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Verification of Thermo-mechanical Model in High Fidelity ATF Fuel Code

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1. Introduction

After Fukushima accident, the demand for safer nuclear fuel led to the innovation of accident tolerance fuel (ATF). One of the near-term promising technology is the use of coated cladding, utilizing multiple-layer, multi-materials.

Traditional fuel performance codes such as FRAPCON [1], FRAPTRAN [2], ROPER [3] have employed finite difference method (FDM) to assess the performance of nuclear fuel. However, conventional finite difference method (FDM) have troubles on analyzing structural deformation in multi-layered multi-material cladding.

To overcome these limitations, finite element method (FEM) based numerical simulation codes, such as BISON from the Idaho National Laboratory (INL) [4, 5] and MERCURY from Korea Atomic Energy Research Institute (KAERI) [6, 7], have been introduced. These FEM based codes employ general physical equations to effectively model the coupled thermo-mechanical behaviors of multi-layered multi-material cladding (e.g. ATF).

For use in the nuclear industry, objective reliability metrics are required, even for software. The Technology readiness level (TRL) serves as a gauge to determine technology maturity. To elevate the TRL of software, various methodologies have been devised to quantify the reliability of software, such as verification and validation [8, 9, 10].

In this paper, we introduce a verification process of thermo-mechanical model in high fidelity ATF fuel code. Detailed procedures of verification are discussed and some of verification cases were studied to verify thermo-mechanical model in the code.

2. Verification Method

In this section we discuss the verification method of high-performance FEM based code. We outline the BISON code and its verification process while also presenting the convergence rate of the FEM.

2.1 Previous fuel performance evaluation codes

From early 1970s, many well-known nuclear simulation codes based on FDM and empirical models were developed. For example, FRAPCON and FRAPTRAN were very popular fuel performance codes developed and maintained by Pacific Northwest National Laboratory (PNNL) [1, 2].

As computational power grew, with its ability to represent complex governing equations and deformation of geometry, FEM became basis for most of these advanced codes.

BISON is a FEM based fuel performance code developed by INL. Although the source code of BISON is concealed, its performance and capabilities are assessed through verification and validation process [11, 12, 13].

2.2 Process of verification

In general, there are two main processes to assess the performance of software: verification and validation. Verification is a process to ensure that the code is functioning correctly, while validation is used to assess the code’s ability with physical problems.

Verification is composed of three components. First one is the software quality assurance (SQA), which is to eliminate coding errors. Version control, defect testing, regression testing, and code-to-code comparison can be used as SQA. Second one is code verification which is to ensure that code can faithfully demonstrate the underlying mathematical model. To achieve the code verification, solution obtained using code and reference solution from underlying mathematical model are compared. The last process is solution validation, which is an assessment of solution’s numerical errors and stability like round-off error, iterative error, and discretizing error.

2.3 Verification Methodologies

As mentioned above, sufficient number of problems should be tested for the code verification. However, those problems must have its reference solution based on its embedded mathematical model.

Let us note $\mathcal{L}$ as system operator of the intended mathematical model. The method of exact solutions (MES) is a method to find the analytic solution $f(\vec{x},t)$, which is a function of space $\vec{x}$ and time *t*, satisfying:

$$\mathcal{L}[f(\vec{x},t)] = 0 \tag{1}$$

However, finding a nontrivial solution for a complex nonlinear differential equation is very complicated and, in most cases, impossible. Therefore, most of MES only involve a single equation of state, varying property, or simple geometry.

Method of manufactured solutions (MMS) can be employed to overcome MES. Unlike MES, MMS works backward to find the solution form. First, one determines a particular solution $\mathcal{M}(\vec{x},t)$, then the remainder solution $\mathcal{R}(\vec{x},t)$ satisfying:

$$\mathcal{L}[\mathcal{M}(\vec{x},t)] = \mathcal{R}(\vec{x},t) \quad (2)$$

Due to its laborious work for finding $\mathcal{R}(\vec{x},t)$, it is highly recommended to choose $\mathcal{M}(\vec{x},t)$ as a continuous and smooth function. However, these functions can be sufficiently complex to assess the coupled complex phenomena of mathematical model. Note that, for verification process, the solution of MES or MMS can be physically unrealistic, as it is only intended to assess the underlying mathematic algorithm.

2.4 Order of Accuracy in Finite Element Method

FEM is a method of finding an approximated solution with finite number of basis functions. For problems with differentiable solutions, the upper bound of error can be estimated and it is called the order of accuracy in FEM. Investing how the discretization error converge to zero with respect to its mesh size can be one of verification process.

