Introduction and research progress of the project of numerical virtual reactor

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Abstract: Various projects on numerical virtual reactor (NVR) are on-going around the world for the advanced modeling and simulation application in nuclear engineering. In this paper, definition of NVR is first made and then the technological solutions for NVR are discussed. Lastly, research progress of the authors' group which is called project of "Research on Key Technology for Numerical Virtual Reactor" is introduced with its development roadmap, and some typical demonstrative results.

Keyword: numerical virtual reactor; modeling and simulation; multi-physics; multi-scales

1. Background[1-5]

Modeling and simulation (M&S) has been an efficient way for scientific research. In nuclear engineering, simulation is often the only method to conduct on research because of the potential radioactive risk. In fact, M&S has played a vital role since 1970s in the design, operation, performance and safety of nuclear power plants. The representative achievements are development of simulators and safety analysis codes which have contributed to improve the design, operation and performance of nuclear power reactors significantly. But the available tools of nuclear M&S today are empirically based ones which are only valid for conditions very close to the original experiments, and in many cases only incremental improvements have been made on old computer codes for a long decades.

In order to predict the performance of nuclear reactors with confidence through comprehensive, science-based modeling and simulation technology, and also to enhance safety, reliability, and economics of nuclear power plant, the U.S Department of Energy has started Consortium for Advanced Simulation of Light Water Reactors (CASL) project in 2010. Consortium has ten core partners which are centered at Oak Ridge National Laboratory. Through new insights afforded by its modeling and simulation (M&S) technology, CASL will address key nuclear energy industry challenges to further accelerating power uprates, higher burnup, and/or lifetime extension while providing with higher confidence on enhancement of nuclear safety. CASL project focused on modeling physics within the reactor vessel and it has six technology areas: Advanced Modeling Applications (AMA), Physics Integration (PHI), Radiation Transport Methods (RTM), Materials Performance and Optimization (MPO), Validation and Uncertainty Quantification (VUQ), Thermal-Hydraulics Methods (THM). The achievement of CASL is offering a Virtual Environment for Reactor Applications (VERA) and its latest edition is VERA-CS. The key physical modeling components in VERA model include neutronics, fluid flow, chemistry heat transfer, and thermo-mechanical performance of fuel and structures. Its infrastructure is included to couple these physics model for specific problems, to provide a common input and output of information, and to support

Received date: October 10, 2015

validation and uncertainty quantification. CASL M&S technology will become the leading nuclear energy industry M&S capability for supporting advanced nuclear steam supply system (NSSS) and nuclear fuel research, development, and deployment. Now CASL has finished “Phase I” (2010-2015) project and will start the extension “Phase II” project.

2. What is “Numerical Virtual Reactor”

Like VERA by CASL project in US, the concept of “Numerical Virtual Reactor” (NVR) had been first proposed in 2011 by Nuclear Power Simulation Research Center (NPSRC), Harbin Engineering University (HEU), in China. The “Numerical Virtual Reactor” is defined as a scientific computing system which is made up of science-based, high-fidelity models of neutron transport, thermal-hydraulics, material performance in reactor vessel (RV) and nuclear steam supply system (NSSS) with efficient and robust solver on and high performance computer (HPC) platform.

The program of Numerical Virtual Reactor aims at attaining the following four goals:

(1) NVR provides comprehensive, science-based, high-fidelity and coupled Modeling and Simulation (M&S) capabilities to deal with the operational, safety and design problems during a whole lifetime of a reactor.

(2) The integrated simulation system can confidently predict the behavior, phenomenon and inherent law in RV and NSSS, and the results are easy to understand through virtual reality (VR) display terminal.

(3) To develop and apply a menu of ways for simulation verification and validation (V&V), and uncertainty quantification (UQ) to enhance the acceptance of prediction.

(4) NVR can support engineering validation, safety evaluation and review, behavior prediction, optimizing design so that it can replace a part of function of large-scale experiment equipment and prototype reactor.

The Numerical Virtual Reactor has great values for Scientific Research**,** Engineering and Institution, as can be summarized as below:

The value for Scientific Research: By developing and applying advanced M&S, the behavior and inherent law of reactor and NSSS can be more realistically revealed by NVR to provide theoretic foundation for design and operation.

The value for Engineering: The NVR can allow safer and more efficient utilization of nuclear energy so that nuclear accidents can be made more preventable with reduced consequences.

The value for Institution: The NVR can allow building up exemplary mutual cooperation by all members in nuclear industry: universities, institutes, power plants, manufacturers, government and the public.

3. Total technology solution and key challenges of NVR

The total technology solution for NVR is illustrated in Fig.1. The core of NVR is the science-based, high-fidelity models for nuclear reactor.

The models in NVR cover the full-scope physical processes in nuclear reactor which include neutron transportation, thermal-hydraulic, fluid-structure interaction, chemical corrosion and irradiation damage of materials. In addition, equipment models of NSSS are built up to calculate the transient of the load side of nuclear power plant. The coupled relationships among these physical processes are considered in modeling procedure. The parallel computational technology is applied in NVR to deal with the very-large-scale computational tasks. But before NVR is used to engineering design, operational supporting or scientific prediction, the works of verification and validation (V&V) for models, codes and results are indispensable, and the uncertainty quantification (UQ) toolkit is one of the important components in NVR. Moreover, an interactive human machine interface (HMI), through which users can operate with the virtual reactor, is necessary for easy understanding of computed results.

