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RELAP5-3D Resolution of Known Restart/Backup Issues

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EXECUTIVE SUMMARY

The state-of-the-art nuclear reactor system safety analysis computer program developed at the Idaho National Laboratory (INL), RELAP5-3D, continues to adapt to changes in computer hardware and software and to develop to meet the ever-expanding needs of the nuclear industry. To continue at the forefront, code testing must evolve with both code and industry developments, and it must work correctly. To best ensure this, the processes of Software Verification and Validation (V&V) are applied.

Verification compares coding against its documented algorithms and equations and compares its calculations against analytical solutions and the method of manufactured solutions. A form of this, sequential verification, checks code specifications against coding only when originally written then applies regression testing which compares code calculations between consecutive updates or versions on a set of test cases to check that the performance does not change.

A sequential verification testing system was specially constructed for RELAP5-3D to both detect errors with extreme accuracy and cover all nuclear-plant-relevant code features. Detection is provided through a “verification file” that records double precision sums of key variables. Coverage is provided by a test suite of input decks that exercise code features and capabilities necessary to model a nuclear power plant. A matrix of test features and short-running cases that exercise them is presented.

This testing system is used to test base cases (called null testing) as well as restart and backup cases. It can test RELAP5-3D performance in both standalone and coupled (through PVM to other codes) runs. Application of verification testing revealed numerous restart and backup issues in both standalone and couple modes. This document reports the resolution of these issues.

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ACRONYMS

BC	Boundary Conditions
CCFL	Counter Current Flow Limiting
CHF	Critical Heat Flux
CPU	Central Processor Unit
DA	Developmental Assessment
ECC	Emergency Core Coolant
HSE	Hydro Static Equilibrium
HTC	Heat Transfer Coefficient
ICONE	International Conference On Nuclear Energy
IEEE	Institute of Electrical and Electronics Engineers
INL	Idaho National Laboratory
LOCA	Loss Of Coolant Accident
NURETH	NUclear Reactor Thermal Hydraulics
PVM	Parallel Virtual Machine
RELAP	Reactor Excursion and Leak Analysis Package
RHS	Right Hand Side
STD	Standard
V&V	Verification and Validation

SYMBOLS

English

b	RHS of Δp Linear System
*d*i	Probability of detecting differences
H_0	Null Hypothesis
H_1	Alternative Hypothesis
N	Number of test cases
P	Probability function
S	Size of the verification file
t_i	Number of timesteps if the i^{th} input case
T	Temperature
T_r	Trip
UP	User-reported Problem
u_f	Liquid internal energy
u_g	Gas internal energy
V_f	Velocity of the Liquid (Fluid)
V_g	Velocity of the Gas
X	Random Variable for the Hypothesis Test that two runs are identical
X_a	Noncondensable Quality
X_i	Random Variable for Test Case i, the i^{th} input deck.
Y	Control Variable
3D	Three dimensional

Greek

α	significance level of a hypothesis test
α_g	Void fraction of gas
β	Probability of committing Type II error in a hypothesis test
Δp	Pressure Drop
Δt	Timestep for Hydrodynamic Advancement
Δt_{kin}	Timestep for Neutron Kinetics Advancement
ε	Sum of RELAP5-3d estimate errors
φ	Neutron Flux
$\boldsymbol{\rho}_b$	Density of Boron

1. INTRODUCTION

The state-of-the-art nuclear reactor system safety analysis computer program developed at the Idaho National Laboratory (INL), RELAP5-3D[1-1], continues to adapt to changes in computer hardware and software and develops to meet the ever-expanding needs of the nuclear industry. In order to continue at the forefront, code testing must evolve with both code and industry developments, and it must work correctly. To best ensure this, the processes of Verification and Validation (V&V), defined in IEEE-STD-610[1-2], are applied. Validation is the process of evaluating a system or component (software) during or at the end of the development process to determine whether it satisfies specified requirements, i.e. will fulfill its intended use. Verification evaluates a system or component (software) to determine whether the products of a given development phase satisfy the conditions imposed at the start of that phase.

A special form of validation testing called Developmental Assessment[1-3] is performed on each new RELAP5-3D release. Verification compares coding against its documented algorithms and equations and compares its calculations against analytical solutions and the method of manufactured solutions. A form of this, sequential verification[1-4], checks code specifications against coding only when originally written then applies regression testing[1-5] which compares code calculations between consecutive updates or versions on a set of test cases to check that the performance does not change.

Small initially, the test set grew as new features and test cases for them were added. As it grew, the diffem[1-6, 1-7] utility was developed to automate the checking process and introduce greater fidelity than visual inspection. Diffem compares the output files from two different RELAP5-3D versions, character-by-character, for each input file in the test set. Thus every difference recorded on the printed output files is detected automatically. However because output file are accurate only to five or more decimal places, this proved insufficient to guarantee the calculations were sufficiently exact when applied to complex models or long-running transients. Therefore enhancements were developed systematically.

Code features relevant to nuclear power plant modeling were identified. RELAP5-3D has numerous features to verify including phenomenological capabilities for thermal fluids trips, controls, heat transfer and neutronics. Additional code features include alternate fluids, general tables, linear equation solvers, time advancement models, special models and correlations, etc. Though these can be employed to model physical systems in a variety of application areas, the original purpose for the verification test suite was to verify RELAP5-3D code for nuclear power plant safety applications. These are listed in Table 1.0.1. The input tests for the verification suite were select to test nuclear-related code features.

Table 1.0.1. RELAP5-3D Primary Variables

Quantity	**In manual**	**On file**
Pressure	p	P
Liquid internal energy	u_f	Uf
Gas internal energy	u_g	Ug
Void fraction of gas	α_g	VOIDg
Noncondensable quality	X_a	QUALa
Density of boron	$\boldsymbol{\rho}_b$	Boron
Liquid velocity	V_f	Vf
Gas velocity	V_g	Vg
Heat Structure Temperature	T	Temp
Neutron flux	φ	Flux
Timesteps sum	Δt, Δt_{kin}	dtsum
Trips	T_r	Trips
Control system value	Y	Cntrl

To improve the accuracy of comparisons, a verification file replaces the RELAP5-3D output file for comparisons. Arrays of primary variables listed in Table 1.0.1 along with some other important quantities are summed and recorded on the file to reduce its size. Verification files of two runs that should produce exactly the same calculations can be compared. If no differences occur for any pair of comparisons in the test suite, the code is sequentially verified. If not, the reason must be found. If it is a code bug, it must be fixed before continuing. If it is justifiable for reasons such as expected improvements due to bug fixes, model enhancements, or changes to the operating system, the code is considered to be sequentially verified.

The new verification process was designed to provide the ability to verify more code capabilities and modes of operation than simple regression testing allows. Null testing compares pairs of runs of the same input deck on two different versions or updates of RELAP5-3D. Process testing compares verification files made with the same RELAP5-3D version run on related input for which the calculations ought to be exactly the same. Related runs include comparisons of a base case run of an input model against a restart run, a run with forced backups, or one where the model is the result of multiple input cases that result in the exact same model.

The original form of Verification Testing went into RELAP5-3D version 4.1.3. It had only the first three categories of testing: null, restart, and backup as shown in Table 1.0.2.

Table 1.0.2. Original verification testing categories

No.	Category	Description
1	Null testing	Check that two code versions produce the same calculations
2	Restart testing	Check that a restarted run produces the same calculations as the original run
3	Backup testing	Check that the code still produces the same calculations with a forced backup

When verification testing was first introduced, many issues were discovered. The identified nuclear-related code features were tested by 43 input decks with 125 input cases among them[1-6, 1-7]. A test deck is considered to fail if there are any differences between two corresponding verification files. This can be broken down further. Verification files make individual dumps on user specified timesteps and dumps within the file are separated by the cases of the input deck whenever the deck has multiple cases. Individual cases within a given verification file may compare perfectly while others have differences. Table 1.0.3 summarizes the failures to compare perfectly, both by input deck in column 2 and by input case in column 3, for RELAP5-3D version 4.3.1.

Table 1.0.3. Issues revealed by original verification testing

Version 4.1.3	Failures in 43 Test Problems	Failures in 125 cases
Null Testing	6/43	6/125
Restart Testing	25/43	52/125
Backup Testing	37/43	62/125

The purpose of this report is to document the improvements made to RELAP5-3D to make all the verification test suite problems run perfectly. Thus whenever pairs of corresponding verification files are compared for version 4.3.1, there are no differences. In the case of null testing, this means 4.3.1 compares perfectly with 4.3.0.

A second purpose of this project is to increase the scope of verification testing. Originally, RELAP5-3D was verified for standalone operation only. This project adds two additional modes of operation. It is also noted that a fourth category of verification testing, multi-case verification, was developed in response to a User Problem. However, since it was not part of this project, it will not be reported in detail.

RELAP5-3D can be run standalone or as a thread or instance under the direction of the PVM (Parallel Virtual Machine) Executive. An instance of RELAP5-3D can run alone under Executive control or coupled with another thread running another code. The latter mode allows RELAP5-3D to communicate with one or more other codes to solve a complex problem that has been split via domain decomposition into pieces that are assigned to the code best-suited to modeling its apportioned part of the problem. As of version 4.3.1, only PVM coupled verification is performed. Moreover in PVM coupled mode, only null and restart testing is performed, as shown in Table 1.0.4.

Table 1.0.4. Categories and modes of verification testing

Category Number	**Category Name**	**Standalone RELAP5-3D**	**RELAP5-3D Coupled to RELAP-3D via PVM Executive**
1	Null	X	X
2	Restart	X	X
3	Backup	X	N/A
4	Multi-case	INL only	N/A

The Section 2 details the verification file and covers the theory of verification testing. Section 3 covers the input decks that were added to test suite to make the verification test more powerful. Section 5 introduces and explains the new modes of testing. Section 6 is coding and scripting for the test. Section 7 is a Bibliography.

