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Abstract – The current generation of reactor safety simulation codes such as RELAP and TRAC are relatively old (approx. 30 years). These codes have been extensively validated for the existing reactors. However, for the advanced reactor designs such as sodium cooled fast reactors (SFR), very high temperature reactors (VHTR) and liquid salt cooled reactors, which tend to have slow and long transients (relative to LWRs) resulting from passive safety features, the performance of these codes is questionable. At INL, we have launched an effort to develop a code named SARAH (Safety Analysis for Reactor Applications with High fidelity) by incorporating the improvements in physical models, numerical methods, software engineering and computer hardware over the last 30 years. The near term applications of SARAH are for SFRs and the code will be extended to VHTRs and LWRs applications in the future. This will be accomplished by employing modern parallel solution algorithms and producing a simulation capability that is second order accurate in space and time. Modern nuclear reactor simulations that incorporate better physics and improve safety analysis and to reduce excessive conservativeness in reactor designs.

I. INTRODUCTION

Physics in a nuclear reactor is a complicated mixture of multiple physical phenomena. The accurate reactor safety evaluation requires integrated analyses involving neutronics, fluid thermal hydraulics, fuel heat conduction, and fuel structural mechanics. Integrated multiphysics computational tools are necessary to simulate these interrelated phenomena. Traditional nuclear reactor system simulators such as RELAP^{1,2}, TRAC³, employ a looselycoupled operator split algorithm. When these codes were originally developed in the 1970s, computers were expensive, slow and had small memories and hence fast running operator split method had to be used. In this approach, each of the physics (fluid flow, heat conduction and neutron diffusion) is solved separately and the coupling terms are done explicitly. With explicit coupling, the values of some of the variables at new time step are calculated based on variables or closure models available at old time step. Changing the nonlinear coupling between physical makes the problem easier processes to solve computationally, but it introduces truncation errors into the simulation⁴. These truncation errors affect the physics of the problem. This loosely coupled approach limits accuracy to first order in time and space at best. This method also

yields low efficiency since the explicit coupling imposes stability restrictions on the time step size. In addition, some physical models in these codes are also out of date. The first example is the two-phase flow model which is illposed. This means that the partial differential equations that describe the physics do not have a unique solution. The codes rely on numerical diffusion from their first order accurate in space discretization to regularize the solution. This prevents modern 2nd order in space methods from being employed since they do not have enough "error" to keep the solution regularized. The second example is the flow regime maps which are based on steady state and fully developed flow assumptions. In fluid flow modeling there are physics that are resolved by the temporal and spatial discretization and subgrid physics (too small or fast) which are not resolved by the grid. The subgrid physics is modeled by closure relations. Even though the subgrid physics is not resolved they still have physical length scales and time scales. The steady state and fully developed assumptions in current flow regime maps remove these length and time scales. This results in physics that are discontinuous in space and time. These discontinuities prevent numerical methods from being more than first order in space and time.

Due to the limited funding in the past two decades, reactor system simulation codes have not evolved much from the perspectives of numerical techniques, fundamental physical models, and software engineering. It should be noted that although current simulation codes contain many questionable models and assumptions, they perform well of simulating existing nuclear reactors. There are two reasons that kept these first order accurate methods applicable to the existing reactors. The first reason is that the existing LWR reactors were designed to have short transients. Hence the error accumulation during the course of a transient has not been significant. The second reason was the availability of large amount of experimental data. These simulation codes have been "tuned" based on large experimental data sets. For example, if a numerical method or physical model causes a pressure drop to be larger than is measured experimentally, the simulation input can be modified to lower the pressure drop until it matches the experiment. Therefore, if there is a large experimental data set that covers the state space that the reactor will operate in, and the simulation code has been "tuned" for that application, the simulation will match the reactor behavior. However, the tuning process generates compensating errors, which limit the applicability of the code to a different set of requirements or designs⁵. The semi-implicit time integration employed by existing codes contains a CFL (Courant Friedricks and Lewy) stability limit. Therefore, the time step size is limited by stability rather than accuracy and consequently makes the codes slow This weakness is further exacerbated when running. applying these codes to new nuclear reactor designs such as SFR or VHTR designs which tend to have slow and long lasting transients (relative to Gen-II or Gen-III LWRs) resulting from passive safety systems.