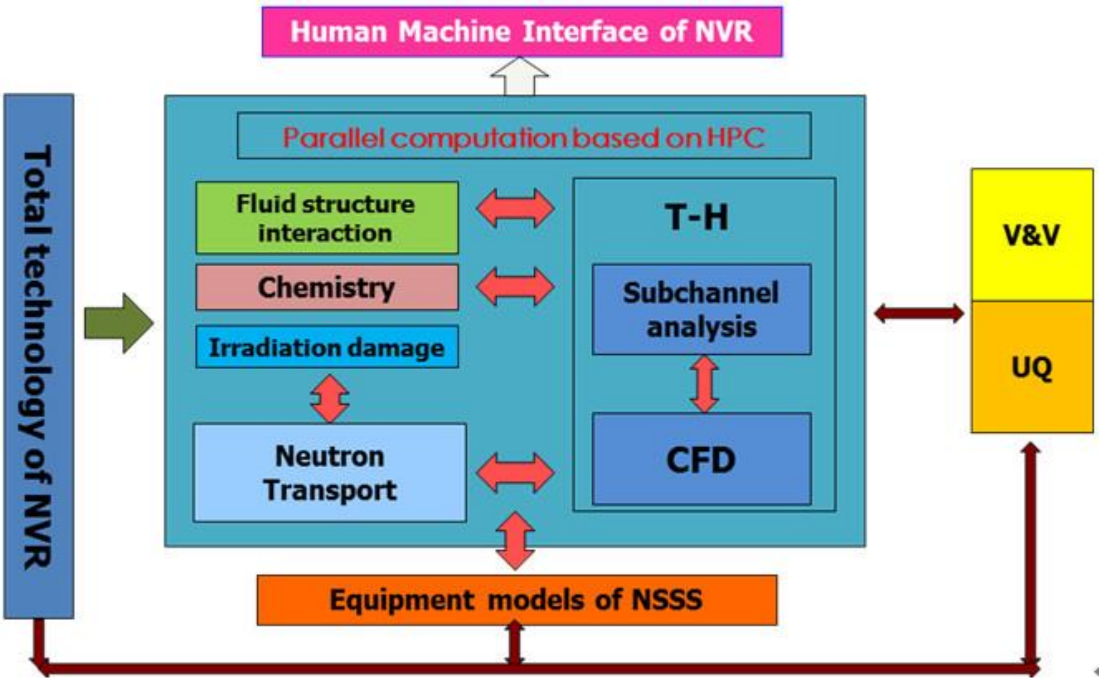

Fig.1 The total technology solution for NVR.

In order to achieve those targets of NVR, the next four key challenges must be tackled as discussed in the subsequent sections.

3.1 Challenges 1: Multi-physics Coupled

In nuclear reactor, physical processes of neutron transport, coolant flow, heat transfer, nuclear fuel and material performance evolution will influence with each other. These coupled relationships are showed in Fig.2. So in NVR the coupled relationships among all models of physical processes should be considered to ensure a realistic description of physical phenomena in nuclear reactor. There are certain requirements to achieve such multi-physics coupled calculation effectively. These requirements are met by the development and implementation of five basic components of coupling methodologies: (i) a deeply insight into the mechanisms that underline those impact mentioned above, (ii) coupling approach(integration algorithm or parallel processing), (iii) spatial mesh overlays and time-step algorithms, (iv) coupling numeric algorithms (explicit, semi-implicit and implicit schemes), and (v) coupled convergence schemes. These principles of the multi-physics simulation in NVR should be elaborately designed.

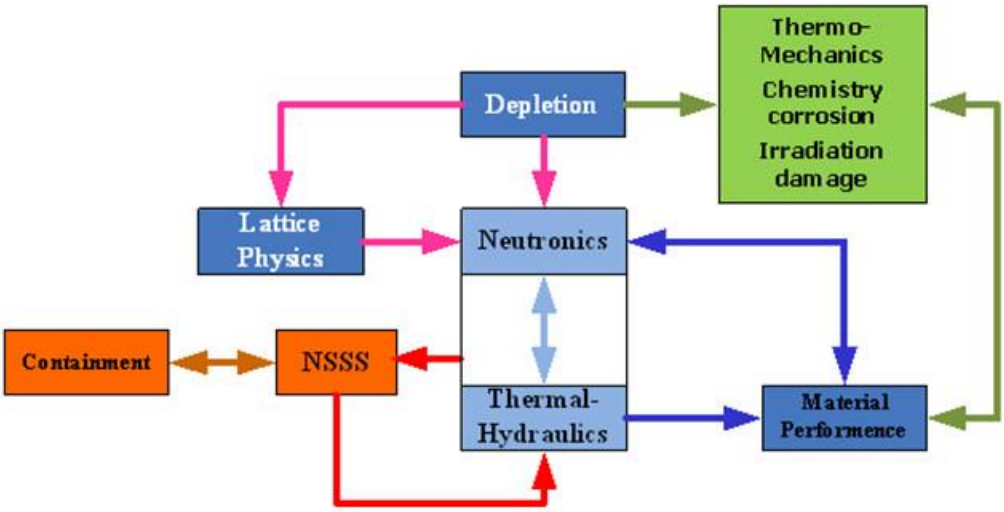

Fig.2 Coupled relationships among different physics process.

3.2 Challenges 2: Multi-scales Coupled

Traditional modeling approach was to focus on one scales because only one physical phenomenon was considered. In contrast, the complex coupled multi-physics processed in nuclear reactor are described by considering models simultaneously at different scales in NVR. For example, to predict nuclear fuel and material performance evolution, the models in meso-scale or micro-scale are often required to obtain the changes of crystal structure. At the same time, the material performance evolution will influence on the macro parameters in heat transfer and neutron transportation such as heat conductivity and macroscopic cross section. But we encounter a tall order in multi-scales coupled simulation: the macroscale are very efficient but are often not accurate enough, or lack of crucial microstructural information that we are interested in. Microscopic models, on the other hand, may offer better accuracy, but they are often too expensive to be used to model whole system of a real nuclear reactor. It would be nice to have a strategy that can combine the efficiency of macroscale models with the accuracy of microscale models.

3.3 Challenges 3: Uncertainty reduction and Validation and Uncertainty Quantification (VUQ)

Figure 3 shows the sources of uncertainty in computer simulation. The first type uncertainty is the modeling error. The second type of uncertainty comes from discretization procedure of mathematical model. This is often called the error of numerical methods or discretization. The third type of uncertainty results from a finite string representation of real values by computer [6]. The difference between the calculated approximation of a number and its exact mathematical value due to rounding is called "round-off error".

And the methods of uncertainties control can be described as follows: to reduce the model error, more science based models are utilized in NVR and the micro and meso scale models are applied to provide for better closure relationships; to deal with the second type of uncertainty, high-order discrete scheme and of fully-implicit schemes should be used for discretization procedure. The tight coupling solution, instead of the loose coupling, is applied to tackle with the multi-physics and multi-scales coupled problem. The calculations are based on the fine meshes which are converted from assembly-wise to pin-wise. Moreover, HPC and an integrated and usable simulation platform are employed to diminish the last error.

