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Code Architect & Manager

To 4.5.2 and Beyond

International RELAP5 User Group Meeting

Battelle Energy Alliance manages INL for the
U.S. Department of Energy's Office of Nuclear Energy

Idaho National Laboratory

RELAP5-3D stays abreast of the ever-changing nuclear and computer industries.

- Where did we come from?
  - History of RELAP5 up to RELAP5-3D
- Where are we now?
  - History from RELAP5-3D Version 1.0 to Version 4.4.2
- What's in the newest released version?
  - Upgrades that went into version 4.5.2
- Where are we going?
  - Some plans for future advancements.

Where did we begin? A Brief History of RELAP5-3D

- **1966: RELAP1** - Revised version of FLASH-1 LOCA analysis code
- Primary system was three lumped volumes with
  - pressure-dependent coolant pumps and a flow-dependent heat exchanger.
- Point kinetics with several reactivity functions
- 2-point heat transfer model with 3 modes
- Interpolated steam tables from 1 to 3200 psia

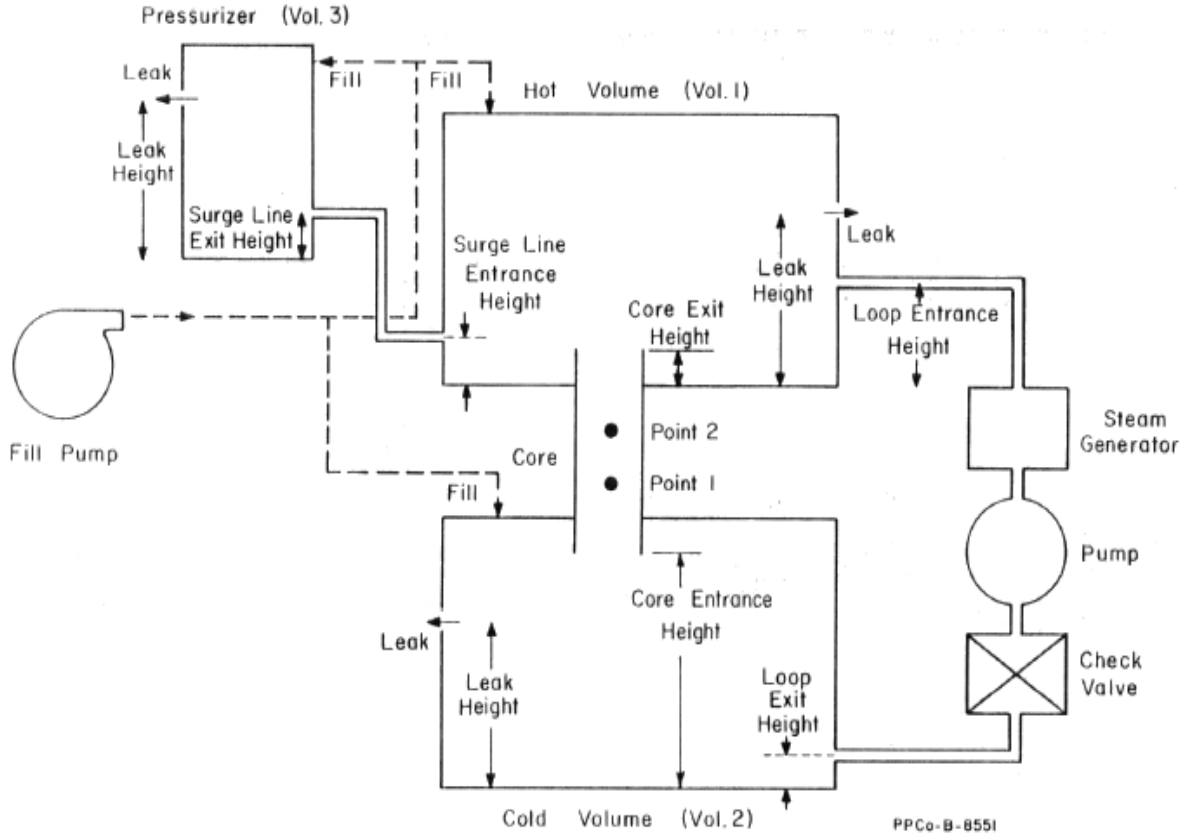

Figure 2 RELAPSE-1 (RELAP1), 1966