1.1 References

1-1 The RELAP5-3D Code Development Team, "RELAP5-3D Code Manual Volume I: Code Structure, System Models and Solution Methods," INL-EXT-98-00834-V1, Revision 4.2, June, 2012.

1-2 IEEE Computer Society Standards Coordinating Committee, IEEE Standard Computer Dictionary, A Compilation of IEEE Standard Computer Glossaries 610, Library of Congress Catalog Number 90-086306, ISBN 1-55937-079-3, The Institute of Electrical and Electronics Engineers, 345 East 47th Street, New York, NY 10017, USA, 1990.

1-3 The RELAP5-3D Code Development Team, "RELAP5-3D Code Manual Volume III: Developmental Assessment," INL-EXT-98-00834-V1, Revision 4.0, Section 8.2, p 8-4, June, 2012.

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1-5 J. Watkins, Testing IT: An Off-the-Shelf Software Testing Process Handbook, ISBN: 052179546X 9780521795463, Cambridge; New York: Cambridge University Press, 2001.

1-6 G. L. Mesina, "RELAP5-3D Restart and Backup Verification Testing," INL-EXT-13-29568, September, 2013.

1-7 G. L. Mesina, D. L. Aumiller, F. X. Buschman, "Automated, Highly Accurate Verification of RELAP5-3D," ICONE22-31153, Proceedings of the 22nd International Conference on Nuclear Engineering, Prague, Czech Republic, July 7-11, 2014.

2. Verification File and Testing Theory

The verification method first released version in RELAP5-3D/4.1.3 has been expanded in three ways: form of the verification file, size of the test suite, and uses of the verification test. However, the method is still built from the same design concepts. Section 2.1 details the file and its changes. Section 2.2 advances the theory. Additions to the suite are covered in Section 3.

2.1 Summary of the Verification File

Software verification testing has two important aspects:

- detection – finding errors in the coding tested
- coverage - percentage of coding exercised by the test set

The first requires the test to have a high probability of *detecting* differences in the calculations of two different code versions *for a given test case*. Coverage requires development of test cases that exercise as much of the code as possible for evaluation.

The verification file was designed to be small, require little maintenance, and detect small changes in code calculations. This is accomplished by recording the sums of primary variables. There are three major categories of data/variables:

1. Primary variables from the five physical phenomena: heat transfer, thermal hydraulics, neutronics, controls and trips are listed in Table 1.0.1. The independent variable time is also primary.
2. Secondary variables derived from primary variables and used in constructing the set of equations solved for the primary variables on the next advancement. E.G. heat capacity, enthalpy, and power.
3. Output-only variables do not feed back into primary or secondary variables. E.G. water packer count.

If a primary variable differs between two code runs, variables in category 2 and 3 that are derived from it will also differ. If a secondary variable differs on a given time step, on the next step it will affect the equations of (at least) one primary variable and thus its value when the equation is solved. The sums of primary variables are also sufficient to catch some output-only variable differences that are not caused by errors in calculating those quantities. However, differences in output-only variables do not affect category 1 or 2 variables. Therefore errors created in output-only variables that are not written on the verification file go undetected by the verification test

The verification file is a versatile tool for comparing the calculations of two RELAP5-3D runs on the input files of the test suite. It provides a basis for comparison of code modeling capabilities, processes such as restart and backup, and modes of operation such as standalone mode and coupled to another code.

Shown in Figure 2.0.1, the major features of the verification file can be seen. The top or header of the file displays the computer program, version and time the executable was created, the machine on which it was run, and the date and time of the run. The footer gives the CPU time and size of the verification file. Everything in-between is the body of the verification file. At the highest level it is organized into input-cases since RELAP5-3D can run several cases in a single input deck. The title of the case is given. Within each case, data from a timestep is dumped onto the file headed by the dump and advancement number and cumulative time. The remainder of the dump displays the L_1-norm of primary variables, and some other important sums. The floating point sums are accumulated in quadruple precision and are displayed in both hexadecimal and 1pe20.16 floating point formats.

Figure 2.0.1. Verification File with 2 Cases for Edward's Pipe

```
RELAP5-3D/Ver:4.1.3   steelers.inl.gov
Time compiled: Aug 13 2013 13:29:15
Date and Time of run: 13/08/14     15:04:49

Case  1  edward's pipe problem base case with extras

Dump     1    Advancement=     109 time=  1.0000E-01
P=      4.9365983737086219E+07 401878A1EFDE58D75B00000000000000
Uf=     1.9649507480408072E+07 40172BD3E37AFC05FEC0000000000000
Ug=     5.4520489485535964E+07 40189FF554BE260AE000000000000000
VOIDg=  7.0158488970410998E+00 4001C103AB179E074A00000000000000
QUALa=  0.0000000000000000E+00                                0
Boron=  0.0000000000000000E+00                                0
Vf=     2.0448213290728118E+02 400698F6DA1FDA3236D4000000000000
Vg=     2.3165076689908255E+02 4006CF4D3151A9C1FEC1000000000000
RHSth=  0.0000000000000000E+00                                0
SOLth=  5.2542461771631456E+04 400E9A7CEC6D54CEA4E0000000000000
Error= -8.5282658356481664E-05 BFF165B38EA0ADAA2000000000000000
Temp=   1.1047897158084513E+05 400FAF8EF8B985B33F57500000000000
Flux=   6.4046362410846550E+10 4022DD2EBDE55B16F000000000000000
dtsum=  3.0000000000000001E-03 3FF689374BC6A7EFA000000000000000
Trips= -3.9020138535691576E+00 C000F37530A0CF29DB80000000000000
Cntrl=  3.7065329809843512E+06 4014C47527D90E52D0F595356B020000
Rdc:Crnt,Extrp,Mass,Prop,Qual=     0     2     0     2     0
Rpt:Air,DelP,Flip,Jpack,Vpack=     0     0     0     0     0

Dump     2    Advancement=     509 time=  5.0000E-01
P=      1.1610017826711973E+07 4016624F43A746CAAC00000000000000
Uf=     1.3706563288757732E+07 4016A24A8693D80DB180000000000000
Ug=     5.3792556235069888E+07 40189A67961E16C52400000000000000
VOIDg=  2.0127747744316551E+01 4003420B4137FFA34180000000000000
QUALa=  0.0000000000000000E+00                                0
Boron=  0.0000000000000000E+00                                0
Vf=     2.8891214895206032E+02 400720E98297FE2E04B8000000000000
Vg=     9.1675057057565303E+02 4008CA6012B255E284C0000000000000
RHSth=  4.2453960924539154E+07 401843E5E476574C8C12980000000000
SOLth=  1.6144078316381101E+05 40103B50643EB635D838000000000000
Error= -9.9606881069212402E-05 BFF1A1C812FC4B5E8000000000000000
Temp=   1.0939814425864978E+05 400FAB5624EE2286FA5FD00000000000
Flux=   2.7820142401306227E+07 4017A8806E66BC014000000000000000
dtsum=  3.0000000000000001E-03 3FF689374BC6A7EFA000000000000000
Trips= -1.6980010000000000E+00 BFFFB2B0318B93469800000000000000
Cntrl=  8.6399604127190748E+05 4012A5DF815219769C2F2BB3AB200000
Rdc:Crnt,Extrp,Mass,Prop,Qual=     0     2     0     2     0
Rpt:Air,DelP,Flip,Jpack,Vpack=     0     0     0     0     0

CPU Time=  3.6094499999999996E-01 size    2764
```

Figure 2.0.2 shows only the first dump of the new format as of RELAP5-3D/4.3.1, The decimal digits are displayed as 1pe27.20 for both time and the L_1-norms. Besides formats, the new row, timesum, is the sum of both the hydrodynamic and heat transfer cumulative times. Also, the sum of time steps, dtsum, now adds the heat-transfer dt to the hydrodynamic and kinetic. An option to print the edit times is coded, but is commented out.

2.2 Statistical Analysis of the Verification System

This section summarizes the statistical theory underlying the verification testing system. Theorems that were proven previously[2-1, 2-2] are restated without proofs. A couple new theorems are proven. This section summarizes the statistical theory underlying the verification testing system. The null and alternate hypotheses of the test are denoted H_0 and A_0, respectively.

$H_{0,i}$: The two runs produce exactly the same calculations for test case i. (2.2.1)

$A_{0,i}$: Code calculations are different for test case i. (2.2.2)

The verification test suite contains N test cases. The statistic used to test the hypothesis for the ith test case, Xi, has a value of 0 if no differences are found between the two runs and 1 otherwise, and X is the maximum of all the Xi. Applying standard statistical methods[12], this is expressed mathematically as:

$$X_i = \begin{cases} 0 & if \quad exactly\ 0\ differences\ are\ found \\ 1 & if \quad at\ least\ one\ difference\ is\ found \end{cases} \quad (2.2.3)$$

$X = \max \{X_i \mid i = 1, 2, \ldots, N\}$ (2.2.4)

H_0: For every test case i, the two corresponding runs produce the same calculations. (2.2.5)

$A_{0,}$: Code calculations are different some test case i. (2.2.6)

Verification Test: Accept the null hypothesis if X = 0, but reject it when X = 1. (2.2.7)

Hypothesis testing potentially commits two kinds of errors. The first, Type I Error or false positive, is the rejection of the null hypothesis when it is true. That means finding differences when there are none. The second kind of error, called Type II Error or a false negative, is to accept the null hypothesis when it is false. That means there are differences that go undiscovered. Table 3 summarizes this.

Table 3. Hypothesis Testing Table for Test (2.2.7)

	H_0 is true No differences exist	**A_0 is true** Differences exist
Accept H_0	*Correct* Report: "No differences"	*Type II Error* Don't find extant differences
Reject H_0	*Type I Error* Detect non-existent differences	*Correct* Report: "Differences found"

The probabilities of committing Type I and Type II Error are denoted α and β. These are all standard definitions[2-3].

