SAND2020-2368C

# Verification: a physics-based procedure with applications to CTF and BISON

N. W. Porter[1], A. Toptan[2], R. Salko[3], and M. Pilch[4]

[1]*Sandia National Laboratories, PO Box 5800 Albuquerque NM 87185-0748*
[2]*Idaho National Laboratories, PO Box 1625 Idaho Falls ID 83415*
[3]*Oak Ridge National Laboratories, 1 Bethel Valley Road Oak Ridge TN 37830*
[4]*M. Pilch Consulting, Tijeras NM 87059*

## INTRODUCTION

In 2010, the U.S. Department of Energy created its first Energy Innovation Hub, which is focused on developing high-fidelity and high-resolution simulation tools for modeling Light Water Reactors (LWRs). This Hub, Consortium for Advanced Simulation of LWRs (CASL), has developed a reactor simulation tool called the Virtual Environment for Reactor Applications (VERA). One thermal hydraulic tool in VERA is CTF [1], which is a specialized version of Coolant Boiling in Rod Arrays-Three Field (COBRA-TF). The fuel performance tool used in VERA is BISON [2], which is a code developed at Idaho National Laboratory using the Multiphysics Object-Oriented Simulation Environment (MOOSE).

To address the reliability and predictive capability of complex simulation tools, it is necessary to establish a pedigree for these tools. This process is accomplished through a series of tasks, which successively add evidence that a tool is reliable [3, 4].

1. Software quality assurance (SQA) minimizes the error introduced by coding mistakes.
2. Code verification ensures that the numerical algorithm is a faithful representation of the underlying mathematical model.
3. Solution verification quantifies all sources of numerical uncertainty.
4. Validation quantifies how faithfully the simulation tool can model a real system.
5. Uncertainty quantification attempts to bound the quantity of interest.

Following recommendations for improving the code verification evidence in CASL [5], additional work was performed for both CTF [6] and BISON [7]. These works are briefly summarized in this paper, and a few examples are provided. For both codes, a series of problems are created and solved. All problems are compared to a known solution and the numerical error is quantified as the spatial and/or temporal mesh is converged. The error behavior is compared to the expected behavior to quantify the success of each problem. A physics-based approach is used to direct development work towards areas of the codes that are lacking. By ensuring that most conservation equations, discretizations, and geometry are tested, this approach maximizes confidence in the numerical algorithms employed by a particular simulation tool.

The next section in this paper discusses the verification procedure. Then a few examples are presented from the CTF and BISON verification matrices.

## METHODS

In this work, convergence studies are used to quantify the behavior of numerical error with mesh refinement.

$$||y - \tilde{y}_h|| = Ch^p \tag{1}$$

Here, $y$ is the analytic solution to some problem, $\tilde{y}$ is the numerical approximation, and $||\cdot||$ indicates a Euclidean norm. The numerical error can be described as a function of an arbitrary constant $C$, the characteristic spatial and/or temporal mesh spacing $h$, and the order of accuracy $p$.

There are techniques for establishing the formal order of accuracy for a particular finite difference or finite element method [8, 9, 10, 11]. The observed order of accuracy is approximated by (1) choosing an analytic model with an analytic or manufactured solution, (2) creating the computational model of the problem, (3) running the computational model on successively refined meshes, and then (4) approximating the observed order using Equation 1. Once the observed order is established, it is required to match the formal order to within ±0.1 [3] to deem the verification process as successful.

In the work summarized in this paper, verification matrices were created for each code. The matrices were constructed such that most conservation equation terms, geometry choices, and discretization options are tested. This vastly improves the confidence in the underlying numerical algorithms.

## CTF DEMONSTRATION

CTF is a thermal hydraulic subchannel code for reactor core analysis [1]. It solves a two fluid, three field formulation of two-phase flow and a conduction equation in solid structures.

$$\underbrace{\frac{\partial \alpha\rho}{\partial t}}_{\text{transient}} + \underbrace{\nabla\cdot(\alpha\rho\vec{u})}_{\text{advection}} - \underbrace{\Gamma}_{\text{mass transfer}} = 0 \tag{2}$$

$$\underbrace{\frac{\partial \alpha\rho h}{\partial t} - \alpha\frac{\partial P}{\partial t}}_{\text{transient}} + \underbrace{\nabla\cdot(\alpha\rho h\vec{u})}_{\text{advection}} - \underbrace{\Gamma h}_{\text{mass transfer}} - \underbrace{q_w}_{\text{convection}} = 0 \tag{3}$$

