Review of Tools for Modeling Core Radial Expansion in Liquid Metal-Cooled Fast Reactors

Nuclear Science and Engineering Division

About Argonne National Laboratory

Argonne is a U.S. Department of Energy laboratory managed by UChicago Argonne, LLC under contract DE-AC02-06CH11357. The Laboratory's main facility is outside Chicago, at 9700 South Cass Avenue, Argonne, Illinois 60439. For information about Argonne and its pioneering science and technology programs, see www.anl.gov.

DOCUMENT AVAILABILITY

Online Access: U.S. Department of Energy (DOE) reports produced after 1991 and a growing number of pre-1991 documents are available free at OSTI.GOV (<http://www.osti.gov/>), a service of the US Dept. of Energy's Office of Scientific and Technical Information.

Reports not in digital format may be purchased by the public from the National Technical Information Service (NTIS):

U.S. Department of Commerce
National Technical Information Service
5301 Shawnee Rd
Alexandria, VA 22312
www.ntis.gov
Phone: (800) 553-NTIS (6847) or (703) 605-6000
Fax: (703) 605-6900
Email: **orders@ntis.gov**

Reports not in digital format are available to DOE and DOE contractors from the Office of Scientific and Technical Information (OSTI):

U.S. Department of Energy
Office of Scientific and Technical Information
P.O. Box 62
Oak Ridge, TN 37831-0062
www.osti.gov
Phone: (865) 576-8401
Fax: (865) 576-5728
Email: **reports@osti.gov**

Disclaimer

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor UChicago Argonne, LLC, nor any of their employees or officers, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of document authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof, Argonne National Laboratory, or UChicago Argonne, LLC.

Review of Tools for Modeling Core Radial Expansion in Liquid Metal-Cooled Fast Reactors

prepared by
Nicholas Wozniak¹, Emily R. Shemon², and James J. Grudzinski¹

¹Experimental Operations and Facilities Division, Argonne National Laboratory

²Nuclear Science and Engineering Division, Argonne National Laboratory

November 30, 2020

Abstract

Core radial expansion in liquid-metal cooled fast reactor systems is a well-known phenomenon that produces strong reactivity feedback effects. It is crucial from a safety standpoint to design a reactor with the proper core restraint system to guide expansion of the fuel assemblies into a formation that produces negative reactivity feedback in accident conditions. However, the modeling of core radial expansion and its associated reactivity feedback is extremely challenging. Liquid metal-cooled fast reactor designers (both industry and commercial) have pointed to improved modeling of core radial expansion as a key modeling challenge for these types of reactors. The Department of Energy Nuclear Energy Advanced Modeling and Simulation (DOE-NEAMS) program has an important role to play in helping to develop a robust, predictive tool for this phenomenon.

A literature review has been performed to identify current simulation capabilities applicable to the prediction of core radial expansion in liquid metal-cooled fast reactors and the resultant reactivity feedback effects. An overview as well as a detailed description of the multi-physics phenomena underlying core radial expansion is given in the first two chapters. The objective of this report is to identify existing software that has been or could be applied to the core radial expansion problem, and then to identify possible paths to develop a robust, coupled multiphysics tool for advanced analysis, in which all three physics (radiation transport, structural mechanics, thermal fluids) are taken into account considering feedback effects from each physics to the other.

Several computer codes and workflows have been developed in the United States and abroad to perform individual aspects of radial expansion calculations or to perform loosely coupled analysis. No code system currently exists which tightly and robustly couples the neutronics, thermal hydraulics, and thermal mechanical physics with enough detail to fully resolve the complex core radial expansion reactivity feedback effects. The future availability of such a code system is of vital importance to fully understanding the reactivity feedback effects that occur due to radial expansion, and consequently to optimizing the design of the core restraint system. A potential code development path forward using MOOSE-based tools is suggested in order to leverage the natural tight coupling and robustness of MOOSE-based applications. Additionally, potential gaps for modeling and common assumptions are listed which require further investigation to ensure accuracy for prediction of deformations.

Contents

Abstract	i
Contents	ii
List of Figures	iv
List of Tables.....	vi
1 Introduction.....	1
2 Mechanics of Deformation	2
2.1 Grid Plate Expansion and Bowing Due to Thermal Gradients	2
2.2 Irradiation Creep and Swelling	4
2.3 Core Restraint System.....	9
2.3.1. Free Flowering	10
2.3.2. Limited Free-Bow	11
3 Codes for Modeling Core Radial Expansion	14
3.1 NUBOW-3D.....	14
3.2 DIF3D/SAS4A/SASSYS-1 Workflow.....	19
3.3 SHARP (PROTEUS, Nek5000, Diablo)	20
3.4 RAINBOW.....	23
3.5 OXBOW	23
3.6 ARKAS / ATLAS	27
3.7 FAST	31
3.8 GeN-Foam.....	32
3.9 IWGFR Participating Codes.....	33
3.10 High-Fidelity Finite Element Method (FEM) Software	33
3.11 Multiphysics Object Oriented Simulation Environment (MOOSE) and MOOSE- Based Applications	34
3.11.1. MOOSE Tensor Mechanics Module	36
3.11.2. MOOSE Contact Module	37
3.11.3. BISON	37

3.11.4.	Grizzly	38
3.11.5.	Systems Analysis Module (SAM)	38
4	Gaps for Modeling Core Expansion and Path Forward	45
4.1	Tight Coupling to Reactivity Feedback	45
4.1.1.	MOOSE-Based Physics Coupling.....	45
4.1.2.	Other Possible Coupling Schemes	46
4.2	Material Properties	46
4.3	Validation of Modeling Assembly Internals	47
4.4	Nozzle Boundary Condition Experimental Validation	47
4.5	Geometric Uncertainties.....	48
5	Summary	49
6	References.....	50
	Appendix A – Description of IWGFR Example Problems.....	55
	Appendix B – Description of Mechanical Contact Models	60

List of Figures

Figure 1. Schematic representing the axial thermal gradient.....	3
Figure 2. Representation of the radial thermal gradient and radial power profile.....	4
Figure 3. Example of swelling strain rate as a function of temperature	5
Figure 4. Schematic of bowing effects, top row without restraint and bottom row with restraint. a) and b) show bowing due to a thermal gradient with irradiation creep, c) and d) show irradiation swelling bowing due to a flux gradient (Adopted from [6])..	6
Figure 5. Representation of the summation of deformation due to multiple mechanical affects for each assembly duct	8
Figure 6. Schematic of Free Flowering core restraint system, (a) ducts at uniform temperature and zero power, (b) outward bow due to thermal gradient and increasing power to flow ratio	11
Figure 7. Schematic of the limited free bow restraint system in a reactor vessel showing the fuel assemblies in elevation view with load pads and restraint rings	12
Figure 8. Schematic of Limited Free-Bow core restraint system, (a) ducts at uniform temperature and zero power, (b) outward bow due to thermal gradient and increasing power to flow ratio, (c) lock-up at the ACLP at full power showing reverse bending in core region.....	13
Figure 9. Schematic showing the centerline deformation of a duct in NUBOW-3D	15
Figure 10. Duct geometry	16
Figure 11. NUBOW code schematic	17
Figure 12. SHARP coupling and iteration workflow.....	22
Figure 13. Assembly deformation in a free-bow sodium-cooled fast reactor design calculated by SHARP (adopted from [23]).....	22
Figure 14. ARMI interface stack schematic showing the reactor model coupled with the physics models (adopted from [28])	25
Figure 15. ATLAS workflow for core bowing reactivity calculations	29
Figure 16. FAST code system structure.....	32
Figure 17. MOOSE Framework.....	35
Figure 18. Example of self-similar pattern of mesh refinement for 1D elements (top row), 2D quadrilateral elements (second row), and 3D hexahedral elements (bottom row) (adopted from [43]).....	36
Figure 19. Tensors required to fully describe a mechanics material (adopted from [43]).....	37
Figure 20. Coupling structure schematic for fuel axial expansion (Adapted from [44]).....	39
Figure 21. Coupling structure schematic for core radial expansion (Adapted from [44]).....	41

Figure 22. Mesh for hollow disk (left) and grid plate (right) (Adopted from [44]).....	41
Figure 23. Grid plate thermal expansion verification results (Adopted from [44]).....	42
Figure 24. Single channel radial expansion reactivity comparing SAM standalone calculations (solid black line) with the coupled Tensor Mechanics results (triangle points) (Adopted from [44])	43
Figure 25. 5 Channel reactivity feedback calculations for the ABTR comparing SAM standalone calculations (solid lines) with the coupled Tensor Mechanics results (dashed lines), (Adopted from [46])	44
Figure 26. Fixed end beam deflection.....	48
Figure 27. Pin-roller with beam overhang deflection	48
Figure 28. Model for example 3A of 60° symmetric core region with a free boundary, represented by the red dashed line. The blue arrow indicates the direction of the thermal gradient induced bow for duct 1 (Adapted from [19] © IAEA).....	57
Figure 29. Model for example 3B of 120° symmetric core region with a free boundary, represented by the red dashed line. The blue arrow indicates the direction of the thermal gradient induced bow for duct 1 (Adapted from [19] © IAEA).....	57
Figure 30. Model for example 4 of 30° symmetric core region, represented by the red dashed line, with a core restraint ring at the TLP and ACLP. The blue arrows indicate the direction of the thermal gradient induced bow for ducts 42, 43, and 44 (Adapted from [19] © IAEA).	58
Figure 31. Core model showing the location where the neutron damage dose is active within the circle, for examples 5, 6, and 8A (Adopted from [19] © IAEA).....	59
Figure 32. Beam model contact, with (a) before contact and initial gap, g, and (b) after contact.....	61
Figure 33. Beam model penalty contact, with (a) before contact with initial gap, g, and spring stiffness, k, and (b) after contact with small penetration, d	63

List of Tables

Table 1. Summary of deformation responses based on the different mechanisms of action within a reactor	2
Table 2. Description of duct geometric parameters at the reference temperature	16
Table 3. NUBOW summary of IWGFR verification results	19
Table 4. Summary of ARMI physics modules and integrated codes (adapted from [28])	25
Table 5. Summary of IWGFR problems analyzed with OXBOW with the average of the assembly displacement differences compared to IWGFR participants	26
Table 6. ARKAS summary of IWGFR verification results (ARKAS data from [32]).....	30
Table 7. Geometric and material properties of grid plate	42
Table 8. IWGFR participating organizations and their codes (adapted from [19] © IAEA) ..	55

1 Introduction

Fast reactor core reactivity is sensitive to core assembly movement. The long mean-free-path of neutrons in a fast spectrum system allows neutrons to leak out of the system through new pathways opened up by even small amounts of core assembly movement. Temperature changes within the reactor cause thermal expansion of the reactor materials, changing the geometry of the reactor and the density of the material within it. In addition, structural deformations can be induced by temperature gradients that result in bowing, by elastic deformation due to high stresses, or by buckling as a consequence of axial restraint on thermal expansion. To design an inherently safe fast reactor, reactivity due to bowing needs to be engineered into the reactor plant to assure a net negative reactivity insertion during transient events [1]. The location and geometry of the fuel assemblies is a driving parameter for this. The reactivity of the core is highly dependent on the position of the fuel elements which are supported in an array within a thin-wall hexagonal duct (Figure 1). Thermal and fast neutron flux gradients within the core cause the assembly ducts to swell and bow. This bowing is both of a transient (elastic thermal strains depending upon power profile) and permanent (inelastic irradiation creep and swelling strains that depend on time and fluence) nature. Transient bowing of core assemblies causes significant changes in reactivity during reactor start-up, transient overpower (TOP), and unprotected loss of flow without scram (ULOF) [2]. During unprotected loss-of-flow (ULOF), P/F can reach double that of nominal conditions [1]. The negative reactivity feedback due to bowing is usually the dominant reactivity feedback during unprotected accidents in advanced liquid metal-cooled reactors (LMR) [3]. The permanent bowing of the ducts changes the reactivity over time and more importantly affects the mechanical forces required to refuel the core because the displacement of some ducts due to bowing is greater than the duct-to-duct clearance.

For both safety and operational reasons, it is important to control the location of the ducts to a small tolerance. A core restraint system that properly constrains the duct location is necessary. It is also necessary however that this system leave a gap between ducts to accommodate irradiation swelling that accumulates over time as a result of the fast neutron fluence. If insufficient clearance exists, the ducts swell into contact with each other and become difficult to remove during refueling operations. The burn-up of the core is then limited by swelling. However, leaving the ducts with too much clearance provides too large of an available reactivity insertion in the event of sudden compaction.

2 Mechanics of Deformation

It is important to understand the physical phenomena that contribute to core radial expansion in order to see how the deformations themselves affect the reactivity. There are two main mechanisms that contribute to the radial expansion. The first is **grid plate expansion** due to heating and thermal expansion of the grid plate, which uniformly separates all of the assembly ducts. The second is **bowing deformation of assembly ducts** driven primarily by changes in temperature and temperature gradients, as well as creep and swelling effects driven by changes in flux and flux gradients throughout the core. Table 1 summarizes the mechanisms that drive core deformation. These mechanisms are explained further in this chapter.