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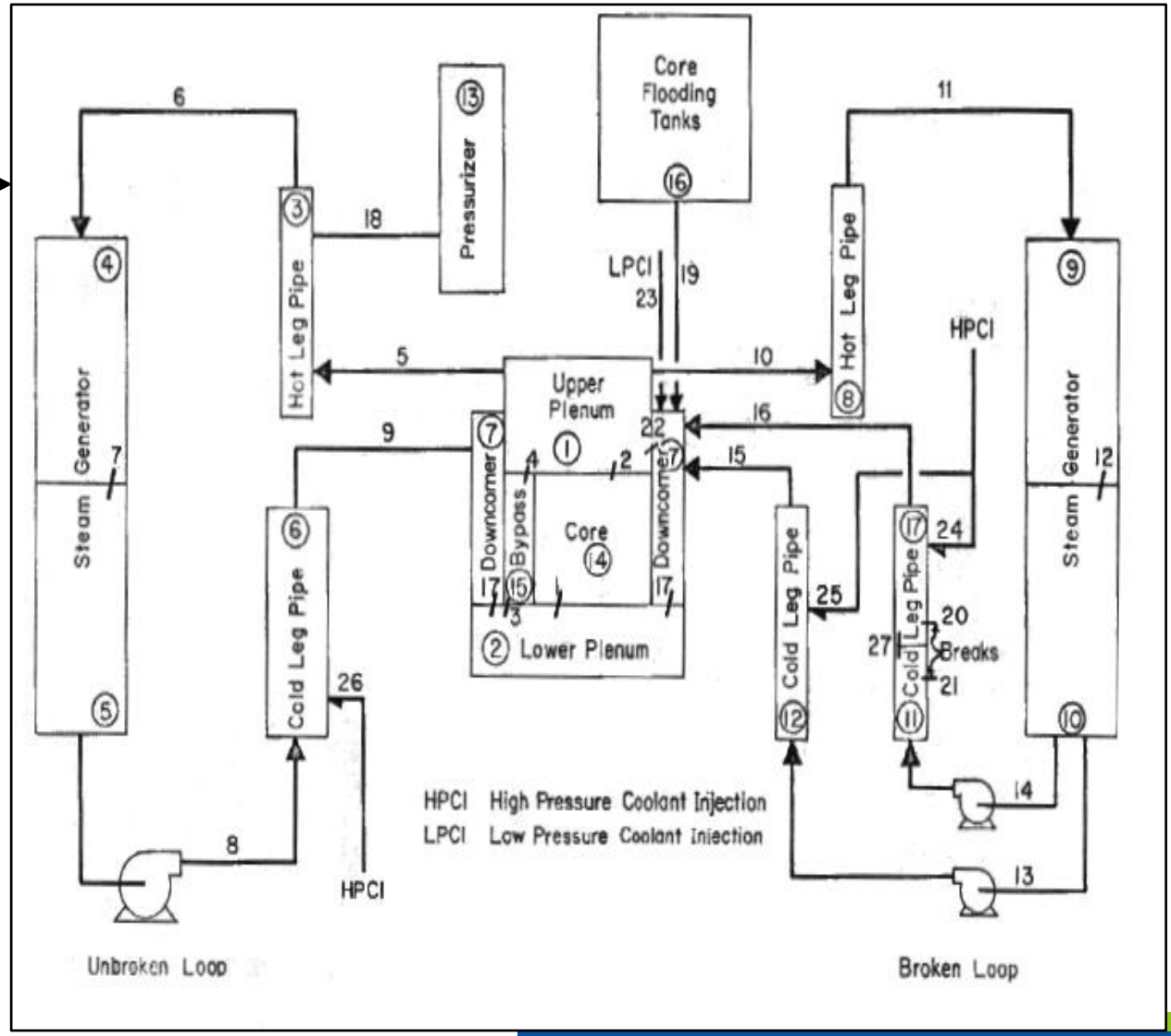
Where did we begin? A Brief History of RELAP5-3D

- **1968: RELAP2** - BWR modeling
- **1970: RELAP3** – up to **20 volumes**,
  - Trip, valve, fuel
  - extended heat convection and conduction models
- **1973: RELAP4** - **100 volumes**
  - True 1-D flow, a momentum flux term dP/dA and form losses
  - 2-fluid slip model
  - molecular nitrogen for the accumulator
  - representation of the secondary system as a flow network
  - reflood heat transfer.
  - SB-LOCA capable



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Where did we begin? A Brief History of RELAP5-3D

- 1979 **RELAP5/MOD 0 - 2-fluid model** w/ governing equations set for liquid and gas phases.
- **Fortran 77**
- **Semi-implicit numerics** for time advancement.
- Other improvements:
  - **Interfacial momentum** terms and mass and energy exchange terms were added
  - **Cross-flow** between 1-D fluid flow channels
  - A **multi-channel fuel rod** model
  - **Trips and controls**
  - Appendix K
  - Solutes and non-condensable gases
  - Many new models, correlations