$$\underbrace{\frac{\partial \alpha\rho\vec{u}}{\partial t}}_{\text{transient}} + \underbrace{\nabla\cdot(\alpha\rho\vec{u}\vec{u})}_{\text{advection}} - \underbrace{\alpha\rho g}_{\text{gravity}} + \underbrace{\alpha\nabla P}_{\text{pressure force}} - \underbrace{\tau_w + \tau_i}_{\text{shear}} = 0 \tag{4}$$

$$\underbrace{\rho c_p\frac{\partial T}{\partial t}}_{\text{transient}} - \underbrace{\frac{\partial}{\partial x}k\frac{\partial T}{\partial x}}_{\text{conduction}} - \underbrace{Q}_{\text{internal generation}} + \underbrace{q_w}_{\text{convection}} = 0 \tag{5}$$

The first three equations are the phasic liquid conservation equations of mass, momentum, and energy. The phase

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

indicators have been omitted, but they represent an equation for each of the three fields in CTF: water, steam, and droplets. The only exception to this is that the droplets are assumed to be in thermal equilibrium with the water, and therefore do not have a separate energy equation. Turbulent mixing and void drift are omitted from the equations, but are included in the code. The final equation is the conduction equation in the solid.

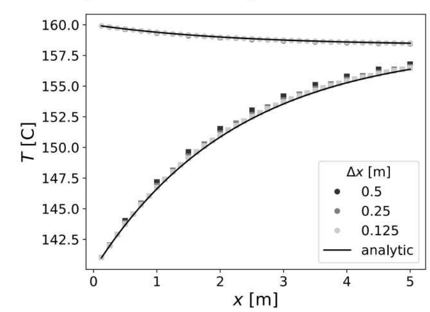
Previously performed code verification studies are documented in the CTF V&V manual [12]. The code verification matrix was previously extended in [13]. New problems added to the CTF verification matrix have been added to the V&V manual and are described in a new CASL report [6]. This section describes two new problems added to the CTF verification matrix: convection and advection.

## Convection

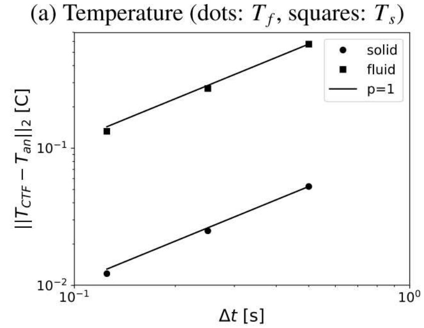
This problem is designed specifically to test wall heat transfer governing the coupling of the CTF solid and fluid equations. A stationary fluid and solid are initially at different temperatures and come to thermal equilibrium over time. The following assumptions are made: (1) the fluid and solid are zero-dimensional, (2) all properties and the heat transfer coefficient are constant, and (3) there is no heat generation. The fluid and solid have initial temperatures $T_{f0}$ and $T_{s0}$, respectively.

$$T_f = \frac{C_f T_{f0} + C_s T_{s0}}{C_f + C_s} + \frac{T_{f0} - T_{s0}}{C_f + C_s} C_s e^{\left(-\frac{hA(C_f+C_s)}{C_f C_s} t\right)} \quad (6)$$

$$T_s = \frac{C_f T_{f0} + C_s T_{s0}}{C_f + C_s} - \frac{T_{f0} - T_{s0}}{C_f + C_s} C_f e^{\left(-\frac{hA(C_f+C_s)}{C_f C_s} t\right)} \quad (7)$$




(a) Temperature (dots: $T_f$, squares: $T_s$)




(b) Convergence plot

Fig. 1: CTF convection problem

Here, $T$ is temperature, $h$ is heat transfer coefficient, $A$ is surface area, and $t$ is time. The thermal capacitance is notated as $C = V\rho c_p$, where $V$ is volume and $\rho$ is density. The subscript indicates the field: fluid $f$ or solid $s$.

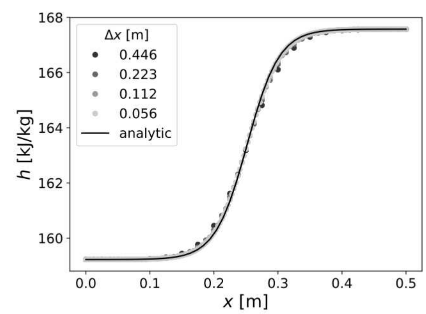
The results are shown in Figure 1a. The thermal capacitance of the solid is larger than the fluid, so the fluid temperature changes more over the transient. Figure 1b is a convergence plot. The error between the code solution and analytic solution converges at approximately $p = 1.06$ for both the solid and fluid solution. This is within $\pm 0.1$ within the formal order; therefore, the code displays the expected first order convergence for the solid-to-liquid coupling.