Mechanism of Action	Deformation Response
Temperature Increase	Grid plate thermal expansion
Thermal Gradient	Duct bowing, in direction of gradient from hotter to colder
Restraint	Limit on the amount of deformation possible, at contact there is a compression force applied at the load pad resisting further deformation
Irradiation (flux)	Irradiation induced creep deformation when restraint present, acting in the direction of the restraint force
	Irradiation induced swelling expansion

Table 1. Summary of deformation responses based on the different mechanisms of action within a reactor

2.1 Grid Plate Expansion and Bowing Due to Thermal Gradients

The grid plate at the bottom of the core holds assemblies in position so that the base of each assembly does not move significantly in the radial or axial direction during operation. Grid plate expansion is driven by an increase in temperature as the reactor transitions from cold to hot condition during startup. As the temperature in the core increases, the grid plate structural material expands which uniformly separates all of the assembly ducts, effectively increasing the assembly pitch. This separation of assemblies has a reactivity feedback effect due to new pathways opened up between assemblies.

At power, the thermal gradient in the core manifests with distributions in both the axial and radial directions. The axial thermal gradient is due to the temperature change of the fuel during radiation bombardment and fission reactions. The axial thermal gradient is impacted by the axial power distribution which generates heat, and the coolant flow rate which removes heat as the

coolant passes axially through the core. The radial temperature gradient is due to radial power distributions and inter-assembly heat transfer between core assemblies; temperature is generally highest in the center region of the active core and decreases radially outward. These radial temperature gradients occur between assemblies and also within any individual assembly. When one wall of an assembly has a higher temperature than another, the wall with higher temperature thermally expands by a greater amount than the lower temperature wall, causing the assembly to deform in the direction of the gradient from higher temperature to lower temperature. This bending deformation is called bowing [4]. LMFBR core environments are subjected to a large temperature rise from the core inlet to the core outlet, with the increase in temperature and temperature gradient occurring primarily in the fuel region [5].

Figure 1 depicts axial thermal gradients on two walls of a ducted assembly. Below the core region (where heat is generated due to fission processes), the temperature is constant and the same on both duct walls. As the elevation in the active core increases, the temperature on one duct wall increases more quickly than on the other wall, such that the two walls have different axial thermal gradients and different temperature at the top of the active core region.

Figure 2 depicts radial thermal gradients for a row of assemblies in a core. Assembly location, flow rate, and radial power distribution all impact these gradients. In the example shown, the assembly walls closer to the core center have higher temperatures and will consequently expand more than the wall further from the core center, driving the assembly to bow away from the core center. Furthermore, the radial thermal gradient is smaller for assemblies near the core center due to flatter radial power distribution.

Figure 1. Schematic representing the axial thermal gradient

Figure 2. Representation of the radial thermal gradient and radial power profile

2.2 Irradiation Creep and Swelling

Irradiation of structural materials by neutrons creates an additional deformation component that is both time-dependent and mostly non-recoverable (inelastic). Irradiation can cause two main modes of additional deformation, swelling and creep.

Irradiation swelling is the rearrangement of the atoms of a material due to neutron interactions, which results in the increase in volume and decrease in density of a material. Creep is an inelastic deformation defined as the gradual deformation of a component under sustained loading; over time, a component will relax the internal stresses induced by the loading and transform them into inelastic creep strains. Creep deformation is a property of many materials and is a function of time and temperature. Normally, steel does not experience creep deformation, except at extremely high temperatures not normally experienced in a nuclear reactor. However, neutron irradiation exposure can influence steel materials to creep under much lower temperatures. Irradiation creep is the gradual deformation due to the sustained loading induced by contact restraints on deformation in a nuclear reactor [5]. Irradiation swelling and creep are unique temperature and flux dependent material properties which depend on the molecular structure of a specific material and require experimental testing to develop material correlations for prediction. The swelling rate as a function of temperature has a common shape, shown in Figure 3. As shown, the swelling peaks at a specific temperature and reduces at high temperatures; for different materials this peak value occurs at different temperatures.

Figure 3. Example of swelling strain rate as a function of temperature

Figure 4 illustrates an example of duct bowing resulting from thermal gradients and flux gradient effects individually. The top row of figures shows the resulting bowed deformation for a single *unrestrained* duct due to a thermal gradient (a&b) and a flux gradient (c&d). The bottom row of figures shows the *restrained* case.

In the unrestrained case (top figures in Figure 4a and Figure 4b), the duct bows outward when subjected to a thermal gradient (at power). The dashed centerline represents the center of the duct in the straight, vertical position, and the solid line represents the duct centerline deformation. The duct returns to the straight, vertical position at uniform temperature (zero power). There is no effect of creep since the duct is free to deform without generating any internal stresses. In the restrained case (bottom figures in Figure 4a and Figure 4b), there is a restraint placed with an initial clearance (gap), allowing the duct to freely deform before contact occurs. The restraint represents the physical boundary set by a restraint ring on the core barrel preventing excessive deformation of an outer row of ducts. At power, the duct bows until it closes the gap between the duct and the restraint, which results in contact forces and induced internal stresses in the duct. The dashed line represents the unrestrained bow, while the solid line represents the restrained bow. Irradiation creep begins to take effect, resulting in some inelastic (permanent) deformations as the stresses induced by the restraint contact start to relax and cause creep strains. At the zero power condition, the duct has a residual inward bowed shape based on the magnitude of the creep strains. The primary factors affecting how much inward bow occurs are the initial duct-restraint gap and the

magnitude of the temperature gradient. A smaller gap or higher temperature gradient will increase the contact force and the internal stresses, resulting in larger creep strains and residual inward bow.

Figure 4c and Figure 4d illustrate the bowing due to swelling gradients. In the unrestrained case (top figures in Figure 4c and Figure 4d), the flux gradient produces an outward bow due to the direction of the swelling gradient. The dashed centerline represents the center of the duct in the straight, vertical position, and the solid line represents the duct centerline deformation. The duct does not return to the straight, vertical position when the flux gradient is removed because the deformation is inelastic (permanent). In the restrained case (bottom figures in Figure 4c and Figure 4d), there is a restraint placed with an initial clearance (gap), allowing the duct to freely deform before contact occurs. If creep is not present, the duct will remain in this position when the flux gradient is removed; if creep is present, some of the swelling strains can be “recovered”, or offset, by the creep strains due to the stresses induced by the restraint contact, resulting in a residual bow. The primary factors affecting the residual bow (outward or inward) are the magnitude of the flux gradient, the swelling gradient, and the creep.

Figure 4. Schematic of bowing effects, top row without restraint and bottom row with restraint. a) and b) show bowing due to a thermal gradient with irradiation creep, c) and d) show irradiation swelling bowing due to a flux gradient (Adopted from [6])

Due to the dependence on flux and temperature [7], the swelling usually acts in the opposite direction of creep deformation. At removal of power and temperature, the ducts deform back in the opposite direction. The resultant bowed shape of the assembly depends on whether swelling or creep is more dominant. Dominance of irradiation creep can completely relax the swelling induced bending stresses and lead to an overall outward radial bowed shape (bowed away from the core

center) during the refueling period. Dominance of swelling can prevent relaxation of swelling induced stresses and lead to a reverse, inward bowed shape during the refueling period [8].

Based on results of irradiation experiments from breeder reactor programs such as EBR-II with pressurized tube tests, relationships for swelling and creep effects (and their interrelation) have been empirically determined for different material properties [9]–[11]. It was also determined that the total effect on deformation can be combined with superposition of the component strains [8]. Superposition is a concept in mechanics which breaks up the problem into “component” deformations, which can be added up to calculate the overall deformation.

Figure 5 shows a representation of the summation of the component deformed shapes due to thermal and irradiation effects. Figure 5a shows the free bow shape (without restraint) when a duct bows due to thermal gradient effects. Figure 5b shows the shape taken by a duct restrained at two locations, the Above Core Load Pad (ACLP) and Top Load Pad (TLP). Figure 5c shows the resultant, restrained thermal bowed shape due to contact between adjacent ducts. Figure 5d shows the thermal bowed shape after the effects of creep deformation due to contact stresses. Figure 5e shows the free bow shape after the effects of swelling deformation. Finally, Figure 5f shows the resultant deformation due to the combined effects of (a), (d), and (e) which is thermal bowed, with the combination of creep and swelling deformations. The resultant inward or outward shape depends on whether creep or swelling is more dominant. This inelastic bowing leads to a situation in which the assemblies can contact each other during off power refueling phases due to residual bowed deformations. If the ducts are in contact during refueling operation, they become harder to remove, due to the contact force and friction coefficient between assemblies adding to the force required to remove the assembly from the reactor.

Figure 5. Representation of the summation of deformation due to multiple mechanical affects for each assembly duct

To calculate the deformed shape of the assemblies, if they remain in the elastic condition, the temperature effects can be evaluated as instantaneous changes. Normally, the base case for the deformation is calculated as “day 0” of the operation.

Irradiation creep and swelling are time-dependent components of the overall bowed deformation, accumulated over a long period of time, usually over the life of the core or the

refueling cycle. Transient events usually cause a large thermal gradient change over a short period of time. The deformation of assemblies in the case of an unexpected transient is usually driven more by this large thermal gradient change than the creep and swelling effects. Thus, the *creep and swelling effects are considered negligible in the deformation change of the reactor due to a transient event*, however, they are still important for predicting future deformed configurations of the core.

2.3 Core Restraint System

The mechanical system for restraining the core assemblies plays a significant role in the structural deformation and radial expansion of the core. The structural support system of the nuclear reactor core is called the Core Restraint System. Generally, each fuel assembly is restrained at the nozzle, which is the primary support point. Each duct also has one or two load pads along the height which are areas designed for contact between fuel assemblies. The inside of the core barrel of the reactor vessel will have one or more restraint rings at the same elevation as the load pads which are designed for contact between the outer fuel assemblies and the core barrel [2]. Two types of passive restraint systems are the **free-flowing** (free-standing) design and the **limited free-bow design** [6]. Previous investigations, [1], [2], [6], have shown that a limited free-bow restraint system (Figure 7) allows for greater negative reactivity insertion during transient events. Mechanical contact plays an important role in the estimation of the restraint ring response and is a difficult phenomenon to model. Appendix B provides some descriptions for different mechanical contact models and considerations.

Objectives of the Core Restraint System

The general requirements of the core restraint system are summarized as:

1. Control Reactivity
 - a. Control core assembly bowing and ensure predictable and safe reactivity response during steady state and transient events [9], [12], [13]
 - b. Provide large enough gaps at the load pads to ensure net negative reactivity feedback during transients [5], [14]
 - c. Limit maximum step reactivity insertion to stay within fuel damage limits [14]
2. Control Rod Movement
 - a. Control core alignment to allow complete insertion and removal of control rods during operation [9], [12]–[14]
3. Refueling Operation
 - a. Limit bowing to prevent excessive contact of assembly ducts to allow refueling [14]

- b. Limit the magnitude of the forces required to remove and insert core assemblies during refueling below the design limits of the core assemblies or the refueling equipment [5], [9], [12]–[14]
- 4. Irradiation Effects
 - a. Limit bowing effects caused by irradiation creep and swelling [9]
 - b. Provide gaps between ducts large enough to accommodate duct dilation (overall diameter change due to thermal expansion, internal pressure, swelling, creep, etc.) [5]
- 5. Structural Limits
 - a. Control and predict the inter-assembly contact forces during operation to keep the assemblies within their structural limits [5], [12]

2.3.1. Free Flowering

In the free-flowering design, depicted in Figure 6, core assembly ducts are rigidly supported from the grid plate, similar to cantilever beams. No restraint ring is present, but the peripheral (outer) assemblies in the core have ducts with greater stiffness and thicker duct walls to provide a “soft spring restraint during excessive top motion” [6]. Load pads are located in and/or above the core to prevent compaction. Figure 6a shows the nominal configuration of ducts at isothermal condition. As power increases and a radial thermal gradient is developed outward from the core center, the ducts bow outward (Figure 6b) and have a constant negative reactivity insertion slope with increasing power-to-flow ratio. The drawback of this design is the lack of a rigid physical bound (restraint ring) to limit the maximum amount of positive reactivity insertion: a free-flowering core can deform outwards more easily than a limited free bow core, and thus can experience significant positive reactivity insertion in the event of core compaction. The second drawback is lack of a restraint against lateral motion due to a seismic event [1].

Figure 6. Schematic of Free Flowering core restraint system, (a) ducts at uniform temperature and zero power, (b) outward bow due to thermal gradient and increasing power to flow ratio

2.3.2. Limited Free-Bow

In the limited free-bow design (Figure 7), ducts are supported at the grid plate to prevent translation in any direction, but are free to rotate, similar to a simply supported beam. Load pads are located above the core (ACLP) and at the top (TLP) of the core assemblies. There are also rigid restraint rings attached to the core barrel at the ACLP and TLP elevations. The TLP clearance is such that only a limited amount of outward bow is allowed before contact. The clearance at the ACLP is just large enough that contact is not made during normal reactor operations. The limited free bow design takes advantage of the thermal bowing/bending action of the ducts to provide an inherent safety mechanism during overpower transient events [6].

Figure 7. Schematic of the limited free bow restraint system in a reactor vessel showing the fuel assemblies in elevation view with load pads and restraint rings

Figure 8a shows the nominal configuration of the ducts at isothermal temperature. As the radial thermal gradient develops (temperature decreases as distance from centerline increases), the ducts begin to bow outward (Figure 8b) in the direction of lower temperatures. Prior to contact with the top core restraint ring, the duct bends away from the core centerline as the temperature increases and therefore causes negative reactivity feedback. After contacting the top restraint ring and as the temperature gradient increases, the center of the duct bows inward which temporarily increases the reactivity. As the gradient increases, the inward bowing continues until the ducts contact at the ACLP. When the interior ducts all contact at the ACLP, the reactor is '*locked-up*' and no further compaction can occur. Subsequent increased thermal gradients cause a reverse bowing below the ACLP moving the core region away from the core center as illustrated in Figure 8c. At this point, the reactivity generally decreases with constant negative slope as temperature increases. The core restraint system is designed to have this lock-up occur below the nominal operating core outlet temperature. *In this way, the core is already locked up during normal operation, and any transient events with increasing temperature will induce further outward bowing in the middle of the core* [6].