α = P(Type I Error) = P(Reject H_0 | H_0 is true) = Level of significance of the test (2.2.8)

β = P(Type II Error) = P(Accept H_0 | H_0 is false) (2.2.9)

Power of the test = $1 - \beta$ (2.2.10)

Some useful statements about the verification test have been proven. These show that the verification test is very powerful and reliable.

THEOREM 1: Verification Test (2.2.7) *always* accepts the null hypothesis when it is true.
Proof: Suppose H_0 is true. Then there are no differences to detect in any test in the entire suite. Thus, for each test in the suite, $X_i = 0$. Therefore, $X = \max \{X_i\} = 0$ always (when H_0 is true). Since X is 0, Test (2.2.7) accepts H_0. Thus, $P(\text{Accept } H_0 \mid H_0 \text{ is true}) = P(X = 0 \mid H_0 \text{ is true}) = 1$. Q.E.D.

COROLLARY: Verification Test (2.2.7) has level of significance, $\alpha = 0$.
PROOF: $\alpha = P(X=1 \mid H_0 \text{ is true}) = 0$. *The test commits no Type I Error. It never detects non-existent differences.*

Interpretation: *If properly programmed, the verification test will never report nonexistent code bugs*. The next two results are proven in exactly the same way.

THEOREM 2: Restart Test (2.2.7) commits no Type I Error. It has significance level, $\alpha = 0$.

THEOREM 3: Backups Test (2.2.7) commits no Type I Error. It has significance level, $\alpha = 0$.

Despite these powerful results, Test (2.2.7) can commit Type II Error. It can miss actual differences. There are three potential causes:

1. On timesteps when verification dumps are not made, the calculations could be different.
2. Two arrays may differ yet have the same L_1-norm.
3. L_1-norms of primary variables catch the differences, but do not account for all output-only variables.

Consider the first issue. In the authors' experience, two runs do not differ on some time-steps but have identical sums on steps when verification dumps are made. For all tests in the verification suite, once the primary variables diverge even slightly, the differences do not disappear on later time advancements. A verification dump always occurs on the final step to catch differences.

Another source of Type II Error is the possibility that significant values in some primary variable array may differ, but the L_1-norms are the same. For example, if velocities of two runs of the same input model were equal but opposite in sign, or if the first and second entry of a primary variable array were swapped between two runs, the L_1-norms would be the same. Such solutions cannot occur for a well-posed system of equations, a RELAP5 topic discussed in many sources[2-4].

The second source of Type II Error cannot be completely eliminated due to finite precision arithmetic. The next result quantifies it.

Consider the sample space of length-N arrays of double-precision numbers. Fortran uses IEEE 754 quadruple-precision floating-point format[2-5, 2-6], binary128. It has 1 sign bit, 15 exponent bits, and a significand (or mantissa) with 113bits (not 112 because the lead bit of the significand is always 1 implicitly, unless the whole fraction part is 0, so the one is not stored). The total precision in decimal digits is $34.02 \approx \log_{10}(2^{113})$. Unit round-off, for which $1.0 + \varepsilon > 1.0$ and $1.0 + \varepsilon/2 = 1.0$, is $\varepsilon = 1.9\times10^{-34}$. In double precision, the significand has 49 bits, the exponent has 15, and unit round-off is $\delta = 2.2 \times 10^{-16}$.

Theorem 4: If (1) **u** and **v** correspond to the same primary variable from different RELAP5-3D runs (satisfy the governing equations), (2) the L_1-norms are calculated in quadruple precision, (3) $N > 3$, then
$P(\|\mathbf{u}\|_1 = \|\mathbf{v}\|_1 \mid \mathbf{u} \neq \mathbf{v}) < 10^{-18}$.
Proof: Consider two distinct double-precision arrays of length two that have the same sum. Divide by the larger value to normalize. If the sums $1.0 + A_0 = 1.0 + A_1$ while $A_0 > A_1$, then $A_0 - A_1 < \varepsilon$. But A_1 and A_0 are double-precision, so $A_0 - A_1 > \delta A_0$, otherwise $A_1 = A_0$. By transitivity $\varepsilon > \delta A_0$, so $A_0 < \varepsilon/\delta = 10^{-18}$.

Let the sample space be arrays of length N of double-precision numbers from ε to 1.0. Represented as a rounded 16 decimal digit number, $A = 10^{-m}\times(a_1 . a_2 a_3 \ldots a_{16})$. The quadruple precision sum, $1+ A$, is:

$1.0 + A = 1.0\ldots0\ a_1\ldots a_{16}\ 0\ \ldots\ 0$ if $A > 10^{-18}$.

$1.0 + A = 1.0\ldots0\ a_1\ldots a_{16-k}$ if $10^{-18-k} > A > 10^{-18-k-1}$.

For $10^{-18-k} > A > 10^{-18-k-1}$, there are 10^k distinct sums and 10^{16-k} indistinct. The numbers of indistinct sums is $S = \sum_{k=1}^{16} 9 \times 10^{k-1} < 10^{16}$. The sample space of length N arrays has $(N-1) \times 10^{34}$ possible sums for $N > 3$. The ratio of indistinct sums to possible sums is $S/[(N-1)\times10^{34}] < 10^{-18}$. **Q. E. D.**

Corollary 2: Under the same hypotheses, P(X = 0 | primary or secondary variables differ) $< 10^{-18}$.

Output-only variables have great importance to training simulators whose alarms may be triggered by one of these variables, and to users who view the printed output files. To check these variables, the verification test can be combined with a test of output-only quantities.

The diffem[6, 7] utility performs a character by character comparison of output-only values in the printed output file. Since 5 or more decimal places are printed, the worst error committed by diffem in output-only variables is due to round-off. The error is $D < 0.5\times10^{-5}$.

The power of the combined test is considered next. Power is 1 – P(Type II Error) and relates to round-off error.

THEOREM 5: For a single test case of a well-posed problem, the combined verification test (2.2.7) and diffem test has Type II Error, $\beta < 10^{-5}$.

PROOF: Two runs of the model are made, either by different code versions or to test different code processes or modes. Consider all variables in RELAP5-3D data for a given input deck on a time step for which verification data is written. P(Type II Error) = P(X = 0 | differences exist between two runs).

Let A = the sets of data for which primary or secondary variables differ.

Let B = the sets of data where Category 3 variables differ, but Category 1 and 2 variables do not.

Let C = the sets of data for which X = 0.

$$\text{P (Type II Error)} = P(C \mid (A \cup B)) = \frac{P\big(C \cap (A \cup B)\big)}{P(A \cup B)} = \frac{P(C \cap A \cup C \cap B)}{P(A \cup B)}$$

$$= \frac{P(C \cap A) + P(C \cap B) - P(C \cap A \cap C \cap B)}{P(A \cup B)}$$

$$< \frac{P(C \cap A)}{P(A \cup B)} + \frac{P(C \cap B)}{P(A \cup B)} < \frac{P(C \cap A)}{P(A)} + \frac{P(C \cap B)}{P(B)}$$

$$= P(C|A) + P(C|B) < 10^{-18} + 0.5 \times 10^{-5}$$

Therefore by Equation (2.2.9), $\beta < 10^{-5}$. **Q. E. D.**

By Equation (2.2.10), the power of the combined verification (2.2.7) and diffem test is 99.999% for a single test case. This theorem means that for the features the input deck is designed to test, there is one chance in 10^5 that the combined test will miss an error if it exists. However, the theorem does not address the power of the combined test to find errors in the code across the entire verification test suite.

2.3 References

2-1 G. L. Mesina, "RELAP5-3D Restart and Backup Verification Testing," INL-EXT-13-29568, September, 2013.

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2-4 V. H. Ransom and V. A. Mousseau, "Convergence and Accuracy Expectations for Two-Phase Flow Simulations," Canadian Nuclear Society International Conference on Simulation Methods in Nuclear Engineering, Montreal, Canada, April 18-20, 1990.

2-5 W. Kahan "IEEE Standard 754 for Binary Floating-Point Arithmetic," Elect. Eng. & Computer Science, Univ. of California, Berkeley CA 94720-1776, p4, October, 1997.

2-6 J. C. Adams, et al, The Fortran 2003 Handbook, The Complete Syntax, Features, and Procedures, ISBN 978-1-84628-378-9, Library of Congress 2008934286, Springer, springer.com, October 31, 2008.

3. Verification Test Suite

As stated previously, there are two fundamental aspects controlling the Type II error of Test (2.2.7), namely, the detection of differences for a given input case, enabled by the verification file, and the coverage of the program provided by the test cases of the Test suite. The second component of verification is coverage. The test suite provides coverage.

Coverage analysis typically examines the lines, functions and subprograms of a code. The verification method developed here examines features of the code instead. The features include the most commonly used features in RELAP5-3D as well as those important for modeling nuclear power plants. The suite can be expanded to include testing of more features in the future.

Section 3.1 summarizes the new verification input tests. Section 3.2 displays them in the verification test matrix.

3.1 Summary of the Verification Tests

The verification test suite expanded in RELAP5-3D version 4.3.1 to include 20 new sets of tests shown in Table 3.0.1. The resulting test suite has three modes of running RELAP5-3D for verification testing, namely standalone, controlled by the Executive, and coupled to another instance of itself through the Executive. In addition, a fourth categories of verification tests, the multi-test case for standalone RELAP5-3D mode, was added to resolve a user problem. Note that multi-case testing is not available in modes involving the PVM Executive because the Executive does not have multi-case capability.

Table 3.0.1. Descriptions of new verification input file.

