planned in the frame of a collaboration among Argonne National Laboratory, EPFL, North Carolina State University, and University of Cambridge. Two parallel paths forward are being pursued. A first possibility is to make use of the current surface-tracking routine of OpenMC, but allowing for the use of OpenFOAM-type meshes. The second, more computationally efficient option is to extend OpenMC to delta-tracking, and to employ mesh-based spatial partitioning algorithms to identify containing cells for particle collision sites and for data transfer schemes. Another project, currently participated by Politecnico di Milano, Texas A&M University and EPFL, aims at the creation of an OpenFOAM library for reduced order modelling. Finally, a small project has been proposed for the creation of a point-kinetics solver in OpenFOAM to allow for simple multiphysics analysis starting from available thermal-hydraulic solvers.

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