MELCOR Code Development Status, Code Assessment, and QA

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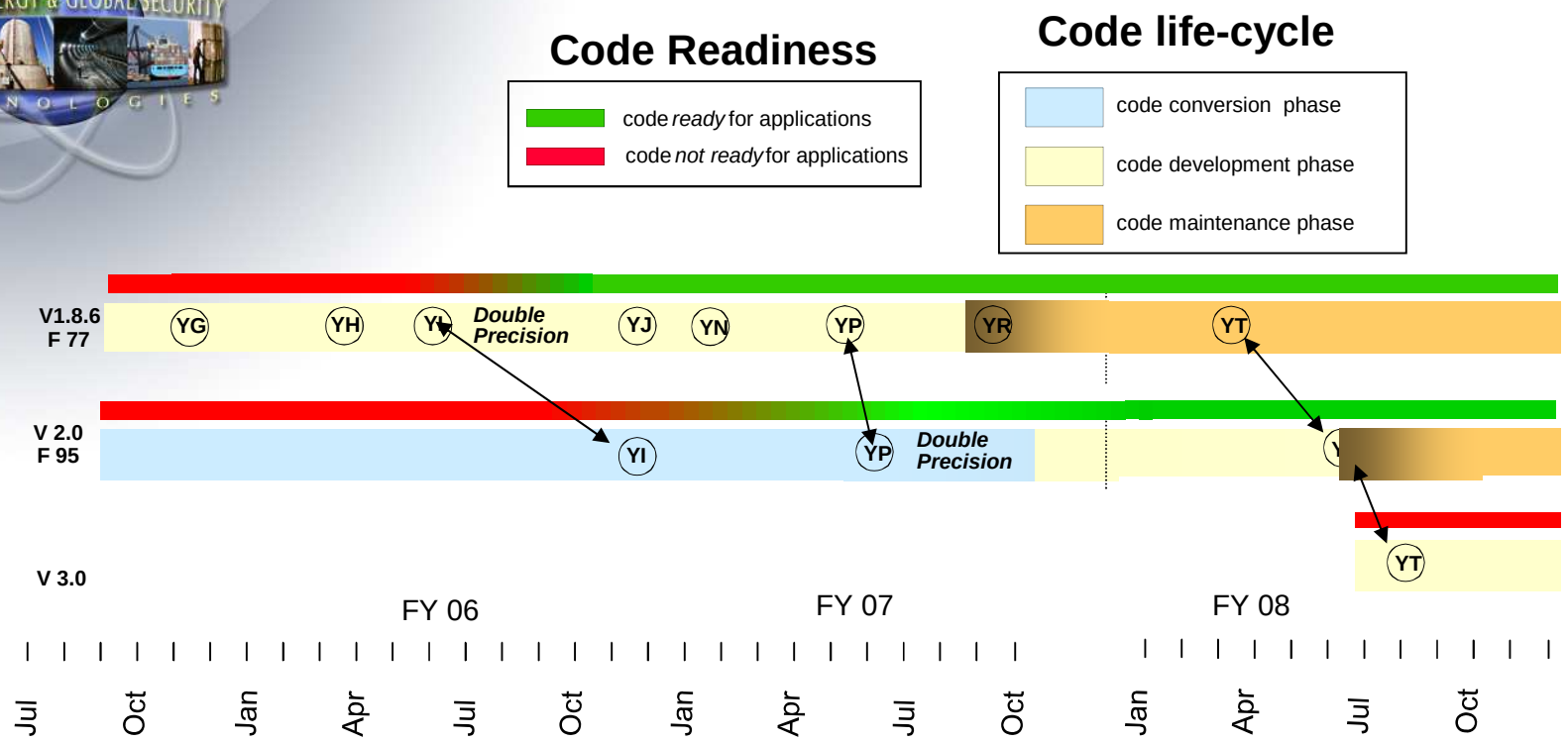
Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Sandia National Laboratories

MELCOR Code Development

- **MELCOR is developed by:**
  - **US Nuclear Regulatory Commission**
  - **Office of Nuclear Regulatory Research**
  - **Division of Safety Analysis (DSA)**
- **MELCOR development is also strongly influenced by the participation of many International Partners through the US NRC Cooperative Severe Accident Research Program (CSARP and MCAP)**
  - **Development Contributions – New models**
  - **Development Recommendations**
  - **Validation**

