Multi-physics coupling simulation in virtual reactors

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Abstract
Nuclear power stations involve a range of complex and interacting multi-physical processes. With the rapid development of high-performance computing technology, accurate multi-physics simulation in virtual reactors has drawn more and more attention in industry and academia. Great efforts have been made toward the simulation of multi-physics coupling processes in reactors. The interpretations of many terms that describe multi-physics simulation vary in different literatures. We organize and discuss some important terms relevant to the multi-physics coupling simulation. We compare the three most frequently used multi-physics coupling strategies: the operator splitting, Picard iteration, and Jacobian-Free Newton–Krylov methods. We summarize three main viewpoints on the degree of coupling of the three strategies (loose, tight, or full coupling). Then we review the coupling software and corresponding coupling strategies in some representative virtual reactor projects. We present the research focuses of Spider coupling platform. The Spider is developed in the China Virtual Reactor (CVR) project. The multi-physics phenomena are considered in the CVR project from three scales: fuel scale, reactor core scale, and system scale. Both loose and tight coupling strategies are supported in the Spider platform.

Keywords
Modeling and simulation, high-performance computing, multi-physics, coupling, virtual reactor

1. Introduction
A nuclear power reactor is a large, complex, and intrinsically multi-physics-coupled system. Simulating multi-physical phenomena is a significant challenge in nuclear engineering.¹ Limited by the computing and storage ability of computers, a multi-physics problem is usually divided into several isolated physical processes in traditional simulation approaches. Each isolated physical process is tackled by a specific software program. The isolated codes are generally based on engineering models (such as homogenized and lumped parameter models), which rely on experimental observations. By introducing approximation and assumption, traditional multi-physics simulation does not require many computing and storage resources (usually desktop workstations are enough). However, in the meantime, approximations and assumptions cause inaccuracy, and they ultimately limit the performance of nuclear stations.

Computer hardware and high-performance computing technology are developing rapidly. The exa-scale supercomputing era is upcoming. Researchers from academia and industry are becoming more and more interested in research into the virtual reactor (which is also called the numerical reactor in some of the literature²–⁴). The virtual reactor is a comprehensive simulating tool for accurate analysis of reactors. It is an interdisciplinary research field that involves nuclear engineering, high-performance computing, applied mathematics, and software engineering. Leveraging powerful supercomputers, accurate models (e.g., computational fluid dynamics (CFD) with a large eddy simulation model rather than the sub-channel method), and state-of-the-art numerical methods, a virtual reactor provides high-fidelity multi-physics simulation better than ever before. By providing a science-based simulation of the multi-physics processes, the virtual

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reactor delivers a better description, understanding, and prediction of crucial phenomena in reactors. The virtual reactor will play a significant role in addressing some intractable problems faced by the commercial nuclear power industry nowadays. It is possible that the virtual reactor will play an important role in uprating power and extending the lifetime for existing reactors and future reactors.

Many countries and international organizations have been carrying out research on multi-physics modeling and simulation in their virtual reactor projects. The USA has launched the Consortium for Advanced Simulation of Light Water Reactors (CASL), Nuclear Energy Advanced Modeling and Simulation (NEAMS), and Centre for Exa-scale Simulation of Advanced Reactors (CESAR) projects. The European Union (EU) has initiated the series of European Simulation Platform for Nuclear Reactor Safety (NURESIM) research. China started the China Virtual Reactor (CVR) project in 2017.

The main contributions of this paper are as follows.

- The interpretations of many terms relevant to the multi-physics simulation vary in different research. We classify some important terms.
- We compare the three most frequently used multi-physics coupling strategies in academia and industrial practice: the operator splitting (OS), Picard iteration, and Jacobian-Free Newton–Krylov (JFNK) methods. There is no widely accepted notion in the spirit of the degree of coupling (loose, tight, or full coupling) of the coupling strategies. We summarize the three main points from many opinions.
- We review the coupling software and their coupling strategies in some typical virtual reactor projects. We analyze those projects from the perspective of multi-physics coupling.
- We present the research focus of the multi-physics simulation in the CVR project and the Spider coupling platform.