Figure 8. Schematic of Limited Free-Bow core restraint system, (a) ducts at uniform temperature and zero power, (b) outward bow due to thermal gradient and increasing power to flow ratio, (c) lock-up at the ACLP at full power showing reverse bending in core region

3 Codes for Modeling Core Radial Expansion

Several codes and associated workflows are currently used to model radial core expansion. These are described here. To the extent possible, each subsection describes how core expansion is determined by the tool by detailing models and approximations used inside the code, input and output data to the code, and any relevant verification and validation.

3.1 NUBOW-3D

NUBOW-3D [15] is a Fortran code developed by Argonne National Laboratory capable of performing structural analysis for liquid metal-cooled fast neutron reactors [16]. NUBOW was originally developed 1974 as a 2D beam analysis code [17], with the intent to expand the domain to 3D calculations, which was first completed in 1978 with the release of NUBOW-3D. A specific version, called NUBOW-FFTF, was used to perform calculations for core management of the Fast Flux Test Facility (FFTF), and had additional features to support core assembly shuffling and rotation [18].

NUBOW-3D calculates the bowing deformation of the reactor core assemblies by modeling the ducts as beam segments undergoing thermal bending. Irradiation creep and swelling as well as duct contact at the load pad locations are also considered in the bowing calculation. NUBOW-3D models ideal contact between the ducts without consideration for friction between load pads or duct rotation about the centerlines. It allows the core restraint ring to act as a boundary condition at the load pad locations and models the inlet nozzle as a pinned support for limited free bow design.

The outputs of NUBOW-3D include the centerline deformation at specified nodes along the length of each duct (Figure 9) and the gaps or contact forces (when gaps are closed) between each duct at the load pad locations.

Figure 9. Schematic showing the centerline deformation of a duct in NUBOW-3D

NUBOW-3D can perform analysis of a full core model or $1/12^{\text{th}}$ symmetric core model. To build the model, NUBOW-3D requires the full geometric description of the core assemblies as inputs for the calculations; these are shown in Figure 10 with a description of parameters in Table 2. NUBOW-3D assumes a hexagonal array for the assemblies and will create the full core, or $1/12^{\text{th}}$ symmetry model, based on the pitch and the number of rows and assemblies. It also requires a description of the temperature and flux distribution of the cross section at certain axial locations along the ducts. Time steps can be included to calculate the irradiation creep and swelling effects during the core lifetime.

Figure 10. Duct geometry

Dimension Parameter	Description
A	Nozzle Length
B	ACLP Elevation
C	TLP Elevation
D	Duct Length (assembly length/height)
E	Nozzle Diameter
F	Duct Wall Thickness
G	ACLP Wall Thickness
	TLP Wall Thickness
H	Duct across flats
J	TLP across flats
K	ACLP across flats
M	Load pad Height
N	ACLP restraint ring clearance
P	ACLP gap clearance
Q	TLP restraint ring clearance
R	TLP gap clearance
	Upper Nozzle Receptacle Diameter
	Lower Nozzle Receptacle Diameter

Table 2. Description of duct geometric parameters at the reference temperature

NUBOW-3D calculates the thermal bowing based on 1D beam elements subjected to thermal loading with hexagonal cross sections. The bending stiffness is assumed to come from the subassembly duct geometry and material only, and NUBOW-3D neglects any stiffening provided by the fuel pin bundle. The assembly displacements are calculated relative to the centerline of the duct and does not take rotation or twisting effects into account. Contact is assumed to act normal to the face of the load pad and frictional effects are neglected. If the reactivity displacement-worth for each duct is provided as input, NUBOW-3D post-processes reactivity change as a linear combination of the reactivity displacement-worth times the displacement. The basic schematic of the NUBOW-3D workflow is provided in Figure 11.

Figure 11. NUBOW code schematic

Validation/Verification

Past versions of NUBOW have gone through some verification and validation but many of the details are no longer available. NUBOW was used at FFTF to manage refueling [18]. The code correctly predicted standby residual bowing shape resulting from inelastic strains and was used to calculate resulting forces due to contact. The experiments produced updated creep and swelling correlations, which provide the necessary material models for NUBOW to correctly predict creep and swelling contributions to bowing. Contact forces matched well with measurements noting that the main cause for error was probably due to modeling the geometry based on theoretical gaps instead of effective gaps. NUBOW was used successfully over 1730 days of reactor operations with over 1000 duct withdrawal/insertion and 20 bow dilation measurements, matching core

dilation creep values fairly well. Duct bow-reactivity feedback measurements were taken during the FFTF acceptance test period. When compared with NUBOW calculations, there were “reasonable agreements in general characteristics” at higher P/F ratios when gaps are closed [18].

For the most recently modified version of NUBOW, a set of verification and validation problems from the International Working Group on Fast Reactors (IWGFR) [19] were modeled with NUBOW. The examples demonstrated the ability of NUBOW to perform calculations for fuel assemblies undergoing free thermal bow, inter-assembly contact, core restraint system interaction, and irradiation dose gradients. The results, summarized in Table 3, agreed fairly well with the other code averages for predicting the displacement and contact forces with the largest difference in displacement prediction occurring in Example 4, but still within 7.5% of the average of the other codes.

Example	Description	Feature	Code Average	Spread	NUBOW	
					Result	Accuracy
1	Free thermal bowing of a single subassembly, Linear Thermal Gradient	Displacement at the top of duct	12.26 mm (code)	1.2%	12.25 mm	-0.1%
			12.25 mm (theory)			0.0%
2	Free thermal bowing of a single subassembly, Non-linear Thermal Gradient	Displacement at the top of duct	16.34 mm (code)	1.6%	16.33 mm	-0.06%
			16.33 mm (theory)			0.0%
3A	Thermal bowing of a S/A into a 60-degree sector array of S/A's	Max Load	52.68 N	5.5%	51.33 N	1.0 %
		Max disp.	8.54 mm	1.0%	8.55 mm	0.1%
3B		Max load	102.0 N	5.9%	100.5 N	-1.5%
		Max disp.	8.10 mm	1.1%	8.05 mm	-0.6%
4	Thermal bowing interactions in a symmetric array, with passive restraint	Max Load				
		ACLP	3192 N	6.2%	3262 N	2.2%
		TLP	1850 N	4.1%	1884 N	1.8%
		Disp. S/A 43				
		TLP	1.60 mm	1.3%	1.55 mm	-3.1%
5	Irradiation bowing interactions in a symmetric array with a passive restraint	ACLP	1.78 mm	1.6%	1.71 mm	-3.9%
		Core Mid	1.59 mm	1.6%	1.47 mm	-7.5%
		Max load at 100 dpa				
		ACLP	989 N	10.7%	936 N	-5.4%
		TLP	1152 N	11.5%	1079 N	-6.3%
		Disp. S/A 43				
		TLP	1.76 mm	0.6%	1.71 mm	-2.8%
		ACLP	1.92 mm	1.9%	1.85 mm	-3.6%
		Core Mid	5.95 mm	1.8%	5.69 mm	-4.4%

Table 3. NUBOW summary of IWGFR verification results

Limitations

While NUBOW can provide detailed calculations of core mechanical behavior through the deformations and contact forces for a full reactor core under thermal loading at multiple time steps throughout the life of the core, the limitations are clear. NUBOW performs the calculations independent of other core modeling simulation codes and requires only a loosely coupled approach to include the temperature and flux distributions as input files. However, reactor state changes are interpolated based on the information provided at the beginning of the NUBOW simulation. This means that any flux or temperature changes that would be induced during core deformation are not included, and the reactivity effects are based only on the final state of the reactor.

Another major limitation of NUBOW is that it is only capable of performing the calculations for a static load scenario.

3.2 DIF3D/SAS4A/SASSYS-1 Workflow

SAS4A/SASSYS-1 provides a detailed, multiple-channel thermal/hydraulic treatment of the reactor core. A SAS4A/SASSYS-1 [20] calculation is performed to calculate the temperature distribution in the core, and the resulting radial expansion reactivity feedback is computed using either a “simple” or “detailed” model [21].

In the simple model, the radial expansion of the core region is determined by interpolating between the expansion of the lower grid plate support and the expansion of the duct walls at the above core load pad. The expansion at the grid plate is assumed to be proportional to the rise in the inlet temperature above the initial steady state-value. The expansion at the ACLP is assumed to be proportional to the change in the average temperature at that location [20]. The reactivity feedback is determined by taking the estimate of the radial expansion of the middle of the active core region and multiplying by the reactivity coefficient obtained from the DIF3D reactor physics code to obtain the reactivity change. The reactivity coefficient from DIF3D is calculated by performing a nominal (undeformed) configuration and a uniformly dilated configuration which yields the change in k -eff per unit of dilation. The simple model does not explicitly account for assembly bowing but attempts to determine a reasonable average core deformation [21].

In the detailed model, SAS4A/SASSYS-1 calculates a deformed shape for a single representative assembly that is an average assembly in the outer row of the core consistent with the limited free-bow core restraint system. The shape of the assembly is determined by evaluating the deformation of a continuous beam subjected to the thermal gradient across the assembly, considering the restraints due to the grid plate, the load pads, and any restraint rings [20]. Then, the reactivity coefficient for uniform dilation is distributed axially along the assembly according

to the normalized power distribution in the active core zone. The axially-dependent deformation is weighted with the axially-dependent reactivity coefficients to obtain the reactivity change. One limitation of this model is that it assumes that deformation of a single assembly represents the average shape of the whole core, so different assembly bowing shapes within the core cannot be simultaneously modeled. [21].

Validation and Verification

The initial radial core expansion model was compared to existing empirical correlations for estimating the reactivity feedback as a function of the normalized power-to-flow ratio (P/F) based on a series of tests from the FFTF reactor. There was good qualitative agreement for $P/F < 1.25$ with discrepancies due to modeling limitations of the core restraint ring [20].

3.3 SHARP (PROTEUS, Nek5000, Diablo)

Simulation-based High-efficiency Advanced Reactor Prototyping (SHARP) [22] is a toolkit developed under the DOE-Nuclear Energy Advanced Modeling and Simulation (NEAMS) program to integrate neutronics, thermal-hydraulics, and structural mechanics through a coupled, multiphysics analysis to quantify the reactivity feedback effects of liquid metal cooled fast reactors [23]. SHARP couples three different high fidelity physics solvers: PROTEUS-SN, Nek5000, and Diablo.

PROTEUS-SN is high fidelity deterministic neutron transport solver that can model deformed configurations directly if the geometrical changes are provided by a mechanics solver. Nek5000 is a computational fluid and thermal dynamics solver responsible for computing temperature and velocity fields. Diablo is a solid mechanics solver developed at Lawrence Livermore National Laboratory that uses implicit, Lagrangian finite-element methods in the application of non-linear structural mechanics and heat transfer problems [24].

Diablo's capabilities include:

- Spatial discretization: low-order hexahedral continuum, quadrilateral shells, and two-node beams.
- Material stress response models: isotropic and orthotropic elasticity, plasticity, simple soil, hyperelastic foam.
- Material thermal response models: isotropic and orthotropic conduction, phase change, enclosure grey-body radiation.
- Material irradiation models: simplified irradiation creep deformation simulation with the capability of easily adding more models for other materials and the inclusion of irradiation swelling if needed.
- Body contact models (unbonded material interfaces): friction, pressure-dependent thermal conductivity, arbitrary interface motion, via mortar contact constraints

- Time integration: Solid mechanics time integration with the Newmark method, thermal mechanics with generalized-alpha method
- Iterative and direction solution parallel linear solver options are available, allowing different methods to be designated for different physics solutions.

SHARP seeks to perform a fully-coupled, multi-physics analysis through a single simulation of the core undergoing radial thermal expansion while modeling the full geometric detail at the continuum scale. The integration of the neutronics, thermal-hydraulics, and structural mechanics in a single, simultaneous, calculations precludes the necessity to perform offline perturbation analyses or passing reactivity coefficients between codes. Instead, the modules work together to inform/influence each other to drive the results through an iterative analysis procedure [23].

SHARP couples the three physics components using in-memory coupling. An inner iteration is performed between neutronics and thermal hydraulics to converge the temperature and power fields, and then the temperature is pushed to the mechanics code (Diablo) which calculates detailed displacements in the mesh and has advanced contact algorithms for handling duct contact at load pad locations and restraint rings. Additional developments are needed in the non-structural mechanics codes to handle geometry which contacts and therefore removes discretized elements. The neutronics code adjusts the geometry based on these displacements, which requires in some cases material densities to preserve mass (for example fuel and structural materials), and in other cases keeping material densities constant (for example liquid sodium). Models are built into the PROTEUS-SN neutronics solver to handle this automatically. Once deformed, the reactivity and power profile of the system changes, which has an impact on temperature fields again. Additional updates can be made to converge the system into its deformed state. Data transfers are made in memory through a MOAB-based interface.