Current MELCOR Development

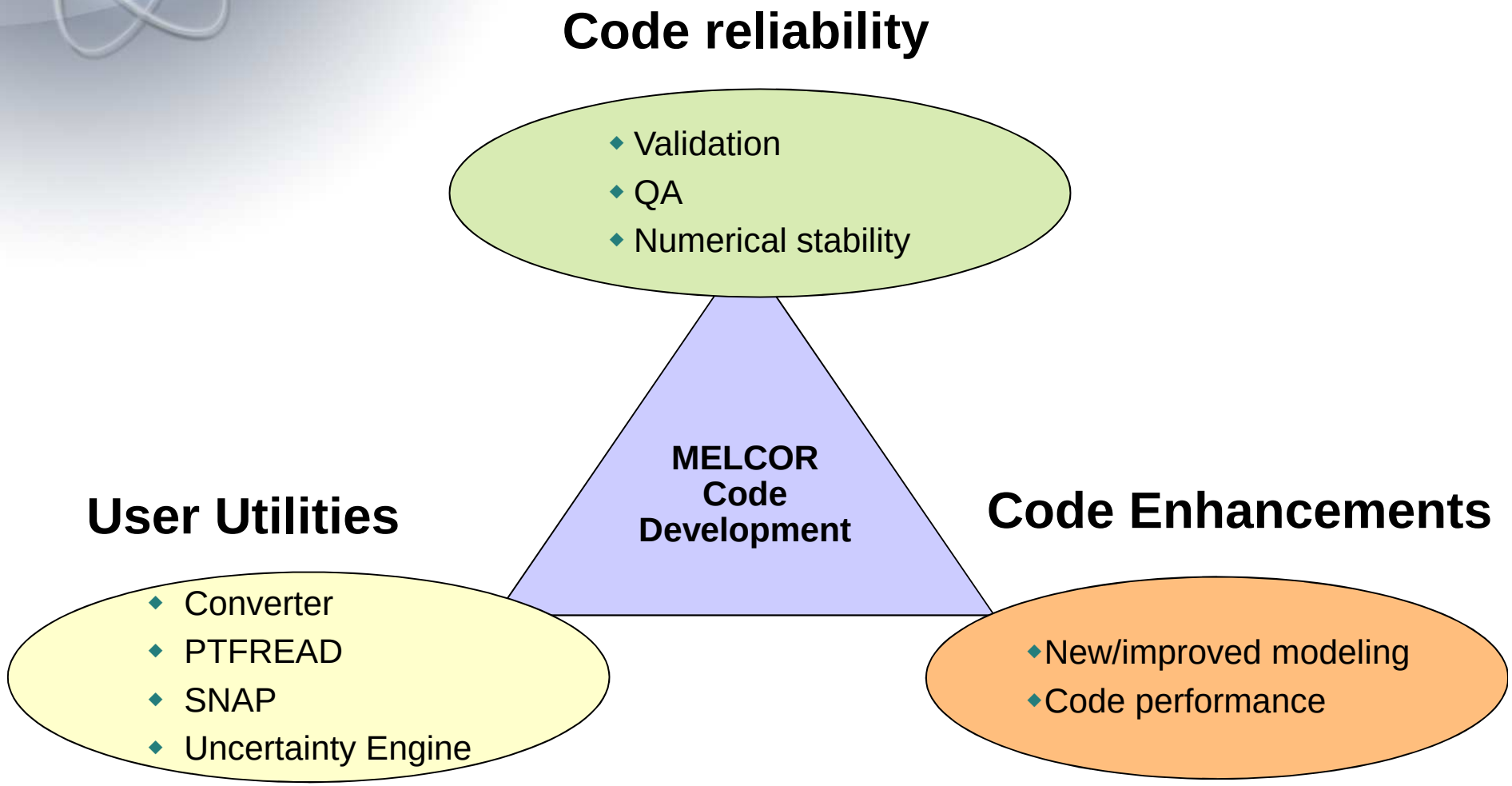


- **MELCOR 1.8.6**
  - Molten pool models
  - Core Package upgrade
  - Released Fall 2005
  - Code Maintenance
  - Current Workhorse