For dealing with the uncertainties which exist in simulation results, the VUQ plays a critical role in achieving goals of NVR. First, the user or engineer of NVR must have an ability to assess whether the predicted results are accurate enough for evaluation of the design and safety margins. Second, the VUQ can help the model developers to find which models have a large contribution to the uncertainties of results. So the developers can pay more attention to development of these models which deal with sensitivity. The basic ways to deal with VUQ can be stated as below:

(1) Utilization of an advanced measurement technology,

(2) Assimilation of extensive data of reactor design, test and operation,

(3) Development or application of mathematical and statistical UQ methods and toolkit, and

(4) Collaboration of an experienced team across different areas of engineering, mathematics and software.

3.4 Challenges 4: Very-large-Scale Computation

The models of NVR are a set of three-dimensional non-linear unstable equations which are solved on the fine meshes, and therefore NVR is a computationally intensive project. Now consider a full core thermal-hydraulic problem of QinShan-I NPP, a brief analysis of very-large-scale computation in NVR is given. There are 121 fuel assemblies in QinShan-I NPP. Each fuel assembly can be divided into the coolant channel, mixing vane and space grid regions when the temperature, velocity and pressure field are solved with CFD method. Table 1 gives the dimension of a fuel assembly and the required number of cell when gird-independent solutions are obtained. It is found that cells in excess of 62 billion are needed even though only the thermal-hydraulic calculation is carried out.

4. Technical areas of NVR

NVR focuses on four technical areas (TAs), (i) advanced model and simulation, (ii) integrated simulation platform, (iii) validation and verification, uncertainties quantification, and (iv)hardware configuration. Those are explained in the subsequent sections.

4.1 Advanced model and simulation (TA1)

The whole subjects in concern are illustrated in Fig.4 for advanced model and simulation, and the condensed summaries of object, short term and long term planning for each subject are given in the subsequent parts.

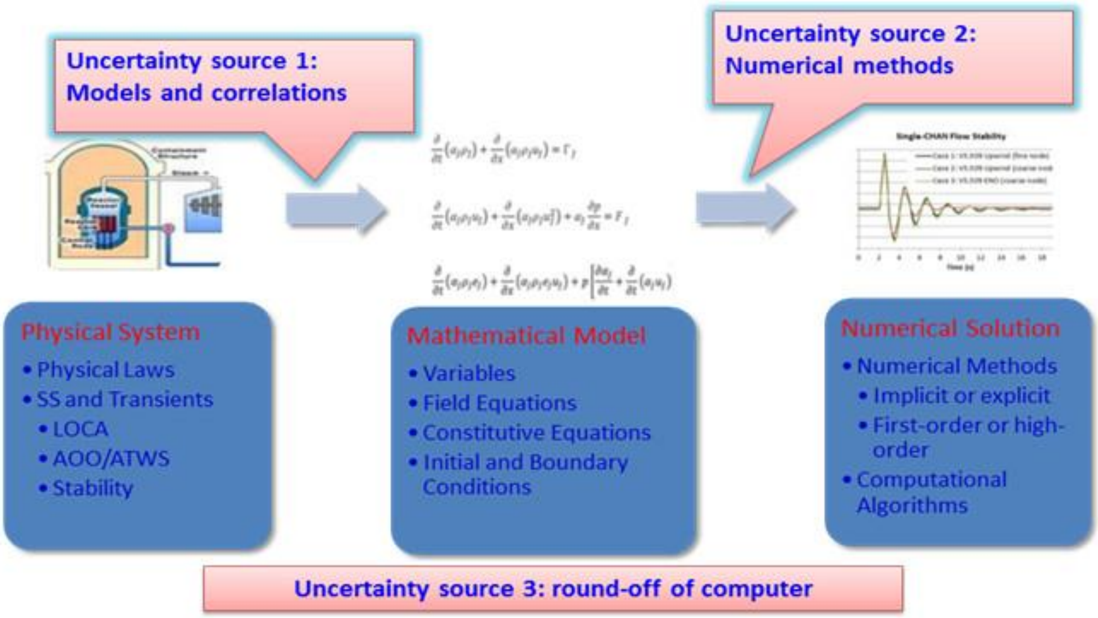

Fig.3 Uncertainty sources in computer simulation.

Table 1 Required cell number in full core T-H calculation for Qinshan-I NPP

Region	Cell number per unit region	Region size of one channel	Channel number of one assemble	Assemble number of one reactor	Total cell number of each region
Coolant Channel	100K/m	3 m	15*15	121	~ 9.85 billion
Mixing Vane	84K/layer	6 layers	15*15	121	~ 10.41 billion
Spacer Grid	194K/layer	8 layers	15*15	121	~ 41.95 billion
Total cell number of a full core： > 62 billion!					

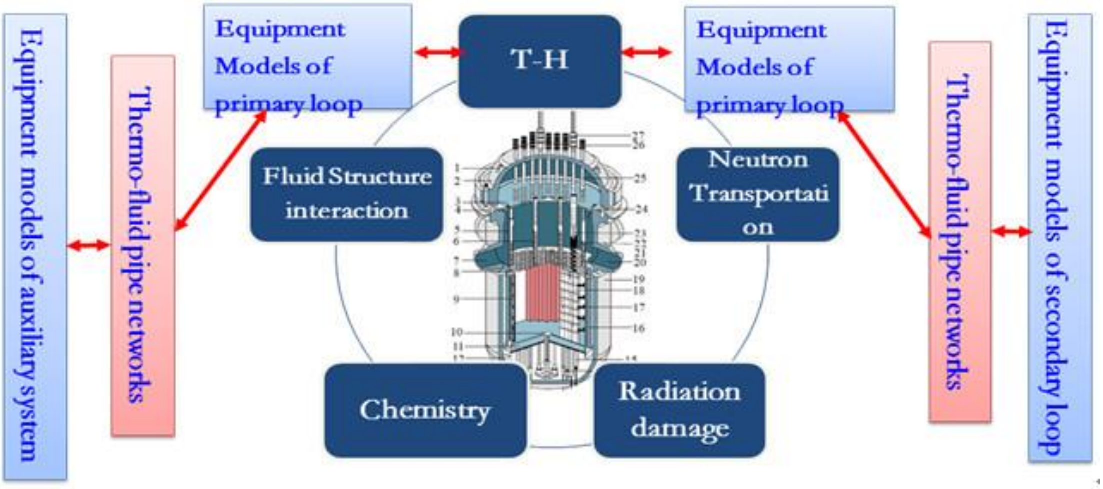

Fig.4 High-fidelity model components in TVA.