## Advection of a Hyperbolic Tangent

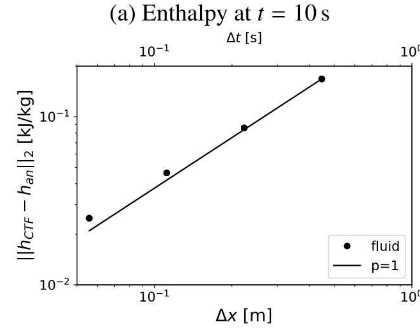
This problem was originally performed for CTF in [14]. Single phase water flows through a horizontal pipe with: (1) constant velocity, (2) constant pressure, and (3) no external sources. The analytic solution to this problem is the advection of the inlet condition with the constant velocity $u$. Three wave shapes are tested in the CTF verification matrix, but here we outline results for the hyperbolic tangent wave.

$$h = \begin{cases} h_o, & ut \leq x \\ \frac{1}{2}\left[(h_o + h_{in}) - (h_o - h_{in}) \tanh\left(\frac{u(t-\tau)-x}{l}\right)\right], & ut > x \end{cases} \quad (8)$$

Here, $h$ is enthalpy, $x$ is the spatial coordinate, initial and inlet conditions are respectively indicated by the subscripts $o$ and $in$. The constant wave velocity is $u$, the wave is offset in time by $\tau$ and its width in space is determined by $l$. The initial and inlet quantities were iteratively selected such that the velocity and pressure are approximately constant.




(a) Enthalpy at $t = 10\,\mathrm{s}$




(b) Convergence plot

Fig. 2: CTF hyperbolic tangent advection problem

Figure 2a shows the enthalpy results for four different mesh sizes and a convergence plot is shown in Figure 2b. The successive refinements show the expected diffusive numerical errors. As the convergence plot shows a observed order of about $p = 0.93$, the verification study is deemed successful.

## BISON DEMONSTRATION

BISON is a fuel performance code which models the thermo-mechanical behavior of nuclear fuel [2]. It solves three fully-coupled equations for energy conservation, mechanics, and species conservation.

$$\underbrace{\rho c_p \frac{\partial T}{\partial t}}_{\text{transient}} + \underbrace{\nabla \cdot (-k\nabla T)}_{\text{conduction}} - \underbrace{e_f \dot{F}}_{\text{fission}} = 0 \tag{9}$$

$$\underbrace{\frac{\partial C}{\partial t}}_{\text{transient}} + \underbrace{\nabla \cdot (-D\nabla C)}_{\text{diffusion}} + \underbrace{\lambda C}_{\text{decay}} - \underbrace{S}_{\text{source}} = 0 \tag{10}$$

$$\underbrace{\nabla \cdot \sigma}_{\text{stress tensor}} + \underbrace{\rho f}_{\text{body force}} = 0 \tag{11}$$

Previously performed V&V work is documented in [15], though most verification work is SQA-oriented. The first BISON code convergence study was introduced in [16]. In the current work, this has been extended to over twenty convergence studies [7]. Here, we summarize two of the new problems: one that uses an exact solution and one with a manufactured solution.

### Conduction with Analytic Solution

A slab with uniform heat generation is exposed to some constant temperature on each side: $T(0) = T_0$ and $T(L) = T_L$. The thermal conductivity varies linearly with temperature $k = k_L(1+\beta T)$. The temperature profile can be obtained [17, pages 129–132] by

$$T(x) = T_L + \frac{1}{\beta}\left[\sqrt{1 + \left(\frac{\beta q''' L^2}{k_L}\right)\left(1 - \left(\frac{x}{L}\right)^2\right)} - 1\right]. \tag{12}$$

The temperature results are shown in Figure 3a for three meshes and two different types of one-dimensional finite elements. The BISON predicted distribution accurately predicts the temperature distribution, even though this is a problem with nonlinear conduction. The convergence plot is shown in Figure 3b for the two different element types. The elements each show the correct order of convergence.