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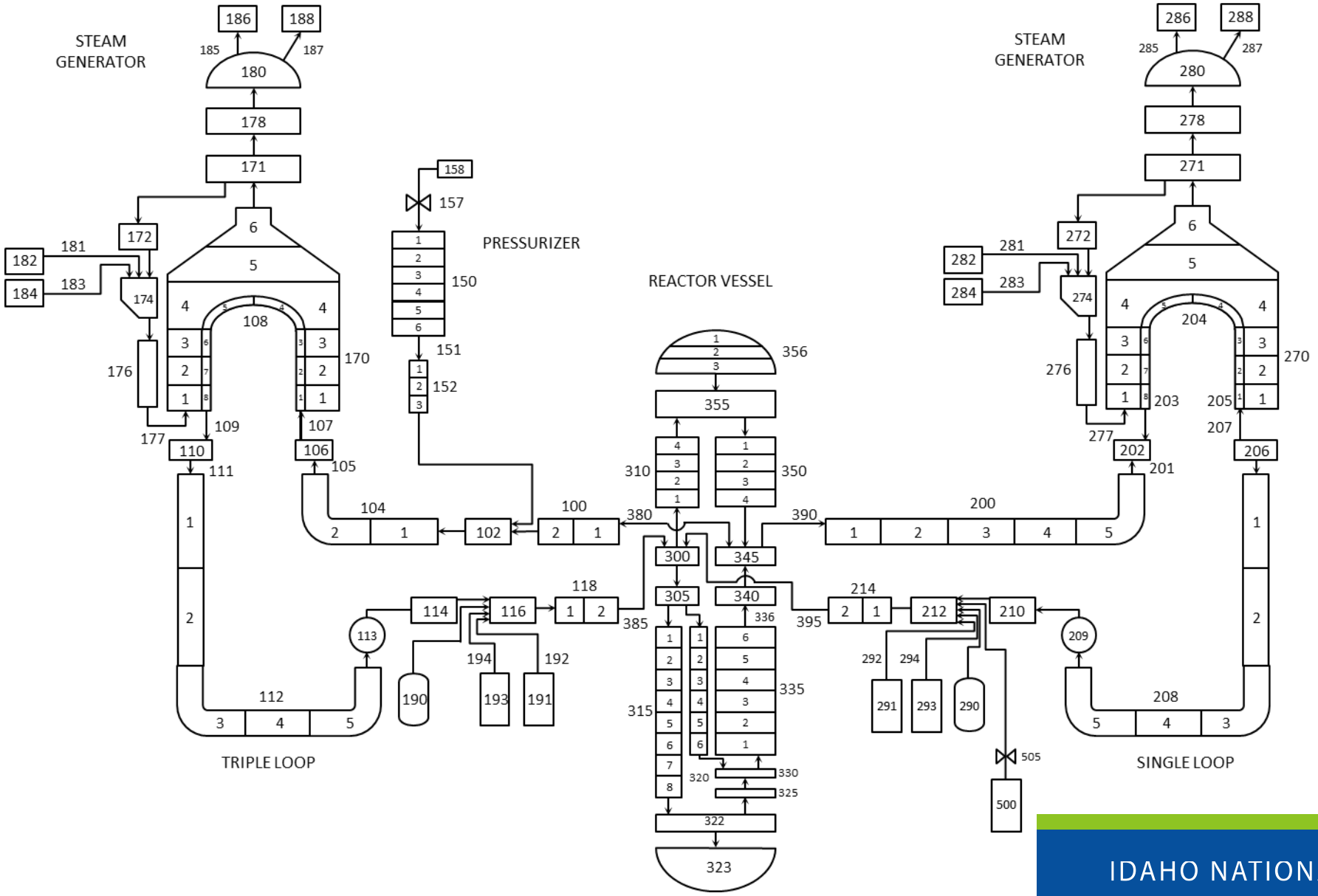
Example RELAP5-3D/Mod 1 Nodalization