The paper is organized as follows: in Section 2, we discuss the three most frequently used coupling strategies. We also organize strong/weak coupling, tight/loose coupling, implicit/explicit coupling, inner and outer coupling, and other important terms concerning multi-physics coupling. In Section 3, we review the coupling software in some representative virtual reactor projects. We analyze those projects from the perspective of multi-physics coupling. In Section 4 we present the research focus of the multi-physics simulation in the CVR project and the Spider coupling platform. The paper is summarized in Section 5.

## 2. Coupling strategies and classification

Multi-physics sometimes refers to multi-physics phenomena in reality and associated equation sets. When the solution of one physics equation has a great influence on another physics equation, the physical processes are strongly coupled, otherwise they are weakly coupled. Multi-physics sometimes means the numerical solution method and related application software that simulate the multi-physics phenomena. The coupling strategies refer to methods that couple the different pieces of mono-physical parts. The OS, Picard iteration, and JFNK methods are the three most frequently used coupling strategies. There are loose, tight, and full coupling classifications for these methods, which will be discussed in Section 2.2.

### 2.1. Coupling strategies

- **OS**
  - OS is a traditional and widely used coupling method. This divide and conquer strategy divides the multi-physics phenomena into several isolated physical processes. The isolated physical processes are treated by specialized simulation codes. When one state of a process is solving, all other states are fixed. The coupling between the mono-disciplinary software is implemented by transferring data at every time-step as boundary conditions in a black-box way. The solving completes when the system convergence is achieved. The method has the following advantages: (1) only minor modifications of legacy codes are required, which makes the method very practical in industry; (2) OS makes full use of legacy codes, which are well verified and validated in years of engineering practice; (3) OS requires a low computation cost in every time-step; (4) OS supports various numerical methods (such as the finite volume method, spectral element method, and finite element method (FEM)), programming languages (C, C++, Fortran), and different types of meshes (tetrahedral or hexagonal) for distinct single physical codes; (5) OS is not restricted to partial differential equation (PDE) or ordinary differential equation (ODE) problems, and is compatible with particle problems (such as molecular dynamics and Monte Carlo); (6) it is effective in simulating weakly coupled phenomena; (7) it requires little knowledge of the single physics component (residuals are not required). However, if the phenomena are two-way strongly coupled, OS will converge in a slow rate, especially when the coupled simulation spans disparate time scales.
OS also has accuracy and stability issues in the simulation of strongly coupled phenomena.\textsuperscript{16,20}

- There are two kinds of OS method according to the iteration mechanic: \textit{Simultaneous OS coupling} and \textit{Staggered OS coupling}. Simultaneous OS coupling uses old values to calculate new ones at each time-step, and it also called the Jacobi coupling iteration by some researchers, such as Tautges\textsuperscript{21} in the CESAR projects. Staggered OS coupling,\textsuperscript{22} which is also called the Gauss–Seidel iteration, uses new values to compute. The OS method is presented in Figure 1.

- \textbf{Picard iteration}
  - The Picard iteration (or fixed-point) has the same advantage over the OS method: it is easy to implement and allows developers to make full use of already developed and verified software programs with slight modifications. Compared to the OS method, the Picard iteration is easier to converge by estimating the convergence. However, the calculation cost is greater than the OS method at every time-step.\textsuperscript{23} The workflow of OS and the Picard iteration is presented in Figure 2.

- \textbf{JFNK}
  - Both OS and the Picard iteration split the multi-physics process into pieces of mono-physical processes. Different codes deal with particular parts of the problem separately. Coupling is performed by transferring the output of one code to another code as the input data.\textsuperscript{23} One alternative coupling strategy is to describe all related physical models into one set of equations, and often a Newton-based method such as the JFNK method is applied to solve the equations.\textsuperscript{25,26} Compared to OS and the Picard iteration, the JFNK method is a tighter and more accurate coupling strategy. The JFNK method solves the physics-related equations (usually PDEs) simultaneously, and simulates multiple physical processes in a monolithic code. The JFNK method solves multi-physics equation sets using the synergistic combinations of Newton-type methods and the Krylov-space method. There is no linearization error caused by iterations between single physical solvers, so the JFNK method preserves higher order accuracy and is able to converge even in strong coupling situations. Using the JFNK method, refactoring or major changes to already developed simulation codes are usually required.

