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INITIAL 1-D SINGLE PHASE LIQUID VERIFICATION OF CTF

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ABSTRACT

Nuclear engineering codes are being used to simulate more challenging problems and at higher fidelities than they were initially developed for. In order to expand the capabilities of these codes, state of the art numerical methods and computer science need to be implemented. One of the key players in this effort is the Consortium for Advanced Simulation of Light Water Reactors (CASL) through development of the Virtual Environment for Reactor Applications (VERA). The sub-channel thermal hydraulic code used in VERA, COBRA-TF (Coolant-Boiling in Rod Arrays - Three Fluids), is partially developed at the Pennsylvania State University by the Reactor Dynamics and Fuel Management Research Group (RDFMG). The RDFMG of version COBRA-TF is referred to as CTF.

In an effort to help meet the objectives of CASL, a version of CTF has been developed that solves the residual formulation of the one dimensional single-phase conservation equations. The formulation of the base equations as residuals allows the for the isoloation of different sources of error and is a good tool for verification purposes. This paper outlines the initial verification work of both the original version of CTF and its residual formulation. The verification problem is a simple 1-D single phase liquid channel with no heat conduction, friction, and gravity. A transient boundary condition is applied that alters the inlet density and temperature while keeping the velocity within the channel constant. The constant velocity simplifies the modified equation analysis and the order of accuracy is readily obtained. A Richardson extrapolation is performed on the problem on the temporal and spatial step sizes to determine the convergence and order of accuracy of the discretization error. While extensive validation work has been present for CTF, there has been little to no verification work previously.

Key Words: CTF, thermal hydraulic, verifiation, residual, Richardson extrapolation, CASL

1 INTRODUCTION

For the past several decades, the primary focus in nuclear engineering within the United States has been focused on light water reactors (LWR). Commercially, all nuclear reactors are either boiling water reactors (BWR) or pressurized water reactors (PWR). Correct computation of the thermal hydraulics within the reactor core leads to efficient design and accuracy in the safety analysis. A popular subchannel code for modelling the hydrodynamics within the reactor core is CTF. This FORTRAN based code solves 8 conservation equations for liquid, entrained droplet, and vapor phases in 3-D dimensions [1]. A 1-D residual formulation of the code has been created. This paper outlines an initial verification of the original version of code as well as the residual version of the code. The verification problem is a single phase 1-D channel with transient inlet density and mass flow rate. The problem will undergo a Richardson's extrapolation in the temporal and spatial domains to verify the convergence and order of accuracy of the error. The study of the order of accuracy is considered one of the more rigorous verification criteria [2].

2 CTF

The thermal hydraulics of a LWR core is an important part of nuclear reactor design. CTF solves 8 conservation equations for liquid, entrained droplet, and vapor phases of water boiling within the rod structure of a LWR reactor core [1]. Currently, the conservation equations analytically reduce into a pressure matrix in a semi-implicit method with rod temperatures solved for explicitly. The residual formulation of the code currently solves the 1-D single phase liquid conservation equations and calculated variables in a residual formulation. While it has the ability to solve the code semi-implicitly or implicitly, only the semi-implicit solution method is considered in this paper. This residual formulation should allow for easier and more in depth verification analysis. This paper details the initial comparison of the residual formulation to the original code.

2.1 Software Quality Assurance

Software quality assurance is a set of tools and procedures that helps ensure that the software is reliable. CTF is managed by GitHub repository setup and maintained by CASL. An extensive test matrix is run before each major push to ensure that the code meets the specified requirements. The test matrix consists of unit tests, code coverage runs, validation problems, and challenge problems. The code documentation consists of a theory manual, a user manual, a developer manual, and a validation manual. Further work might involve using auto documentation tools to keep an up to date developers manual. This paper will be the beginning of a verification manual, integrating this verification problem directly into the test matrix.

2.2 1-D Single Phase Liquid Conservation Equations

The finite volume structure in CTF in figure 1 is for a one-dimensional channel in the axial direction with n number of cells. The first and last cells at 0 and $n + 1$ are ghost cells and act as the boundary conditions for the problem. Pressure, enthalpy, and density are averaged over the cell

volume and are located at the center of the cell. Mass flow rate and velocity are located at the faces in between cells. The cells are represented with an index i, and the faces with indexes of $i + \frac{1}{2}$ or $i - \frac{1}{2}$. This project will initially focus on this 1-D configuration. Usually the code is 3-D, with channels connecting to each other in two more dimensions.