Major Features of RELAP5, Decades 2 and 3

- 1987: RELAP5/MOD2 – Adaptation to **Cray**, **vectorization**
- 1992: RELAP5/MOD2 – **Portability** to all Unix platforms, **parallelization**
- 1995: RELAP5/MOD3.2.1.2 – Last version of RELAP5/MOD series at INL
- 1997: RELAP5-3D/Ver. 1.0 – Full **3D hydrodynamics**
- 1998: International RELAP5 user group (IRUG) formed
- 2001: RELAP5-3D/Ver. 2.2 – Completed **PVM coupling** to other codes
- 2002: RELAP5-3D/Ver. 2.3 – **Windows OS** compatible
- 2011: RELAP5-3D/Ver. 3.0 – **Fortran 90** Alpha Test Version
- 2012: RELAP5-3D/Ver. 4.0 – **Fortran 90** V&V'ed Version

- Many other upgrades went into these; see next slide

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Some Other RELAP5-3D Code Architecture Upgrades

- Code coupling via the R5EXEC program
- Synchronized integer-based time-step control
- Decoupled thermal-hydraulic and kinetic time steps
- Fortran 95
- Strongly modular through structured programming
- Open MP parallel directives
- Fast hydrodynamic linear equation solvers for larger problems: BPLU and PGMRES
- Machine-independent binary fluid and plot files
- RGUI (RELAP5-3D Graphical User Interface)
- Fortran 2003