Major performance and code maintenance issues have been identified in the current implementation, making the set of codes difficult to apply for realistic, large systems. SHARP is no longer being developed or maintained regularly but was successful in its mission to demonstrate that high fidelity codes could indeed be directly coupled for this type of problem.

Figure 12. SHARP coupling and iteration workflow

Verification and Validation

SHARP's fully coupled solver has only been demonstrated for very preliminary, coarse mesh configurations of a limited-free bow system based on thermal response without the inclusion of irradiation creep or swelling. These models are referred to as the 2D and 3D ABTR mini-core and full core models. No verification or validation studies have been performed.

Figure 13. Assembly deformation in a free-bow sodium-cooled fast reactor design calculated by SHARP (adopted from [23])

3.4 RAINBOW

ReActivity Induced by assembly BOWing (RAINBOW) is a code developed by Purdue University under a DOE-sponsored NEUP grant using the perturbation theory method for evaluation of the reactivity change in sodium cooled fast reactors due to assembly bowing [25]. Assembly bowing is modeled by shifting axially discretized assembly segments, and heterogeneous assembly configurations are represented by unstructured finite element meshes. Perturbation theory calculations are performed by following material movements. RAINBOW calculates the reactivity changes for the displacements of axial assembly segments in each of six directions normal to the duct wall surfaces [26].

Validation/Verification

RAINBOW benchmark tests were performed using 2D and 3D mini core models derived from the ABTR core design [27]. MCNP6 was used to obtain reference solutions using Monte Carlo simulations, and PROTEUS-SN was used for deterministic solutions. RAINBOW showed good results calculating the displacement worth of both the 2D and 3D models when statistically compared with MCNP6 with deviations being due to the underestimated standard deviations reported by the MCNP6 calculations. The same models were also compared with deterministic calculations from PROTEUS-SN and the 2D models agree with the reference solutions to within one pcm. Using an extrapolation scheme for the 3D model mesh convergence for the PROTEUS-SN solution, the RAINBOW results agreed very well. Thus, it is shown that RAINBOW can calculate the displacement worths of axial assemblies relatively well.

Limitations

While RAINBOW has demonstrated the ability to calculate reactivity changes in SFRs due to assembly bowing, it is not a structural mechanics code and is not capable of calculating the deformed shape or the radial expansion values. Thus, to be effective to calculate the reactivity feedback due to core radial expansion (and other combined effects), RAINBOW would need to be coupled with a structural mechanics code which can provide the deformation response for the entire reactor.

3.5 OXBOW

TerraPower, LLC has developed a tool for simulating the radial expansion of reactors called OXBOW. OXBOW is a high fidelity, long-running finite element analysis code which calculates stresses, elastic and plastic strains, geometric distortions as functions of power, flow, and irradiation history [28]. OXBOW employs the framework of the commercially available finite element software Abaqus [29] and the Abaqus Standard solver, calculating the mechanical response using the 8-node reduced-integration continuum shell element, SC8R. To perform the

calculations, OXBOW requires the input temperature, dose, and flow histories of one of the collections of assemblies, which it receives from the ARMI system. User-defined subroutines are used to implement custom material models, especially for irradiation response models. Contact between ducts is modeled via the direct “hard” contact method in Abaqus. The option to use the penalty method for modeling contact is also available for ease of convergence [30].

OXBOW functions as part of an interface for the coupled simulation of advanced nuclear reactors: The Advanced Reactor Modeling Interface (ARMI) code system which “leverages seamless communication, coupling, automation, and continuous development, allowing key performance metrics to be linked explicitly to the design inputs” [28].

ARMI Architecture

The ARMI framework is made up of two main entities, the reactor model and the interface stack. The reactor model comprises the main system description for all the physical details of the reactor including the geometry, material properties, power, temperatures, etc. The interface stack is the system that couples together the different physics modules, performing the simulation modeling and calculations, and updating the reactor model as necessary. ARMI is an object oriented architecture that allows full coupling of the reactor physics while allowing decoupling of the source code for each physics module [28]. ARMI contains external code adapters to ANL fast reactor physics codes including MC², DIF3D and REBUS. For the transient analysis, ARMII contains an adapter for the SASSYS/SAS4A code. The reactivity module automatically calculates the necessary reactivity coefficients including the radial expansion coefficient and writes the core sections of the SASSYS input file. With the complete SASSYS file, ARMI can run multiple SASSYS cases, perturbing the reactivity and performing statistical sampling of the reactivity coefficients to determine target values of input uncertainty [28].

Figure 14. ARMI interface stack schematic showing the reactor model coupled with the physics models (adopted from [28])

Physics Modules	Codes
Neutronics Adapter	MC2/DIF3D/REBUS MCNPX
Thermal-Hydraulics	COBRA MONGOOSE
Fuel Performance Fuel Management	CRUCIBLE ALCHEMY
Safety and Transient	SASSYS/SAS4A DIF3D-K RELAP5
Core Mechanical	OXBOW

Table 4. Summary of ARMI physics modules and integrated codes (adapted from [28])

Verification

TerraPower selected seven of the verification problems from the IWGFR problems [19] to run with OXBOW as the Phase 1 benchmarking test. The examples demonstrated the ability for OXBOW to perform the analysis of fuel assemblies under fundamental behaviors such as free

thermal bow, inter-assembly contact, core restraint system interaction, and irradiation dose gradients [30]. The OXBOW results matched well for Examples 1, 2, 3a, 3b, and 5 showing that displacement results for single assembly thermal free bow (Examples 1 and 2), thermal bowing in a pseudo-free flowering configuration (Examples 3a and 3b), and limited free bow core restraint with bowing due to irradiation dose gradients (Example 5) were consistent with those of the IWGFR participants. The examples are summarized with OXBOW displacement difference averages compared to the IWGFR participants in Table 5.

Example	Description	Displacement Difference Average
1	Free thermal bowing of a single subassembly, linear thermal gradient	0.7%
2	Free thermal bowing of a single subassembly, non-linear thermal gradient	0.7%
3a	Thermal bowing of a S/A into a 60-degree sector array of S/A's, corner-to-corner direction	1.2%
3b	Thermal bowing of a S/A into a 60-degree sector array of S/A's, flat-to-flat direction	5.0%
4	Thermal bowing interactions in a symmetric array, with restraint ring	23.5%
5	Irradiation bowing interactions in a symmetric array with a restraint ring	7.2%
8a	Assembly free dilation under internal pressure and irradiation	20.0%

Table 5. Summary of IWGFR problems analyzed with OXBOW with the average of the assembly displacement differences compared to IWGFR participants

Examples 4 and 8a show substantial differences between the IWGFR participant averages and the OXBOW calculations, as seen in Table 5. Example 4 modeled a 60° section of the core with one row of core assemblies experiencing thermally induced bowing in a limited free bow core restraint configuration. According to [30], the displacement results from OXBOW varied 15-50% from the IWGFR participant averages at the core-mid and ACLP locations. This deviation was attributed to a bridging phenomenon, in which the thermally activated ring compacts and develops a load path tangential to the core center, preventing inward movement at the ACLP. Upon further investigation it was concluded the bridging response was caused by the thermal expansion at the ACLP decreasing the gap between the assemblies. Another difference that contributed could be the hard contact formulation employed by OXBOW, which was investigated by changing the contact formulation to the penalty method. With the penalty contact method, the bridging response was mitigated, and the results were closer to the IWGFR averages.

Example 8a modeled the assembly free dilation under internal pressure and irradiation. According to [30], the results from OXBOW were 15-25% lower than the OWGFR participants

averages. The differences between the OXBOW model results and the IWGFR averages are attributed to higher fidelity finite element models employed by OXBOW. The IWGFR results are based on linear beam theory, with fixed supports at the corners, to estimate the total deflection on the duct wall. Abaqus Standard solver, used by OXBOW, accounts for geometric nonlinearities with “large displacement” formulations, and stress relaxation due to irradiation under constant pressure.

3.6 ARKAS / ATLAS

ARKAS is a three-dimensional finite element code originally developed by NAIG Nuclear Research Laboratory in Japan, supported by Toshiba, for the simulation and analysis of core distortion mechanical behavior for fast spectrum reactors [31].

ARKAS contains two separate models for describing the sub-assemblies, a simple beam model and a thin, folded plate shell model (figure available in [32]). In each model, the support nozzle is modeled as a simple beam with joint elements to represent the support conditions at the lower and upper grid plate support locations. The elements are subdivided into a user-specific number of elements in the axial direction, assuming homogeneous, isotropic, elastic material properties. Each element includes six degrees-of-freedom (three translations and three rotations) per node. It also requires a description of the temperature and flux distribution of the cross section at certain axial locations along the ducts. Time steps can be included to calculate the irradiation creep and swelling effects during the core lifetime [31].

A unique feature of ARKAS is the inclusion of a fictitious element developed specifically to model the nonlinear stiffness between neighboring ducts, called a joint element. The joint element is capable of modeling partial and angled contact, as well as frictional effects. The joint elements are normally located at all load pad locations, ACLP and TLP, as well as the nozzle tip and base locations, and between the outer ducts and restraint rings [31].

At each time step, ARKAS calculates the 3D rotations and displacements for each subassembly, as well as the inter-assembly contact forces including friction effects. The nonlinearity due to contact and separation from assembly motion is solved based on the Newton-Raphson method in a step iterative procedure. In each step, the linear matrix equation is reconstructed and solved directly, using the substructure method. The block successive over-relaxation (SOR) method is used to solve the linear matrix equation. The strain due to swelling, creep, and thermal expansion is calculated at all six duct corner mid-wall points and at all user-specified duct face mid-wall points. The load vectors are calculated by assuming a linear variation circumferentially between neighboring mid-wall points in each axial plane [32].

ARKAS_cellule is an improvement on the original ARKAS simplified shell model developed to model each sub-assembly with multiple shell elements (figure available in [33]) instead of one thin plate per hexagonal face [34].

More information on the derivation of the analytical and finite element methods employed can be found in [31], [33], [34].

Integration of ARKAS into ATLAS

ARKAS was integrated into the code system ATLAS in 1994 to perform a multiphysics, consistent calculation of the reactivity feedback effects of core bowing along with three other codes: CITATION, ATHENA, and VEGA [35].

CITATION is an older, and at the time a commonly used, 3D diffusion reactor physics code for calculating power and neutron flux distributions.

ATHENA is a software to predict the thermo-hydraulic behavior for a large number of assemblies based on the porous body model proposed by Khan [36]. The model can handle multiple boundary conditions including mirror and rotational symmetry as well as a full core.

VEGA is a 3D reactivity worth map code which integrates the inner product of displacement and material reactivity worth gradient with respect to volume over the whole core. The model uses first order perturbation to calculate the fuel worth distribution with respect to the homogenized composition.

The workflow for core bowing reactivity feedback calculations is shown in Figure 15. Given the full core inputs, CITATION calculates the neutron flux and power distributions. ATHENA takes the flux and power distributions and performs the thermo-hydraulic calculations to obtain the temperature distributions along the ducts. ARKAS takes the temperature and flux distributions to calculate the core-bowing effects due to thermal expansion and irradiation creep and swelling. And finally the reactivity change is calculated by passing the assembly deflections and the flux and adjoint flux values to VEGA [35].

Figure 15. ATLAS workflow for core bowing reactivity calculations

Validation/Verification

ARKAS was one of the codes that was used by NAIG in the verification problems from the IWGFR problems [18]. Due to the way the problems were posed, in which the load pads were assumed to have uncoupled stiffness on each of the duct faces, the shell model was assumed to be inadequate. Thus, all the verification problems were solved with the beam model [32]. A summary of some key results is shown in Table 6. The results agreed very well with the other code averages for predicting the displacement and contact forces under free bowing, simple thermal bowing of multiple sub-assemblies with passive core restraint, and irradiation bowing interactions in full core assemblies with passive core restraint.

Example	Description	Feature	Code	Spread	ARKAS	
			Average		Result	Accuracy
1 Theory	Free thermal bowing of a single subassembly, Linear Thermal Gradient	Displacement at the top of duct	12.26 mm (code)	1.2%	12.33 mm	0.6%
			12.36 mm (theory)			-0.2%
2 Theory	Free thermal bowing of a single subassembly, Non-linear Thermal Gradient	Displacement at the top of duct	16.34 mm (code)	1.6%	16.44 mm	0.6%
			16.48 mm (theory)			-0.2%
3A	Thermal bowing of a S/A into a 60 degree sector array of S/A's	Max Load	52.68 N	5.5%	53.20 N	1.0 %
3B		Max disp.	8.54 mm	1.0%	8.56 mm	0.2%
		Max load	102.0 N	5.9%	103.0 N	1.0%
		Max disp.	8.10 mm	1.1%	8.11 mm	0.1%
4	Thermal bowing interactions in a symmetric array, with passive restraint	Max Load				
		ACLP	3192 N	6.2%	3261 N	2.2%
		TLP	1850 N	4.1%	1878 N	1.5%
		Disp. S/A 43				
		TLP	1.60 mm	1.3%	1.60 mm	0.0%
		ACLP	1.78 mm	1.6%	1.77 mm	-0.2%
5	Irradiation bowing interactions in a symmetric array with a passive restraint	Core Mid	1.59 mm	1.6%	1.58 mm	-0.9%
		Max load at 100 dpa				
		ACLP	989 N	10.7%	1018 N	2.8%
		TLP	1152 N	11.5%	1186 N	3.0%
		Disp. S/A 43				
		TLP	1.76 mm	0.6%	1.76 mm	0.2%
6	Irradiation bowing interactions in a full core array with 127 S/A's with a natural restraint	ACLP	1.92 mm	1.9%	1.93 mm	0.7%
		Core Mid	5.95 mm	1.8%	5.93 mm	-0.3%
		Max load at 100 dpa				
		Disp. S/A 53				
		TLP	10.16 mm	1.7%	10.26 mm	0.9%
		ACLP	3.25 mm	1.3%	3.27 mm	0.6%
		Core Mid	2.82 mm	3.3%	2.83 mm	0.4%
		Creep disp. S/A 53				
		TLP	5.71 mm	5.7%	5.72 mm	0.2%
		ACLP	2.92 mm	5.8%	2.93 mm	0.2%
		Core Mid	0.33 mm	8.7%	0.33 mm	0.0%
		Swell Disp. S/A 53				
TLP	26.20 mm	3.4%	26.53 mm	1.2%		
ACLP	13.11 mm	3.3%	13.26 mm	1.2%		
Core Mid	1.20 mm	7.1%	1.22 mm	2.4%		

Table 6. ARKAS summary of IWGFR verification results (ARKAS data from [32])

ARKAS_cellule has undergone validation testing with experimental data from the NNC's Core Restraint Uni-Planar Experimental Rig (CRUPER) which was designed to simulate compaction of sub-assemblies at the above core restraint plane [33]. To study compaction sequences in arrays of sub-assemblies, CRUPER represented a horizontal slice through a fast reactor core containing a restraint plane. The model represented 91 'sub-assemblies' (in five rings) of the UK commercial fast reactor (CDFR) core, which could be compacted by 30 exterior rams [33].