4.1.1 Neutron transport

Object: Direct full-core integral transport calculation. Pursue the deterministic and stochastic transport methods to develop 3D pin-by-pin calculation capability.

Short term Planning:

- 3D diffusive calculation for real-time simulation
- 2D MOC +1D SN coupling method
- Pin level T/H feedback by coupling with CFD
- Subgroup method for “Resonance Treatment”
- Efficient parallel algorithm

Long term Planning:

- 3D MOC and parallel computation
- Transport calculation in sub-pin level
- Monte Carlo method
- Transportation/CFD coupled in full core

The 2D MOC +1D S_N coupling method is employed to solve the neutron transport problem with the illustration of this method given in Fig. 5.

In Fig.5, the specific characters of 2D MOC +1D S_N coupling method [7] are

- To use MOC transport in radial directions, and
- To use nodal transport /diffusion in axial direction, to realize
- More accurate than by nodal methods but less computational resource cost than by fully 3D transport.

Traditional “Two-step method” is replaced by “One-step method”. Fine lattices in cell are applied for whole core.

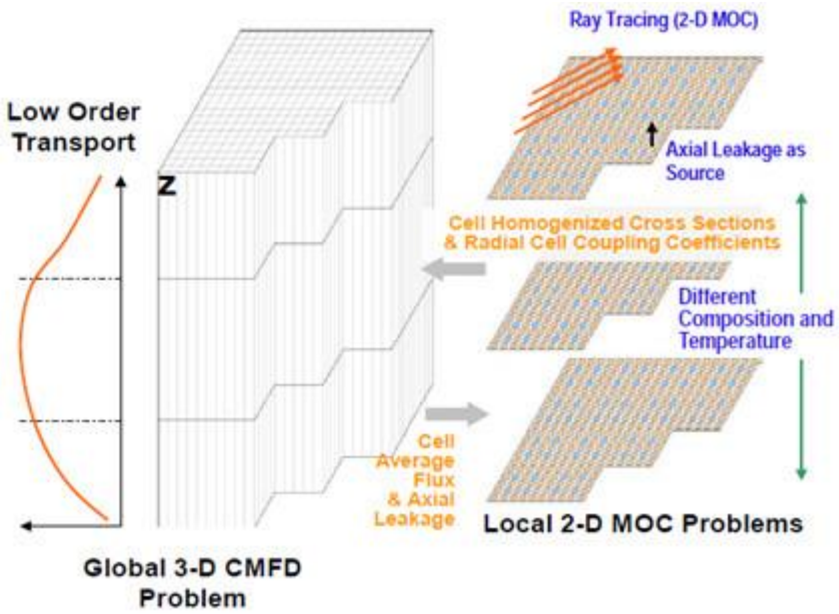

Fig.5 2D MOC +1D S_N coupling method.

4.1.2 Thermal-hydraulic

Object: Deliver 3D single and two phase flow and heat transfer calculation capabilities based on CFD technology, including advanced closure correlations for boiling.

Short term planning:

- To develop the next-generation sub-channel code and explore parallel solution
- To research on mesh optimization
- Single-phase transient calculation in a whole assembly based on CFD
- To utilize advanced measurement for code validation
- To include severe accident analysis model

Long term planning:

- Fundamental understanding of two phase flow and heat transfer
- To develop closure correlations for boiling based on reliable data
- To develop confident and stable 3D turbulent model for boiling
- Two-phase steady calculation in a whole assembly based on CFD
-

Characters of the next-generation sub-channel code

➢ 3D two-fluid flow and heat transfer models of the two-phase flow include:
- Mass equations (liquid and vapor)
- Energy equations (liquid and vapor)
- X-direction, y-direction and z-direction equations (liquid and vapor)
- Non-condensable gas mass equation
- Boron tracking model

➢ Flow-regime dependent closure correlations
- Inter-phase friction and heat and mass transfer
- Wall drag and heat transfer

➢ Pin conduction model

➢ Parallel solution

CFD technology is employed to obtain the fine flow and temperature fields in reactor core. The research focuses on the following areas:

- Mesh generation technology for complex geometries and mesh optimization technology
- High-order scheme application
- CFD models for two phase flow
- Influence of boundary condition
- Results validation
- Parallel solution

4.1.3 Fluid Structure interaction

Object: Develop capabilities of high-fidelity thermo-fluid-structure analysis to predict turbulent excitation, structure vibration and wear.

Short term Planning

- To develop fluid-structure interaction model
- To calculate, with confidence, turbulent flow excitation
- To predict rod vibration and fretting wear
- Implicit 3D finite element method

Long term Planning

- To consider other sources of stress, fission gas, corrosion, *etc*.
- To consider the effects of irradiation damage

4.1.4 Chemistry

Object: Develop models of chemistry transportation and reaction to predict behavior of fuel and structure corrosion and crud growth.

Short term Planning

- Fundamental understanding of reaction between material and chemistry
- To develop model of chemistry/thermodynamics/fluid and explore general non-linear equations solution
- Develop constitutive relations about chemistry

Long term Planning

- Crud growth simulation
- To be coupled with fluid structure interaction and irradiation damage

4.1.5 Radiation damage

Object: Reveal the behavior of fuel, reactor internal and reactor vessel under strong radiation. Evaluation of the operating margin and lifetime limits of material.

Short term Planning

- To carry out radiation damage experiment and assimilate experiment data.
- To develop basic material data libraries
- To develop the model of radiation damage based on molecular dynamics

Long term Planning

- To be coupled with fluid structure interaction and structure corrosion
- To support design of advanced fuel

4.1.6 Equipment &Thermo-fluid pipe networks models

Object: Develop physics-based, real-time models of equipment and pipe networks to complete the simulation of a whole NPP.