\subsection*{2.2. Classification of key terms describing multi-physics coupling}

As mentioned before, multi-physics coupling refers to both nature multi-physics phenomena and numerical solution...
strategies. The classification of multi-physics phenomena coupling is as follows.

- **Degree of nature physics coupling**: strong coupling and weak coupling. Strong and weak coupling describe the interdependence nature of coupling phenomena. If a change to a solution variable in one physics equation has great influence on another physics equation, the corresponding multi-physics phenomena are strongly coupled. Conversely, if a change to a solution variable in one physics has negligible effect on another physics equation, the corresponding multi-physics phenomena are weakly coupled.

- **Direction of nature physics coupling**: one-way and two-way coupling. One-way coupling exists where one set of physics equations depend on another equation set but not vice versa. Two-way coupling exists where two physics equations depend on each other.

- **Mathematical relation of nature physics coupling**: linear and nonlinear. If the changes to a solution variable in one physics lead to linearly proportional effects on the solution variable on the other physics, then the coupling is regarded as linear coupling. Otherwise, the coupling is nonlinear.

A classification of numerical solution coupling is as follows.

- **Degree of numerical solution coupling**: loose, tight, and full coupling. There is no widely accepted definition and classification of loose, tight, and full coupling. We summarize three main opinions.

  1. Keyes et al.\textsuperscript{27} put forward the definition that loose and tight coupling should be classified according to whether the state variables over different models are well synchronized at all times. In a tightly coupled strategy, all the state variables should change in as synchronized manner as possible across different numerical models at all time-steps; in a loosely coupled strategy, the state variables could be shifted by one time-step or stumbled with a fraction of time-steps.\textsuperscript{27} According to this point, OS and the Picard iteration are loose coupling strategies, whereas the JFNK method is a tight coupling strategy. A similar view is taken by Schmidt\textsuperscript{10} in a report about LIME (Lightweight Integrating Multiphysics Environment for coupling codes) coupling software: the explicit operator split method and the implicit Picard iteration are loosely coupled methods, and the implicit Newton or JFNK method are tightly coupled methods. Novascone et al.\textsuperscript{18} and Williamson et al.,\textsuperscript{28} who are researchers in the BISON project, hold similar opinions. In this opinion, OS and the Picard iteration are loosely coupled methods because the individual physics processes are solved separately in a divide and conquer schema, while using the JFNK method to solve equation sets simultaneously in BISON is a tightly coupled strategy. Park et al.\textsuperscript{29} implemented a tight multi-physics coupling simulation for pebble bed reactors using the JFNK method.

  2. OS is a loose coupling strategy. The Picard iteration and the JFNK method are tight coupling strategies because they converge the nonlinearities among distinct physics at every time-step to achieve a tightly coupled solution that is consistent with the nonlinear systems of PDEs.\textsuperscript{30} The tight coupling strategies are unconditionally stable and preserve high-order accuracy. The loose coupling strategy is only conditionally stable. Researchers

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\caption{The workflows of operator splitting and the Picard iteration.}
\end{figure}
from the Simulation-based High-efficiency Advanced Reactor Prototyping (SHARP) project, such as Mahadevan et al.,\textsuperscript{23} share a similar opinion that the Picard iteration, which they use in the SHARP project, is tightly coupled just like the JFNK method, and OS is a loosely coupled strategy.