Comparison between ARKAS_cellule and the CRUPER experimental results show good agreement between the ram loads at low compaction states where the array is flexible. As the core compacts further, changing the stiffness of the load plane by increasing the contact faces of the assemblies, the ARKAS_cellule and CRUPER results diverged at a number of rams, with a mean relative difference of +8.2% with a standard deviation of 25.5% without the effects of friction included. With friction calculation using the friction coefficient of 0.15 the mean relative difference was reduced to +3.2% with a standard deviation of 24.4%.

3.7 FAST

Fast-spectrum Advanced Systems for power production and resource management (FAST) is a project established at Paul Scherrer Institute (PSI) to develop a new tool to analyze the static and dynamic behavior of a whole reactor system for advanced fast-spectrum reactor concepts [37].

FAST is a code system assembled from a set of stand-alone codes with the goal of coupling the multi-physics simulation in as generic a way as possible to be applicable to many Generation IV reactor concepts. The main codes coupled in the current system (Figure 16) are:

- ERANOS and PARCS reactor statics and kinetics codes
- TRAC/AAA thermal hydraulics code
- FRED fuel rod thermal-mechanics code

Due to insufficient information on FAST, its applicability to the core radial expansion problem is undetermined, but it has been included here for further investigation.

Figure 16. FAST code system structure

3.8 GeN-Foam

GeN-Foam [38] is a new solver developed at the Paul Scherrer Institute (PSI), as a supplement to the FAST group's efforts in fast reactor analysis, to tightly couple multiphysics effects without the use of legacy solvers. It is based on OpenFOAM, an open source C++ library for solving partial differential equations using finite-volume discretization, which is developed to couple thermal-hydraulics, displacement-based thermal-mechanics, multi-group neutron diffusion, and a finite-different sub-scale fuel model for coarse mesh simulations. The thermal-mechanics solver in GeN-Foam is based on the solidDisplacementFoam solver available from OpenFOAM 2.3.0, which is a displacement-based finite-volume solver for linear-elastic, small-strain deformation of solid, isotropic bodies. The main modification to the original solidDisplacementFoam solver is to expand the heterogeneous material solver by the inclusion of multiple homogenous zones with associated properties. This thermo-mechanical solver is used to calculate the temperature-induced deformations of the main structures, and to determine the radial displacement of the core.

A GeN-Foam based thermal-mechanical analysis of the ESFR-SMART core design was performed to demonstrate the capabilities and determine reactivity feedback based on local deformation of the assembly geometry [39]. The assemblies were modeled as separate bodies with

the contact between bodies simulated by a boundary condition developed for the OpenFOAM-based OFFBEAT solver, which uses the OpenFOAM Arbitrary Mesh Interface to evaluate the distance between two bodies and applies a contact pressure when the bodies begin to penetrate (closing the gap). The authors note the difficulty in coupling the neutronics calculations with the deformed mesh due to thermal-mechanical behavior, as well as the difficulty in modeling the assembly gaps due to being very thin regions. The results showed the capability of the thermal-mechanics solver in determining the core shape due to deformation but noted the reactivity feedback required computationally expensive models and are limited for distorted assemblies. Future work would include verification and validation [39].

3.9 IWGFR Participating Codes

The following is a list of codes participating in the IWGFR benchmark problems discussed in previous tables, for which code-average values were displayed.

- HARMONIE/SOLO – France, CEA de Cadarache
- HARMONIE/SISCO – Italy, ENEA/VEL, Bologna
- CRAMP – UK, NNC Ltd, Risley
- SABOW/MABOW – India, IGCAR
- STRAW – Belgium, Belgo Nuclearie
- DDT/DDTR/DDAB – Germany, Interatom GmbH
- ACME – USSR, Inst. PPE
- HIBEACON – Japan, PNC/Hitachi
- RAINBOW-X – Mitsubishi API

3.10 High-Fidelity Finite Element Method (FEM) Software

In addition to specific software developed for nuclear reactor cores, high-fidelity FEM software, such as Abaqus [31], ANSYS Mechanical [40], and COMSOL Multiphysics [41] can be used to create very detailed models of the core geometry for thermal-mechanical analysis. Due to the complex geometry of a reactor core, it would require a significant effort to create the models, so scripting techniques built-into or added onto the software would be necessary to automate the model generation. These models could also be used to evaluate and verify the physics employed in other software, such as NUBOW-3D.

3.11 Multiphysics Object Oriented Simulation Environment (MOOSE) and MOOSE-Based Applications

Multiphysics Object Oriented Simulation Environment (MOOSE) is a parallel computational framework developed at Idaho National Laboratory (INL) to solve systems of coupled, nonlinear partial differential equations (PDEs) using the finite element method [42]. MOOSE uses an object-oriented design to provide a user-friendly interface for scientists and engineers to rapidly develop efficient finite element-based software without needing expert levels of programming experience [43].

MOOSE typically solves for the full set of coupled physics models in a single nonlinear system of equations. It allows for the use of multiple solution techniques to do this, but the most commonly used technique is the Jacobian-free Newton-Krylov (JFNK) method. The JFNK method is often preferred because analytically expressing the Jacobian matrix can be difficult, especially for the terms that couple different physics. Krylov iterative solvers such as the generalized minimum residual (GMRES) algorithm only require the matrix-vector product between the Jacobian and the solution state vector, which can be estimated with a finite-difference approach [42]. MOOSE also has a recently-developed capability that allows for the use of automatic differentiation to directly compute an accurate Jacobian matrix, which can give improved solution convergence with minimal development effort.

MOOSE is built on a modular architecture which simplifies adding physics to the simulation as well as coupling physics together. It is based on a layered approach with the physics modules, called kernels, at the top to drive the physics simulation, libMesh below the kernels with MOOSE providing core functionality to integrate the physics into the finite element solution approach, and at the lower level is the solver interface which uses the PETSc to solve the matrix equations.

Figure 17. MOOSE Framework

MOOSE is a powerful framework that utilizes different coding packages to make the simulation generation as user-friendly as possible, while still leveraging advanced capabilities for generating finite element equations and solutions. MOOSE models are generally independent of dimensionality, meaning most modules can be used in one, two, or three-dimensional simulations with no changes to the code. All programs built with MOOSE are also parallel by design; the same code can run on one processor or more. Another advanced feature built into MOOSE is mesh adaptivity. MOOSE uses h-adaptivity to refine or coarsen the mesh in areas of high or low error, respectively, using a “self-similar” approach; the current element is split into elements of the same type. For example, if a quad element is used, it will be split evenly into four smaller quad elements, shown in Figure 18.

Figure 18. Example of self-similar pattern of mesh refinement for 1D elements (top row), 2D quadrilateral elements (second row), and 3D hexahedral elements (bottom row) (adopted from [43]).

MOOSE is open-source and community developed. While it is possible to take the general MOOSE framework and add independently-created physics equations, many standard modules have already been developed by the community to be used in any simulation. Some of the physics modules include: Chemical reactions, Contact, Fluid Properties, Heat Conduction, Navier-Stokes, and Tensor Mechanics. Of particular relevance to the radial core expansion problem is the Tensor Mechanics module of MOOSE. The following sections describe modules within MOOSE, as well as specific MOOSE-based applications that have already been developed, which are relevant to the core radial expansion problem considered in this paper.

3.11.1. MOOSE Tensor Mechanics Module

The Tensor Mechanics Module is a library of code modules based on MOOSE used in continuum mechanics simulations, which models the mechanical deformation and stresses of solids. It can be used in pure mechanics simulations or in multiphysics simulations with other MOOSE modules such as heat transfer, phase field, contact, porous flow, and XFEM (the extended finite element method used to treat PDEs with discontinuities). The tensor mechanics system can be used to simulate both linear and finite strain mechanics, including elasticity and Cosserat elasticity, plasticity and micromechanics plasticity, creep, and damage due to cracking and property degradation. It supports both small and finite strain formulations. There are also multiple classes for calculating elastic stress, plastic stress, creep stress, and a combination of stress calculation methods.

The constitutive models in Tensor Mechanics are implemented in a modular fashion, with a standard set of models for the various calculations leading up to computing the current stress. Figure 19 shows the basic set of calculations required for stress calculations problem: the strain, constitutive/elasticity (C_{ijkl}), and stress tensors. In addition, the module allows for eigenstrains and

extra stress definitions. Eigenstrains are defined as mechanical deformation not caused by external stresses such as thermal expansion or deformations due to dislocations. An extra stress is typically a residual stress. Multiple formulations for each of these computations are available, and can be used interchangeably, permitting a wide variety of combinations of calculation types.

Figure 19. Tensors required to fully describe a mechanics material (adopted from [43])

3.11.2. MOOSE Contact Module

The MOOSE Contact Module enforces mechanical constraints between surfaces in the finite element mesh for preventing penetration and developing contact forces. The types of physical contact models available are glued, frictionless, and coulomb (frictional). Glued contact does not allow slip between the elements once contact occurs. Frictionless contact allows slip between elements during contact, often used when smooth surfaces are assumed. Coulomb (frictional) contact considers the friction force along the interface during sliding and assumes force tangential to the contact interface.

Contact formulations used to enforce contact constraints are through either the node to face approach with the penalty and kinematic methods or through a face to face approach with mortar-based contact. In the node to face approach a geometric search determines which secondary nodes have penetrated primary faces. For those secondary nodes, forces are computed on the appropriate primary faces and are distributed to primary nodes by employing the finite element shape functions. In the mortar method, a face to face constraint is applied without the requirement that elements at the contact interface have the same overlapping mesh. Currently, the penalty and kinematic formulations are well developed, and work is still being done to fully develop the mortar-based contact formulation as it currently does not work in three dimensions [43].

3.11.3. BISON

BISON is an engineering-scale nuclear fuel performance code based on MOOSE. BISON typically simulates the coupled thermal/mechanical response of fuel systems in the reactor environment but can also simulate other physics such as species diffusion. BISON relies heavily on the foundational capabilities provided by the Tensor Mechanics, Heat Conduction, and Contact modules in MOOSE and provides models for the materials used in a variety of fuel forms. Because

it is based on a finite element framework, BISON can be used to model a variety of fuel geometries and has been applied to LWR fuel (both standard and advanced concepts), metallic fuel, and TRISO fuel. The material models in BISON represent the irradiation and temperature dependent thermal and mechanical behavior of fuel and cladding/coating materials, including effects such as thermal and irradiation-induced creep, instantaneous plasticity, swelling, thermal expansion, and fracture.

3.11.4. Grizzly

Grizzly is a MOOSE-based code that simulates progression of aging mechanisms in nuclear power plant components and the integrity of these components subjected to degradation during normal and off-normal loading conditions. Grizzly is a superset of BlackBear, which is an open-source code that has non-nuclear specific models. Grizzly is intended to ultimately address a broad range of materials and components, but development has primarily focused on three main systems: LWR reactor pressure vessel embrittlement and fracture, environmentally-induced degradation of reinforced concrete structures, and high temperature creep in alloys relevant to advanced reactors. Like BISON, Grizzly relies heavily on the foundational capabilities of the MOOSE physics modules.

3.11.5. Systems Analysis Module (SAM)

Systems Analysis Module (SAM) is a MOOSE-based modeling and simulation tool developed at Argonne National Laboratory for advanced reactor safety analysis [44], in particular sodium-cooled fast reactors (SFRs), lead-cooled fast reactors (LFRs), fluoride-salt-cooled high temperature reactors (FHRs), and molten salt reactors (MSRs). SAM calculates the reactivity feedback during transient simulations due to the following effects: fuel Doppler, coolant density changes, axial fuel expansion, and core radial expansion [44]. This section will focus on the axial and radial expansion capabilities.

SAM considers reactivity feedback effects due to thermal deformation such as *thermal expansion of the fuel* and *core radial expansion*. The changes in dimensions are then used to determine the change in reactivity during the transient. SAM can calculate the thermal deformations either with built-in SAM standalone model or by coupling to the MOOSE Tensor Mechanics Module through the MultiApp tool.