Mission

- To develop primary-loop equipment models which include steam generator and pressurizer
- To develop secondary-loop equipment models which include turbine, condenser, deaerator, and separator
- To develop general equipment models which include centrifugal pump, shell-pipe heat transfer, and valves
- To develop 1D compressive-thermo-fluid pipe networks model

4.1.7 Severe accident simulation

Motivation:

- After Fukushima accident, it has been realized that we have much to learn, or rather relearn about severe accidents to prevent from or to mitigate its consequence.
- To develop revolutionary safety designs that have significantly higher margins to severe accidents
- Many NPP will be built in China inland. The potential risk of radioactive release to off-site must be eliminated in design

Capability:

- Severe accidents refer to T-H, fuel and structure behavior, chemical reaction, radioactive transportation, *etc*. NVR has an integrated simulation environment to predict various phenomena caused by severe accidents

4.2 Integrated simulation platform (TA2)

An integrated simulation platform is required which supports the database management, code execution, geometry and mesh generation, results demonstration and provides the data exchange interfaces. The structure of the platform for NVR in short term planning is shown in Fig.6.

Moreover in the long term planning, a fully integrated simulation platform will be developed which integrates the models, pre/post processors, solvers for PDEs and linear/nonlinear systems, material and cross section library, *etc*. The platform will borrow from merits of the Multi-physics Object-Oriented Simulation Environment (MOOSE). It will provide a high-level interface to some of the most complex multi-physics and multi-scale coupled problems, and the simulation platform can runs on the state of art supercomputers. The scientists and engineers could pay more attention to the establishment of models rather than development of solver and data interface. So the coupled solution of models and codes for different physics processes in nuclear reactor is easily achieved under the support of the platform. The structure of the platform for NVR in long term planning is shown in Fig.7.

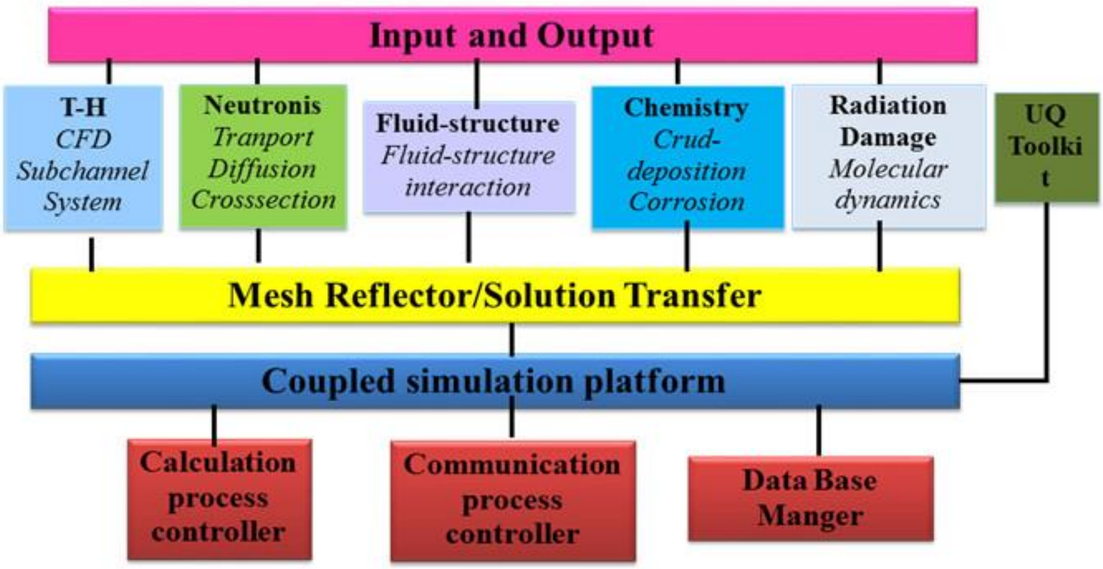

Fig.6 The structure of the platform for NVR in short term planning.

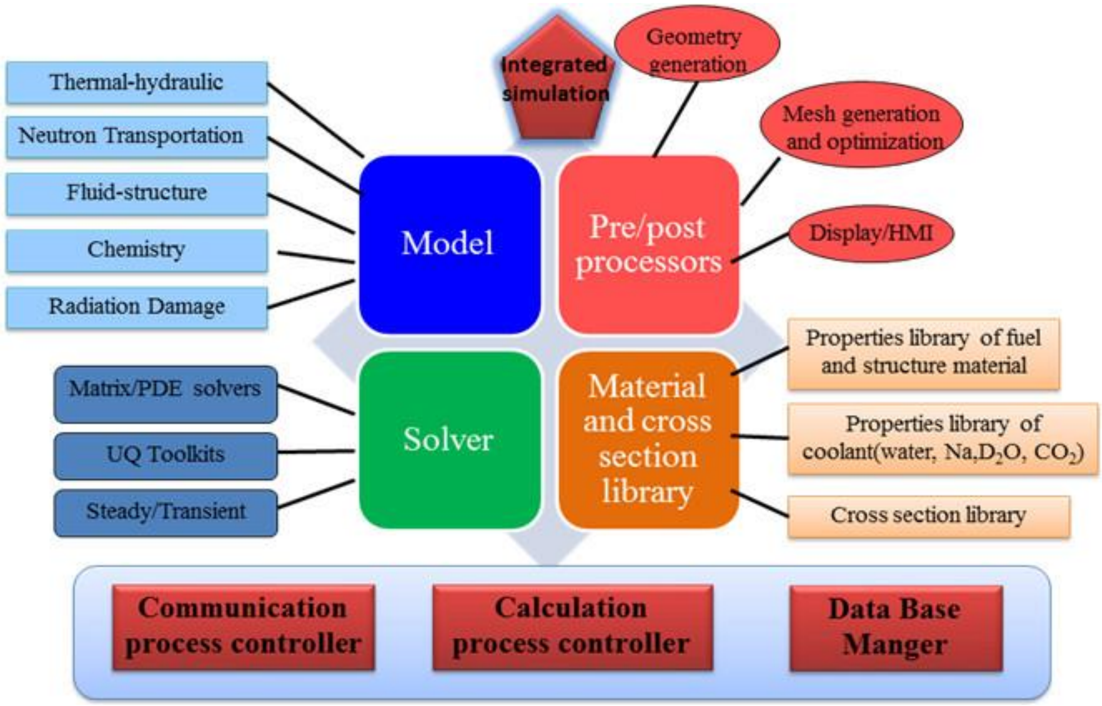

Fig.7 The structure of the platform for NVR in long term planning.