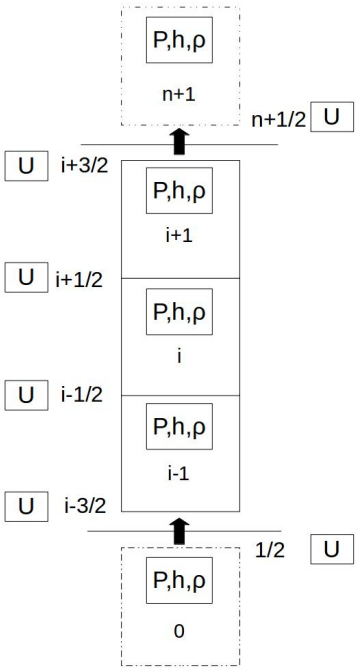

Figure 1. The finite volume structure for CTF

The single phase Euler partial differential equations for mass (1), momentum (2), and energy (3) correspond to the unknown variables density ρ, velocity u, pressure P, and enthalpy h. The first terms in each of the equations are temporal terms. The rest of the terms are steady state spatial terms.

$$\frac{\partial \rho}{\partial t} + \bigtriangledown \rho u = 0 \tag{1}$$

$$\frac{\partial \rho u}{\partial t} + \bigtriangledown \rho u^2 + \bigtriangledown P - \rho g = 0 \tag{2}$$

$$\frac{\partial \rho h}{\partial t} - \frac{\partial P}{\partial t} + \bigtriangledown (\rho u h) = 0 \tag{3}$$

2.3 Residual Formulation and Jacobian Construction

A residual is simply the difference between the value at some future time $n + 1$ and the value at the current iteration k. This can be applied to desired variables and equations. For example,

the residual for density, $\delta\rho_i$, is the difference between iterate levels $n+1$ and k, $\rho_i^{n+1} - \rho_i^k$. The residuals for the equations are determined by substituting the residuals into the discretized equations, which should effectively change all $n+1$ into k. Each cell will have three residual variables and three residual equations. For the entire solution, we will then have a residual variable array δX, and a residual function array $F(X)$ which defines a linear system $J\delta X = -F(X)$.

The Jacobian matrix is defined as the derivative of each response of the function F_j with respect to each variable X_i. The derivative can be calculated numerically as shown by equation (4) where ϵ is a small numerical value. For CTF the equations are linear, and this numerical approximation of the Jacobian matrix is exact. This should produce the same Jacobian matrix that CTF currently generates analytically.

$$J_{i,j} = \frac{\partial F_j(X)}{\partial X_i} \approx \frac{F_j(X_i + \epsilon) - F_j(X)}{\epsilon} \tag{4}$$

To build the Jacobian matrix, an object oriented class was created that contains three arrays. An array that points to the residual functions, an array that points to the position within a target variable array, and an array that has the index that the function is to be evaluated at. These lists can be appended in any order, but they have to be appended simultaneously such that variables and functions correspond with each other. Then to construct the Jacobian matrix, the residual function and residual variable arrays can each be looped over to numerically build the Jacobian matrix as seen in figure 2.

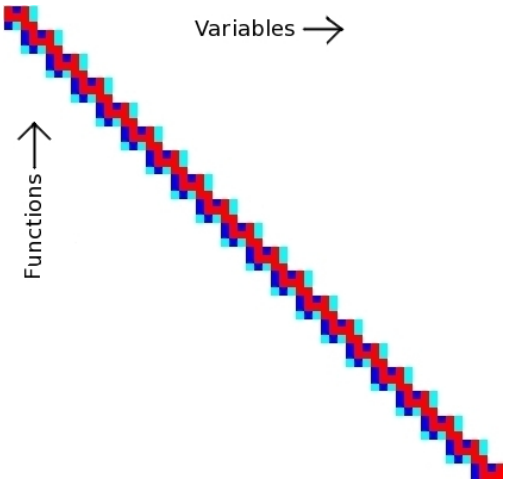

Figure 2. Structure of the Jacobian matrix for single phase liquid

3 ISOKINETIC SINE WAVE ADVECTION

Code verification is the set of procedures set in place to ensure that the code was written properly. The procedures can use the following as code verification criteria from least to most rigorous are expert judgement, error quantification, consistency / convergence, and order of accuracy [3]. For

this work, the Richardson Extrapolation will be used to check for convergence and order of accuracy of the error in space and time. The error should converge to zero, and the order of accuracy should converge to the values obtained through the modified equation analysis at the end of this section.