For advanced reactor designs, there usually does not exist a large experimental data base that covers their operation like the over billion dollars investment in large scale integral experiments performed at INL site several decades ago for the existing LWRs. The predictability of utilizing existing simulation tools with loosely coupled approaches is questionable. For example, sodium cooled fast reactors have compact core geometry coupled with the long neutron mean free path, which result in a much higher neutron leakage fraction than that for a typical commercial light water reactor. This high leakage fraction implies that the reactivity effect impacts the reactor as a whole rather than locally for a LWR and the reactor reactivity is sensitive to small geometric changes. As the temperature increases causing materials to expand, negative reactivity feedback is inherently introduced. Conversely, positive reactivity is introduced as the temperature decreases. This type of tightly coupled system requires tightly coupled multiphysics simulation with high fidelity predictability. Reactor system simulation tools which utilize modern

numerical methods, that have high temporal and spatial accuracy (and quantifiable uncertainty), and better physical models, that have realistic physical length scales and time scales, can be used to predict the reactor behavior where experimental data does not exist. Due to the exponential growth of computer speed and memory while the price held affordable and the rapidly growing cost of conducting experiments, high fidelity simulations are becoming increasingly important for advanced reactors. This requirement for predictability is the motivation for a large scale overhaul of all of the models and assumptions in transient nuclear reactor safety simulation software.

At Idaho National Laboratory, we have launched an effort to simultaneously address the main obstacles in the existing nuclear reactor simulation codes. Over the past few decades, significant progress has been made to develop innovative fully coupled algorithms for solving the partial differential equations describing strongly coupled and complex phenomena. These new algorithms provide a mechanism to remove operator splitting and to allow the coupled equations to be solved implicitly to improve accuracy and efficiency⁶⁻¹⁴. In addition, the nonlinear solution software packages such as PETSc (Portable, Extensible Toolkit for Scientific Computation)¹⁵ are readily available for free. These algorithms and scalable software packages will be utilized to facilitate the developmental Modern well posed two-phase flow models will effort. employment of more accurate spatial allow the Improved closure models that include discretization. physically realistic length scales and time scales will improve the physical model accuracy as well as the spatial and temporal accuracy. Our long term objective for this effort is to develop a high fidelity system analysis code named SARAH (Safety Analysis for Reactor Applications with High fidelity) that employs modern physical models, numerical methods, and computer science for transient safety analysis of generation IV nuclear reactors.

This paper provides an overview of the developmental effort. The current status of the development effort as well as some results from analyzing a simplified primary system of a conventional pool type sodium cooled fast reactor¹⁶ will be presented. Various simplified transient analyses are performed with this simplified SFR model to study two fundamental issues related to system analysis codes – accuracy of numeric algorithm and efficiency from the perspective of CPU time needed to achieve the same level of accuracy.

II. SARAH DEVELOPMENT CONSIDERATIONS

In order to have a successful development of the SARAH project, three broad areas will be addressed – software engineering, physical modeling and numeric

method development. Fig. 1 illustrates the paradigm of the SARAH code development. From the software engineering perspective, modern code infrastructure and design pattern should be employed such that the code can be easily extended and maintained. The code should have a user friendly interface. From the physical models development perspective, the partial differential equations used will be in well posed and conservative format. It should be noted that the two-phase flow equations used in TRAC and RELAP are not well posed. Because of the numerical viscosity induced by the first order upwind advection scheme employed in the discretization of these equations, the discrete solution of these ill posed equations are used.

The subgrid physics modeled by closure models developed in the context of the PDEs will have physically realistic time scales and length scales. The last but not the least is the availability of robust grid generation capability. Grid generation is an essential aspect of all numerical methods that employ finite differences, finite volumes and finite elements for the solution of PDEs. Shortly put, it consists in subdividing bounded or unbounded domains into elements. The topic of grid generation has become a field on its own. A good grid can accelerate the convergence of the solution, while a bad grid can even lead to a divergent solution. Advanced multiphysics methods have to work in conjunction with high quality grids to provide accurate solutions.



Fig. 1. The paradigm for SARAH development.