3. Researchers such as Tautges\textsuperscript{21} in the CESAR project hold the view that OS is a loose coupling approach, the Picard iteration is a tight coupling approach, and the JFNK method is a full coupling approach. Montgomery\textsuperscript{31} and Senecal and Wei\textsuperscript{32} support this view by coming up with the idea that the JFNK method simulates the multi-physics problem simultaneously in a fully coupled manner. In a report on the Virtual Environment for Reactor Applications (VERA), Montgomery et al.\textsuperscript{31} consider that using the Multiphysics Object-Oriented Simulation Environment (MOOSE), which is based on the JFNK method in the BISON project, to study fuel performance is a fully coupled strategy. Gaston et al.\textsuperscript{16,33} in the MOOSE project also consider that MOOSE, which solves multi-physical associated PDEs simultaneously, is a fully coupled software. Figure 3 presents the three main points on classifying loose, tight, and full coupling strategies.

- **Software architecture of numerical solution coupling: bottom-up and top-down.**
  - Tautges et al.\textsuperscript{34} in the SHARP project state that there are two approaches to conduct a multi-physics coupled simulation application. One is to integrate some existing isolated physical codes into an overall system, which is known as the bottom-up or small-f (f) framework approach. The SHARP project uses this approach and it will be discussed in Section 3.3. The other is to develop new software pieces simulating relevant single physics into an integrated framework, and this is called the top-down and large-f (F) framework approach. MOOSE software in the BISON project uses the top-down approach and it will be analyzed in Section 3.3 too.

- **Data transfer method: file transfer and memory transfer.**
  - With the file transfer method, the data transfer among different programs is implemented by exchanging input and output files. This file-exchange-based coupling method is also called offline coupling\textsuperscript{35} or outer coupling in some research. In coupling applications that require large amounts of exchange information, such as full core pin-by-pin neutronics and thermal-hydraulics simulation, the Hierarchal Data Format (HDF5)\textsuperscript{36} or binary format files are often used to manage data more effectively.\textsuperscript{37,38} With the memory transfer method, the data exchange among programs is carried out by direct memory access. The memory transfer method is also called online coupling\textsuperscript{35} or inner coupling.

- **Time integration of numerical solution coupling: explicit and implicit.**
  - The state variable in the present time-step can be calculated using values in the last time-step in an explicit coupling schema.\textsuperscript{27} An example is forward Euler iteration $y_{n+1} = y_n + \Delta t F(y_n)$. This schema has fewer computations at each time-step, but has inferior stability. The implicit coupling schema is not straightforward. The state variable in the present time-step is not only associated with values in the last time-step but also with the present ones. An example is backward Euler iteration $y_{n+1} = y_n + \Delta t F(y_{n+1})$. This schema has more
calculations at each time-step but it has better stability. OS belongs to explicit schema. The Picard iteration and the JFNK method are implicit coupling schemas.

All the coupling key terms discussed above are shown in Figure 4.

3. Coupling software in virtual reactor projects

Great efforts have been made in the research toward the multi-physics coupling.25,39–46 In this section, we discuss some coupling software in several representative virtual reactor projects.

3.1. Brief introduction to representative virtual reactor projects

The major achievement of CASL is VERA, which is a software application environment47 for nuclear reactor core behavior simulation.48–50 VERA consists of two main components47: (1) physics components, such as mechanics, thermal hydraulic, and neutronics simulating programs; (2) infrastructure components, such as LIME, MOOSE, and PIKE (Physics Integration KErnels)51,52 programs used for coupling simulation. The NEAMS workbench is organized into three product lines53–55: the Fuel Product Line (FPL), Reactor Product Line (RPL), and Integration Product Line (IPL). The CESAR project56 starts with mature, peta-scale simulating legacy programs to prepare for exa-scale simulating codes. The excellent peta-scale codes investigated in CESAR are Nek5000 for thermal-hydraulics simulation, UNIC for deterministic neutron transport simulation, and OpenMC for Monte Carlo neutron transport simulation. Typical virtual reactor projects in the EU are the series of NURESIM projects. The research is planned into several stages: NURESIM, NURISP, and NURESAFE.