Test ID	#	Description
1. 2phspump	12	Tests two-phase pump head degradation as a function of void fraction alone and as a function of void fraction and pressure.
2. 3dflow	18	Simulates 3-D flow of single-phase liquid, single-phase vapor, or two-phase flow in a 3x3x3 Cartesian grid with either 1-D or 3-D momentum equations.
3. ans	9	Tests decay heat options with the point kinetics model, fission power types, fission product types available with each ANS standard, and the G-factor contribution to the decay heat.
4. boronm	4	Tracks a square wave in boron concentration through a constant area pipe with and without Godunov method.
5. crit	4	Tests Ransom-Trapp and Henry-Fauske critical flow models for a range of stagnation conditions including subcooled, two-phase, and superheated in a small horizontal pipe. Also tests cases with no choking allowed and homogeneous flow.
6. cyl3	1	Tests the metal water reaction model for steam flowing past the right surface of a cylindrical heat structure.
7. duklerm	5	Tests the CCFL model using Dukler-Smith air-water countercurrent flow data. Wallis, Kutateladze, and Bankoff correlations are tested.
8. eccmix	1	Models a portion of the cold leg of a typical PWR during ECC injection.
9. edhtrkm	5	Edward's pipe simulates a rapid blowdown of a pipe. Includes extras: reactor kinetics, heat structure cosine temperature problems, and all control variables types, but shaft. Cases use fluids: h2o, d2o, h2on, h2o95, hen, and an air/water mixture.
10.eflag	2	Simulates blowdown of one vessel into another to check the effect of the e-flag on the thermodynamic state in the downstream vessel.
11.enclss	1	Steady-state calculation of a graphite stack using the heat conduction enclosure model.
12.fric	14	Tests various single-phase wall and junction friction models. Cases include turbulent flow with and without heated wall effect, laminar flow with and without shape factors, abrupt area change options, and user input equations for wall and form friction.
13.fwhtr	1	Represents a tube-in-shell feedwater heater.
14.gota27	1	Simulates rod-to-rod radiation in a 64-rod bundle in low-pressure steam using radiation enclosure model.

15.hse	3	Simulates two-phase flow through a horizontal tee with offtakes coming off the top, bottom, or side face of the horizontal pipe.
16.httable	3	Simple model of a pipe and heat structure exercising structure BC related to heat flux and heat transfer coefficient.
17.httest	9	Simple model of a pipe and heat structure that varies IC and BC to achieve various heat transfer regimes for heat transfer packages 1, 111, and 134. Also tests the non-equilibrium volume option.
18.hxco2m	2	Models a once-through heat exchanger with PbBi on the shell side and supercritical carbon dioxide inside the tubes. Tests the normal and alternate heat structure-fluid coupling models in steady-state.
19.jetjun	2	Simulates insurges and outsurges of liquid into a pressurizer with and without the jet junction model.
20.jetpmp	1	Tests jet pump performance over a range of suction and driveline flows.
21.l31acc	1	Represents the accumulator response during a slow depressurization during LOFT Experiment L3-1.
22.l2-5-emA 23.(1)	1	Tests Appendix K options during a LOFT Experiment L2-5, which simulates a loss-of-coolant accident initiated by a large break.
24.neptunus	2	Models pressurizer insurge/outsurge experiment with spray.
25.pack	4	Vertical fill problem tests water packing model when subcooled liquid is injected into superheated steam from below. Uses semi- and nearly-implicit timesteps.
26.pitch	1	Tests an inertial check valve with movement.
27.radial	1	Models pure radial, symmetric flow problem in a 2D hollow cylinder. There is no azimuthal flow.
28.rcpr	1	Tests the performance of a recompressing compressor in a supercritical CO2 cycle.
29.refbun	1	Tests two-phase flow and heat transfer with horizontal and vertical bundles that exercise the Groeneveld and PG CHF correlations and correlations for narrow, rectangular channels.
30.regime	22	Tests the standard horizontal and vertical flow regimes by adjusting flow boundary conditions through a simple pipe. Both the pre-CHF and post-CHF regimes are tested for the vertical pipe.
31.rigidbody	1	Models pure azimuthal, symmetric flow problem in a 2D hollow cylinder. There is no radial flow.
32.rtheta	1	Models flow in a 2D hollow cylinder with symmetric flow in both the radial and azimuthal flow directions.
33.rtsampnm	1	Based on typpwr, tests radio-nuclide transport model and the axial heat source options using nodal kinetics.
34.rtsamppm	1	Based on typpwr with uses point kinetics, tests various axial heat source options, including those from tables, control variables, and reactor kinetics. Tests the radio-nuclide transport model too
35.slab3	1	Tests the metal water reaction model for steam flowing past the right surface of a rectangular heat structure.
36.sphere3	1	Tests the metal water reaction model for steam flowing past the right surface of a spherical heat structure.
37.state	24	Tests various fluid states, including subcooled liquid, two-phase, superheated vapor, high-pressure liquid, high-temperature vapor, and supercritical, for h2o, h2on, d2o, and new helium.
38.todcnd	1	Models heat transfer from hot wall with the reflood and two-dimensional heat conduction models.
39.turbine9	1	Multi-stage steam turbine with moisture separation. All four types of turbines are tested.
40.typ12002	1	Models small-break LOCA in a typical pressurized water reactor for 1200 s.
41.typ_kindt	2	TYPPWR input model with nodal kinetics, Krylov solver, and independent kinetics timestep.
42.valve	5	Models opening and closing of all valves, except relief.
43.varvol2	1	Uses the variable volume model and a general table to vary the fluid volume of a single liquid-filled volume.
New Tests Introduced in this project		
44.cpl_det	1	A simplified version of TYPPWR (test 40) that tests the detector model with pt. kinetics
45.cpl_det_new	1	Same as cpl_det (test 51) with modified weighting factors and attenuation coefficients.
46.cpl_new_sa	1	A version of TYPPWR (test 40) that tests the detector model with nodal kinetics
47.cpl_pvm_core	1	Christensen model domain decomposed into two semi-implicitly coupled regions, one with the center of the pipe representing the core, the other with the upper and lower portions.
48.cpl_pvmcs	1	Edward's pipe problem adapted to test control system coupling
49.cpl_pvmeda	1	Edward's pipe problem split in half to test asynchronous coupling
50.cpl_pvmedca	1	Edward's pipe problem split in half to test asynchronous explicit conserving coupling
51.cpl_pvmedcs	1	Edward's pipe problem split in half to test synchronous explicit coupling
52.cpl_pvmnd	1	A version of TYPPWR (test 40) that tests nodal kinetics coupling
53.cpl_pvmnonc	1	Parallel pipes tests multiple connections to a coupling TDV and multiple noncondensables
54.cpl_pvmpt	1	A version of TYPPWR (test 40) that tests point kinetics coupling
55.det	1	Tests the detector model.
56.det_new	1	Tests the detector model.
57.do_nothing	1	Tests if zero flow and zero heat transfer are maintained in a rectangular solid of 3x5 vols. constructed of 5

		volume pipes connected by multiple junctions.
58.ht_expl_fluid	1	Tests explicit fluid-to-heat structure coupling
59.ht_imp_fluid	1	Tests implicit fluid-to-heat structure coupling
60.nothing_trans	1	Tests moving problems translational acceleration specified by both periodic and table input in a 3x3x5 rectangular solid built of 5 volume pipes connected by multiple junctions.
61.pvmcore	1	Tests ability of RELAP5-3D to run the vessel interior of a modified Christensen model[8, 9].
62.pvmcs	1	Edward's pipe problem adapted to test control system
63.pvmnonc	1	Parallel pipes tests multiple connections to TDV and multiple noncondensables
64.pvmpt	1	A version of TYPPWR (test 40) that tests point kinetics
65.tdvtdj	1	Tests multiple connections to a TDV.

3.2 Features and Cases Matrix

A review of the code's capabilities and features that are commonly used in performing reactor and associated system simulations was performed. The important categories of code features and models included hydrodynamic components, volume and junction options, heat structure types, correlations, boundary conditions, trips, tables, control variables, reactor kinetics, Appendix K, and user choices that affect the way the code operates. Among user choices are time advancement scheme, solver, card 1 options and many others.

Features identified in the initial report are the same ones used for this report with a few extras.

Input cases include those from the original report and a number of new cases of interest. Because of the additional cases, Features-Cases Matrix is too long and wide to represent legibly across a page. To accommodate the information, the features are broken into 6 sub-tables. The cases are broken in half with the old cases presented in part "a" of each sub-table followed on the next page by the new cases reported in sub-table "b." For example, Table 3.2.1a holds the components for the original cases and Table 3.2.1b has the 22 new cases. Since the automated system does not detect everything, there are many blank rows.

Both Fortran and Linux script coding was improved to find more of the tested features and place them in the CSV version of the Features-Cases Matrix. Still, not all features are detected automatically. For those that are, an 'M' for Machine-identified is placed beneath the case name in the row of the feature detected. As always, an "X" in Column two indicates the feature is tested by at least one member of the suite of cases and an "X" in Column three indicates feature is restarted. These marks are "carried over" from the rest of the matrix, and indicate testing among all 65 cases, not just the new cases. Items marked in purple are not tested and, though of some value in modeling some nuclear power plants, are of lesser importance, have very few applications, or can be modeled through other means with RELAP5-3D.