3.1 Problem Setup

The verification problem is defined as a single horizontal channel with base parameters listed in table I. Channel area and perimeter are constant across the entire height of the channel. No grid spacers are present, and frictional losses are set to zero. Velocity and pressure are assumed to be constant, but small fluctuations may occur due to coding mistakes or numerical roundoff. The channel geometry and operating conditions approximate a standard PWR. The inlet of the channel has a constant velocity with a fluctuating enthalpy that corresponds to a 37.5 °C temperature change. The length of the transient was defined to be quadruple the time needed for the liquid at the inlet to advect to the outlet.The frequency of the sine wave was defined to generate a full period of a spatial wave across the height of the channel.

Table I. Problem Parameters

Parameter	Symbol	Value	Unit
Axial Height	H	3.6586	m
Channel Area	A_{ch}	4.94E-005	m^2
Wetted Perimeter	P_w	1.49E-002	m
Velocity	V_o	7.35	$\frac{m}{s}$
Pressure	P_o	155.00	bar
Temperature 1	T_1	289.500	°C
Temperature 2	T_2	327.00	°C
Enthalpy 1	h_1	1281.55	$\frac{kJ}{kg}$
Enthalpy 2	h_2	1497.21	$\frac{kJ}{kg}$
Mass Flow Rate 1	$\dot{m}_1$	0.2713	$\frac{kg}{s}$
Mass Flow Rate 2	$\dot{m}_2$	0.2399	$\frac{kg}{s}$
Final Time	t_f	2.00	sec
Wave Frequency	ω	1.00	Hz

The lookup table to vary the inlet enthalpy h and inlet mass flow rate, $\dot{m}$, are genererated from equations 5 and 6 respectively. The trignometric functions assume constant axial spacing, Δx, and time step size, Δt, where i and j are the spatial and temporal indices. These equations should also behave as the known solutions throughout the entire domain of the problem. The enthalpy and mass flow rate vary proportionally to the density such that an isokinetic boundary condition is created at the inlet. However, this is dependent on the steam tables used in generating the input and calculating the EOS. A python script was used to generate the data tables according to trignometric equations using lookup tables that mimic the IAPWS-97 steam tables used by the code [4].

$$h(i,j) = \frac{1}{2}\left((h_1 + h_2) + (h_1 - h_2)cos\left(\omega\left(j\Delta t + \frac{i\Delta x}{V_o}\right)\right)\right) \tag{5}$$

$$\dot{m}(i,j) = \frac{1}{2}\left((\dot{m}_1 + \dot{m}_2) + (\dot{m}_1 - \dot{m}_2)cos\left(\omega\left(j\Delta t + \frac{i\Delta x}{V_o}\right)\right)\right) \tag{6}$$

The comparison between the data table and the output in CTF are shown for enthalpy and mass flow rate in figures 3 and 4, respectively. The CTF output was read from hdf5 data files at each point in time, which omitted the actual ghost cell where these values were applied. The CTF values are located at the nearest node to the inlet, and will be slightly out of phase to the exact values. For large mesh sizes this small discrepancy is not noticeable.