We will briefly introduce the relation between discretization error and mesh size. The exact solution $U(x)$ near $x = \hat{x}$ can be expressed using Taylor expansion:

$$U(x) = \sum_{n=0}^{\infty} \frac{1}{n!} \frac{d^n U}{dx^n}\bigg|_{\hat{x}} (x-\hat{x})^n \quad (3)$$

The approximated solution with polygonal basis order up to p can be expressed as:

$$\widetilde{U}(x) = \sum_{n=0}^{p} a_n (x-\hat{x})^n, \quad (4)$$

where a_n are the coefficients that needs to be found.

When the mesh size, $h \geq |x-\hat{x}|$, is sufficiently small, the error can be express using the remaining terms with order higher than $p+1$ and coefficients C_n:

$$U(x) - \widetilde{U}(x) \rightarrow \sum_{n=p+1}^{\infty} C_n (x-\hat{x})^n, \text{ as } h \rightarrow 0 \quad (5)$$

Consequently, the upper bound of discretization error norm is:

$$\left\| U - \widetilde{U} \right\| = C h^{p+1}, \quad (6)$$

where C is a problem-dependent arbitrary constant.

The equation above shows the relation between discretization error and size of element h. In general, it is required to show the solution convergence of element size vs. error graph in log-log scale and the result should show constant slope as calculated from Eq. 6.

3. Benchmark problem

We introduce a set of benchmark problems for verification of high fidelity ATF fuel code. 14 benchmark problems are selected from verification problem set of BISON [13] and well-known commercial software ANSYS [14].

Here, we demonstrate a problem from BISON verification [13] and its result. As illustrated in Fig. 1, the infinite hollow cylinder with inner radius r_i and outer radius r_o is exposed to two constant temperatures: T_i and T_o on its inside and outside faces, respectively. When it reached the thermal equilibrium, the analytic solution of temperature distribution T along radius r is:

$$T(r) = \frac{T_0 \ln(r_i) - T_i \ln(r_0)}{\ln(r_i/r_0)} + \frac{(T_i - T_0)}{\ln(r_i/r_0)} \ln(r) \quad (7)$$

The 4-node finite element of cylindrical coordinate system is used to model the problem with the high fidelity code. The cross-section is discretized into N-by-N finite elements (N=2, 4, 8, 16, 32, and 64, respectively).

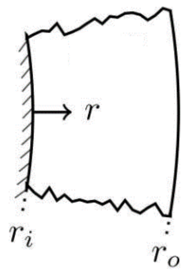

Fig. 1. Hollow cylinder with Dirichlet boundary conditions.

Table I. shows the relative error and its convergence curve are illustrated in Fig. 2. It shows that results using FEM based high fidelity code converge to the exact solution with the correct order of accuracy, as predicted in Eq. (6). In other words, the proposed code exhibits the best computational efficiency for the problem.

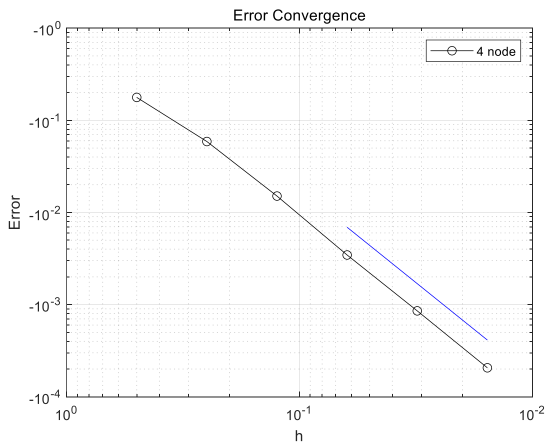

Fig. 2. Convergence curve for hollow cylinder with Dirichlet boundary conditions. The blue line represents the optimal convergence rate. Note that the optimal convergence rates are different depending on basis' polynomial order of element.

Table I: Relative errors in the hollow cylinder with Dirichlet boundary conditions

No. Elems	h	Error
2×2	0.5	1.77288×10^{-1}
4×4	0.25	5.88798×10^{-2}
8×8	0.125	1.50702×10^{-2}
16×16	0.0625	3.45581×10^{-3}
32×32	0.03125	8.55430×10^{-4}
64×64	0.015625	2.06199×10^{-4}

4. Conclusions

The code assessment procedures are crucial for software development. Verification and validation process with proper benchmark problems ensures that code is free of coding mistakes and accurately represents the reality. The verification process of FEM based BISON code is introduced, and verification process of newly developed FEM based high-fidelity performance code is demonstrated through benchmark problems. As a result, a convergence curve that showed an optimal convergence rate demonstrate that the thermo-mechanical model in the code was verified against the theoretical model in compliance with FEM verification procedure.

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