4.3 Validation and verification, uncertainties quantification (TA3)

Verification and validation, uncertainty quantification are for gaining confidence to the result of simulation.

Object: Develop and apply a general method for NVR verification and validation, through experimental and operational data identification and assimilation, sensitivity analysis, error analysis and improvement, uncertainty quantification.

Approach:

- Validation through experimental data
- Validation through operational data of NPP
- Validation through benchmark problem
- Sensitivity analysis and UQ
- Calibration of software development process and assessment of quality of software
- Acceptable experiment and precise measurement are also necessary for the validation of simulation

Motivation:

- To validate simulation results
- Fundamental understanding
- Large uncertainties are hidden in current closure relations. A set of better alternatives are needed
- Traditional measurement cannot meet the requirement of NVA

4.4 Hardware configuration (TA4)

Figure 8 shows the hardware configuration of NVR. The hardware system is composed of a high-performance computer, small severs, graphic workstations, engineering stations, internet exchangers and a display terminal. The high-performance computer is the core equipment which is used to solve the most sophisticated models and to save the mass data. Small severs are used to solve the simple models such as equipment models, control system models. The function of graphic workstations is to process complex pictures of geometry, meshes and results. Engineers can develop, modify, maintain and upload models and develop computer codes through the engineer stations.

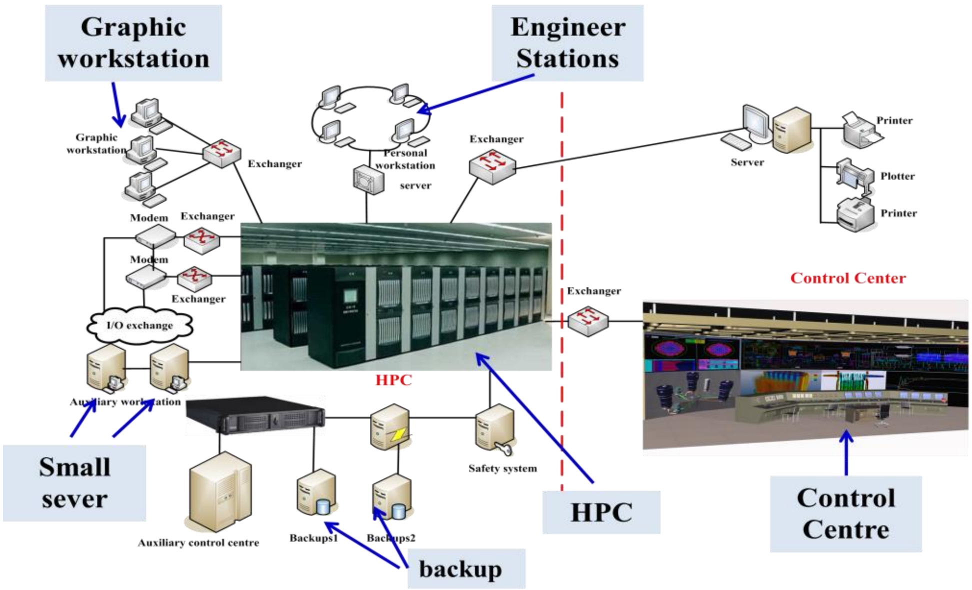

Fig.8 Hardware configuration of NVR.

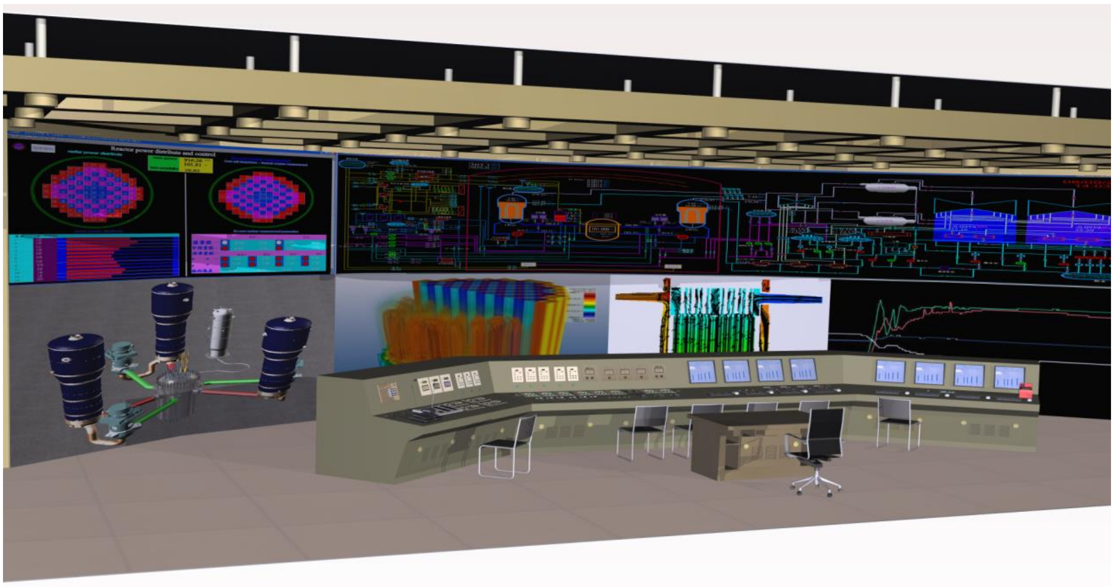

Fig.9 Display terminal of NVR.