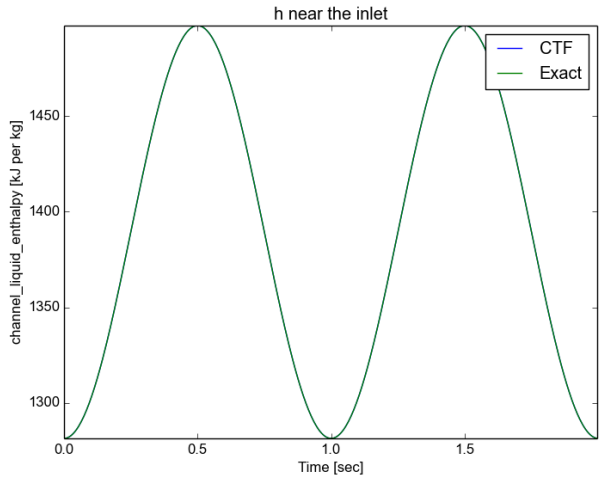

Figure 3. Enthalpy Near the Inlet and the Analytical Solution

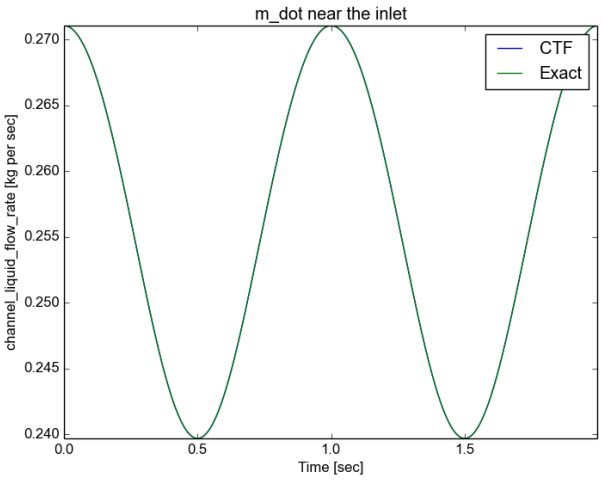

Figure 4. Density Near the Inlet and the Analytical Solution

For the original version of CTF, there is a small discrepancy in the way the density is calculated at the inlet that causes the velocity to be non-constant. This is considered small for this problem and should not greatly affect the order of accuracy. The residual formulation was coded in such a

way as to avoid this problem and has considerably less fluctuation in the inlet velocity. The hdf5 output files allow for a high level of precision, reducing round off error in the output.

3.2 Code Convergence

The current version of CTF uses global code convergence criteria that are used to estimate the error associated with the solution of the code for transient and steady state problems as shown in figure 5. The mass terms are in units of $\frac{kg}{s}$, and the energy terms in units of kW. For this problem, the solid energy storage is zero since there are not any heat structures present. The fluctuating values represent differences between the energy and mass entering and leaving the system.

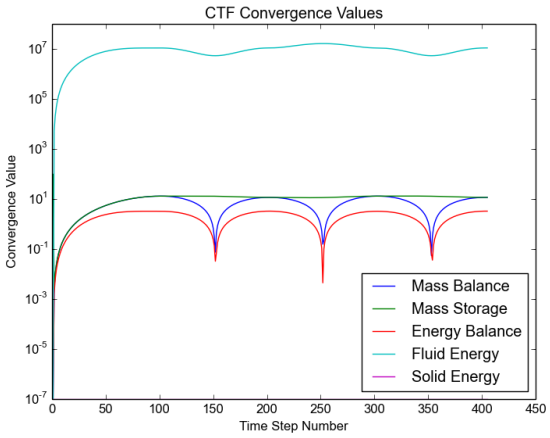

Figure 5. Code Convergence Criteria for the Original Version of CTF

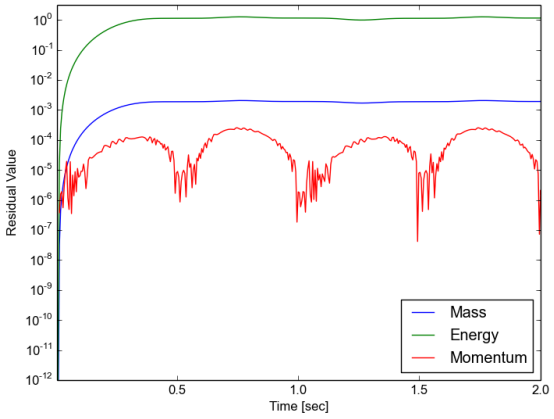

Figure 6. Summation of the Residuals for the Residual Version of CTF

The residual formulation prints out the summation of the equation residuals across the domain to an output file for each time step and can be seen in figure 6. The mass equation residual is in units of $\frac{kg}{m^3 s}$. The energy equation residual is in units of $\frac{kW}{m^3}$. The momentum residual is in units of $\frac{kg}{m^2 s^2}$. The mass balance and energy balances present in the code convergence criteria are much

smaller for the residual formulation. These residuals provide a much better indication as to the level of error present in the solution of the system. They can even be expanded to provide convergence information at every position, variable, and equation.