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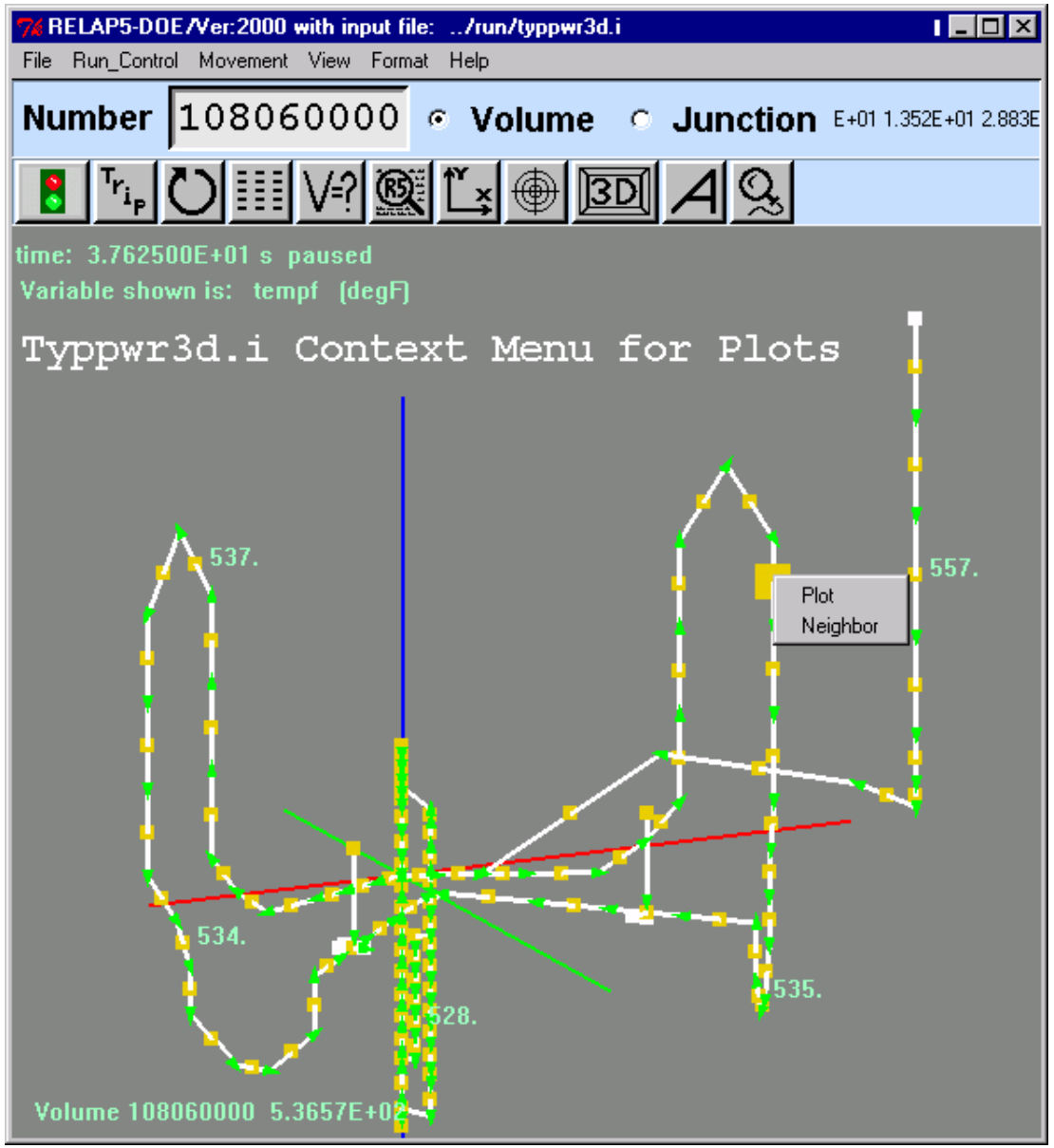
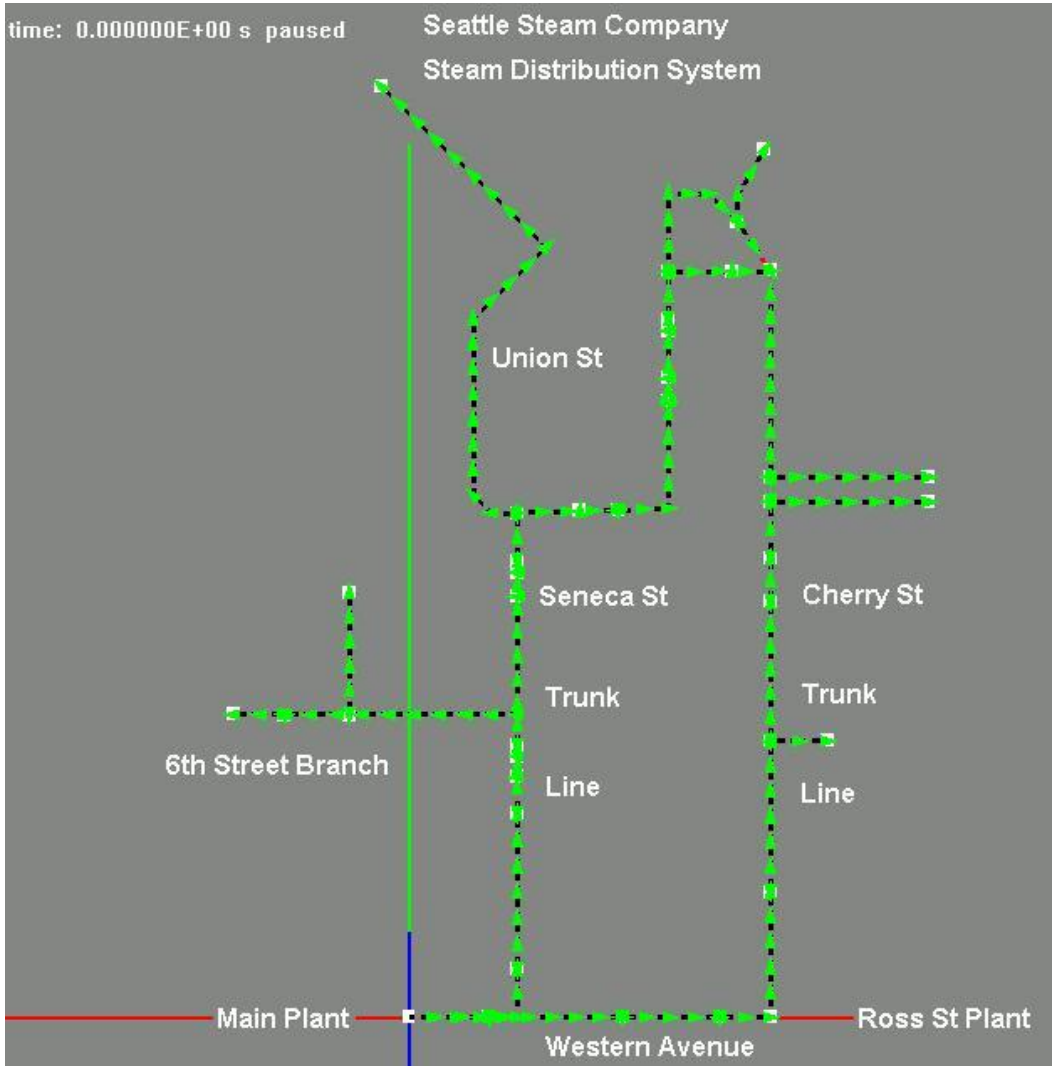
Screens from RGUI: RELAP5-3D Graphical User Interface