Display terminal, also called control center, can demonstrate the results with an easily understanding way. The rendering picture of display terminal of NVR is shown in Fig.9. The screen is divided into several parts on which the system schematic, virtual reality of equipment, 3-D results, power distribution in reactor core, transient curves of main parameters are displayed.

5. The Roadmap and research progress of NVR

Tables 2 and 3 give the roadmap of NVR for each interesting technical area during the period 2016-2020. Since 2012, NPSRC had been in charge of the project of “Research on Key Technology for Numerical Virtual Reactor” which is supported by Chinese government. Aims of the project are as follows:

- To make a breakthrough on key technology for multi-physics and multi-scales coupled
- Based on 2D MOC +1D S_N coupling method, models and codes for pin-by-pin neutron transportation computation are developed.
- To develop the next-generation sub-channel code and CFD technology is employed to obtain the high-fidelity flow and temperature results in a fuel assembly with complex structures.
- To achieve neutron diffusion and thermal-hydraulic sub-channel analysis coupled solution in a whole reactor core. Complete neutron transport and thermal-hydraulic CFD analysis coupled solution in a fuel assembly.
- To research on V&V and UQ of simulation results and develop the toolkit of UQ.
- To breakthrough key technologies of large-scale parallel computation

Table 2 Roadmap of NVR - Part 1

TA	2016	2017	2018	2019	2020
Neutron Transport	● Overall design for 3D transport program based on one-step method ● Full core CMFD and 1D nodal method	● Complete 2D MOC, 3D steady state calculation based on assumed cross section	● Resonance Computational modules development	● Multi-groups（70 or more）cross section library development	● Full core 3D transport code development with one-step method based on refined 2D MOC and 1D SN
Thermal-hydraulic	● Rod-assembly reactor 3D thermal-hydraulic analysis program ● Single phase CFD calculation in a whole assembly	● Rod-assembly reactor 3D thermal-hydraulic analysis cprogram ● Couple CFD to subchannel code	● Develop confident and stable 3D turbulent model for boiling	● Two-phase steady calculation in a whole assembly based on CFD	● Refine two-phase flow capability
Fluid Structure interaction	● Evaluate of existing fluid-solid coupling calculation capabilities ● Select the fluid-solid coupling solution scheme	● Two-way fluid-solid coupling calculation	●Develop fluid-structure interaction model ●Calculation, with confidence, turbulent flow excitation	● Implicit nonlinear wear calculation, capability	● Consider other sources of stress, fission gas, corrosion
Chemical corrosion	● Core chemical corrosion mechanism research	● Fuel cladding scaling and growth mechanism research	● CIPS/CILC phenomena and mechanism research	● establish the chemical corrosion model of fuel ● Establish fuel crud depositing, scaling and growth model	● Evaluate the existing chemical corrosion calculation capabilities ● Determine the solution scheme for core chemical corrosion calculation

Table 3 Roadmap of NVR - Part 2

TA	2016	2017	2018	2019	2020
Irradiation damage	● Fundamental experiment study for irradiation dam-age	● Fundamental experiment study for irradiation dam-age	● Mechanism research of fission gas caused by irradiation	● Calculation of fuel irradiation damag e based on LAMMPS	● Calculation of reactor vessel irradiation damag e based on LAMMPS
Coupling	● Management platform development for multi-physics multi-scale coupling calculation	● Method research for thermal-hydraulic multi-scale coupling calculation	● Method research for NT and CFD) coupling calculation in pin resolved	● Method research for Multi-physics coupling calculation	● Full core neutron transport-CFD-Fuel vibration coupling calculation
Uncertainty analysis	● Framework and method research for uncertainty analysis of NVR	● Uncertainty analysis for physical, thermodynamic local independent model ● General physical computing uncertainty analysis program development	● Uncertainty analysis for physical, thermodynamic global independent model	● General thermodynamic computing uncertainty analysis program development	● Uncertainty analysis for neutron physics and thermal-hydraulic coupling system
Validation	● Determine validation experiment and measurement method ● Establish fundamental experimental conditions	● Single phase validation experiment on 7*7 assemble	● Two-phase validation experiment on 7*7 assemble ● Neutron calculation results validation by MCNP	● Neutron-T/H coupling experiment	● Validation based on practical measured data of PWR NPPs

The completed research contents are shown below:

- 3D real-time neutron diffusion code for square lattice and hexagonal lattice
- 3D high-fidelity neutron transport calculation for a rod fuel assembly
- Equipment models and thermo-fluid pipe networks model for real-time computation
- Research on CFD mesh generation and optimization method
- Sub-channel analysis code for plate fuel assembly
- 5*5 rod assembly T-H calculation based on CFD
- Sub-channel(plate fuel) /diffusion coupled calculation in whole core by using loose couple method

The researches of the following contents are in progress:

- 3D high-fidelity neutron transport calculation for a plate fuel assembly
- Sensitivity and uncertainty analysis (SUA) of transport calculation
- 3D high-fidelity whole-core integral transport calculation
- Sub-channel analysis code for rod fuel assembly
- A whole rod assembly T-H calculation based on CFD
- Results validation
- Sub-channel(rod fuel) /diffusion coupled calculation in whole core using loose couple method
- CFD/Transport coupled calculation on pin-resolved
- Research on tight couple method

Lastly, some typical 3D results of thermal-hydraulic based on CFD are introduced in Figs.10-13.

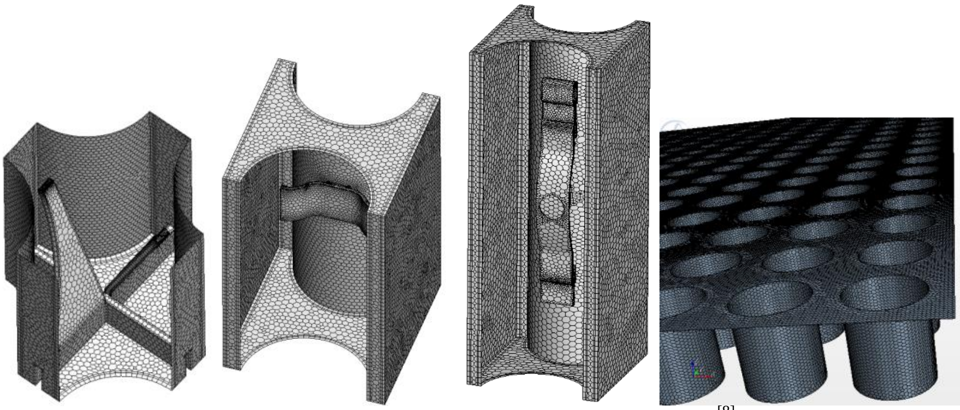

Fig.10 Meshes of fuel assembly for CFD computation[8].