The SAM *axial thermal expansion model* considers two cases: 1) fuel pellet is in free expansion, and 2) fuel pellet and cladding are in the eutectic condition. In case (1), the cladding is ignored, while in case (2) the fuel rod is constrained by the cladding in the radial direction and expand together through some interaction. In each case, simple linear thermal expansion is assumed. The axial expansion reactivity feedback is calculated as:

$$R_A(t) = \int_{z=0}^{z=L} \rho_f(z, t) \times r_f(z) \times A dz$$

Where $\rho_f(z, t)$ is the fuel density during the transient at time t , $r_f(z)$ is the fuel reactivity coefficient, A is the fuel cross section area, and L is the fuel length. The radial expansion coefficient can be calculated with a code such as PERSENT [45].

If the axial displacements are not provided, SAM performs a standalone calculation with the following equation:

$$u_i(z) = \int_0^z \alpha_i \times (\bar{T}_i - T_{0,i}) dz, i = 1, 2$$

where, u_i is the displacement field (axial expansion), α_i is the thermal expansion coefficient, $\bar{T}_i$ is the area-averaged temperature, and $T_{0,i}$ is the stress free temperature, where subscript $i=1$ represents the fuel and $i=2$ represents the cladding.

The coupling structure for the fuel axial expansion is shown in Figure 20. The SAM temperature distribution is passed to the Tensor Mechanics module at each time step to calculate the axial displacement field. The axial displacements are passed back to the SAM point kinetics model for the reactivity calculation, where the difference between the transient and initial values is used to calculate the fission power.

Figure 20. Coupling structure schematic for fuel axial expansion (Adapted from [44])

The SAM *core radial expansion model* considers uniform radial thermal expansion of the constraint systems (e.g. grid plate) at different axial positions. The axial expansion reactivity feedback is calculated as:

$$\Delta R_{RC}(t) = \sum_n^N \left(\frac{\Delta R}{R} \right) \times w_n \times \rho_{RC,n}$$

where $\Delta R/R$ is the relative change in the radius of the core, $\rho_{RC,n}$ is the core radial expansion reactivity coefficient at position n , w_n is a user-defined weight factor, and N is the total number of constraint systems. The radial expansion reactivity coefficients can be calculated with a code such as PERSENT [45].

SAM's standalone model for core expansion considers uniform radial expansion at multiple axial locations, with the temperature equal to the coolant temperature at the same elevation. Therefore, it can calculate an axial profile for the expansion, but does not consider a radial thermal gradient or calculate structural mechanical interactions between ducts. Each axial location, (e.g. the grid plate or the constraint system at the load pads) is assumed as a uniform hollow disk. Then the expansion is calculated as a displacement field linear with the radial location, r .

$$u(r) = \alpha \Delta T r$$

The coupling structure for the core radial expansion is shown in Figure 21. SAM can model the core radially as a series of “core channels” which represent different regions in the reactor (e.g. inner/outer fuels, reflector, or shielding assemblies). The core is modeled axially by segmenting the channels between restraints locations (e.g. grid plate, ACLP and TLP) and approximating the core restraints as grid plates, one at the lower region (inlet) and one at the upper region (outlet). The temperatures at each level are considered equivalent to the coolant temperature at the same elevation. At each time step, the inlet and outlet temperatures are passed to the Tensor Mechanics module to calculate the radial displacement, which is considered to vary linearly between the inlet and outlet locations for each segment. The relative change in the core radius at different locations is calculated, $(\Delta R/R)_i$, and passed back to SAM for the reactivity calculation.

Figure 21. Coupling structure schematic for core radial expansion (Adapted from [44])

The radial thermal expansion model in SAM was verified using the ABTR grid plate design model [44]. The model geometry and mesh are shown in Figure 22 with the hollow disk model on the left side and the grid plate geometry on the right side. The geometry and material properties are given in Table 7.

Figure 22. Mesh for hollow disk (left) and grid plate (right) (Adopted from [44])

Parameter	Value
Outer Radius, R_0 (m)	0.75
Assembly Pitch, P (cm)	14.598
Gap Width, G (cm)	0.4
Thermal Expansion Coefficient, α (m/m/K)	1.60×10^{-5}
Reference Temperature, T_{ref} (K)	293.15
Thermal Conductivity, k (W/m K)	15.0
Young's Modulus, E (GPa)	200.0
Poisson's Ratio, ν	0.3

Table 7. Geometric and material properties of grid plate

For the test, a uniform temperature of 638.15 K was applied to the grid plate and the SAM model was compared with simulation results for both the hollow disk and the grid plate geometry models. The results are shown in Figure 23. The simulation results match very well with the model prediction, with the authors noting that the mean relative difference between results was less than 0.1%.

Figure 23. Grid plate thermal expansion verification results (Adopted from [44])

The reactivity feedback modeling was simplified from the ABTR model to test the individual reactivity feedback models. The test used a single channel model with inlet coolant temperature increasing from 628.15 K to 728.15 K during a 100s transient. The geometry and material properties were the same as Table 7. The results for the radial expansion reactivity are given in

Figure 24 showing comparison between the standalone SAM radial expansion model and the coupled analysis between SAM and the Tensor Mechanics module. There is good agreement between the results showing that the coupling system works as expected.

Figure 24. Single channel radial expansion reactivity comparing SAM standalone calculations (solid black line) with the coupled Tensor Mechanics results (triangle points) (Adopted from [44])

The heat transport system of the ABTR with 5 core channels was used to test the reactivity feedback calculations of both the SAM standalone calculations and the coupled Tensor Mechanics calculations [46]. The results are shown in Figure 25 with the solid lines indicating the SAM calculations and the dashed lines indicating the coupled calculations. The calculations match very well, with the largest differences coming from the axial expansion model. The error is noted by the authors to come from the approximations in calculating the axial displacements, specifically the area-averaged temperature assumption.

Figure 25. 5 Channel reactivity feedback calculations for the ABTR comparing SAM standalone calculations (solid lines) with the coupled Tensor Mechanics results (dashed lines), (Adopted from [46])

4 Gaps for Modeling Core Expansion and Path Forward

This report has so far described the tools currently in existence that can be used to model some aspects of the radial core expansion phenomenon. This section summarizes the gaps for developing a fully coupled, high fidelity multiphysics simulation capability for the radial core expansion problem.

4.1 Tight Coupling to Reactivity Feedback

There are many codes which exist to analyze different aspects of a nuclear reactor system, thermal hydraulics, neutronics, deformation response, etc., but they currently exist in a completely uncoupled, or very loosely coupled system currently. There is no current code system which effectively couples the multiphysics response of a nuclear reactor deformation code with the reactivity feedback. For example, codes such as NUBOW and ARKAS can calculate a detailed deformation response of a single assembly or entire core restraint system and RAINBOW can take a deformation curve for an assembly and calculate the reactivity change, but there is no interface between these different codes to automate the process of reactivity calculations. While a loosely coupled approach might allow an approximation of the response, an issue arises when each time step of physics response impacts the input for the next time step. An example is when the reactor starts deforming, the radial expansion and reactivity feedback can affect the power and temperature of the reactor, changing the state to update the temperature gradients which would then update the deformation response and so on. Thus, a more tightly coupled structural response may be required for the desired accuracy. The SHARP toolkit was the first known attempt to create a tightly coupled code system for high fidelity multiphysics modeling of all three physics (neutronics, thermal fluids, and solid mechanics), but development of this coupled code was terminated before code performance issues could be resolved, which were related to the specific coupling interface used and its limitations.

4.1.1. MOOSE-Based Physics Coupling

In order to solve the complex problem of radial core expansion/bowing in fast reactors and the resultant reactivity feedback, a high fidelity software capable of performing coupled multiphysics simulations consisting of neutronics calculations, thermal-hydraulic analysis, and structural mechanics is required. Leveraging MOOSE-based physics tools is a top candidate for such a capability, as MOOSE is capable of easily coupling different physics simulations together, has a wide range of already developed physics modules for use, and allows new modules to easily be created and integrated. The neutronics code must be capable of high-fidelity geometrical modeling with a flexible, deformable geometry option based on MOOSE framework. The discrete ordinates solvers within the Griffin code (developed under NEAMS) meet the criteria, and near-term efforts are planned to improve computational efficiency to enable high fidelity full core simulation.

Griffin could be coupled to MOOSE-based structural mechanics and thermal/fluids modules. Several options are available for the thermal-hydraulics analysis: SAM, Pronghorn, or a combination of native MOOSE modules such as the Porous Flow and Heat Conduction modules. The best option for structural mechanics moving forward would be the Tensor Mechanics module as it already has the foundations implemented for finite deformation mechanics and is readily extensible to permit adding material-specific models. Further development would be needed in order to capture the irradiation creep and swelling material properties of the reactor components, but that would only require developing extra material properties for evaluating eigenstrains (thermal expansion and swelling) and the irradiation creep in the components and would not require re-tooling the Tensor Mechanics module base code. Similar models have already been developed in the BISON and Grizzly codes and could either be directly used for this application or used as a starting point for the development of models specific to this application.

4.1.2. Other Possible Coupling Schemes

As the development of a high fidelity radial expansion and reactivity feedback simulation capability in MOOSE will take significant time to develop moving forward (including upgrades required in the solvers for both physics and performance), it is beneficial to take advantage of the current software available. In the near term, NUBOW is a very useful software for calculating the thermal-mechanical response of a full reactor given the proper thermal gradient and flux inputs, and it can calculate the reactivity feedback given the reactivity displacement-worths of the assemblies. Many different codes exist which simulate the thermal hydraulics and could output the thermal gradients for use in a software like NUBOW, such as SE2, SAM, Nek5000, etc., but some of those options might require extensive coupling or data pre-processing efforts to be used within NUBOW. And finally, a high fidelity neutronics code with a deformable geometry option would be required to evaluate the reactivity feedback effects. RAINBOW appears to be a solid candidate as it can evaluate the radial expansion reactivity effects based on perturbed geometry. PROTEUS-SN is another potential candidate since it can be used with deformed mesh geometry. The main challenges in using these separately-developed tools involve developing workflows and managing information transfer between the tools in a consistent way to capture the correct physics.

4.2 Material Properties

The general deformation response of the duct material for the reactor assemblies is based on material properties correlations developed through experimental testing and mathematical regression analysis. The governing material properties for an assembly in a reactor core are Young's modulus, coefficient of thermal expansion, irradiation swelling strain, and irradiation creep strain. These properties vary based on the molecular composition of the material and vary with temperature, and are well understood properties. The material properties with the most uncertainty are those which vary within a neutron flux environment. To determine the response

due to irradiation creep and swelling, material correlations need to be developed, and have been done for specific reactor design materials, such as HT9 and AISI 316 stainless steel. More data with further experimental testing and statistical analysis can reduce the uncertainties by updating the correlations to provide for better approximations of the deformations.

4.3 Validation of Modeling Assembly Internals

Bending of beams is a well understood phenomenon and can be described using Bernoulli beam theory equations which relate the deformation of a beam to the internal bending moment induced by the applied load (contact or thermal bending), young's modulus, and the cross section moment of inertia. For a fuel assembly, a major concern is how to quantify the moment of inertia. Current assumptions regard the moment of inertia of the assembly equal to the moment of inertia of the hexagonal duct, neglecting any additional stiffness from the fuel elements [6]. A validation experiment was performed as part of the IWGFR Stage 2 to relate a force at the tip of the duct to the deformation [19]. The experiment showed a linear relationship between the force and the deformation, consistent with beam bending deformation for a cantilever, and that the flat-to-flat deformation was equal to the corner-to-corner deformation proving the moments of inertia for the two directions are equal. Because of the limited data available for the experiment, specifically how they defined the moment of inertia for the sections, more modern experimentation is required to check the assumptions stated above. One such test was performed by [47] which reached the same conclusion that the load orientation (face or corner contact) has little effect on the deformation. This conclusion supports the assumption that the moment of inertia of the duct can be taken as equal to the cross section, neglecting contributions from the fuel, because the moment of inertia of a hexagon is equal along any axis that crosses the center. Further experimentation would be needed to fully support this assumption.

4.4 Nozzle Boundary Condition Experimental Validation

Another major modeling concern is the nozzle boundary condition. All of the IWGFR code comparison problems neglected the nozzle boundary condition, assuming a fixed boundary for the ducts [19]. However, the boundary condition of the nozzle would play an important role in determining the total deformation of the assembly under load. Figure 26 and Figure 27 show examples of the deformation curve under a concentrated load for a fixed end beam and a pin-roller beam with overhang (representing the nozzle), respectively. Neglecting the nozzle and considering a fixed end condition (Figure 26) would result in a smaller deflection amount due to the lack of rotation at point B. Meanwhile, considering the nozzle as a pin-roller beam with the overhang representing the duct of the assembly (Figure 27) allows some rotation at point B increasing the overall deflection of the duct. *Understanding the actual boundary conditions in a reactor and which of the two end conditions correctly represents the assembly is crucial to modeling the deformation correctly.* The experiment in [47] also tested these assumptions and concluded the

nozzle definition needed to be considered. Further experimentation and testing would be needed with a more complete definition of a reactor assembly to test these boundary conditions.