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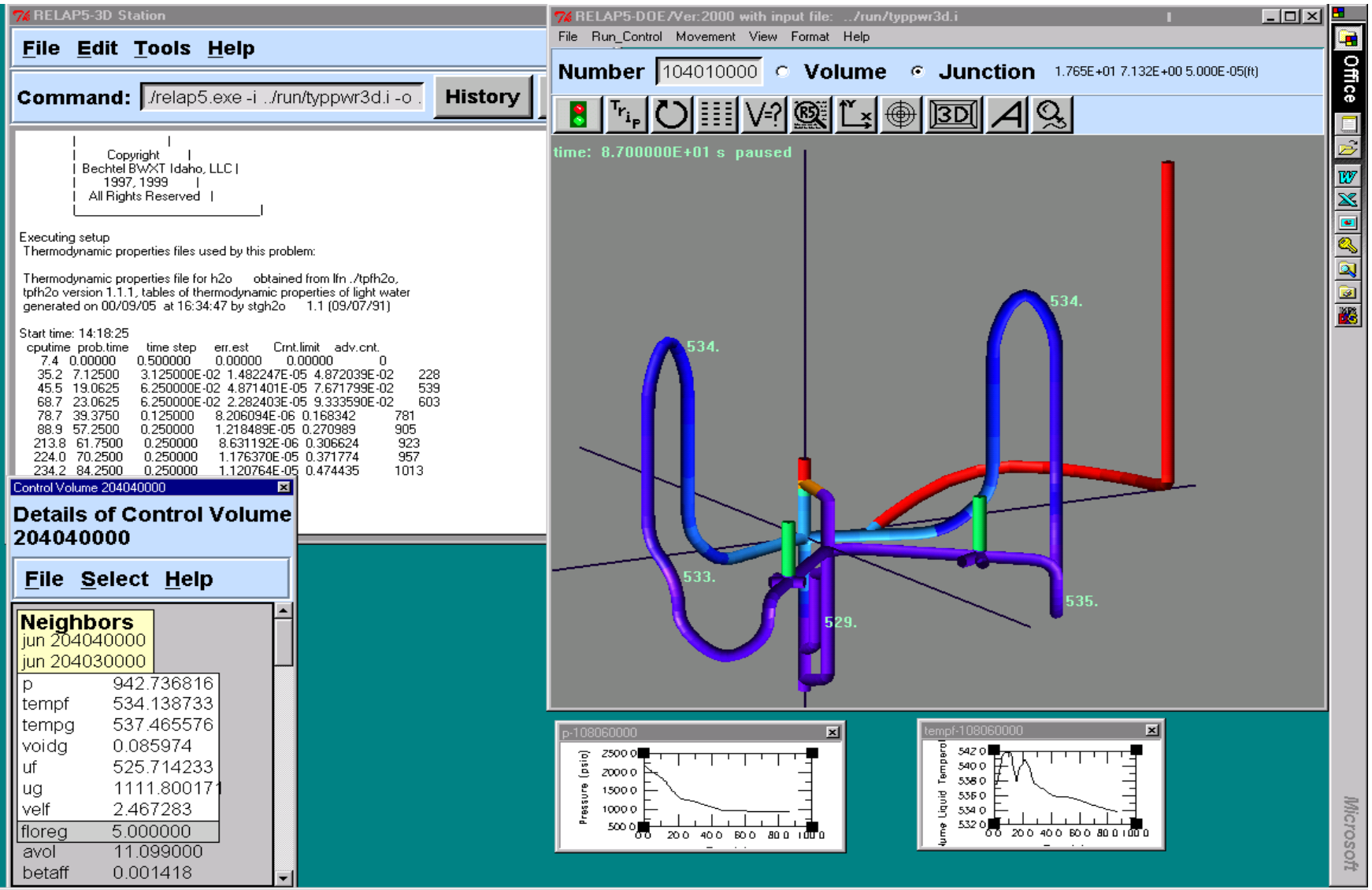