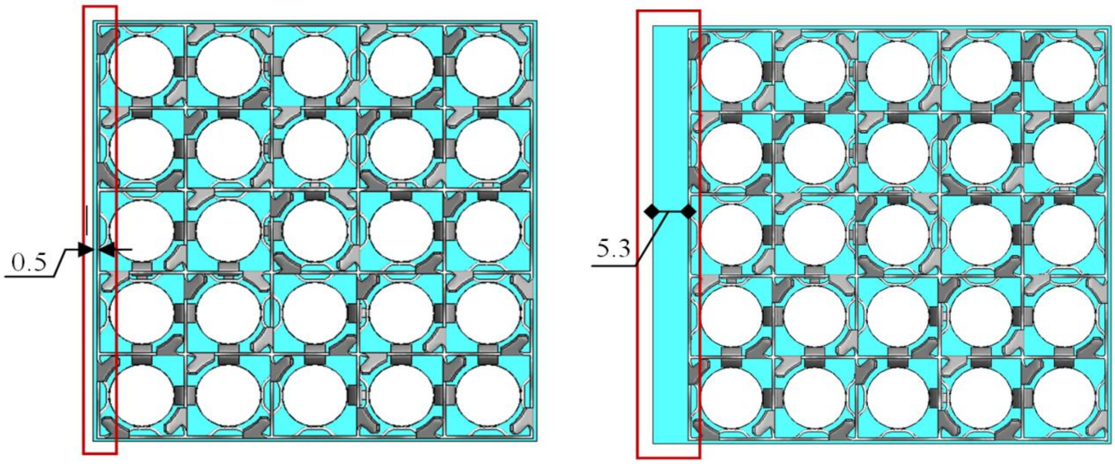

Fig.11 Geometry of 5*5 fuel assembly.

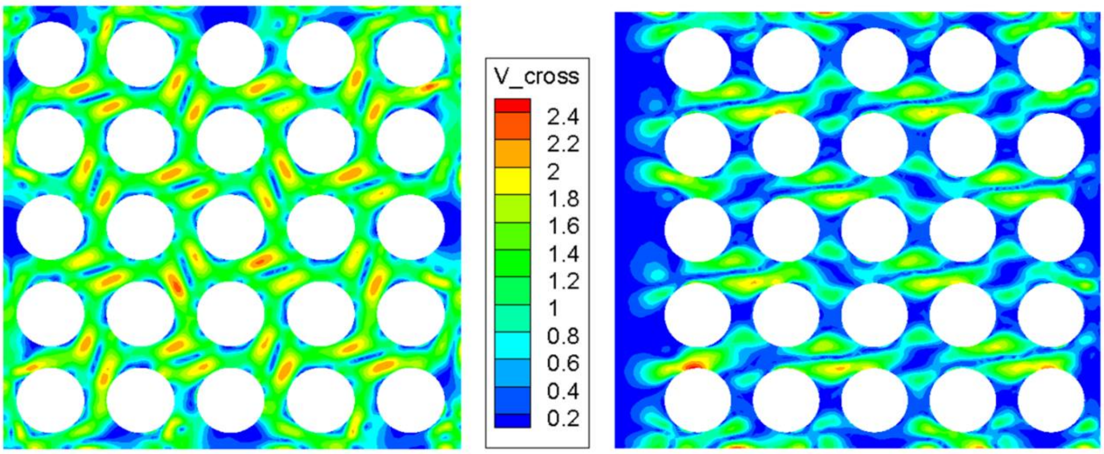

Fig.12 Velocity fields in 5*5 fuel assembly.

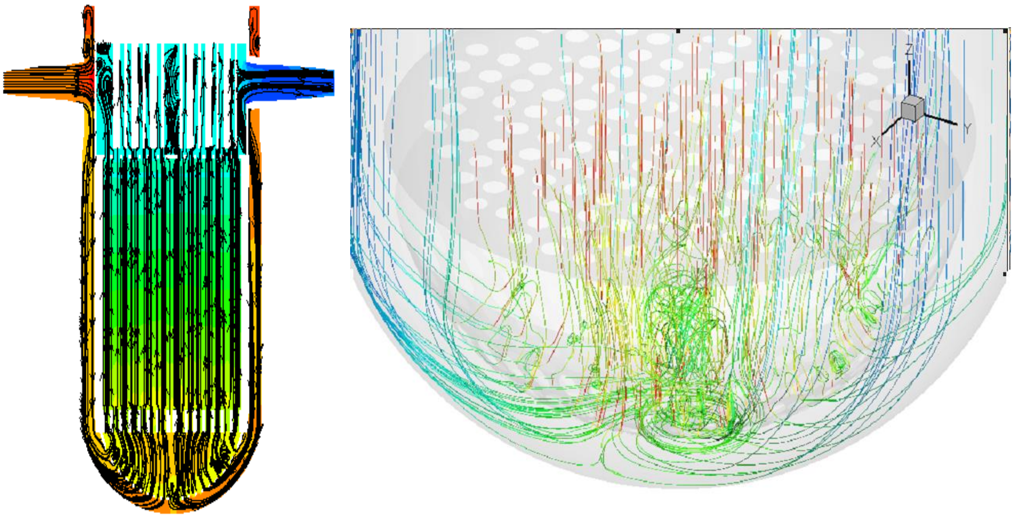

Fig.13 Streamline in vessel and lower plenum[8].

6. Conclusion

Many projects on numerical virtual reactor (NVR) have been in progress around the world for the advanced modeling and simulation application in nuclear engineering. In this paper, the objective, methods and the progress of the authors' on-going project on "Research on Key Technology for Numerical Virtual Reactor" were introduced with its development roadmap, and some typical demonstrative results.

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