Table 3.2.1a. Features-Cases Matrix – Hydrodynamic Components

Features	Present	Restart	2phspump.i	3dflow.i	ans.i	boronm.i	crit.i	cyl3.i	Drift N/A	duklerm.i	eccmix.i	edhtrkm.i	eflag.i	enclss.i	fric.i	fwhtr.i	gota27.i	hse.i	httable.i	httest.i	hxco2m.i	jetjun.i	jetpmpm.i	12-5-emA.i	131acc.i	neptunus20m.i	pack.i	pitch.i	radialm.i	rcpr.i	refbunm.i	reflecht.i	regime.i	rigidbodym.i	rthetam.i	rtsampnm.i	rtsamppm.i	slab3.i	sphere3.i	state.i	todcnd.i	turbine9.i	typ12002.i	typ_kindt.i	valve.i	varvol2.i
	#	#	1	2	3	4	5	6		7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43
Hydro-Component																																														
SNGLVOL	X	X	X							X			X			X						X	X	X						X						X	X					X	X	X		X
TMDPVOL	X	X	X	X		X	X	X		X	X	X		X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X			X	X	X	X	X
SNGLJUN	X	X	X			X	X	X		X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X		X	X		X	X	X	X			X	X	X	X			X	X	X	X	X
TMDPJUN	X	X	X			X		X		X	X			X	X	X	X		X	X	X	X	X	X		X			X			X	X	X	X	X	X	X	X				X	X		
PIPE	X	X			X	X	X	X		X	X	X	X	X	X	X	X	X	X	X	X	X		X	X		X	X			X	X	X			X	X	X	X	X	X	X	X	X	X	
ANNULUS	X	X																						X												X	X						X	X		
PRIZER	X	X																								X																				
BRANCH	X	X								X											X			X						X	X					X	X						X	X		
SEPARATR	X	X																						X												X	X						X	X		
Black box	X	X																																									X			
GE																																														
JETMIXER	X	X																					X																							
TURBINE	X	X																																								X				
FWHTR	X	X														X																														
ECCMIX	X	X									X																																			
VALVE	X	X														X								X				X								X	X						X	X	X	
CHKVLV	X	X																																											X	
TRPVLV	X	X																						X												X	X						X	X	X	
INRVLV	X	X																										X																	X	
MTRVLV	X	X																						X												X	X						X	X	X	
SRVVLV	X	X														X																													X	
RLFVLV																																														
PUMP	X	X	X																					X												X	X						X	X		
CPRSSR	X	X																												X																
MTPLJUN	X	X		X																									X					X	X											
ACCUM	X	X																						X	X											X	X						X	X		
MULTID	X	X		X																									X					X	X											
SNGLFW																																														
MTPLFW																																														
Variable volume	X	X																																												X
Moving System	X	X																										X																		

Table 3.2.1b. Features-Cases Matrix – Hydrodynamic Components

Features	Present	Restart	cpl_detc.i	cpl_det_newc.i	cpl_det_sas.i	cpl_pvmcorec.i	cpl_pvmcsc.i	cpl_pvmedac.i	cpl_pvmedcaf.i	cpl_pvmedcsl.i	cpl_pvmndc.i	cpl_pvmnoncl.i	cpl_pvmptc.i	det.i	det_new.i	do_nothing.i	ht_expl_fluid.i	ht_imp_fluid.i	nothing_trans.i	pvmcore.i	pvmcs.i	pvmnonc.i	pvmpt.i	tdvtdj.i
	#	#	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65
Hydro-Component																								
SNGLVOL	X	X	M	M	M	M					M		M	M	M					M			M	
TMDPVOL	X	X			M		M	M	M	M		M		M	M		M	M		M	M		M	M
SNGLJUN	X	X	M	M	M	M				M	M	M	M	M	M		M	M		M	M		M	M
TMDPJUN	X	X			M		M	M	M					M	M		M	M					M	M
PIPE	X	X	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M
ANNULUS	X	X			M									M	M								M	
PRIZER	X	X																						
BRANCH	X	X			M									M	M								M	
SEPARATR	X	X			M									M	M								M	
Black box	X	X																						
GE																								
JETMIXER	X	X																						
TURBINE	X	X																						
FWHTR	X	X																						
ECCMIX	X	X																						
VALVE	X	X			M									M	M								M	
CHKVLV	X	X																						
TRPVLV	X	X			M									M	M								M	
INRVLV	X	X																						
MTRVLV	X	X			M									M	M								M	
SRVVLV	X	X																						
RLFVLV																								
PUMP	X	X			M							M		M	M							M	M	
CPRSSR	X	X																						
MTPLJUN	X	X														M			M					
ACCUM	X	X			M									M	M								M	
MULTID	X	X																						
SNGLFW																								
MTPLFW																								
Variable volume	X	X																						X
Moving System	X	X																	M					

Table 3.2.2a. Features-Cases Matrix – Component Control & Specification

Features	Present	Restart	2phspump.i	3dflow.i	ans.i	boronm.i	crit.i	cyl3.i	Drift N/A	duklerm.i	eccmix.i	edhtrkm.i	eflag.i	enclss.i	fric.i	fwhtr.i	gota27.i	hse.i	httable.i	httest.i	hxco2m.i	jetjun.i	jetpmpm.i	12-5-emA.i	131acc.i	neptunus20m.i	pack.i	pitch.i	radialm.i	rcpr.i	refbunm.i	reflecht.i	regime.i	rigidbodym.i	rthetam.i	rtsampnm.i	rtsamppm.i	slab3.i	sphere3.i	state.i	todcnd.i	turbine9.i	typ12002.i	typ_kindt.i	valve.i	varvol2.i
	#	#	1	2	3	4	5	6		7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43
Volume Flags																																														
t – thermal stratification	X	X																								X																				
l – mixture level	X	X																				X				X																				
p – water packing	X	X																									X																			
v – vertical stratification	X	X																								X																				
b – bundle	X	X												X						X											X	X									X					
f – wall friction	X	X													X																															
e – equilibrium	X	X																		X																										
Wall friction options																																														
Turbulent friction	X	X													X																															
Laminar friction	X	X													X																															
Shape factor	X	X													X																															
Viscosity ratio	X	X													X																															
User defined	X	X													X																															
Frictionless	X	X													X																															
Junction Flags																																														
j – jet junction	X	X																				X																								
e – modified PV	X	X											X																																	
f – CCFL	X	X								X														X																						
Wallis	X	X								X																																				
Kutataledze	X	X								X																																				
Bankoff	X	X								X																																				
v – HSE	X	X														X		X																												
Top offtake	X	X																X																												
Bottom offtake	X	X																X																												
Side offtake	X	X																X																												
c – choking	X	X					X																																							
Sub-cooled	X	X					X																																							
Two phase	X	X					X																																							
Super-heated	X	X					X																																							
a – abrupt area	X	X	X				X	X		X	X		X		X	X		X	X	X	X			X		X		X		X	X	X				X	X	X	X				X	X	X	
h – homogeneous	X	X					X			X																							X									X				
s – momentum flux	X	X													X			X						X							X											X				
Junction form loss																																														
Constant	X	X													X																															
Reynolds dependent	X	X													X																															
Abrupt area change	X	X													X																															
Flow regimes																																														
Horizontal	X	X																															X													
Vertical pre-CHF	X	X																															X													
Vertical post-CHF	X	X																															X													
High mixing	X	X	X																																											
ECC mixer	X	X									X																																			
Drift flux models																																														

Table 3.2.2b. Features-Cases Matrix – Component Control & Specification

Features	Present	Restart	cpl_detc.i	cpl_det_newc.i	cpl_det_sas.i	cpl_pvmcorec.i	cpl_pvmcsc.i	cpl_pvmedac.i	cpl_pvmedcaf.i	cpl_pvmedcsl.i	cpl_pvmndc.i	cpl_pvmnoncl.i	cpl_pvmptc.i	det.i	det_new.i	do_nothing.i	ht_expl_fluid.i	ht_imp_fluid.i	nothing_trans.i	pvmcore.i	pvmcs.i	pvmnonc.i	pvmpt.i	tdvtdj.i
	#	#	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65
Volume Flags																								
t – thermal stratification	X	X																						
l – mixture level	X	X																						
p – water packing	X	X	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M
v – vertical stratification	X	X	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	
b – bundle	X	X																						
f – wall friction	X	X	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M
e – equilibrium	X	X																						
Wall friction options																								
Turbulent friction	X	X																						
Laminar friction	X	X																						
Shape factor	X	X																						
Viscosity ratio	X	X																						
User defined	X	X																						
Frictionless	X	X																						
Junction Flags																								
j – jet junction	X	X																						
e – modified PV	X	X																						
f – CCFL	X	X																						
Wallis	X	X																						
Kutataledze	X	X																						
Bankoff	X	X																						
v – HSE	X	X																						
Top offtake	X	X																						
Bottom offtake	X	X																						
Side offtake	X	X																						
c – choking	X	X	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M
Sub-cooled	X	X	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M
Two phase	X	X																						
Super-heated	X	X																						
a – abrupt area	X	X			M									M	M							M	M	
h – homogeneous	X	X																						
s – momentum flux	X	X																						
Junction form loss																								
Constant	X	X																						
Reynolds dependent	X	X																						
Abrupt area change	X	X																						
Flow regimes																								
Horizontal	X	X																						
Vertical pre-CHF	X	X																						
Vertical post-CHF	X	X																						
High mixing	X	X																						
ECC mixer	X	X																						
Drift flux models																								

Table 3.2.3a. Features-Cases Matrix – Heat Transfer Specification

Features	Present	Restart	2phspump.i	3dflow.i	ans.i	boronm.i	crit.i	cyl3.i	Drift N/A	duklerm.i	eccmix.i	edhtrkm.i	eflag.i	enclss.i	fric.i	fwhtr.i	gota27.i	hse.i	httable.i	httest.i	hxco2m.i	jetjun.i	jetpmpm.i	l2-5-emA.i	l31acc.i	neptunus20m.i	pack.i	pitch.i	radialm.i	rcpr.i	refbunm.i	reflecht.i	regime.i	rigidbodym.i	rthetam.i	rtsampnm.i	rtsamppm.i	slab3.i	sphere3.i	state.i	todcnd.i	turbine9.i	typ12002.i	typ_kindt.i	valve.i	varvol2.i
	#	#	1	2	3	4	5	6		7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43
Type Heat Structure																																														
Rectangular	X	X																																				X								
Cylindrical	X	X						X																																						
Spherical	X	X																																					X							
Heat transfer modes																																														
Forced convection	X	X																		X																										
Nucleate boiling	X	X																		X																										
Condensation	X	X																		X																										
Film boiling	X	X																		X																										
Transition boiling	X	X																		X																										
Reflood heat transfer	X	X																																							X					
2D heat conduction	X	X																																							X					
Heat structure BC types																																														
Adiabatic	X	X																																									X			
Convective	X	X																																									X			
Wall temperature	X	X													X																															
Heat flux (table)	X	X																	X																											
Heat flux (control var.)	X	X																	X																											
HTC vs. time	X	X																	X																											
HTC vs. Temp	X	X																	X																											
Alternate coupling	X	X																		X																										
Heat structure heat source options																																														
Radial	X	X																																			X									
Table	X	X																																			X									
Control variable	X	X																																			X									
Point kinetics	X	X																																			X									
Nodal kinetics	X	X																																		X										
Gap conductance model																																														
Metal-Water																																														
Rectangular	X	X																																				X								
Cylindrical	X	X						X																																						
Spherical	X	X																																					X							
Material Prop																																														
Built in	X	X										X																																		
Input	X	X										X																															X			
Function	X	X										X																																		
Enclosure																																														
Conduction	X	X												X			X																													
Radiation	X	X															X																													