From the numerical methods perspective, the solution algorithm will be based on the physics-based preconditioned⁶⁻⁸ Jacobian-free Newton-Krylov⁹⁻¹¹ (JFNK) solution methods. In this approach all of the physical

models are solved implicitly and simultaneously in a single nonlinear system. This includes the coolant flow, nonlinear heat conduction¹², neutron kinetics (including precursors)¹³, and thermal radiation¹⁴ including all of the nonlinear

coupling mechanism such as conjugate heat transfer and neutron cross section feedback mechanisms. Including modern physical models and accurate space and time discretizations will allow this code to be 2nd order accurate in space and time. The JFNK nonlinear solver algorithm provided by PETSc will be utilized. PETSc is a versatile nonlinear solver library developed at Argonne National Laboratory, which provides object-oriented data structures and solvers for scalable scientific computation on parallel computers. PETSc provides algorithms that compute the JFNK matrix-vector product within its Krylov solvers. The library is extremely flexible and extensible providing data structures for user-defined algorithms such as physicsbased preconditioning, which is easily instrumented within the PETSc preconditioning shell. The JFNK algorithm will be accelerated with the adaptation of the physics-based preconditioning. The spatial accuracy and the temporal accuracy of the discretized from of the PDEs will be 2nd order accurate. Highly efficient sensitivity analysis will be obtainable with the problem solutions¹⁷.

III. BRIEF REVIEW OF JFNK METHOD AND PHYSICS-BASED PRECONDITIONING

The JFNK method is an efficient method to solve nonlinear equations. It is a nested iteration method consisting of four levels. The outermost level is the implicit time stepping with time steps chosen to accurately simulate the transients. Within the time stepping level are multiple Newton iterations (nonlinear solver) required to converge nonlinearities and these iterations are building up Krylov iterations (linear solver) out of which each Newton correction is drawn. The overall efficiency of the JFNK method is dominated by the convergence rate of the Krylov iterations. Interior to the Krylov iteration, a preconditioner is usually implemented to accelerate the convergence rate of the Krylov iteration.

Over the past decade, application of JFNK method has been investigated to solve fully coupled system of equations. First introduced by Brown and Saad¹⁸ in 1994, the JFNK algorithm avoids the explicit computation and storage of the Jacobian matrix used in the Newton's method to solve a coupled nonlinear system of equations through a numerical approximation of the Jacobian matrix and a Krylov vector product performed within iterative Krylov solvers. By eliminating the need to compute and store an explicit Jacobian matrix, the algorithm provides computational savings both in memory and computational time. The technique has gained popularity within the numerical methods development community, particularly in models simulating coupled nonlinear multiphysics problems. The following part presents a brief overview of the JFNK methodology and physics-based preconditioning.

Let us consider a set of implicitly time discretized nonlinear system of equations of the form

$$f(x) = 0 \tag{1}$$

where f represents a vector valued function of nonlinear residuals for the conservation equations, such as conservation of mass, momentum, energy, and neutron diffusion etc., and x represents a vector containing all of the state variables such as density, momentum, energy, temperature and neutron fluxes, etc..

$$f = \{f_1, f_2, ..., f_i, ..., f_n\}^T$$
(2)

$$x = \{x_1, x_2, \dots, x_i, \dots, x_n\}^T$$
(3)

where i represents the component index. Applying Newton's method to solve this nonlinear system iteratively involves solving a sequence of linearized problems defined by

$$J^{k} \delta x^{k+1} = -f(x^{k}) \tag{4}$$

where J represents the Jacobian matrix, the superscript k is the Newton iteration index, δx^{k+1} is the update vector and $\delta x^{k+1} = x^{k+1} - x^k$. The (i,j)th element (*i*th row, *j*th column) of the Jacobian matrix is the derivative of the *i*th equation (f_i) with respect to the *j*th variable (x_j) . A Jacobian matrix is generated by computing derivatives of the function with respect to all degrees of freedom

$$J_{i,j} = \frac{\partial f_i}{\partial x_i} \tag{5}$$

Finding each element of the Jacobian matrix can be both error-prone and time consuming process for many problems. Eq. (4) is solved for δx^{k+1} and the new Newton iteration value for vector x is then computed from