3.3 Modified Equation Analysis

Because the velocity is constant, it can be pulled out of the spatial derivative as shown in equation 7. Using upwinding, the finite difference can be written to look like equation 8. A second order Taylor series approximation can be used for ρ_i^{n+1} and ρ_{i-1}^n as shown in equations 9 and 10 respectively. The higher order terms ($O(\Delta x^2, \Delta t^2)$) are not taken into account for this approximation. The Taylor series approximations can then be substituted into 8 to yield 11. This is the beginning of the modified equation analysis. The goal will be to isolate the original PDE and define the truncation error.

$$\frac{\partial \rho}{\partial t} + U_0 \frac{\partial \rho}{\partial x} = 0 \tag{7}$$

$$\frac{\rho_i^{n+1} - \rho_i^n}{\Delta t} + U_0 \frac{\rho_i^n - \rho_{i-1}^n}{\Delta x} = 0 \tag{8}$$

$$\rho_i^{n+1} = \rho_i^n + \frac{\partial \rho}{\partial t}\Delta t + \frac{1}{2}\frac{\partial^2 \rho}{\partial t^2}\Delta t^2 + O(\Delta t^3) \tag{9}$$

$$\rho_{i-1}^n = \rho_i^n - \frac{\partial \rho}{\partial x}\Delta x + \frac{1}{2}\frac{\partial^2 \rho}{\partial x^2}\Delta x^2 + O(\Delta x^3) \tag{10}$$

The lengthy equation 11 can be reduced to equation 12 since the ρ_i^n terms subtract out and the Δt and Δx terms in the denominator cancel out. This reduced equation can the be re-written into equation 13, with the original PDE followed by the truncation terms.

$$\frac{\left(\rho_i^n + \frac{\partial \rho}{\partial t}\Delta t + \frac{1}{2}\frac{\partial^2 \rho}{\partial t^2}\Delta t^2\right) - \rho_i^n}{\Delta t} + U_0 \frac{\rho_i^n - \left(\rho_i^n - \frac{\partial \rho}{\partial x}\Delta x + \frac{1}{2}\frac{\partial^2 \rho}{\partial x^2}\Delta x^2\right)}{\Delta x} + O(\Delta x^2, \Delta t^2) = 0 \tag{11}$$

$$\frac{\partial \rho}{\partial t} + \frac{1}{2}\frac{\partial^2 \rho}{\partial t^2}\Delta t + U_0\left(\frac{\partial \rho}{\partial x} - \frac{1}{2}\frac{\partial^2 \rho}{\partial x^2}\Delta x\right) + O(\Delta x^2, \Delta t^2) = 0 \tag{12}$$

The terms to the right of the original PDE are the first order accurate truncation terms. Notice how the truncation error is dependent on both the on the second derivatives of density with respect

to space and time, and on the numerical spacing Δt and Δx. Since the truncation error is linearly dependent on Δt and Δx, the order of accuracy is 1 with respect to time and space. When the energy equation undergoes a similar modified eqution analysis, the order of accuracy is also 1 for time and space. The momentum conservation equation should does not apply for this problem since the velocity is constant.

$$\frac{\partial \rho}{\partial t} + U_0 \frac{\partial \rho}{\partial x} + \frac{1}{2}\frac{\partial^2 \rho}{\partial t^2}\Delta t - U_0 \frac{1}{2}\frac{\partial^2 \rho}{\partial x^2}\Delta x + O(\Delta x^2, \Delta t^2) = 0 \tag{13}$$

4 RICHARDSON EXTRAPOLATION

The richardson extrapolation was performed by refining the spatial and temporal step sizes by a factor of 2 for a set number of times. The spatial and temporal studies are refined separately in their own study in order to isolate the spatial and temporal affects on the solution. The generation of the inputs, running of the codes, and analysis of the output were automated with a python script in order to reduce user input errors and increase repeatability. With each additional refinement level, the amount of computational resources doubles. For this analysis, a significant amount of information was added to the hdf5 output files. The spatial refinements require more computational resources that the temporal refinements due to the need to keep the study in the asymptotic range. In order to keep the computational resources needed to perform this analysis reasonable, fewer spatial refinements were performed compared to the temporal analysis.