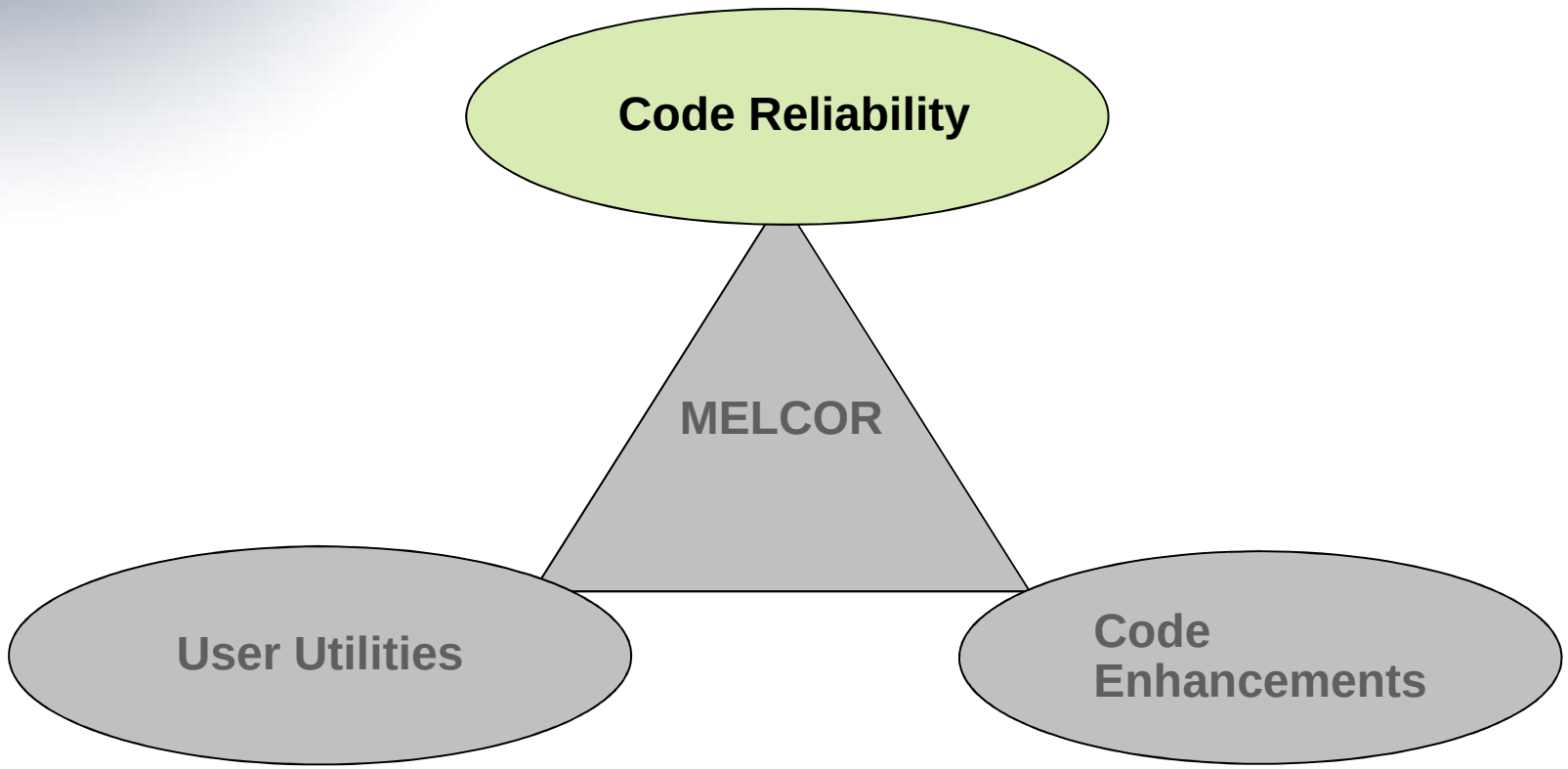
- **MELCOR 2.1**
  - FORTRAN 95
  - New input
  - 2.0 beta version released Sept 2006
  - 2.1 Release Sept 2008