$$x^{k+1} = x^k + d\delta x^{k+1} \tag{6}$$

where *d* is a damping parameter that is computed to keep the components of *x* in physically realizable space and the same damping value is applied to all of the updates. The state variables are updated and the residuals are recalculated. This iterative process continues until either the norm of the nonlinear residuals or the δx vector is less than a specified tolerance. The linear system of equations (Eq. 4) is then solved using an iterative Krylov solver such as GMRES¹⁹. The GMRES (Generalized Minimum RESidual) method, introduced by Saad and Schultz, is a popular and efficient Krylov subspace method used to solve nonsymmetric system of equations. The GMRES algorithm generates a sequence of orthogonal vectors, and because the matrix being inverted is not symmetric, short recurrence relations cannot be used as in the case of the Conjugate Gradient algorithm²⁰. Instead, all previously computed vectors in the orthogonal sequence have to be retained. One matrix-vector product is required per Krylov iteration, as in

$$w = Jv \tag{7}$$

With JFNK, the Jacobian-vector product in Eq. (7) is approximated through a perturbation or finite differencing of the residuals in the direction of the Krylov vector

$$Jv \approx \frac{f(x + \mathcal{E}v) - f(x)}{\mathcal{E}}$$
(8)

Where ϵ is a small parameter used to control the magnitude of perturbation. The matrix-free approximation introduced in Eq. (8) is used to create the Jacobian-free framework. Detailed information on the exact numeric algorithm and implementation of GMRES in the JFNK framework as well as the optimal equation for choosing the perturbation parameter ϵ has been shown in reference 12.

JFNK has several advantages, including avoiding the expensive operation of computing and storing the Jacobian matrix. In addition, the numerical approximation prevents programming or coding errors often introduced by computing derivatives analytically to generate the Jacobian matrix. However JFNK is often slower for solutions requiring a large number of Krylov iterations per Newton iteration since repeated evaluation of the perturbed residuals becomes more expensive than processing the Jacobian matrix. Therefore, to fully realize the benefit of JFNK, it must be combined with efficient preconditioning to reduce the number of Krylov iterations can be accomplished by right preconditioning the linear system

$$J^{k}P^{-1}P\delta x^{k+1} = -f(x^{k})$$
(9)

Where P is the linear preconditioning process. The solution of this system can be divided into two steps by first solving the system

$$J^{k}P^{-1}s = -f(x^{k})$$
(10)

for *s*, where $s=P\delta x^{k+1}$, and then back-solving to obtain δx^{k+1} from the equation

$$P\delta x^{k+1} = s \tag{11}$$

With respect to a Krylov solver such as GMRES, an ideally preconditioned matrix ($P^{I}J$ or $J^{I}P$) is the one that is close to normal and whose eigenvalues are tightly clustered around some point away from the origin²¹. Obviously if P=J, the preconditioned matrix would be the identity matrix and GMRES would converge in a single iteration. However, although P should be a good approximation to J, the cost of constructing P should be minimal and solving the system

$$P\delta x = -f(x) \tag{12}$$

should be much easier than solving the original system. Therefore, P should be a simplified approximation to J. The traditional approach to preconditioning is to construct the preconditioning matrix P which approximates the Jacobian matrix J and then compute P^{-1} in a fast manner.

An efficient preconditioning technique has been developed called "physics-based" preconditioning based on the recognition that there exist numerous operator split methods to solve non-linear equations. These methods, though fast but inaccurate, do provide some insights into the time scales or physical behavior of the problem. These traditional methods can be coupled to an accurate method such as JFNK to provide a hybrid method that is fast and accurate. The traditional operator split method such as RELAP used, which has problems with stability and accuracy, can be used to provide a good estimate of the solution. The JFNK method, in turn, can converge to the correct solution with a small amount of computational work. Detailed discussion of physics based preconditioning can be found in references 6, 7, 8 and 12.

IV. DYNAMIC TIME STEP CONTROL

The appropriate time steps used in the solution methods should resolve the dynamic timescales of the physics in the problem¹⁰. Since the timescales in the problem are changing as the problem is evolving over time, an efficient algorithm would adjust the time step to adapt to the changing dynamic timescales. That means short time steps should be taken when the problem is changing rapidly while large time steps be taken when the problem is changing slowly.

In order for the traditional operator split approaches which use semi-implicit solutions to be numerically stable, the time step is constrained by the material Courant limit. The material Courant limit dictates that in order to achieve numerical stability, a particle of fluid may not pass through a calculational cell during a single time step. This leads to a certain maximum time step size that can be used in the simulations. The weakness of this type of time step control is that it does not consider the varying timescales of the state variables in the problem except for the velocity. Time steps dictated by the material Courant limit may be much smaller or much larger than those required to capture the timescales of the physics in the problem resulting in excessive computation or inaccurate results respectively.