Table 3.2.3b. Features-Cases Matrix – Heat Transfer Specification

Features	Present	Restart	cpl_detc.i	cpl_det_newc.i	cpl_det_sas.i	cpl_pvmcorec.i	cpl_pvmcsc.i	cpl_pvmedac.i	cpl_pvmedcaf.i	cpl_pvmedcs1.i	cpl_pvmndc.i	cpl_pvmnonc1.i	cpl_pvmptc.i	det.i	det_new.i	do_nothing.i	ht_expl_fluid.i	ht_imp_fluid.i	nothing_trans.i	pvmcore.i	pvmcs.i	pvmnonc.i	pvmpt.i	tdvtdj.i
	#	#	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65
Type Heat Structure																								
Rectangular	X	X			M									M	M	M	M	M	M		M		M	M
Cylindrical	X	X	M	M	M	M	M	M	M	M	M		M	M	M	M			M	M	M		M	
Spherical	X	X			M									M	M	M							M	
Heat transfer modes																								
Forced convection	X	X																						
Nucleate boiling	X	X																						
Condensation	X	X																						
Film boiling	X	X																						
Transition boiling	X	X																						
Reflood heat transfer	X	X																						
2D heat conduction	X	X																						
Heat structure BC types																								
Adiabatic	X	X																						
Convective	X	X																						M
Wall temperature	X	X																						
Heat flux (table)	X	X																						
Heat flux (control var.)	X	X																						
HTC vs. time	X	X																						
HTC vs. Temp	X	X																						
Alternate coupling	X	X																						
Heat structure heat source options																								
Radial	X	X																						
Table	X	X																						
Control variable	X	X																						
Point kinetics	X	X																						
Nodal kinetics	X	X																						
Gap conductance model																								
Metal-Water																								
Rectangular	X	X																						
Cylindrical	X	X																						
Spherical	X	X																						
Material Prop																								
Built in	X	X					M	M	M	M						M			M		M			
Input	X	X																						
Function	X	X																			M			
Enclosure																								
Conduction	X																							
Radiation	X																							

Table 3.2.4a. Features-Cases Matrix – Tables and Kinetics

Features	Present	Restart	2phspump.i	3dflow.i	ans.i	boronm.i	crit.i	cyl3.i	Drift N/A	duklerm.i	eccmix.i	edhtrkm.i	eflag.i	enclss.i	fric.i	fwhtr.i	gota27.i	hse.i	httable.i	httest.i	hxco2m.i	jetjun.i	jetpmpm.i	12-5-emA.i	131acc.i	neptunus20m.i	pack.i	pitch.i	radialm.i	rcpr.i	refbunm.i	reflecht.i	regime.i	rigidbodym.i	rthetam.i	rtsampnm.i	rtsamppm.i	slab3.i	sphere3.i	state.i	todcnd.i	turbine9.i	typ12002.i	typ_kindt.i	valve.i	varvol2.i
	#	#	1	2	3	4	5	6		7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43
Radionuclide transport	X	X																																		X	X									
Reactor kinetics																																														
Point	X	X										X																									X						X			
SEPARABL	X	X										X																									X									
TABLE3																																														
TABLE4																																														
TABLE3A																																														
TABLE4A																																														
Scram (table)	X	X										X																																		
Scram (control var.)																																														
Power history	X	X										X																																		
Nodal	X	X																																		X										
RAMONA																																														
HWR																																														
GEN	X	X																																		X										
Control Rod	X	X																																		X										
Decay Heat																																														
NO-GAMMA	X	X			X																																									
GAMMA	X	X			X																																									
GAMMA-AC	X	X			X																															X	X									
ANS73	X	X			X																																									
ANS79-1	X	X			X																																									
ANS79-3	X	X			X																															X	X									
ANS94-1	X	X			X																																									
ANS94-4	X	X			X																																									
ANS05-1	X	X			X																																									
ANS05-4	X	X			X																																									
G factor	X	X			X																																									
Detector																																														
Alternate fluids	X	X																		X	X									X										X			X	X		
Noncondensable	X	X						X		X	X	X		X				X		X	X			X	X				X	X			X	X	X	X	X	X	X		X		X	X		
Valve open and close	X	X																																											X	
Boron tracking	X	X				X																		X																						

Table 3.2.4b. Features-Cases Matrix – Tables and Kinetics

Features	Present	Restart	cpl_detc.i	cpl_det_newc.i	cpl_det_sas.i	cpl_pvmcorec.i	cpl_pvmcsc.i	cpl_pvmedac.i	cpl_pvmedcaf.i	cpl_pvmedcsl.i	cpl_pvmndc.i	cpl_pvmnoncl.i	cpl_pvmptc.i	det.i	det_new.i	do_nothing.i	ht_expl_fluid.i	ht_imp_fluid.i	nothing_trans.i	pvmcore.i	pvmcs.i	pvmnonc.i	pvmpt.i	tdvtdj.i
	#	#	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65
Radionuclide transport	X	X																						
Reactor kinetics																								
Point	X	X																			M		M	
SEPARABL	X	X																			M		M	
TABLE3																								
TABLE4																								
TABLE3A																								
TABLE4A																								
Scram (table)	X	X																						
Scram (control var.)																								
Power history	X	X																						
Nodal	X	X			M									M	M									
RAMONA																								
HWR																								
GEN	X	X			M									M	M									
Control Rod	X	X																						
Decay Heat																								
NO-GAMMA	X	X																						
GAMMA	X	X			M									M	M						M		M	
GAMMA-AC	X	X			M									M	M						M		M	
ANS73	X	X																						
ANS79-1	X	X			M									M	M								M	
ANS79-3	X	X																						
ANS94-1	X	X																						
ANS94-4	X	X																						
ANS05-1	X	X																						
ANS05-4	X	X																						
G factor	X	X																						
Detector		X												X	X									
Alternate fluids	X	X																						
Noncondensable	X	X																						
Valve open and close	X	X																						
Boron tracking	X	X																						

Table 3.2.5a. Features-Cases Matrix – Trips and Controls

Features	Present	Restart	2phspump.i	3dflow.i	ans.i	boronm.i	crit.i	cyl3.i	Drift N/A	duklerm.i	eccmix.i	edhtrkm.i	eflag.i	enclss.i	regime.i	fric.i	fwhtr.i	gota27.i	hse.i	httable.i	httest.i	hxco2m.i	jetjun.i	jetpmpm.i	12-5-emA.i	131acc.i	neptunus20m.i	pack.i	pitch.i	radialm.i	rcpr.i	refbunm.i	reflecht.i	rigidbodym.i	rthetam.i	rtsampnm.i	rtsamppm.i	slab3.i	sphere3.i	state.i	todcnd.i	turbine9.i	typ12002.i	typ_kindt.i	valve.i	varvol2.i
	#	#	1	2	3	4	5	6		7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43
Trips	X	X	X							X		X									X		X		X	X	X				X					X	X					X	X	X	X	X
Control variables																																														
SUM	X	X	X					X		X		X			X	X	X		X	X		X			X	X					X		X			X	X	X	X			X	X	X	X	X
MULT	X	X						X		X		X			X	X			X	X		X			X						X				X			X	X			X				
DIV	X	X						X		X		X			X	X			X	X		X			X	X					X							X	X			X				
DIFFRENI	X	X										X																																		
DIFFREND	X	X										X														X																				
INTEGRAL	X	X						X		X		X													X											X		X	X					X		
DELAY	X	X								X		X																																		
FUNCTION	X	X								X		X			X																X					X								X		
STDFNCTN	X	X						X		X		X			X				X						X													X	X						X	
ABS	X	X								X		X			X				X																										X	
SQRT	X	X						X		X		X			X																					X		X	X					X		
EXP	X	X						X				X																										X	X							
LOG	X	X										X																																		
SIN	X	X										X			X																															
COS	X	X										X			X																															
TAN	X	X										X																																		
ATAN	X	X										X																																		
MIN	X	X										X			X																															
MAX	X	X						X				X			X										X													X	X							
TRIPUNIT	X	X								X		X													X						X					X								X		
TRIPDLAY	X	X										X																																		
POWERI	X	X										X																																		
POWERR	X	X										X			X											X																				
PROP-INT	X	X										X					X																												X	
LAG	X	X										X																																		
LEAD-LAG	X	X										X																																		
CONSTANT	X	X						X				X			X	X				X																X	X	X	X					X		
SHAFT	X	X																													X											X				
PUMPCTL	X	X										X																																		
STEAMCTL	X	X										X																																		
FEEDCTL	X	X										X																																		
INVKIN	X	X										X																																		

Table 3.2.5b. Features-Cases Matrix – Trips and Controls

Features	Present	Restart	cpl_detc.i	cpl_det_newc.i	cpl_det_sas.i	cpl_pvmcorec.i	cpl_pvmcsc.i	cpl_pvmedac.i	cpl_pvmedcaf.i	cpl_pvmedcsl.i	cpl_pvmndc.i	cpl_pvmnoncl.i	cpl_pvmptc.i	det.i	det_new.i	do_nothing.i	ht_expl_fluid.i	ht_imp_fluid.i	nothing_trans.i	pvmcore.i	pvmcs.i	pvmnonc.i	pvmpt.i	tdvtdj.i
	#	#	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65
Trips	X	X			M		M	M	M	M		M		M	M						M	M	M	
Control variables																								
SUM	X	X	M	M	M		M	M	M	M			M	M	M						M		M	M
MULT	X	X						M	M	M											M			
DIV	X	X																			M			
DIFFRENI	X	X																						
DIFFREND	X	X																						
INTEGRAL	X	X			M		M							M	M						M			
DELAY	X	X					M														M			
FUNCTION	X	X			M		M							M	M						M			
STDFNCTN	X	X					M														M			
ABS	X	X																						
SQRT	X	X																						
EXP	X	X																						
LOG	X	X																						
SIN	X	X					M														M			
COS	X	X																						
TAN	X	X																						
ATAN	X	X																						
MIN	X	X																						
MAX	X	X																						
TRIPUNIT	X	X			M		M	M	M	M				M	M						M			
TRIPDLAY	X	X					M														M			
POWERI	X	X					M														M			
POWERR	X	X					M														M			
PROP-INT	X	X					M														M			
LAG	X	X					M														M			
LEAD-LAG	X	X					M														M			
CONSTANT	X	X			M		M							M	M						M			
SHAFT	X	X																						
PUMPCTL	X	X					M														M			
STEAMCTL	X	X					M														M			
FEEDCTL	X	X					M														M			
INVKIN	X	X																						

Table 3.2.6a. Features-Cases Matrix – Code Operation Control & Misc.