4.1 Convergence of Error

The relative difference at each point for a particular time step was calculated between each iteration for each quantity of interest. For the spatial refinement, the lower iterate values were numerically integrated to match the shape of the initial domain. The errors were then summed over the entire domain to yield a total error for each variable. The total error for enthalpy is plotted in figures 7 and 8 as a function of temporal and spatial step size respectively.

The data points where chosen to be outside of the asymptotic range as shown by the good power fit with an exponent near 1. The fit shows that as the temporal and spatial step sizes are reduced, the numerical error approaches zero. The discretization error between the original version of CTF is relatively small and is most likely due to the small fluctuations in the velocity present in the original version of the code. While only the enthalpy is shown here, the mass flow rate and the density showed similar trends.

4.2 Order of Accuracy

The order of accuracy for this verification problem is first order as shown by the modified equation analysis. This can be considered to be the exponent on the power fits as seen in figures 7. However the order of accuracy p can be calculated by using equation 14 where f_1, f_2, f_3 are

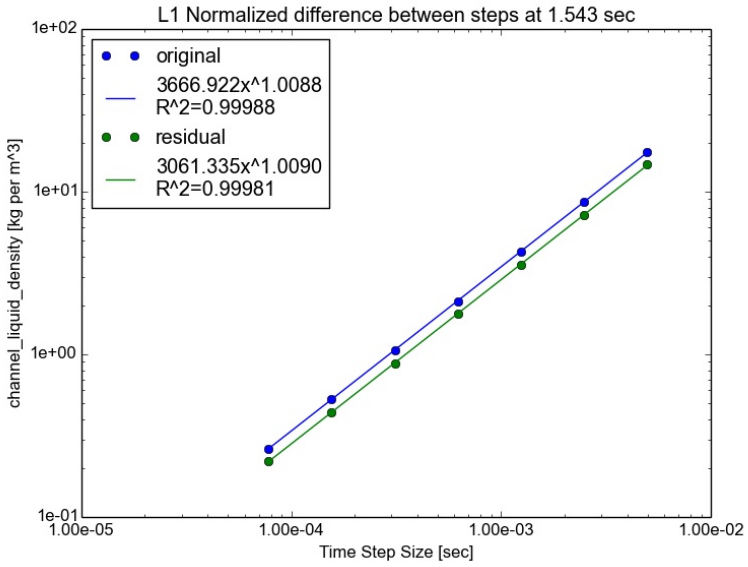

Figure 7. Difference Between Successive Temporal Refinements for Density

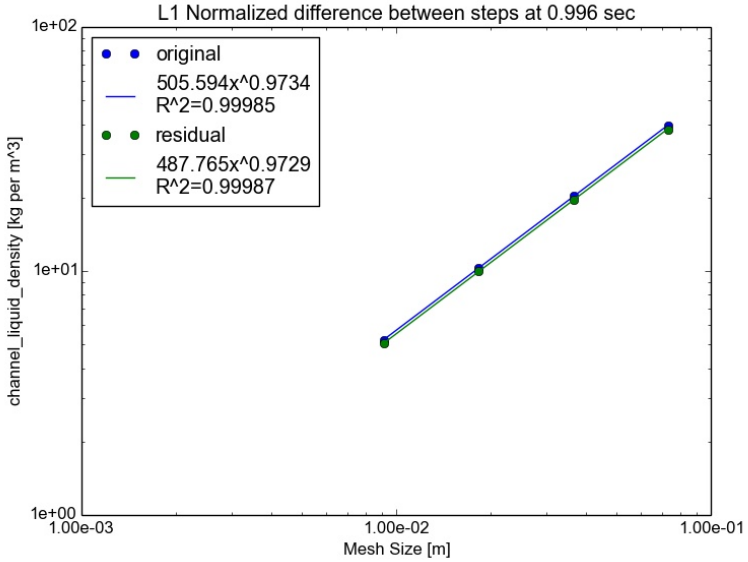

Figure 8. Difference Between Successive Spatial Refinements for Density

consecutive levels within the same Richardson extrapolation study. The refinement factor, R, has the constant value of 2 for both the spatial and temporal studies.

$$p = \frac{ln\left(\frac{f_3 - f_2}{f_2 - f_1}\right)}{ln(R)} \tag{14}$$

The order of accuracy for all of the variables are presented for the temporal analysis and spatial analysis in figures 9 and 10 respectively. The temporal order of accuracy is well within the asymptotic range for the whole analysis, and moves closer to 1.0 with decreasing time step size. The spatial order of accuracy is a little bit outside the asymptotic range, but also approaches an order of accuracy of 1.0 with decreasing mesh size.