- **MELCOR 3**
  - Current developmental version

MELCOR 3.0 Code Development Thrust Areas



Code Development: Code Reliability



Intel Visual FORTRAN Compiler

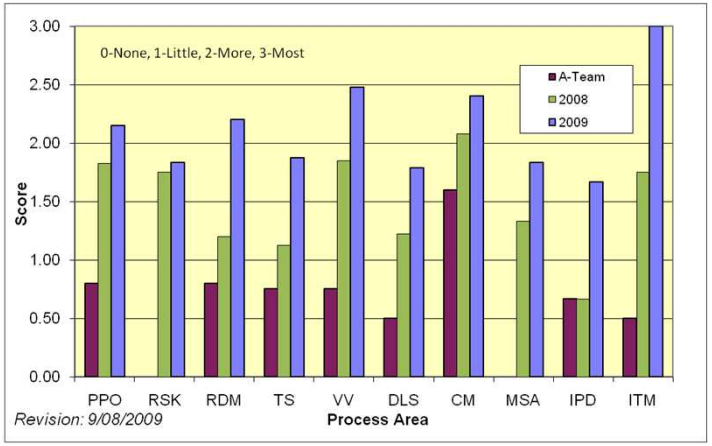
- **Intel Visual FORTRAN has replaced Compaq Visual FORTRAN as our standard development platform**
  - **Did not want to make any changes until after 2.1 was released**
  - **Technical support for CVF no longer available**
  - **Problems with CVF rebuilding entire project**
  - **Problems with error checking**
- **Advantages to Intel Compiler**
  - **Able to build true 64-bit code for 64-bit operating systems**
    - **Performance improvements**
  - **Better support for F95 code**
    - **Improved error checking**
  - **More consistent support for Linux**
  - **Improvements to the programmer interface (Visual Studio.NET)**
    - **Automatic keyword completion**
    - **Integration with subversion**
  - **Capability to automatically convert CVF projects**
- **Have a lot of experience now with compiler options and are able to get identical results on Windows, Mac, and Unix systems with both debug and optimized builds**
  - **MELCOR 2.1 now builds with check:all without any errors!!**

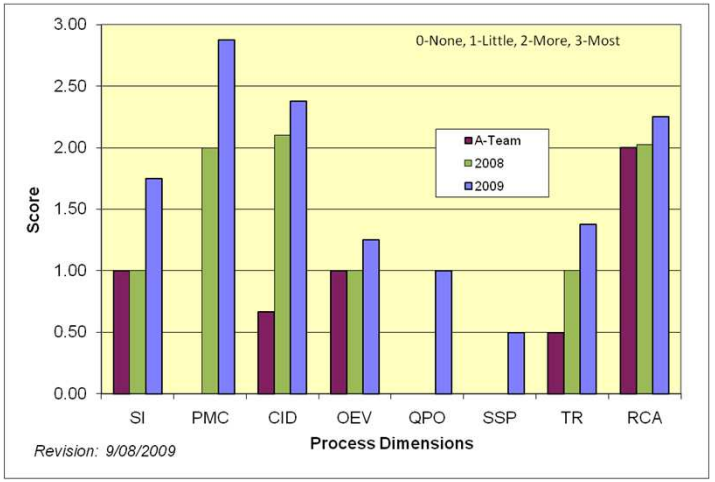
Software Quality Assurance

- **Sandia Corporate Process Requirement 001.3.6 (CPR 001.3.6)**
- **The software management framework adapted from two internationally recognized standards**
  - **the Capability Maturity Model Integration (CMMI) ®**
  - **and ISO 9001**
  - **These standards provide elements of traceability, repeatability, visibility, accountability, roles and responsibilities, and objective evaluation**
- **Areas showing improvement**
  - **Code Review (Code Collaborator)**
  - **Requirements Management**
  - **Configuration Management (Automated Build & Test)**
  - **Further Development of Internal Wiki**
  - **Development of SQA training materials**
- **Areas needing improvement**
  - **Improve debugging response time**
  - **Improve user access to documentation updates**
  - **Explore possibility of external Users' Wiki**
- **Sandia's commitment to SQA**