Features	Present	Restart	2phspump.i	3dflow.i	ans.i	boronm.i	crit.i	cyl3.i	Drift N/A	duklerm.i	eccmix.i	edhtrkm.i	eflag.i	enclss.i	fric.i	fwhtr.i	gota27.i	hse.i	httable.i	httest.i	hxco2m.i	jetjun.i	jetpmpm.i	12-5-emA.i	131acc.i	neptunus20m.i	pack.i	pitch.i	radialm.i	rcpr.i	refbunm.i	reflecht.i	regime.i	rigidbodym.i	rthetam.i	rtsampnm.i	rtsamppm.i	slab3.i	sphere3.i	state.i	todcnd.i	turbine9.i	typ12002.i	typ_kindt.i	valve.i	varvol2.i
	#	#	1	2	3	4	5	6		7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43
Tables																																														
POWER	X	X						X																																						
Temperature	X	X																	X																											
HTRNRATE	X	X																	X																						X					
HTC-T	X	X										X		X										X																						
HTC-TEMP *																																														
REAC-T	X	X			X							X				X		X				X		X		X				X			X			X	X						X	X		
NORMAREA	X	X																						X																						
NORMVOL	X	X																																												X
Equation Solvers																																														
BPLU	X	X	X	X	X	X	X	X		X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X		X	X	X	X	X	X	X	X	X	X		X	X	X	X	X	X	X	X
MA18 (35)	X	X				X			X																		X											X								
PGMRES (34)	X	X				X			X																		X											X								
LSOR	X	X																																		X										
Krylov	X	X																																										X		
Timestep options																																														
Steady-state	X	X												X			X				X																									
Semi-implicit	X	X	X	X	X	X	X	X		X	X	X	X		X	X		X	X	X		X		X	X	X		X	X	X	X	X	X	X	X	X	X		X	X	X	X	X	X	X	X
Nearly-implicit	X	X												X			X				X		X																							
Hydro-heat explicit	X	X			X			X	X			X	X	X	X				X	X	X	X	X		X	X	X	X		X	X		X	X			X	X	X							
Hydro-heat implicit	X	X	X	X		X	X			X	X					X	X	X											X						X	X					X					
Kinetics timestep																																												X		
Card 1 options																																														
11 Supercritical	X	X																			X									X																
15 $\Delta t_{Courant}$	X	X			X																											X													X	
23 Godunov	X	X				X																																								
27 MULTID testing	X	X																																X	X											
41K-loss energy dissipation	X	X			X																											X													X	
50 No flip flop	X	X				X																														X								X		
51 No water packing	X	X																									X																			
54 Void truncation	X	X			X																											X													X	
55 Annular mist	X	X			X																											X													X	
Appendix K																																														
Decay heat																								X																						
Metal water reaction																								X																						
Critical flow																								X																						
CHF																								X																						
Post-CHF heat transfer																								X																						

Table 3.2.6b. Features-Cases Matrix – Code Operation Control & Misc.

Features	Present	Restart	cpl_detc.i	cpl_det_newc.i	cpl_det_sas.i	cpl_pvmcorec.i	cpl_pvmcsc.i	cpl_pvmedac.i	cpl_pvmedcaf.i	cpl_pvmedcsl.i	cpl_pvmndc.i	cpl_pvmnoncl.i	cpl_pvmptc.i	det.i	det_new.i	do_nothing.i	ht_expl_fluid.i	ht_imp_fluid.i	nothing_trans.i	pvmcore.i	pvmcs.i	pvmnonc.i	pvmpt.i	tdvtdj.i
	#	#	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65
Tables																								
POWER	X	X																						
Temperature	X	X				M														M				
HTRNRATE	X	X																			M			
HTC-T	X	X																						
HTC-TEMP *																								
REAC-T	X	X			M		M							M	M						M		M	
NORMAREA	X	X																						
NORMVOL	X	X																						
Equation Solvers																								
BPLU	X	X	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M
MA18 (35)	X	X																						
PGMRES (34)	X	X																						
LSOR	X	X			M									M	M									
Krylov	X	X																						
Timestep options																								
Steady-state	X	X																						
Semi-implicit	X	X				M											M			M				
Nearly-implicit	X	X	M	M	M		M	M	M	M	M	M	M	M	M	M		M	M		M	M	M	M
Hydro-heat explicit	X	X																						
Hydro-heat implicit	X	X																						
Kinetics timestep																								
Card 1 options																								
11 Supercritical	X	X																						
15 $\Delta t_{Courant}$	X	X																						
23 Godunov	X	X																						
27 MULTID testing	X	X																						
41K-loss energy dissipation	X	X																						
50 No flip flop	X	X	M	M	M	M					M	M	M	M	M					M		M	M	
51 No water packing	X	X																						
54 Void truncation	X	X																						
55 Annular mist	X	X																						
Appendix K																								
Decay heat	X	X																						
Metal water reaction	X	X																						
Critical flow	X	X																						
CHF	X	X																						
Post-CHF heat transfer	X	X																						

3.3 Verification Directory and Makefiles

The Test suite is organized into a verification directory, “verify,” with subdirectories of tests. The running of the tests is controlled by Makefiles. There are 6

The main Verify directory contains a single subdirectory for each test case listed at the top of the Features-Decks Matrix. It also contains the principle Makefile, its include files, the template Makefile, set_Makefile, for each of the subdirectories, directories for utility scripts. Within the subdirectories reside the input files for Category 1 and 2 testing, namely the original input deck and a restart deck. There is no Category 3 (or Category 4) input file; Category 3 (and 4) decks are generated from Category 1 decks via scripts. Initially, the only other files that may be present are APT Plot script files.

The new cases that perform coupling mode testing required new directory structure and script programming.

The PVM cases have a collection of at least 5 input decks. If the ABC problem is being run, the types and names of the decks can be:

1. PVM-Executive input deck, ABCx.i
2. Parent base input deck, ABCp.i
3. Parent restart input deck, ABCp.r.i
4. Child base input deck, ABCc.i
5. Child restart input deck, ABCc.r.i

The kind of coupling determines the non-Executive names, which is indicated by the final letter of the deck name. For example: parent-child (p and c as above), client-server (c and s), and leader-follower (l and f).

The Makefiles had to be upgraded to run both RELAP5-3D standalone and coupled modes. The Make.inp direction files had to include new keywords. The main Makefile had to include options to run both modes separately and individually, individual categories (null, restart, backup) within a mode, and even to perform all tests. The set_Makefile that links to each test directory had to expand similarly. It was modified to leave the printed-output file in the directory for debugging purposes until ‘clobbered.’

The Makefile also has targets for comparing restart and backup runs as explained in Sections 4 and 5. It produces files in the MACHNAME directory named NOTREST and NOTBACK which list the names of the input tests that failed each kind of testing. The Makefile allows the Category 1, 2, and 3 tests to be run separately or all three at once. When testing succeeds, the Makefile gives the following messages:

- For null testing: ‘verified’.
- For restart testing: ‘Successful Restart Tests’.
- For backup testing: ‘Successful Backup Tests’.

For failed tests, the corresponding directory will contain a file of differences created by the Linux “diff” function. For restart differences, the file has extension “vdif” and for backup differences, the extension is “b_dif.” These files are useful for debugging purposes.

4. FIXING VERIFICATION TESTING

The initial implementation revealed errors in both restart and backup for RELAP5-3D running in standalone mode. Some user problems were resolved before this project began; however, many remained and more were uncovered during the project. Comparison of verification files from coupled runs revealed new issues relating to PVM communication. Even the programming of the testing method itself proved errant, the placement of the verification backup call allowed some backup errors to go undetected and had to be moved from inside subroutine HYDRO to just after it.

Section 4.1 covers restart testing. Section 4.2 covers backup testing. Section 4.3 covers issues with the overall testing process.

4.1 Restart Resolutions

Most differences in the restart cases had the same root cause, inaccuracy in the last bit of the timestep or a cumulative time on restart. A few resulted from a variable missing from the restart file. Addition of coupled cases to the test suite revealed inaccuracy in edit times calculated by paired processes, including the explicit exchange time between processes.

Differences in the final bit of the cumulative time variable caused many restart problems to differ very slightly at startup. The time for the restart problem was taken directly from the timecard and its floating point representation was as exact as possible. The corresponding time on the base run was calculated after many time steps and sometimes its floating point representation differed from the restart timecard value in the final bit. This caused some problems to drift apart but had no effect on many others.

Many solutions were considered. One that recalibrates cumulative time at every minor or major edit, restart or plot file write, and explicit exchange using quadruple precision to convert between the underlying integer time and floating point time was proposed and implemented. When implemented in the DTSTEP routines of both RELAP5-3D and the PVM Executive program, it eliminated all differences that resulted from mismatched cumulative times in coupled processes.