Figure 26. Fixed end beam deflection

Figure 27. Pin-roller with beam overhang deflection

4.5 Geometric Uncertainties

Another important aspect to consider in the simulation of reactors is the large variety of potential uncertainties in the analysis. While much detail has gone into studying the mechanical response in a reactor deterministically, there are uncertainties associated in the manufacturing process that could directly affect the deformations, and thus the reactivity feedback. Some work was performed in [48] which shows large distributions of assembly deformations based on slight variations in the geometric parameters such as the size of the load pads. Further investigation on how much this could affect the reactivity feedback could be useful in helping to qualify the radial expansion reactivity effects.

5 Summary

This paper summarizes (1) the key physical mechanisms which drive core radial expansion, and (2) the current advanced modeling and simulation tools which have been used or could be used to solve parts of the core radial expansion phenomenon. While some multi-physics code systems have been applied to this problem recently, there is currently no computationally robust, fully coupled, geometrically-detailed multi-physics tool which can be used to iterate on restraint ring design and compute detailed core displacements. The goal of this report is to serve as a reference for future development of an advanced code system to fulfill this purpose. The recommendation of the authors is to examine MOOSE-based tools to understand the development needed within structural mechanics, neutronics, and heat transfer solvers in order to solve the large-scale core radial expansion problem. The MOOSE framework provides a robust computational foundation for detailed physics computation and is based on an unstructured finite element mesh framework ideal for computing core deformations. Additional work will be needed to adapt the current mechanics solvers in MOOSE to large-scale core radial expansion problems. Neutronics and fluid dynamics / thermal hydraulics codes are also being developed in MOOSE and/or connected to the MOOSE framework. Future work will start with assessing the state of the mechanics modules for solving large scale deformations with contact.

6 References

- [1] S. A. Kamal and Y. Orechwa, “Bowling of Core Assemblies in Advanced Liquid Metal Fast Reactors,” Argonne National Lab., CONF-860724--2, 1986. Accessed: Jul. 17, 2018. [Online]. Available: http://inis.iaea.org/Search/search.aspx?orig_q=RN:17089609.
- [2] T. J. Moran, “Core Restraint Contributions to Radial Expansion Reactivity,” Argonne National Lab., IL (USA), CONF-860724-12, Jan. 1986. Accessed: Jul. 05, 2018. [Online]. Available: <https://www.osti.gov/biblio/5111665>.
- [3] R. A. Wigeland and T. J. Moran, “Radial Core Expansion Reactivity Feedback in Advanced LMRs: Uncertainties and Their Effects on Inherent Safety,” Argonne National Lab., Seattle, WA, CONF-8804155--1, Apr. 1988. Accessed: Jul. 16, 2018. [Online]. Available: http://inis.iaea.org/Search/search.aspx?orig_q=RN:19106410.
- [4] R. A. Wigeland, “Radial Core Expansion Reactivity Feedback: Current Understanding and the SASSYS/SAS4A Model,” Argonne National Laboratory, ANL/RAS 88-6, Sep. 1988.
- [5] J. E. Kalinowski, “The Effect of Irradiation Induced Structural Material Deformations on Core Restraint Design,” *J. Eng. Power*, vol. 104, no. 4, pp. 907–912, Oct. 1982, doi: 10.1115/1.3227364.
- [6] J. J. Grudzinski and C. Grandy, “Fuel Assembly Bowing and Core Restraint Design in Fast Reactors,” in *Proceedings of the ASME 2014 International Mechanical & Engineering Congress & Exposition*, Montreal, Canada, Nov. 2014, p. V06BT07A026, doi: 10.1115/IMECE2014-38331.
- [7] J. P. Foster, W. G. Wolfer, A. Biancheria, and A. Boltax, “Analysis of irradiation-induced creep of stainless steel in fast spectrum reactors,” Westinghouse Electric Corp., Madison, Pa. (USA). Advanced Reactors Div., CONF-721115-6, Jan. 1972. Accessed: Jul. 19, 2018. [Online]. Available: <https://www.osti.gov/biblio/4324066>.
- [8] J. P. Foster, J. E. Kalinowski, D. V. Swenson, and A. Boltax, “Technical basis for swelling-irradiation creep opposition testing,” *Nucl. Eng. Des.*, vol. 61, no. 3, pp. 399–413, Dec. 1980, doi: 10.1016/0029-5493(80)90009-6.
- [9] A. Boltax, “Incorporation of Irradiation Effects in Design: A Review of Experience from the Breeder Reactor Program,” *Fusion Technol.*, vol. 21, no. 3P2B, pp. 1921–1926, May 1992, doi: 10.13182/FST92-A30000.
- [10] K. Ehrlich, “Irradiation creep and interrelation with swelling in austenitic stainless steels,” *J. Nucl. Mater.*, vol. 100, no. 1, pp. 149–166, Sep. 1981, doi: 10.1016/0022-3115(81)90531-6.
- [11] E. R. Gilbert and F. A. Garner, “The influence of cold-work level on the irradiation creep and swelling of AISI 316 stainless steel irradiated as pressurized tubes in the EBR-II fast reactor,” *J. Nucl. Mater.*, vol. 367–370, pp. 954–959, Aug. 2007, doi: 10.1016/j.jnucmat.2007.03.059.

- [12] J. N. Fox and B. C. Wei, "Core Mechanics and Configuration Behavior of Advanced LMFBR Core Restraint Concepts," General Electric Co., GEFR-SP--063, 1978. Accessed: Aug. 13, 2018. [Online]. Available: http://inis.iaea.org/Search/search.aspx?orig_q=RN:12592617.
- [13] J. A. Shields, "Bow in Experimental Breeder Reactor II Reflector Subassemblies," *Nucl. Technol.*, vol. 52, no. 2, pp. 214–227, Feb. 1981, doi: 10.13182/NT81-A32666.
- [14] W. H. Sutherland, "Overview of core designs and requirements/criteria for core restraint systems," Hanford Engineering Development Lab., Richland, WA (USA), HEDL-SA-3211-FP; CONF-8410199-2, Sep. 1984. Accessed: Mar. 12, 2020. [Online]. Available: <https://www.osti.gov/biblio/6282120-overview-core-designs-requirements-criteria-core-restraint-systems>.
- [15] G. A. McLennan, "NUBOW-3D (inelastic): A FORTRAN program for the static three-dimensional analysis of bowed reactor cores, including irradiation creep and swelling," *Trans Am Nucl Soc U. S.*, vol. 30, Jan. 1978, Accessed: Oct. 23, 2018. [Online]. Available: <https://www.osti.gov/biblio/6527555-nubow-inelastic-fortran-program-static-three-dimensional-analysis-bowed-reactor-cores-including-irradiation-creep-swelling>.
- [16] A. J. Brunett and T. H. Fanning, "U.S. Sodium Fast Reactor Codes and Methods: Current Capabilities and Path Forward," p. 12, Jun. 2017.
- [17] G. A. McLennan, "NUBOW: A FORTRAN-IV Program for the Static Elastic Structural Analysis of Bowed Reactor Cores," p. 94.
- [18] S. L. Hecht and R. G. Trenchard, "Fast Flux Test Facility core restraint system performance," Feb. 1990.
- [19] "Verification and Validation of LMFBR Static Core Mechanics Codes Part I," International Atomic Energy Agency, Vienna, IWGFR/75, 1990.
- [20] T. H. Fanning, A. J. Brunett, and T. Sumner, "The SAS4A/SASSYS-1 Safety Analysis Code System," Argonne National Laboratory, ANL/NE-16/19, Mar. 2017.
- [21] E. R. Shemon, M. A. Smith, C. H. Lee, T. K. Kim, and T. H. Fanning, "Direct Neutronics Modeling Approach for Deformed Core Analysis using PROTEUS," presented at the International Conference on Mathematics & Computational Methods Applied to Nuclear Science & Engineering, Jeju, Korea, Apr. 2017, Accessed: Jun. 21, 2018. [Online]. Available: https://www.kns.org/files/int_paper/paper/MC2017_2017_1/P014S01-01ShemonE.pdf.
- [22] A. Siegel *et al.*, "(PDF) Software design of SHARP," Monterey, California, Apr. 2007, Accessed: Mar. 02, 2020. [Online]. Available: https://www.researchgate.net/publication/228503475_Software_design_of_SHARP.
- [23] E. Merzari *et al.*, "Multi-Physics Demonstration Problem with the SHARP Reactor Simulation Toolkit," Argonne National Lab. (ANL), Argonne, IL (United States), ANL/NE-15/44, Dec. 2015. doi: 10.2172/1236454.

- [24] N. E. Hodge, R. M. Ferencz, and J. M. Solberg, "Implementation of a thermomechanical model for the simulation of selective laser melting," *Comput. Mech.*, vol. 54, no. 1, pp. 33–51, Jul. 2014, doi: 10.1007/s00466-014-1024-2.
- [25] T. Jing and W. S. Yang, "Development of the RAINBOW code to evaluate assembly bowing reactivity coefficients in sodium-cooled fast reactors," *Ann. Nucl. Energy*, vol. 129, pp. 289–297, Apr. 2019, doi: 10.1016/j.anucene.2019.02.004.
- [26] J. Wharry and W. S. Yang, "Steady-State Thermal-Hydraulic Analysis and Bowing Reactivity Evaluation Methods Based on Neutron and Gamma Transport Calculations," 15–7983, 1493700, Dec. 2018. doi: 10.2172/1493700.
- [27] T. Jing, "Evaluation of Reactivity Feedbacks Due to Core Deformation in Fast Reactors," Doctoral, Purdue, West Lafayette, Indiana, 2018.
- [28] N. W. Touran, J. Gilleland, G. T. Malmgren, C. Whitmer, and W. H. Gates, "Computational Tools for the Integrated Design of Advanced Nuclear Reactors," *Engineering*, vol. 3, no. 4, pp. 518–526, Aug. 2017, doi: 10.1016/J.ENG.2017.04.016.
- [29] Dassault Systemes, *Abaqus*. 2020.
- [30] J. B. Meng and F. Deleo, "Considerations from the Benchmark Comparison of OXBOW against IWGFR Mechanical Analysis Codes," in *2018 International Congress on Advances in Nuclear Power Plants (ICAPP 2018)*, Charlotte, NC, Apr. 2018, p. 9.
- [31] M. Nakagawa, "ARKAS: A Three-Dimensional Finite Element Program for the Core-Wide Mechanical Analysis of Liquid-Metal Fast Breeder Reactor Cores," *Nucl. Technol.*, vol. 75, no. 1, pp. 46–65, Oct. 1986, doi: 10.13182/NT86-A15976.
- [32] M. NAKAGAWA, "Verification of Core Mechanical Performance Code ARKAS with IAEA Benchmark Problems," *J. Nucl. Sci. Technol.*, vol. 28, no. 11, pp. 973–994, Nov. 1991, doi: 10.1080/18811248.1991.9731461.
- [33] H. Ohta and T. Yokoo, "Development and Validation of ARKAS_cellule: An Advanced Core-Bowing Analysis Code for Fast Reactors," *Nucl. Technol.*, vol. 146, no. 2, pp. 131–142, May 2004.
- [34] M. Nakagawa, T. Yokoo, H. Ohta, and S. Matsuyama, "Development of an Advanced Core Bowing Code ARKAS_cellule," in *International Association for Structural Mechanics in Reactor Technology (IASMiRT)*, Washington, DC, Aug. 2001, p. 8.
- [35] M. Nakagawa, H. Endo, and M. Kawashima, "Development of the core-bowing reactivity analysis code system ATLAS and its application to a large FBR core," *Nucl. Eng. Des.*, vol. 157, no. 1, pp. 15–26, Jul. 1995, doi: 10.1016/0029-5493(95)00981-H.

- [36] E. U. Khan, W. M. Rohsenow, A. A. Sonin, and N. E. Todreas, “A porous body model for predicting temperature distribution in wire-wrapped fuel rod assemblies,” *Nucl. Eng. Des.*, vol. 35, no. 1, pp. 1–12, Jan. 1975, doi: 10.1016/0029-5493(75)90076-X.
- [37] K. Mikityuk, S. Pelloni, P. Coddington, E. Bubelis, and R. Chawla, “FAST: An advanced code system for fast reactor transient analysis,” *Ann. Nucl. Energy*, vol. 32, no. 15, pp. 1613–1631, Oct. 2005, doi: 10.1016/j.anucene.2005.06.002.
- [38] C. Fiorina, I. Clifford, M. Aufiero, and K. Mikityuk, “GeN-Foam: a novel OpenFOAM® based multi-physics solver for 2D/3D transient analysis of nuclear reactors,” *Nucl. Eng. Des.*, vol. 294, pp. 24–37, Dec. 2015, doi: 10.1016/j.nucengdes.2015.05.035.
- [39] C. Fiorina, S. Radman, M.-Z. Koc, and A. Pautz, “DETAILED MODELLING OF THE EXPANSION REACTIVITY FEEDBACK IN FAST REACTORS USING OpenFOAM,” Illinois, Aug. 2019, pp. 1434–1442.
- [40] ANSYS Inc., *ANSYS Mechanical*. 2020.
- [41] COMSOL Inc, *COMSOL Multiphysics*. 2020.
- [42] D. Gaston, C. Newman, G. Hansen, and D. Lebrun-Grandié, “MOOSE: A parallel computational framework for coupled systems of nonlinear equations,” *Nucl. Eng. Des.*, vol. 239, no. 10, pp. 1768–1778, Oct. 2009, doi: 10.1016/j.nucengdes.2009.05.021.
- [43] “MOOSE Framework.” <https://www.mooseframework.org/> (accessed Jul. 23, 2020).
- [44] G. Hu, G. Zhang, and R. Hu, “Reactivity Feedback Modeling in SAM,” Argonne National Laboratory, ANL-NSE-19/1, Feb. 2019.
- [45] M. A. Smith, C. Adams, W. S. Yang, and E. E. Feldman, “VARI3D & PERSENT: Perturbation and Sensitivity Analysis,” Argonne National Laboratory, ANL/NE-13/8, Aug. 2018. Accessed: Nov. 20, 2020. [Online]. Available: <https://publications.anl.gov/anlpubs/2018/08/145701.pdf>.
- [46] R. Hu, G. Hu, L. Zou, G. Zhang, B. Hollrah, and M. Gorman, “SAM Developments to Support Transient Safety Analysis of Advanced non-LWRs,” ANL/NSE-19/31, 1577423, Sep. 2019. doi: 10.2172/1577423.
- [47] Z. Ma *et al.*, “Experimental research on assembly section stiffness and bending stiffness for sodium-cooled fast reactor,” *Ann. Nucl. Energy*, vol. 135, p. 106994, Jan. 2020, doi: 10.1016/j.anucene.2019.106994.
- [48] N. Wozniak, “Structural Uncertainty Analysis of Nuclear Reactor Core Load Pads,” Doctoral, Illinois Institute of Technology, Chicago, Illinois, 2019.
- [49] T. A. Laursen, “Mortar-based surface-to-surface contact algorithms in large deformation solid mechanics,” in *Analysis and Simulation of Contact Problems*, P. Wriggers and U. Nackenhorst, Eds. Berlin, Heidelberg: Springer Berlin Heidelberg, 2006, pp. 39–47.