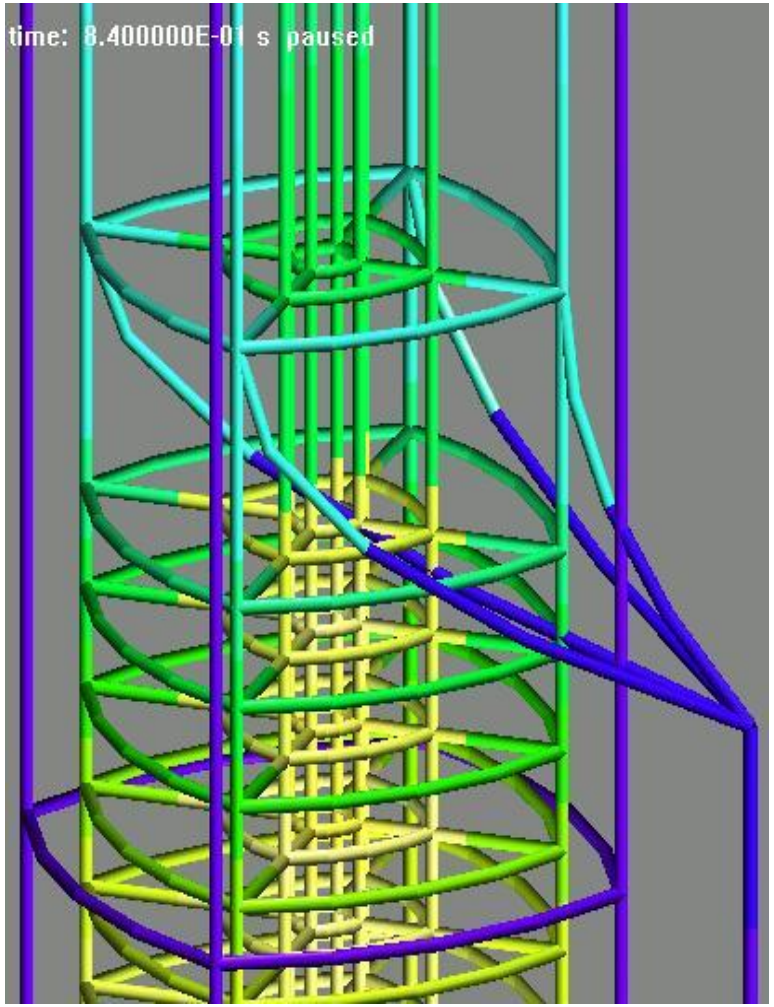

From 4.0.3 to 4.4.2

- CSV format on plot files
  - Increase plot file size beyond 2GB
- Machine-dependent strip of restarted files
- Correction of memory leaks
- Initialization ad pointer nullification improvements
- Flexible Wall component
- Neutronics
  - Face-albedos
  - Neutron velocity
  - Parallelized 3D kinetics
  - Automatic neutronics time-step

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From 4.0.3 to 4.4.2

- Multi-deck restart
- Consistent fluid updates, linpolate
- Foolproof order of operations
- Special connection to STAR-CCM+
- Automated verification to 32-decimal places!
- Fluid property files flucommon and other changes
- Allocation & initialization & module changes
- Windows and various Linux updates
- Jacobian refactoring changes
- Groeneveld 2006 improvement

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Where we are now: Updates from 4.4.2 to 4.5.2

- **Remote RELAP5-3D** (important opportunity) for 4.4.2 onward
- Adaptation to "**Forever**" GNU **Fortran** (huge change) in 4.5.0
- Addition of the **Dissolved Gas Model** (huge change) in 4.5.1
- **Molecular diffusion** model increased to 5 NC working fluids
- **Uniform physical units** throughout code (Calculations change!)
- Change from static to dynamic libraries for New O/S & containers
- Nitrogen and Hydrogen accuracy and range upgrades
  - For advanced reactors

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Information about Remote RELAP5-3D

- Previously, users had to have copy of RELAP5-3D on own computer
- **USER Container** access to Remote RELAP5: **module load relap53D**
  - Uncopiable RELAP5-3D executable, relap5.x
  - Runs as if it were a Linux command
  - The fluid property files are also provided.
- Advantages of Remote RELAP5-3D in INL Enclave
  - Access to three massively parallel supercomputers, each replaced after its third year of operation to maintain state-of-the-art computing.
  - Access to over 3 petabytes of disk storage, 616 terabytes of memory, and 155,000 compute cores.
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Information about Remote RELAP5-3D

- Advantages of INL Enclave (Continued)
  - Access to over 3 petabytes of disk storage, 616 terabytes of memory, and 155,000 compute cores.
  - Fast: INL provides TOP500 list machines.
    - Sawtooth's LINPACK rating is 5.6 PFLOPS.
  - Access HPC library of advanced and commercial software for rendering and analyzing data, and for coupling with RELAP5-3D.
  - The most recent publicly released version of RELAP5-3D is automatically available.
  - No more license files.
  - Security: The HPC is a protected environment that allows users to access only specific directories. Users cannot access other users' files.
  - Availability: when one supercomputer is down for upgrades or repair, the others remain available.