The China Institute of Atomic Energy is the lead institution of the CVR project. The research group of the CVR consists of nuclear research institutions, nuclear power plant companies, universities, and high-performance computing research institutions. The simulating programs in the CVR project are designed to leverage existing supercomputers (such as the Sunway TaihuLight supercomputer and Tianhe supercomputer) and future exa-scale supercomputers. The first phase of the CVR project is planned to build the five essential parts (neutronics, thermal-hydraulics, mechanics, material, and fuel performance analysis packages) and a coupling platform. The purpose of the simulating programs is to provide comprehensive and refined analysis for current and future advanced commercial nuclear reactors. Table 1 introduces the research
group, object, core achievement, and coupling tools of several representative virtual reactor projects from the USA, EU, and China.

### 3.2. Coupling software in CASL

The VERA environment of the CASL project is composed of physics components and infrastructure components. There is a build/test system, coupling tools, Validation and Uncertainty Quantification (VUQ) tools, unified input/output, and strategy for restart in the infrastructure components. The coupling tools that will be discussed below (LIME, MOOSE, and the Data Transfer Kit (DTK)) belong to the infrastructure components in VERA.

VERA adopts two approaches to couple those codes. One is to tightly couple multi-physics codes in an application-oriented framework. This approach is for problems that are well-defined with well-understood numerical methods and have similarly designed codes. For other coupling problems, a more lightweight and loose coupling strategy is applied by using general-purpose coupling tools (such as LIME and DTK) to integrate the physics components, which are not designed to work together.

- **LIME**
- LIME is developed by the Sandia National Laboratories. LIME is designed to be very useful to create multi-physics simulation applications using existing individual programs, such as neutronics, fuel performance, and thermal-hydraulics simulating programs. When developed to LIME...
LIME has two primary sub-packages: LIMELite and LIMEImplicit. LIMELite is a lightweight version of LIME. It uses the Picard iteration to couple existing simulating programs in a loosely coupled manner. LIMEImplicit uses block-implicit and nonlinear-elimination Newton methods to couple multi-physics in a tightly coupled way. LIME has been used in CASL to couple sub-channel thermal-hydraulics software CTF and neutronics software Insilico to implement a full PWR (Pressurized Water Reactor) core simulation.

Figure 5 illustrates how LIME uses its key components to couple three physical codes. The multi-physics driver is customized by users according to the requirements of the coupling application. The multi-physic is typically very small. It is used to instantiate, configure, and invoke the LIME Problem Manager. The Problem Manager is at the center of all the components. It is responsible for packaging multiple Model Evaluators, and controlling different coupling strategies (both Picard iteration- and JFNK-based coupling). The Model Evaluator is designed to wrap stand-alone physics codes into a call-back subroutine, so that the codes are able to work with the Problem Manager. Physics codes are programs that are used to be coupled into LIME. The physics codes can be written in C, C++, Fortran, or other standard programming languages.

- **MOOSE**
  - MOOSE is developed by Idaho National Laboratory. Except for being used in CASL, MOOSE is used in BISON and MARMOT of the NEAMS projects, and extends to other research fields. MOOSE uses the JFNK method to solve PDEs in the simulation of multi-physics coupled phenomena. The hierarchical structure of MOOSE is presented Figure 6. Multiple physics modules (such as the phase field, mechanics, and heat conduction) are abstracted as kernels. Kernels are easy to add, remove, and combine to make new coupling applications. MOOSE is below the kernel level. MOOSE provides residual and Jacobian
evaluation to solve large systems of PDEs using the FEM simultaneously. Libmesh gives functionalities for FEM-based massively parallel computation. PETSc, Trilinos, and other numerical libraries are included to help calculate effectively. Building a tightly coupled simulation software usually requires the development of new software or a major modification of legacy software, which is very time-consuming. The MOOSE framework minimizes the programming efforts needed to create coupling applications.

- **DTK**
- DTK\textsuperscript{17,69} is developed by Sandia National Laboratories. DTK employs the Rendezvous algorithm\textsuperscript{70–72} to map different meshes and share data among multiple simulation domains in parallel. Every physics code needs to register the state variables they offer (such as temperature, density, and power), the geometry, and the mesh. Simulation programs are also required to register the state variables they need in DTK. DKT uses the registered information to map data among physics codes based on Rendezvous algorithms.