### Conduction with Manufactured Solution

This problem utilizes the BISON capability for using the Method of Manufactured Solutions (MMS). The manufactured solution is a simple trigonometric form:

$$T(x) = \sin(a\pi x). \tag{13}$$

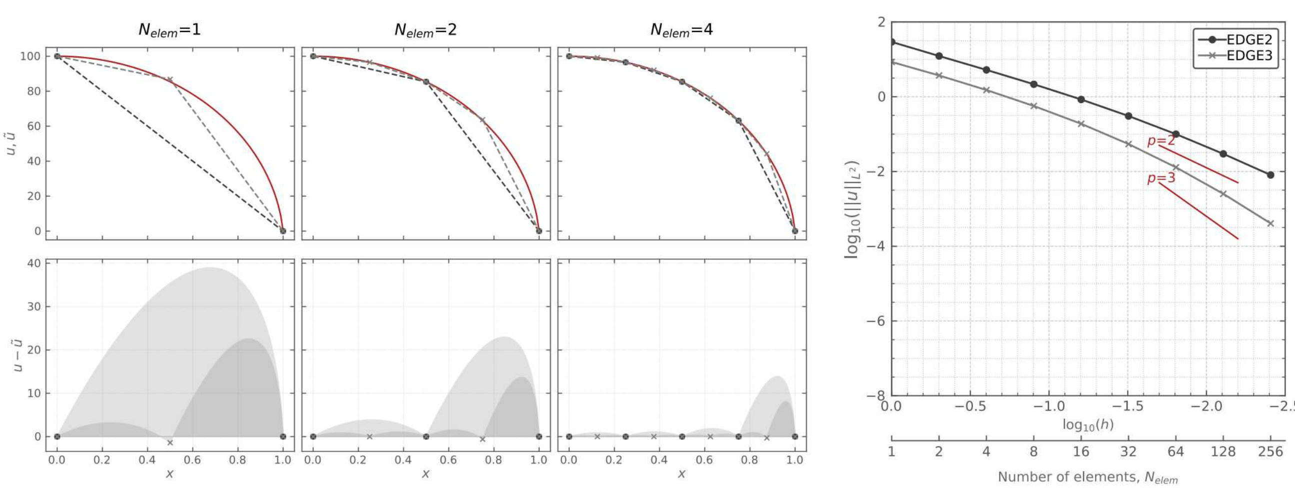
With this manufactured solution the source added to the conduction equation becomes:

$$Q = a^2\pi^2 \sin(a\pi x). \tag{14}$$

In the manufactured problem solved here, the arbitrary constant $a = 2$. This manufactured solution is solved in BISON using one-dimensional Cartesian coordinates. The results are shown in Figure 4a. BISON accurately predicts the temperature distribution. Figure 4b is a convergence plot, which shows the correct order of accuracy for this problem. Therefore, BISON is capable of utilizing the MMS for code verification.

## CONCLUSIONS

New CTF and BISON code verification work is summarized in this work. Verification matrices are created for




(a) Temperature distribution for different meshes and finite elements

(b) Convergence plot

Fig. 3: BISON conduction problem with analytic solution ($u$ indicates temperature)

each code which cover conservation terms, geometry, and discretization choices. New problems are selected to fill existing gaps in these matrices. Though neither of the matrices are fully covered, this work establishes a more thorough pedigree of these codes.

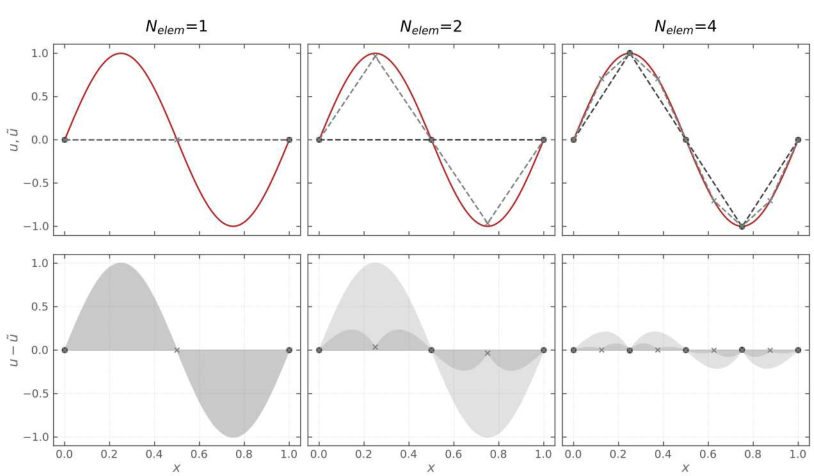
In addition to the creation of the verification matrices and addition of new verification studies, these processes were also automated in both CTF and BISON. This will enable any future verification studies performed for these codes. In the future, the verification matrices will be expanded to examine *combinations* of conservation terms and coupling between different equations. This could reveal numerical bugs that are hidden when only individual terms are tested.