Because of the fully implicit nature in JFNK methodology, there is no numerical stability limit and consequently the time step sizes can be determined based on the rate at which state variables change and the error control. The time step used here is called dynamical time step size control. The dynamical time scales for a generic state variable θ is given by

$$\tau = \left(\frac{1}{\theta} \frac{\partial \theta}{\partial t}\right)^{-1} \tag{13}$$

For a system that contains multiple equations in multiple variables and in multiple control volumes, a dynamical time scale is computed for each variable in each control volume. The time step is then based on the minimum of all the dynamical time scales for all control volumes.

The dynamical time scale for each variable in each control volume is given by

$$\tau^{n+1} = \left| \frac{0.5(\theta^n + \theta^{n-1})\Delta t^n}{\theta^n - \theta^{n-1}} \right|$$
(14)

Taking the minimum across all control volumes and all variables, we obtain

$$\Delta t^{n+1} = \min[\tau^{n+1}, \alpha \Delta t^n]$$
(15)

where α controls the maximum rate at which the time step is allowed to grow.

V. A SIMPLIFIED SFR MODEL ANALYSIS

In this section, the analysis results for a simplified SFR primary system model of are presented as an example of the SARAH application. The efficiency and accuracy (efficacy) studies were performed to highlight the importance and necessity of developing high fidelity reactor system safety analysis.

Fig. 2 provides a schematic view of the simplified primary system of a typical pool type SFR. This simplified model only considers the reactor core, the hot pool, intermediate heat exchangers (IHX), primary pumps and the cold pool. For the results present below, the IHX and the reactor core are modeled as one-dimensional components. The hot pool and the cold pool are modeled as zero dimensional components.



Fig. 2. Schematics of the simplified primary system of a pool type SFR.

Isothermal transients were run with the 1st and 2nd order method and various time steps for the above model, where the cold pool level is set lower than the hot pool level as illustrated in Fig. 2, with the wall friction set equal to zero and the pump model turning off. Fig. 3 plotted the cold pool level calculated with the 1st order in time method with time steps of 1/2 second and 1/16 second and 2nd order in time method with time step of 1/2 second. The first order method results were plotted in green while the second order method results in red. During the transient, the sodium flows from the hot pool to the cold pool and then back to the hot pool. Since there is no friction and no energy source or sink, the total energy of the system is conserved. The level of the hot pool and the cold pool keeps oscillating and the oscillation does not damp (similar to the manometer problem in RELAP developmental assessment and the U-tube developmental assessment problem in TRAC). As shown in Fig. 3, the 2nd order method preserves the magnitude of the cold pool level while the 1st order method damps that. Clearly the second order method provides a more accurate solution, though the first order method becomes more accurate when the time step is made smaller (the 1/2 second case shown by square symbols versus the 1/16 second case shown by circles). Very small time steps have to be taken in order for the 1st order method to match the same accuracy with the 2nd order method with much bigger time steps. For the high temperature gas cooled reactor with which transients could last up to two weeks, the operator split codes could have significant accumulated errors.



Fig. 3. Cold pool level as a function of time with 1st & 2nd order methods.

The cause of this problem is shown in Fig. 4 where the total energy (kinetic plus potential) of the system is plotted. Without friction, the potential energy is converted to kinetic energy and then back to potential energy like a pendulum. Here one can see that the 2nd order in time method conserves the total energy of the system while the 1st order in time method removes energy from the system due to the truncation error. The larger time step results bigger truncation error for the 1st order in time method and consequently renders the energy loss at faster rate. This simple test problem from the simplified primary system model of a SFR clearly demonstrates the importance of having high order accuracy simulation for nuclear reactor simulation. It is sometimes argued that inaccuracy in simple test problems (with no friction and total energy is conserved) does not imply inaccuracy in a "real" problem (with friction).



Fig. 4. Total energy of the system versus time with the 1st and 2nd order methods.