### 3.3. Coupling software in NEAMS

Many software packages in NEAMS are intrinsically multi-physics coupled. BISON uses the JFNK method to solve multi-physics PDEs simultaneously. It is a tightly coupled fuel performance simulating software. SHARP uses coupling tools (mesh-oriented database (MOAB) for mesh modification and CouPe for coupling management) to integrate existing multi-physics software (PROTEUS for neutron transport, Nek5000 for thermal-hydraulics, and Diablo for structural mechanics and thermo-mechanical simulation) in a loose way.

- **MOAB, MBCoupler, and CouPE in SHARP**
- SHARP is developed by Argonne National Laboratory. It is a reactor core-scale product in the FPL in NEAMS. SHARP\textsuperscript{73,74} integrates thermal-hydraulics, neutronics, and structure mechanics simulating codes to implement multi-physics coupled simulating for fast sodium-cooled fuel assembly. SHARP uses the small-f or bottom-up framework which was discussed in Section 2.2. This approach makes full use of legacy software programs. The three existing codes SHARP uses are PROTEUS (for neutron transport simulation), Nek5000 (for Large Eddy Simulation based thermal-dynamics simulation), and Diablo (for structural mechanics and thermo-mechanical simulation).\textsuperscript{23,73}

- To couple the three legacy codes, the SHARP research group develop CouPE (multi-physics driver library). CouPE provides a framework to control the coupling process, which includes the following: (1) a coupling strategy (loose or tight coupling); (2) data transfer; (3) termination iteration when the whole system is converged. In CouPE, both loose coupling (based on the Picard iteration) and tight coupling (based on the JFNK method) are available. The literature in 2013 shows that loose coupling strategy development has been completed, while tight coupling functionality is still in development.\textsuperscript{34}

- In addition to the control of the iteration process, implementation of coupling needs to solve mesh mapping and data transferring issues. SHARP uses MOAB as the data-back. MOAB is a library to query and modify mesh (structures and unstructured meshes) and data in the mesh.\textsuperscript{34,75,76} MBCoupler is developed based on MOAB to transfer solution data in parallel. MBCoupler assigns computing cores between the source and target solvers, making multiple solvers work effectively simultaneously. MBCoupler also maps source meshes to target meshes, for example, mapping the spectral elements meshes in Nek5000 to finite elements meshes in PROTEUS.

- **MOOSE in BISON**
- BISON is developed by Idaho National Engineering Laboratory, and it belongs to the FPL in NEAMS. Compared to SHARP, which uses coupling tools to couple legacy multi-physics software in a bottom-up approach, BISON uses a top-down approach.\textsuperscript{77} BISON solves mechanics equations, heat conduction equations, and other associated PDEs simultaneously. As discussed in Section 2.2, some researchers\textsuperscript{18,78} regard the coupling method used in BISON as a tight coupling strategy and some researchers\textsuperscript{16} regard it as a full coupling strategy. BISON adopts MOOSE, which is based on the JFNK method, to solve PDEs.

- BISON solves the multi-physics problem using the tight method, sometimes called the full coupling method, by default. However, loose coupling is also realizable in BISON. In loose coupling implementation, BISON uses the JFNK method to solve heat conduction equations with the result of structure mechanics being fixed. Then BISON uses the JFNK method to solve structure mechanics equations with the result of heat conduction being fixed.\textsuperscript{78} The iterations repeat until the systems
converge. Figure 7 illustrates the workflow of loose coupling in BISON.