Software Quality Assurance Annual Re-evaluation

- **Process areas**
  - **Project planning and oversight, PPO**
  - **Risk Management, RSK**
  - **Requirements Development and Management, RDM**
  - **Technical Solution, TS**
  - **Verification and Validation, VV**
  - **Development and Lifecycle Support, DLS**
  - **Configuration Management, CM**
  - **Measurement and Analysis, MSA**
  - **Integrated Product, IPD**
  - **Integrated Teaming, ITM**
- **Process Dimensions**
  - **Stakeholder Involvement , SI**
  - **Ongoing Process Monitoring and Control, PMC**
  - **Collected Improvement Data, CD**
  - **Objective Evaluations, OEV**
  - **Quantitative Objectives Defined for Processes, QPO**
  - **Stable Subprocess Performance, SSP**
  - **Training , TR**
  - **Problem Reporting & Corrective Action, RCA**





MELCOR Code Testing

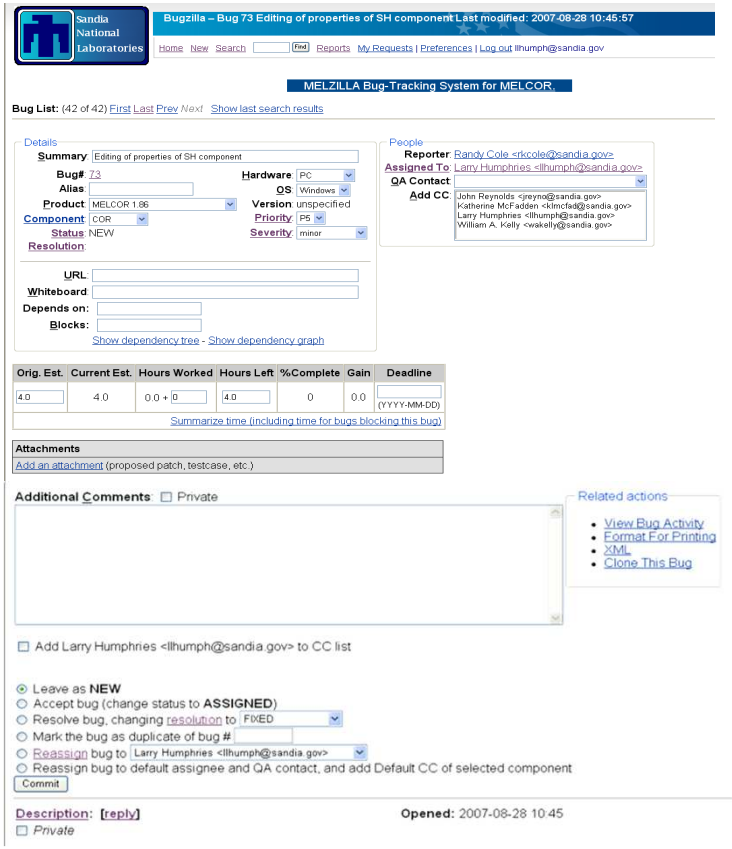
- **Build Testing**
  - **Automated to perform Nightly Builds**
    - **MELCOR 1.8.6 Windows Compaq Visual FORTRAN (CVF)**
    - **MELCOR 2.X Windows CVF**
    - **MELCOR 2.X Windows Intel Visual FORTRAN (IVF)**
    - **MELCOR 1.8.6 Linux IVF**
    - **MELCOR 2.X Linux IVF**
  - **Using CMAKE to generate Makefiles for use on Unix variants to extend building on other platforms**
- **Code Testing**
  - **Performed Daily (at least frequently)**
    - **Dedicated machine for performing auto testing to**
  - **Standard test cases chosen for physics coverage ~14 test cases**
    - **New cases will be added as validation calculations are run**
    - **Debug & optimized versions tested**
    - **Unix versions not tested as frequently (will test more frequently in future)**
  - **Comparison of results**
    - **Windows system**
      - **Latest 1.8.6 (CVF) and YT, 2.X(CVF)**
      - **Latest 2.X (CVF) and Latest 1.8.6 (CVF)**
      - **Latest 2.X (IVF) and latest 2.X (CVF)**
    - **Linux System (not yet realized)**
      - **Latest 2.X (IVF Windows) Latest 2.x (IVF Linux)**
- **Optimization Testing (not yet realized)**
  - **Run automated optimization studies to determine effects of optimization**
    - **Many routines can be optimized with no impact on answers**
    - **Order of arithmetic will mean some routines should not be optimized**