Additional solutions include: resetting the cumulative time to the restart time only when restarts are written and keeping a permanent quadruple precision variable for the cumulative and copy it into the double precision variable for use in the rest of the code.

For coupling cases that differed because of issues with edit times, the same concept provides the solution. All edit time conversions between integer and real were promoted to quadruple precision, just as was done for cumulative time. This resolved most issues for hydrodynamic time in coupled calculations.

A similar issue was discovered for heat transfer time in coupled mode. Heat transfer time has its own cumulative time and time-step variables that can be independent of the hydrodynamic time. Again, calculating the heat transfer cumulative time in quadruple precision resolved the issue.

* * *

It is noted here for future use, that *keeping permanent copies of cumulative and exchange times results in more accurate timekeeping.* It reduces temporal error in transients that use extreme numbers of advancements. It may become necessary, even for the timestep variable, in complex applications. If quadruple precision variables are kept, the code may still use the double precision quantities outside the timestep subroutines.

* * *

A few issues remained. Improving the way time variables were initialized solved a few issues. Some issues resulted from a variable needed after restart being absent from the restart file. Adding it to both the restart read and write routines solved those issues. An example is the decay heat mode variable. In a few cases, variables were read correctly but were overwritten during input processing by calculations that should only be performed when the hydrodynamic system actually changes despite the fact that the system had not changed. Most of these relate to cards the input manual states should not be included in restart decks, such as 100, 115, 119, and 120-129 cards. The subroutines that read these, RNONCN and RMFLDS have been modified to write a message and set the fail flag so that the problem will not run if one of these is present on restart.

At the end of the project, all restart issues are resolved.

4.2 Backup Resolutions

If water packing[4-1], flow reversal[4-2], or a noncondensable appears[4-3] in a volume or junction, a better solution is possible if the system of equations is modified to account for the condition in the control volume or junction associated with it[4-4, 4-5]. Therefore, the code backs up to the beginning of the timestep, rebuilds the equations with adjustments for the backup condition, and solves the new system. A time-step backup requires the values in data to match the values at the end of the previous timestep. Therefore, old-time variables record these values at the end of each timestep.

Backup issues related to these old-time variables. The differences, between base case and runs that force an artificial backup on successful advancements, arose from four primary causes:

1. An old time variable did not exist
2. An old time variable did not receive its updated value at the end of the previous timestep
3. The old time variable was backed up in the wrong place
4. The old time was not used to restore the new time variable when backup was invoked.

Ideally, all transfers of data between current-time and backup copies occur in subroutine MOVER, either to store backup copies after an advancement or to restore data into current-time variables due to a backup. Unfortunately, MOVER is not the correct place for every transfer. Special cases had to be resolved by storing or restoring elsewhere.

For some variables, such as DFRONT, it is necessary to have not just one backup copy, but two. This is because intermediate calculations can change the value of the first backup before the actual backup takes place.

Just as with restart differences, coupling provided special backup issues. The primary issue was:

5. The PVM transferred data was not stored in old time variables after it was received.

This resulted in the code using values from before the PVM data transfer which caused differences.

All of the required backup issues have been tracked down and solved. These cases involve standalone RELAP5-3D, not coupled calculations.

4.3 Testing Process Issues

Two primary issues for testing are the decision point in the flow logic where backup determination is made, and the problem of an artificial backup causing the code to perform an extra real backup that is not otherwise performed in the base case.

4.3.1 Backup Decision Location and Timing

The initial implementation of backup testing left several issues hidden because the decision point for backup determination was misplaced. Subroutine VERFBACKUP was moved just after the velocity calculating subroutines, VFINL and VIMPLT. This placement prevented detection of some backup issues, such as DFRONT as mentioned in Section 4.2. Moreover, a protection clause was added to allow backup testing only after the first advancement was completed and subroutine MOVER had copied new time values into the old time variables.

Both changes were made to eliminate backup comparisons that seemed to make no sense. For example, it makes no sense to try to compare new and old time values before old time values are recorded, hence the change to only begin backup comparison on the second successful advancement, *after* old time values are initialized by the first call to MOVER. In fact, after coupled cases were added, it became clear that some backup copies were not initialized until the second advancement in the leader-follower couplings, and so the protective clause for VERFBACKUP was changed to NCOUNT > 2.

However, the code does perform backups on the first advancement in some cases; Edward's Pipe is a notable example. Since backups do occur during the first advancement, it is important to detect failures to properly initialize old time variables during that advancement.

To account for the issues described above the call to VERFBACKUP was moved to immediately after the call to HYDRO, though it can be equivalently placed just before the return from HYDRO. The situation with NCOUNT was reduced to three cases, NCOUNT > 2, NCOUNT > 1, and NCOUNT > 0. Since NCOUNT starts at 1, the third case is actually unnecessary and can be removed as a protective clause altogether. These three situations were resolved in the order listed above. All of these issues fell into the 5 categories of issues identified in Section 4.2. However, the implementation of NCOUNT > 0 revealed serious issues.

The code initializes a great many state properties at I-LEVEL through subroutine ISTATE. The subroutine that calculates those state properties in the transient, STATEP, though it uses mathematically equivalent forms, produces different values due to finite precision arithmetic. Tracking down each of these differences and resolving them was deemed beyond the scope and funding of the project, though a valuable future endeavor.

One means to resolve the differences is to call STATEP during I-LEVEL. However, this results in code failures; there is a reason ISTATE was written in the first place. Another solution is to call MOVER which calls STATEP immediately before the transient begins. This worked successfully after a few small changes. Calling MOVER early also initializes the old-time variables as is needed for backups whent NCOUNT equals 1.

At this point, all issues involving the location and timing of the backup decision have been resolved.

4.3.2 Artificial Backup Effect

When a true backup occurs, the code sets logical flags and then backs up. When the system of equations is built, the logical flags are always checked first and indicate how to modify the system. The flags are reset to false after the hydrodynamic calculation is deemed successful.

However, when an artificial backup occurs after a flow reversal backup, the logical flags are also reset. In flow regions with multiple hydrodynamic systems, the systems are solved independently of each other. What if a velocity flip-flop occurs in a second system after the original one has been rebuilt, succeeded, and followed by an artificial backup? In that case, the flags are reset in the system that originally had a backup, but then are set for the other. This causes the code to take another backup, one that the base case will not take. The solutions will diverge from that advancement forward.

This divergence does not detect an actual code problem causing the difference, but in essence creates an artificial divergence. *It is a testing issue, not a code issue*.

One solution is to store the logic flags before an artificial backup and restore them after the call to MOVER in DTSTEP when the advancement is deemed successful. Another solution is to recognize that this is a testing issue and not even allow an artificial backup on an advancement that has a real backup.

The former method seeks to force an artificial backup after each successful backup. Under current code logic, this does not work because the code is limited to three backups before cutting the timestep. A sequence of real-artificial-real backups makes three, so the third cannot be followed by an artificial backup. To resolve this, either artificial backups must not be counted, or the limit must be increased.

The alternate method does not force artificial backups after real ones and therefore does not enforce the "artificial backup after each successful backup" rule. Is it possible that some backup error might go undetected with this limitation of artificial backups? The artificial backup following a flow reversal would occur immediately afterwards on the next timestep, if the next advancement initially succeeds just as it did in the base case.

Currently, the former method of saving the old-time logic flags has been implemented without any change to the number of backups before cutting the time step in half.

4.3.3 Remaining Issues

The following are items that were not resolved during this task but do relate to verifying RELAP5-3D calculations and the correctness of verification testing. These have varying levels of importance.

1. Resolve the artificial backup effect of Section 4.3.2.
2. Resolve the PGMRES solver differences. On the first timestep of a restart or backup of the BORONM test case, a difference in the last bit of the right hand side occurs. This results in persistent differences.
3. Change the calculations in ISTATE and STATEP to produce identical results.
4. Resolve the differences in reduction counts occur in a few verification test cases. Since these are output-only variables and not primaries, they have been ignored.
5. Program an algorithm for coupled problem backup testing.

Item 1 is an artifact of testing that has more possible resolutions than the ones listed above; it requires a decision at some future time. Item 2 is handled by recommending that PGMRES not be used for now. Item 3 was worked round by the early call to MOVER. Item 4 has no bearing on calculations and can be ignored safely for now. Item 5 will become important, but is not part of the workscope.

4.4 Conclusion

The restart/backup task has been completed and the code modifications included in RELAP5-3D Version 4.3.1. With the exception of PGMRES, all verification test cases run with no differences in the verification files. The PGMRES and reduction count differences have been recorded as user problems in the electronic ticket system for future resolution.

All the updates for fixing issues with restart and backup verification have been transmitted to the customer. The customer has installed them and reported that their code now verifies properly on all the test cases of the verification test suite.

4.5 References

4-1 The RELAP5-3D Code Development Team, "RELAP5-3D Code Manual Volume I: Code Structure, System Models and Solution Methods," INL-EXT-98-00834-V1, Revision 4.0, Section 8.2, p 8-4, June, 2012.

4-2 The RELAP5-3D Code Development Team, "RELAP5-3D Code Manual Volume I: Code Structure, System Models and Solution Methods," INL-EXT-98-00834-V1, Revision 4.0, Section 8.2, pp. 8-3 to 8-4, June, 2012.

4-3 The RELAP5-3D Code Development Team, "RELAP5-3D Code Manual Volume I: Code Structure, System Models and Solution Methods," INL-EXT-98-00834-V1, Revision 4.0, Section 3.4, pp. 3-271 to 3-274, June, 2012.

4-4 G. L. Mesina, "RELAP5-3D Restart and Backup Verification Testing," INL-EXT-13-29568, September, 2013.

4-5 G. L. Mesina, D. L. Aumiller, F. X. Buschman, "Automated, Highly Accurate Verification of RELAP5-3D," ICONE22-31153, Proceedings of the 22nd International Conference on Nuclear Engineering, Prague, Czech Republic, July 7-11, 2014.