### Coupling Software in CESAR

- The goal of CESAR is to exploit exa-scale supercomputers to solve crucial reactor simulation problems. The research plan of CESAR is to explore the performance of excellent peta-scale (10^15 flops) software and develop exa-scale simulation software. Reports from CESAR show that the software CESAR starts with Nek5000 (for thermal-hydraulics), UNIC (for deterministic neutron transport), and OpenMC (for Monte Carlo neutron transport). Taking Nek5000 as an example, a mini-application Nekbone skeleton application is developed. Nekbone is used to investigate the scaling, communication, storing, and other performance issues of Nek5000. By carrying out in-depth research, CESAR aims to enable those mature peta-scale code scales to be well prepared for future exa-scale platforms.

- On one hand, CESAR investigates the individual simulation codes; on the other hand, CESAR takes the coupling issue into consideration. CESAR investigates CouPE, which was discussed in Section 3.3, when discussing SHARP. The mesh mapping tool CIAN in CESAR is intended to map difference meshes among multi-physics simulation programs. Four steps are required in CIAN solution transfer, which are initialization, point location, interpolation, and normalization.

### 3.4. Coupling software in virtual reactor projects in the EU

The EU has launched virtual reactor projects since 2000. There are three stages of the projects: NURESIM (2005–2008), NURISP (2009–2011), and NURESAFE (2013–2015). NURESIM promotes and incorporate the latest achievements in neutronics, two-phase thermal-hydraulics, and fuel performance simulation. NURESIM is followed by the NURISP project. The main research objects of NURISP are generation II and generation III PWRs, Boiling Water Reactors (BWRs), and Water-Water Energetic Reactors (VVERs). The NURESAFE projects aims at providing advanced and reliable safety analysis for present and future LWRs (Light Water Reactors).

All the software in NURESIM are integrated into the SALOME platform. SALOME is co-designed and co-developed by EDF, The French Alternative Energies and Atomic Energy Commission (CEA), and OpenCascad. SALOME provides a friendly platform for users to make coupling applications. The YACS (dynamic parallel coupling supervisor) module, which replaced the Supervisor coupling module in version 5x, is responsible for the coupling function. YACS couples existing simulation programs in as non-invasive a way as possible. Users use diagrams or Python subscripts to customize their own application workflows. The workflow defines the coupling codes, transferring data, and coupling strategy. YACS uses the explicit coupling approach. The data transfers among programs in the forms of dataflow or datastream in YACS. In the form of dataflow, a code has to wait for the data from other codes before it starts. In the form of datastream, codes are able to run and exchange data simultaneously.

### 4. Multi-physics coupling in China Virtual Reactor projects

Spider is a coupling platform developed within the CVR projects. The research focus of Spider is on the following three parts: modeling, software implementation, and infrastructure building. The layered research focus is illustrated in Figure 8.

As is illustrated in Figure 9, the multi-physics phenomena are considered in the CVR from three scales: the fuel scale, reactor core scale, and system scale. In the fuel scale, the fuel performance is evaluated and predicted by considering all the interacting phenomena comprehensively. The fuel performance is affected by many correlative processes, such as fission gas release, fuel densification, heat transfer, fuel irradiation swelling, corrosion, etc. Simulating the multi-physics processes will provide a capability to help better understand the fuel behaviors and the cause of the behaviors.

The multi-physics processes in the nuclear core scale are considered from the following four aspects in the CVR.
**Neutronics and thermal-hydraulics coupling.** In a reactor core, neutronics and thermal-hydraulics interplay with each other. The change of temperature and density of the coolant has an effect on the neutron flux and neutron spectrum. In return, the variation of the power distribution also has an effect on the coolant temperature and density.

**Neutron transport calculation and depletion calculation coupling.** Coupling neutron transport and depletion plays an important role in accurately analyzing burnup. The interaction information between depletion and transport includes the neutron spectrum, source strength, reaction rates, fission products, and initial nuclide density and its variation. Usually, the transport calculation provides neutron fluxes, the weighted cross-section, and lattice physics parameters using a set of nuclide concentrations. The depletion calculation provides the nuclide concentration.

**Thermal-hydraulics and structural mechanics coupling.** The flow-induced vibration (FIV) phenomenon has been a major concern for nuclear reactor safety. The FIV that happens in fuel rods is especially critical. The random pressure fluctuation of the coolant often results in the vibration of fuel rods. Thermal-hydraulics and structure mechanics coupling is adopted to analyze the FIV of fuel rods.

