Selected Opt Level 1 and 2 Improvements for RELAP5-3D

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Introduction

- Plot file improvements
- Strip file improvements
- Optimization Levels 0 and 1

Plot File Improvements

- Can specify that a given volume variable will go to the plot file for all control volumes
- Plot file has three formats
  - ASCII plot file
  - Machine-dependent plot file
  - Machine Independent plot file
- On a restart, the plot file must be read
  - The new plot file must gain all information from old plot file up to the point of the restart.
  - If not, all data from start of initial run to restart point is absent on the new plot file
- The code needs to know the format of the plot file on restart.

Plot File Improvements

- Card 103 specifies format of the incoming plot file
  - This can be any one of the allowable formats
  - CMPRESS and NCMPRESS are kept for backwards compatibility

103, Word 2	Incoming Plot file format
ASCII	ASCII
BINARY	Machine Independent XDR binary
CMPRESS	Machine Independent XDR binary
NCMPRESS	Machine Independent XDR binary
MBINARY	machine dependent binary

Plot File Improvements

- Card 104 specifies format of the outgoing plot file
  - This format can differ from the incoming plot file
  - Can name the outgoing plot file with card 104, word 2
  - can be any one of the allowable formats

104, Word 1	Incoming Plot file format
ASCII	ASCII
BINARY	Machine Independent XDR binary
CMPRESS	Machine Independent XDR binary
NCMPRESS	Machine Independent XDR binary
MBINARY	machine dependent binary

Strip File Improvements

- New “all” option
  - Can specify that a given volume variable will go to the strip file for all control volumes of the plot file
  - Invoked when 1001-1999 card, word 3 is “all”
- Outgoing strip file has same 3 available formats as Incoming plot file
  - ASCII
  - Machine-dependent binary
  - Machine Independent binary
- New format for Outgoing Strip file:
  - Comma Separated Value (CSV) ASCII format
  - Opens directly with MS Excel

Strip File Improvements

- Cannot have machine INdependent XDR on both plot and strip files.
- This table summarizes the combinations of plot and strip files
  - Available means it is implemented in 4.0.3.
  - Allowed means we will implement if there is sufficient user interest

Outgoing strip file format	Incoming Plot XDR	Incoming Plot Machine dependent	Incoming Plot ASCII
ASCII	Available	Available	Available
Machine dependent	Available	Available	Available
XDR machine INdependent	Not Possible	Allowed, not available	Allowed, not available
CSV (Comma Separated Values)	Next release	Next Release	Next Release

Optimization Level Differences

- Programs should produce the same calculation at low optimization.
  - Optimization level 0 interprets each operation (add, compare, etc.) as if it's the only operation when changing to machine language
    - Lots of wasted memory fetches and stores
  - Optimization level 1 eliminates this kind of waste and does very little more
  - With aggressive optimization, compilers perform shortcuts that change computations.
- RELAP5-3D/Ver:4.0.3 does not produce the same calculations at optimization levels 0 and 1.

Optimization Level Differences

- Typically these are difficult to find and resolve
  - No core dump
  - No error message
  - Use of debugger generally makes difference disappear
  - Diagnostic write statements generally makes difference disappear

- RELAP5-3D printed output file (default installation runs) occur in:
  - 3dflow.p
  - edhtrkd.p
  - All 73 PVM test case output files
- There could be others that printed output does not reveal.

Optimization Level Differences

- 3dflow is a 3x3x3 cube which runs 18 cases
  - The first 9 cases use crossflow junctions to allow crossflow
  - Cases 10 through 18 use true multi-dimensional physics
  - The latter requires far more information
- Cause of failure: Key information arrays were not deallocated after each case was run.
  - Cases 1-9 use the same memory. Case 10 needs much more.
- Solution: Force deallocation of these arrays at end of each case.

Optimization Level Differences

- The EDHTRKD test case is Edward's Pipe with heavy water.
- Differences: only in Volume 21 in input edit section of printed output.
  - SOUNDE = 416.0 for opt 1
  - SOUNDE = 446.0 for opt 0
- *Use of debugger OR diagnostic writes causes opt 1 SOUNDE=446*.
- Subroutine ISTATE: SOUNDE is set according to QUALE.
  - For QUALE = 0.0 or 1.0, homogenous sound speed is calculated from standard homogeneous frozen formula (Vol. 1, Eq. 3.2-24)
  - For 0.0 < QUALE < 1.0, ISTATE uses (Vol. 1, Eq. 3.2-20)
- QUALE is different
  - QUALE = 0.99999999996 for opt 1
  - QUALE = 1.00000000000 for opt 0.

Optimization Level Differences

- X_e = QUALE = the equilibrium quality used in sound speed calculation

  $\mathbf{X_e = [\, XU_g + (1\text{-}X)U_f - U_f^s \,] / (U_g^s - U_f^s)}$

  where $\mathbf{X = (\alpha_g \rho_g)/(\alpha_g \rho_g - \alpha_f \rho_f)}$ is the static quality.
- ISTATE in 2-phase region: if (VOIDF<10^{-10}) VOIDF=0.0
  - $\mathbf{\alpha_f}$ = VOIDF = 0.0 => $\mathbf{\alpha_g}$ = 1.0 => **X** = 1.0
  - $\mathbf{X_e = (U_g - U_f^s) / (U_g^s - U_f^s)}$ = 1.0 at saturation
- ISTATE does not also reset QUALE when it resets VOIDF.
  - Creates inconsistency.
- Fix: FOR HEAVY WATER ONLY:
  - Reset QUALE = 1.0 in saturation when VOIDG reset to 0.0

- All known Opt level 0/1 differences resolved.

Optimization Level Differences: PVM cases

- Solving the 73 PVM cases
  - 50 output files differ in the number of computer cycles.
    - Varies with computer's workload. Not a true difference.
  - Ignoring cycles, 23 files show differences
    - 22 are PVM Executive output files that differ on CPU time
    - Varies based on a computer's load.
  - Only true differences: CJFAILTEST.
- CJFAILTEST checks that improper "coupling junction" input is caught.
  - First difference: *choking flag*
    - off with Opt 1
    - on with opt 0
  - Tracked to uninitialized array in RCPLJUN

Opt Level Debug: PVM 2nd Difference

- The actual problem has only 2 hydrodynamic loops
  - Opt 1 finds only 2
  - Opt 0 identifies 3. *Surprising!*
- Tracked to subroutine IMLP array MARKV
  - MARKV(13) = 0 at opt 1, MARKV(12:13) = 0 at opt 0
- *Use of debugger OR diagnostic writes made error disappear*.
- Cause: allocated memory issues creating an overwrite
- Fix: Prevent overwrite: Move some memory to IMLPMOD
  Move some coding to internal subroutines
- **PVM differences eliminated**.

This fix also improves some values in TYPPWR test cases

Subroutine	Problem fixed
RCPLJUN	Initialization
IMLP	Allocated memory usage

Conclusions

- In 4.0.3, plot and strip file have new formats
  - ASCII plot file
  - Machine-dependent plot file
  - Machine Independent plot file
- In next release, strip file will have extra format: CSV
- 4.0.3 can strip any plot files into strip files of any format except XDR
- 4.0.3 produces different calculations at opt levels 0 and 1
- These have been resolved beginning in version 4.1.0