## ACKNOWLEDGMENTS

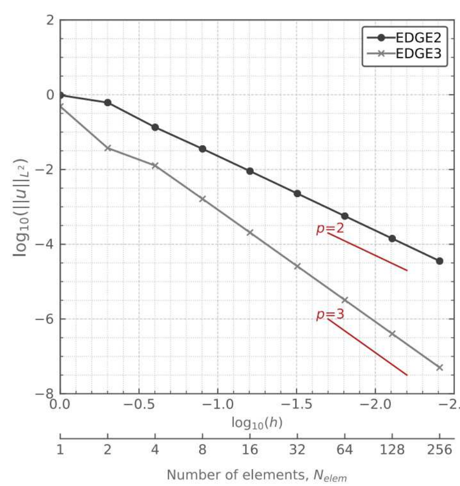
Thanks to Vincent Mousseau and Aaron Krueger for their technical reviews of this document. Sandia National Laboratories is a multi-program laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525. This paper describes objective technical results and analysis. Any subjective views or opinions that might be expressed do not necessarily represent the views of the U.S. Department of Energy or the United States Government.

## REFERENCES

1. R. K. SALKO ET AL., "CTF Theory Manual," Tech. Rep. CASL-U-2019-1886, CASL (2019).
2. J. D. HALES ET AL., "BISON Theory Manual: the equations behind nuclear fuel analysis," Tech. Rep. INL/EXT-13-29930 Rev. 1, Idaho National Laboratory, Idaho Falls, Idaho (2014).
3. W. L. OBERKAMPF and C. J. ROY, *Verification and Validation in Scientific Computing*, Cambridge University Press, Cambridge, UK, first ed. (2010).
4. P. J. ROACHE, *Verification and Validation in Computational Science and Engineering*, Hermosa Publishing, Albuquerque, NM (1998).
5. M. PILCH, A. HETZLER, V. MOUSSEAU, and J. MULLINS, "Review of V&V Documentation," Tech. Rep. SAND2018-4612R, CASL (2018).
6. N. W. PORTER, R. K. SALKO, and M. PILCH, "CTF Code Verification," Tech. rep., CASL (2020).
7. A. TOPTAN, N. W. PORTER, ET AL., "BISON Code Verification by the Method of Exact and Manufactured Solutions," Tech. rep., CASL (2020), manuscript under preparation.
8. R. F. WARMING and B. J. HYETT, "The Modified Equation Approach to the Stability and Accuracy Analysis of Finite-Difference Methods," *Journal of Computational Physics*, **14**, *2*, 159–179 (1974).
9. D. S. BURNETT, *Finite Element Analysis: from Concepts to Applications*, Addison-Wesley Publishing Company, Reading, MA, chap. 9 (1987).
10. J. D. RAMSHAW and J. A. TRAPP, "Characteristics, Stability, and Short-Wavelength Phenomena in Two-Phase Flow Equation Systems," *Nuclear Science and Engineering*, **66**, *1*, 93–102 (1978).
11. V. S. MAHADEVAN, J. C. RAGUSA, and V. A. MOUSSEAU, "A Verification Exercise in Multiphysics Simulations for Coupled Reactor Physics Calculations," *Progress in Nuclear Energy*, **55**, 12–32 (2012).
12. R. SALKO ET AL., "CTF Validation and Verification Manual," Tech. Rep. CASL-U-2019-1887, CASL (2019).
13. M. PILCH and R. K. SALKO, "CTF Code Verification and Solution Verification," Tech. Rep. CASL-U-2019-1919, CASL (2019).
14. N. PORTER, V. MOUSSEAU, and M. AVRAMOVA, "Solution Verification of CTF and CTF-R Using Isokinetic Advection Test Problems," in "International Conference on Mathematics and Computational Methods




(a) Temperature distribution for different meshes and finite elements




(b) Convergence plot

Fig. 4: BISON conduction problem with manufactured solution ($u$ indicates temperature)

Applied to Nuclear Science and Engineering (M&C-2017)," Jeju, Korea (4 2017).
15. BISON TEAM, "Assessment of BISON: A Nuclear Fuel Performance Analysis Code," Tech. Rep. INL/MIS-13-30314 Rev. 4, Idaho National Laboratory (2017).
16. R. GARDNER and D. MCDOWELL, "Automation of Solution Verification in BISON," Tech. Rep. CASL-U-209-1853-000, CASL (2019).
17. V. S. ARPACI, *Conduction Heat Transfer*, Addison-Wesley Publishing Company, Reading, MA (1966).