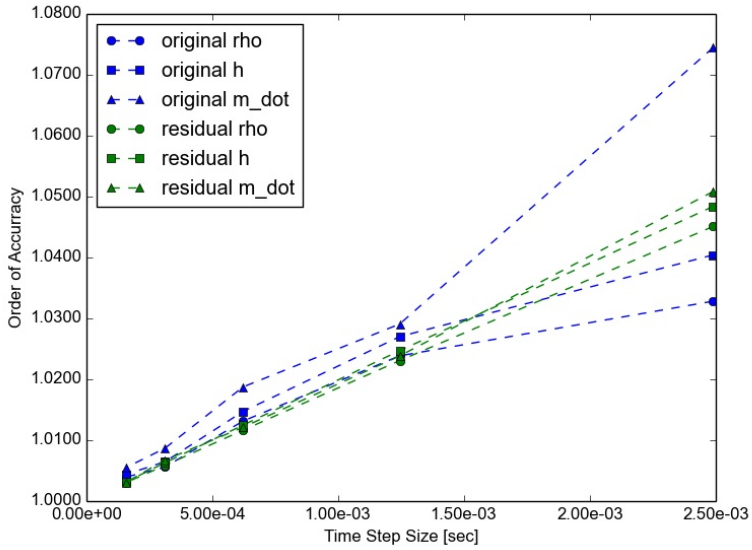

Figure 9. Temporal Order of Accuracy

The slight differences between the original version of CTF and the residual formulation might be due to the different solution methods and back substitution of variables. Despite the small differences, both versions of the code exhibit order of accuracies very close the values obtained through the modified equation analysis.

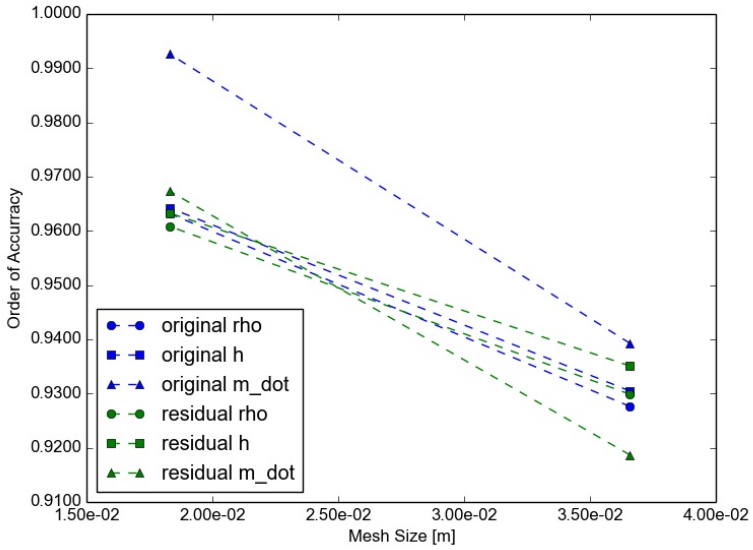

Figure 10. Spatial Order of Accuracy

5 CONCLUSIONS

The residual formulation of CTF allows for a numerical computation of the multivariable Jacobian matrix compared to the original analytical derivation of a pressure matrix. The 1-D isokinetic single phase liquid verification problem was shown to be a good verification problem through its isolation of the order of accuracies through modified equation analysis. The discretization error for both versions of the code converged to zero with decreasing time step and axial mesh size. The order of accuracy for the temporal and spatial refinements matched very closely with the modified equation analysis for both codes. For all of these data points, the residual formulation of the code showed discretization errors that were very close with the original version of the code. Future work might be comparing the results with CFL number of 1 to the known solutions of the code. This would be a less rigorous study, but would be a quick verification problem that could be easily integrated into the CTF test matrix.

6 ACKNOWLEDGMENTS

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