**Fuel performance analysis coupled with neutronics and thermal-hydraulics.** The fuel performance model describes and estimates the thermal-mechanical performance, fission energy generation, fission product production process, and irradiation behavior of fuel rods. The thermo-mechanical behavior of fuel rods is coupled with the thermal-hydraulics behavior of the coolant. At the same time, the fuel performance analysis needs power distribution from the neutronics. Figure 10 presents the coupled processes between fuel performance analysis with neutronics and thermal-hydraulics, in which fuel performance requires power distribution from the neutronics and coolant conditions from the thermal-hydraulics.

As far as the coupling strategy is concerned, the CVR project shares the same opinion as the first point (which is discussed in Section 2.2): OS and the Picard iteration are loose coupling strategies and the JFNK method is a tight coupling strategy. Both loose and tight coupling strategies are introduced to the Spider platform. Modeling and
Implementation in a tight coupling strategy are depicted in blue in Figure 9. Modeling and implementation in loose coupling strategy are depicted in orange. In the tight coupling strategy, the multi-physics phenomena are considered comprehensively. The multi-physics application is implemented in one monolithic software. The software is composed of pieces that reflect single-physical processes. In the loose coupling strategy, multi-physical phenomena are modeled using several independent single-physics models. Every single model reflects a single-physical phenomenon and is implemented in one stand-alone code. To implement multi-physics simulation, the stand-alone codes are loosely integrated. For example, in the loose multi-physics coupling simulation of neutronics and thermal-hydraulics, the stand-alone software programs ANT-MOC and CVR-PASA are integrated. ANT-MOC is a neutronics simulating software based on method of characteristics and CVR-PASA is a thermal-hydraulics software based on the sub-channel method. The single-physics simulation software in the CVR includes newly developed software programs and legacy ones. For examples, CVR-PASA and ANT-MOC are newly developed in the CVR project, and material performance simulation software molecular dynamics software programs CrystalMD92,93,95 and Kinetic Monte Carlo software CrystalKMC94 are legacy software programs.

Infrastructures are necessary in the implementation of multi-physic simulation. The infrastructure of the Spider coupling platform includes the following tools: (1) a data transferring tool that restructures the solution variables of one single-physics code into a form that can be accepted by other single-physics codes; (2) a mesh mapping tool that interpolates between nonconforming source and target meshes; (3) a load balance controller that schedules the computing resources for single-physics codes in a parallel simulation; (4) a common database that can be used to manage in input data, output data produced after the simulation, and data generated in the simulation process (which

**Figure 9.** Multi-physics processes in nuclear systems.
are usually used for verification of the simulation codes; (5) a numerical analysis library that provides a parallel solution for linear or nonlinear equations; (6) a coupling strategy management tool that controls the entire coupling process and includes reading input data, initializing single-physics codes, managing the iteration process, estimating if the system convergence is met, stopping the coupling process in normal or exception cases, and writing output data; (7) a visualization tool that provides a post-processing capability for the coupling simulation results. Some of the tools are legacy software and open-source libraries (such as BLAS, which provides basic linear algebra operations). Some of the tools are developed in the CVR project, such as the mesh mapping tool used in the coupling of thermal-hydraulics and mechanics applications.

5. Summary

It is significant and challenging to simulate the complex multi-physical behaviors in nuclear systems. The virtual reactor is an interdisciplinary research field that arises with the rapid development of high-performance computing technology, advanced applied mathematics, and science-based models. Great efforts have been made toward the multi-physics coupling simulation in the research field of virtual reactors. In this paper, we review the coupling software in some representative virtual reactor projects: CASL, NEAMS, NURESIM, CESAR, and CVR. We classify some important items relevant to the multi-physics coupling simulation and we analyze the three most frequently used multi-physics coupling strategies. Lastly, we present the research focuses of the Spider coupling platform that is developed in the CVR project.

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