Information about Developer's Remote RELAP5-3D

- For researchers and dissertations
  - Same capabilities as Analysts Access
- Developer receives whatever RELAP5-3D coding is minimally required
  - E.G. Fluids coding to create a new fluid
- Developer modifies coding and may add new subprograms
- To test developments, running the build script creates a new executable
  - Includes username appended to relap5 executable.
    - This allows comparison to original relap5 calculations
  - It is also an uncopiable RELAP5-3D executable

Updates from 4.4.2 to 4.5.2

- Dissolved Gas Model (DGM), Presentation #3
  - Allows NC-gases to go in and out of solution based on partial pressures compared to the phasing pressures.
- Uniform Physical Units, Presentation #4
  - Make all constants and conversion factorsthe same level of accuracy throughout the code
- Molecular diffusion (MD) model improvements, Presentation #5
  - Increased from 2 to 5 NC working fluids
  - Mostly applies to accident scenarios
- Creation of air as a working fluid
  - Useful for modeling experiments and air-cooled constructs.

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Updates from 4.4.2 to 4.5.2

- Inclusion of Molten Salt Reactor kinetics model
  - Uranium salt is both fuel and coolant
  - Reaction continues and diminishes outside the core
- Updated CHF table to 2006 standard
  - Modernizes the Critical Heat Flux calculation
- Cladding improvements
  - Modelling for thin cladding coating
  - Cladding rupture model minor edits

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Updates from 4.4.2 to 4.5.2

- Operating Systems
  - Adaptation to Windows 10
  - Adaptation to Rocky Mountain Linux O/S
  - Adaptations for Containers
- GIT Version Control
- Uncertainty Quantification capability for reflood via Raven.
- Many User Trouble Report fixes

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RELAP5-3D – GNU (Forever) Fortran Upgrade

- “Forever Fortran”
  - Adapted RELAP5-3D to GNU Fortran
  - How and why it is “forever”
    - GNU translates Fortran into intermediate C-language before compiling
      - GNU does this with all its compilers
    - Compiles the C to generate the RELAP5-3D executable
    - Almost every operating system is now written in C-language
- Code compiles in both Intel and GNU Fortran
  - Modified over 1000 subprograms and took 1 full year
  - Many conflicts between the compilers were resolved

Planned Improvements going forward from 4.5.2

Consortium forming between INL, NNL, and ISL

- Merge RELAP5-3D with Bettis and ISL versions
- Plan to work together on many new capabilities

Non-consortium plans

- Addition of “new” fluid property tables
  - Helium-3, air, and new molten salts
- New MODERN Graphical User Interface
  - Currently under development by the INL HPC
- Resynch RELAP5-3D Manuals with Code

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Moving BEYOND from 4.5.2

- Use of CIVET (Continuous integration testing and acceptance)
  - INL's tool that tests code regularly at different pre-specified levels
  - Reports failures of various kinds to prevent including new code with errors
- File-transfer-based coupling with MOOSE
  - Initially, RELAP5-3D will couple memory-to-memory with BISON
  - This runs faster then file-to-file transfer
- BEPU (Best Estimate Plus Uncertainty) updates
  - Updates were developed by Carlo Parisi

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Summary

- History of RELAP5 up to RELAP5-3D
- History from there to RELAP5-3D Version 4.4.2
- Upgrades that went into version 4.5.2
- Some plans going forward.

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Future Ideas to Improve RELAP5-3D

- New and/or improved correlations
  - From relatively recent experimental work
  - From ongoing International Benchmarks when available
- Capabilities for new kinds of reactors
  - Space
  - Undersea
- Simulators – RELAP5-3D as the TH Engine
  - For New Reactor Types
  - Possible addition of artificial Intelligence

Future Ideas to Improve RELAP5-3D

- Verify that the manuals match the code, update manuals where needed.
- Increased validation
  - Gas cooled reactors / Liquid metal reactors / Molten salt reactors
  - Small modular reactors / Micro-reactors / Space reactors
  - Research and test reactors
  - Generic thermal-hydraulics phenomena analyses
- Add validation sections to Volume 3
  - High-temperature gases
  - Certain formulations of liquid metals and molten salts

Future Coding Ideas to Improve RELAP5-3D

- Eliminate “dead” pre-compiler directives and associated dead code
- Increase application of the “only” clause on “use” statements
- Eliminate all equivalence statements
- Reduce bit-packing
- Stick to the RELAP5-3D Style Guide
  - This is a living document that will be updated as needed, at least annually

Future Coding Speedup Ideas to Improve RELAP5-3D

- Additional Features of Fortran 2003 & 2008
  - Allow “forall” loops for improving parallelism
  - Allow “where” loops for potential speedup by reduction of passes
  - Declare subprograms pure and elemental if applicable
  - Allow Submodules to save compile complexity and time
    - Defines the body of a module procedure in a “child” submodule whose interface is in the parent module.

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