Transients with 1st order and 2nd order methods were run for the same model that includes friction at fixed time step of $\frac{1}{2}$ second. The system total energy with and without friction is shown in Fig. 5. Here the friction results are in dashed lines and the no friction results are solid lines. The difference between the solid red line and the dashed red line is due to the physical damping calculated with 2nd order in time method resulted from the added friction term. However, the 1st order in time method calculated much smaller physical damping effect as shown by the solid and dashed green lines. One can see that the numerical (truncation) error introduced by the first order method dominates the physical damping in the problem. The 1st method generates results that are not sensitive to the friction variations. The commonly used uncertainty quantification method is the "black box" approach, with which a large number of cases have to be run. Large time steps have to be taken in order to get the cases run at reasonable amount of time. The results may fall into the domain that is discussed here in which the "unphysical" numerical (truncation) error has become the dominant physics in the transient. This implies that if uncertainty quantifications were to be performed with the "black box" approach using a traditional operator split code, misleading results could be obtained. Conversely, the 2nd order in time method has very small numerical error and correctly captures the physical damping effect. Hence, meaningful uncertainty quantifications can be performed with a 2nd order accurate method.

Another point to be made with Fig. 5 is that it is an example of where "tuning" comes in. The first order numerical error had the same effect as making the friction

larger. Therefore to match data with the first order method one has to lower the correct friction and produce a compensating error. However, if a test problem has no analytical solution or experimental data, one does not know how to "tune" the model.



Fig. 5. Total energy of the system versus time with and without friction.

The above accuracy studies carried out by comparing the second order method with the first order method show that numerical errors in the first order method are large and it is very difficult to distinguish numerical errors from physical modeling errors. On the other hand, second order method yields small numerical errors and it is very easy to spot physical modeling errors. Therefore, having second order method enables us to focus more on better physical modeling to provide accurate predicative simulation capability.

The previous studies addressed accuracy issue associated with reactor system analysis and the following studies will address the efficiency issue. As discussed above, the operator split method used in the current generation of nuclear reactor simulation tools reduces the accuracy to first order in time but also introduces stability restrictions caused by the explicit coupling. A good example of this is the semi-implicit method employed by RELAP. In this method the pressure gradient in the momentum equation, is operator split from the advection term which results in a stability limit that requires that a particle of fluid cannot cross a control volume in a single time step (the CFL stability limit).

The efficiency study was carried out in the next simulation with the wall friction turned on and the pump

model enabled. The transient starts with an initial level difference of two meters between the cold pool and hot pool, with a constant pump head of one meter.



Fig. 6. Total energy of the system versus time with and without friction.

The pool levels as a function of time are shown in Fig. 6. Note that this is a log-linear plot and that time is logarithmic and level is linear. Here one can see the levels coming to a new equilibrium as the pump head levels off at one meter.



Fig. 7. Comparison of the dynamic time step and the time step according to the CFL stability.

The time steps for the fully implicit solution method and the CFL stability limit method are compared. The time step for the transient shown in Fig. 6 is given in Fig. 7. Here one can see that the fully coupled, implicit method can run time steps 10,000 times larger (shown in red) than the stability based time step required by operator split codes (shown in green). Note here that both time and timestep are on a logarithmic scale. The dynamic time steps used in a fully implicit method adjusts the time step to resolve the time scales during the various stages of a long lasting transient. This will make a computer code based on fully implicit methods run more efficiently than a CFL stability limit method code like RELAP, in which a particle of fluid cannot cross a control volume in a single time step.

VI. CONCLUSIONS

We have launched an effort to develop a system analysis code with high fidelity for advanced Gen-IV reactors at INL, starting from SFR and will be extended to VHTR and advanced LWRs in the future. The new developmental effort will incorporate state-of-the-art numerical methods, physical models and computing technology. The example problems shown in this paper demonstrated the importance of high fidelity simulation to provide accurate predicative simulation for sodium cooled reactors. Much more efforts are needed to realize the SARAH goals and make it applicable to safety analyses for advanced reactor systems.

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ACRONYMS

- CFL the Courant Friedricks and Lewy limit
- GMRES Generalized Minimal RESidual algorithm
- IHX Intermediate Heat Exchanger
- JFNK Jacobian-free Newton-Krylov method
- PDE Partial Differential Equation
- PETSc Portable, Extensible Toolkit for Scientific Computation
- SARAH Safety Analysis for Reactor Applications with High fidelity
- SFR Sodium cooled fast reactor
- VHTR Very High Temperature Reactor

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