Appendix A – Description of IWGFR Example Problems

The International Atomic Energy Agency (IAEA) organized a working group for the verification and validation of Liquid Metal Fast Breeder Reactor (LMFBR) analysis codes called the International Working Group on Fast Reactors (IWGFR). The coordinated work was performed by eleven participating agencies in nine different countries, listed in Table 8 below and referenced in section 3.9 [19].

Country	Organization	Code
Belgium	BelgoNucleaire	STRAW
CzechoslovakSSR (CSSR)	NRI, Rez	SANDRA/CORDIAL
France	CEA de Cadarache	HARMONIE/SOLO
Fed. Rep. of Germany	INTERATOM GmbH	DDT/DDTR/DDAB
India	IGCAR, Kalpakkam	SABOW/MABOW
Italy	ENEA/VEL, Bologna	HARMONIE/SISCO
Japan	PNC/Hitachi	HIBEACON
	Mitsubishi, API	RAINBOW-X
	NAIG/Toshiba	ARKAS
USSR	Inst. PPE, Obninsk	ACME
UK	NNC Ltd, Risley	CRAMP

Table 8. IWGFR participating organizations and their codes (adapted from [19] © IAEA)

Below are summaries of the IWGFR example problems referenced in the V&V sections of various codes including NUBOW, OXBOW, and ARKAS.

Example 1

This example examined the free (unrestrained) thermal bowed deformation of a single, hexagonal assembly of 4000 mm in height, fixed at the bottom. The assembly had a linearly varying thermal gradient along the axial height in the active core region. Below the core, all the corners had the same temperature of 400 °C which varied linearly from the core inlet to 550 °C at

Corner 4, 537.5 °C at Corners 3 and 5, 512.5 °C at Corners 2 and 6, and 500 °C at Corner 1; the temperature remained at these constant temperatures from the top of the core to the top of the duct.

Example 2

This example examined the free (unrestrained) thermal bowed deformation of a single, hexagonal assembly of 4000 mm in height, fixed at the bottom, similar to Example 1. The difference is the assembly had a non-linearly varying thermal gradient along the axial height in the active core region. Below the core, all the corners had the same temperature of 400 °C which varied non-linearly from the core inlet to 500 °C at Corners 1, 2, and 6 and 550 °C at Corners 3, 4, and 5; the temperature remained at these constant temperatures from the top of the core to the top of the duct.

Example 3A

This example examined the behavior of a single duct thermally bowing into a 60° symmetric sector of a core with free boundaries around the symmetric lines (Figure 28). The dashed red lines indicate the location of the free boundary, and the blue arrow indicates the direction of the thermal bow, corner to corner along the duct cross section. The desired outputs were the interactions between ducts at the ACLP and TLP contact locations.

Figure 28. Model for example 3A of 60° symmetric core region with a free boundary, represented by the red dashed line. The blue arrow indicates the direction of the thermal gradient induced bow for duct 1 (Adapted from [19] © IAEA).

Example 3B

This example examined the behavior of a single duct thermally bowing into a 120° symmetric sector of a core with free boundaries around the symmetric lines (Figure 29). The dashed red lines indicate the location of the free boundary, and the blue arrow indicates the direction of the thermal bow, flat to flat along the duct cross section. The desired outputs were the interactions between ducts at the ACLP and TLP contact locations.

Figure 29. Model for example 3B of 120° symmetric core region with a free boundary, represented by the red dashed line. The blue arrow indicates the direction of the thermal gradient induced bow for duct 1 (Adapted from [19] © IAEA).

Example 4

This example examined the behavior of a 30° symmetric core region with an outward temperature gradient applied to row 5 of the core. The temperature gradient of example 1 is used but in the directions shown in Figure 30. The core and numbering are the same as in example 3 but with the addition of a restraint ring with a clearance equal to the clearance between assembly

load pads (0.5 mm). The desired outputs were the interactions between ducts at the ACLP and TLP contact locations.

Figure 30. Model for example 4 of 30° symmetric core region, represented by the red dashed line, with a core restraint ring at the TLP and ACLP. The blue arrows indicate the direction of the thermal gradient induced bow for ducts 42, 43, and 44 (Adapted from [19] © IAEA).

Example 5

This example used the same core restraint system and 30° symmetric region as example 4 but replaced the thermal bowing with irradiation swelling and creep behavior. The damage dose field, shown in Figure 31, decreased with radius until the circle noted in the figure. For this example, swelling was only activated on ducts 42, 43, and 44 (the same as for the thermal bowing). The desired outputs were the interactions between ducts at the ACLP and TLP contact locations for irradiation damage instead of thermal bowing behavior.

Figure 31. Core model showing the location where the neutron damage dose is active within the circle, for examples 5, 6, and 8A (Adopted from [19] © IAEA).

Example 6

This example examined the irradiation behavior of the entire 127 assembly core shown in Figure 31. It was identical to example 5 without the symmetry section.

Example 8A

This example examined the free dilation (bulging) of assemblies 1, 23, 42, and 44 from example 5 under the same damage dose. The expected outputs were the values of the dilation of the cross section at the core midplane region.

Appendix B – Description of Mechanical Contact Models

In structural analysis of mechanical assemblies, a major concern is capturing the interaction between unbonded material interfaces, referred to as ‘contact’. For the purposes of this report, ‘contact’ refers to mechanical contact, which is differentiated from ‘thermal contact’, which is a process of energy/heat exchange in thermal dynamics problems. Contact problems are very difficult to solve due to the inherent non-linearity presented at the contact interface prior to and post contact. Empirical solutions for contact problems exist for only the simplest of geometry. Research has been ongoing for decades for seemingly fundamental areas of contact: inclusion of friction, contact detection, methods of removing or smoothing the geometric discontinuities, and more accurate representations of the contact pressure.

Mechanical contact between deformable bodies is based on enforcement of the following requirements:

$$\begin{aligned}t_n &\geq 0, \\g &\leq 0, \\t_n g &= 0.\end{aligned}$$

Where the surface traction (understood in the present context to represent contact force normal to the contact surface), t_n , which resists surface penetration must be positive normal to the contact face; the gap, g , must not be positive; and the work done by the traction must be 0 (either the gap is 0 or the traction is 0) at all times. While seemingly non-intuitive to define $g < 0$, in many methods, the gap value is used to scale the contact force in the direction normal to the contact surface. Thus, if the contact is normal to the target face, a positive value for the gap (which indicates penetration of the contact surfaces) multiplied in the normal direction gives a properly directed contact force.

There are many different model assumptions about the contact behavior depending on the physical situation that are chosen either to simplify the analysis or better match the physical situation. The primary differentiations are listed below in order of computational complexity:

- **Bonded Contact:** Contact between two surfaces/elements that are not allowed to separate or slide past each other during contact; the elements act as one body. This is not really a contact problem but a way of joining two distinct bodies and distinct meshes. It can also provide a straightforward method for extracting joint loads.
- **Glued/Rough Contact:** After contact is initiated between two surfaces, no slipping is allowed during contact, but the contact interface can separate.
- **Frictionless Sliding:** Surfaces are allowed to slip along the contact interface with no resistance; usually when surfaces are assumed as smooth.

- Coulomb (Frictional Sliding): Surfaces are allowed to slip along the contact interface, but there is resistance due to friction effects between the surfaces.

Common Solution Techniques

The complexity in solving contact problems arises from the fact that even in linear elastic problems, the contact imposes a nonlinearity into the solution. Also, in unbonded contact problems, there exists an initial gap between the contacting bodies, so an iterative solution approach is necessary to check if the gap closes and contact occurs. Contact problems between multiple bodies that are initially separated and not otherwise completely constrained require those bodies to be brought into contact or require the use of dynamic methods. There are many different solution methods to enforce contact constraints used in finite element solutions with the main methods being: penalty method, Lagrange multipliers, augmented Lagrangian, kinematic method, and mortar-based methods.

To explain the differences between the methods, a simple 2-D beam element representing a fuel assembly and single contact element representing a restraint point are shown in Figure 32. The beam is fixed at the bottom and subject to a concentrated force at the top, with an initial gap, g , between the beam and the restraint point.

Figure 32. Beam model contact, with (a) before contact and initial gap, g , and (b) after contact

Lagrange Multipliers

The method of Lagrange multipliers is a mathematical algorithm used to find the maxima and minima of an equation, $f(x)$, subject to a constraint, $g(x) = 0$, with the general form

$$\mathcal{L}(x, \lambda) = f(x) - \lambda g(x)$$

where λ is the Lagrange multiplier. In the context of finite element contact analysis, λ corresponds to the traction force required to enforce the contact constraint. An advantage of this solution scheme is that in contact such as Figure 32, the contact constraint is enforced exactly with no penetration. Some disadvantages are that enforcing the contact constraint exactly could over constrain the solution to the problem, causing instability of the solver. It also requires the addition of extra equations to enforce all the contact constraints, so adding more degrees of freedom would add many more equations to the system to solve.

Kinematic

FEA solvers that use the kinematic contact enforcement method uses a predictor/corrector algorithm to check if the bodies make contact during the analysis step and strictly enforces no penetration conditions. First the simulation advances the kinematic state of the model into a predicted configuration without considering the contact conditions. A contact search is performed to determine if any nodes on the body penetrated the contact target. The depth of each penetration, the mass of the body, and the time are used to determine the force required to resist the penetration. Then acceleration corrections are determined to obtain a corrected configuration in which the contact constraints are enforced, and no penetration occurs.

Penalty Method

The penalty method changes the hard constraint into a contact element such as a linear spring with an associated stiffness value, k , called the penalty stiffness. The contact node violates the contact constraint by an amount proportional to the penalty stiffness, d , such that if k is sufficiently large, the penetration is sufficiently small. The schematic for this approach is shown in Figure 33.

Figure 33. Beam model penalty contact, with (a) before contact with initial gap, g , and spring stiffness, k , and (b) after contact with small penetration, d

The penalty method allows for a less stringent enforcement of contact by allowing some small amount of penetration which is countered by an opposing traction proportional to the stiffness of the contact element. The use of the linear spring and allowance of minimal penetration removes the discontinuity in the contact force and provides numerical softening as compared with the Lagrange multiplier method. The penalty method can mitigate over-constraint issues and reduce the number of iterations required in an analysis. The penalty method is well-suited for general contact types and situations including: 1) multiple contact per node, 2) contact between rigid bodies, and 3) contact of surfaces also involved in other types of constraints. One of the downsides of this method is that if the penalty parameter is too large, the matrix system can become ill-conditioned and difficult to solve; while if the penalty parameter is too small, the penetration amount becomes too large.

Augmented Lagrange

The augmented Lagrange method combines the methods used in the Lagrange multiplier (which produces exact constraints) and penalty (which allows for some violation of the contact) methods. The Lagrange multiplier method can be difficult to implement with additional degrees of freedom, while the penalty method can lead to an ill-conditioned matrix with too large of a penalty parameter. The augmented Lagrange method seeks a balance by combining the Lagrange multiplier method in series with a penalty parameter. While iterating the solution, incremental

amounts of penetration are added, which can help reduce the penetration while also helping to avoid the hard non-linearity of the Lagrange method alone.

Mortar-Based Method

The mortar-based methods are used to enforce contact constraints on non-overlapping subdomains; the meshes on each element in contact do not have to match node-for-node at the contact locations so surface-to-surface contact can be enforced. Mortar-based methods usually use Lagrange multiplier method to enforce the contact constraints. Mortar-based methods are extremely useful in deformable contact problems with large deformations or sliding, where they are usually more robust and stable than traditional contact methodologies [49].

Nuclear Science and Engineering Division

Argonne National Laboratory
9700 South Cass Avenue
Argonne, IL 60439

www.anl.gov

Argonne National Laboratory is a U.S. Department of Energy
laboratory managed by UChicago Argonne, LLC