Case	BUR	CAV	CF	COR	CVH	DCH	FCL	FDI	FL	HS	NCO	PAR	RN	SPR
M-8-1 NoMix			X		X				X	X	X			
M-8-1 SYM			X		X				X	X	X			
Lace7			X		X	X			X	X	X		X	
Lace8			X		X	X			X	X	X		X	
Vanam-M3			X		X				X	X	X		X	
Molten Salt			X	X	X				X	X	X			
PHEBUS-B9			X	X	X				X	X	X			
FPT1			X	X	X	X			X	X	X		X	
LOFT			X	X	X	X			X	X	X			
Test Inow	X	X	X	X	X	X	X	X	X	X	X	X	X	X
SURRY (LBLOCA)	X	X	X	X	X	X	X	X	X	X	X		X	X
Zion (SBO)		X	X	X	X	X	X	X	X	X	X	X	X	X
PeachBottom (SBO)	X	X	X	X	X	X			X	X	X		X	X
Grand Gulf (SBO)	X	X	X	X	X	X		X	X	X	X		X	

Table 1-1: Physics Package Coverage

Bug Statistics

MELCOR 1.8.6 (since 7/07)	
Number of Bugs Reported	**105**
Number of Bugs Resolved:	**72**
Number of Bugs Unresolved:	**33**
Number of Bugs Reported (this year):	**36**
Number of Bugs Resolved (this year):	**27**
Number of Bugs Unresolved (this year):	**9**
Number of Unresolved User Bugs :	**15**
MELCOR 2.1 (since 9/07)	
Number of Bugs Reported	138
Number of Bugs Resolved:	98
Number of Bugs Unresolved:	40
Number of Bugs Reported (this year):	84
Number of Bugs Resolved (this year):	77
Number of Bugs Unresolved (this year):	7
Number of Unresolved User Bugs :	15



Recent Code Corrections

- **Bug 708 – Oxidation of PD is not calculated.**
  - **When oxidation of unblocked PD was calculated, the conglomerate surface area was used to calculate oxidation. Since no conglomerate had yet been formed, no oxidation was calculated.**
  - **Corrected in revision 2264 (MELCOR 2.x) and 2426 (MELCOR 186)**
- **Numerous changes made to molten pool behavior were made to the 2.x code base.**
  - **Corrections to radiation term from molten pool surface to core support or upper HSs**
  - **Corrections made to the debris settling/displacement model**
  - **Corrections made to heat transfer from crust to lower head / water**
  - **Corrections made for AP1000 calculations modeling ex-vessel cooling**

Documentation

- **MELCOR 186 Manuals were never officially published as NUREGS**
  - **Because of the 'imminent' release of 2.0, it was decided to wait until 2.0 was officially released**
  - **Code issues with 2.0 delayed release of manuals further**
  - **Draft versions of the manuals have been distributed**
- **We are currently reviewing all manuals and will publish them this summer**
  - **This will include the User Guide, Reference Manual, and Assessment Guide.**

Assessments

- **Currently reviewing all Volume III assessments**
  - **See following slide for potential assessments**

- **Participating in Phebus FPT3 benchmark**
- **Participating in the recent OECD generic plant sequence.**

MELCOR 2.1 Volume III Assessment Report

Will be in Vol III report

- **Separate Effects Tests**
  - NUPEC M-8-1
    - FP release & transport
  - NUPEC M-8-2
    - FP release & transport
  - LACE LA-4
    - FP release & transport
  - VANAM-M3
    - FP release & transport
  - CORA13
    - Core heatup, degradation & FP release
  - LOFT LP-FP-2
    - Core heatup, degradation & FP release
  - PHEBUS B9
    - Core heatup, degradation & FP release
  - PHEBUS FPT-1
    - Core heatup, degradation & FP release
- **Plant Decks**
  - SURRY LBLOCA
  - ZION LBLOCA

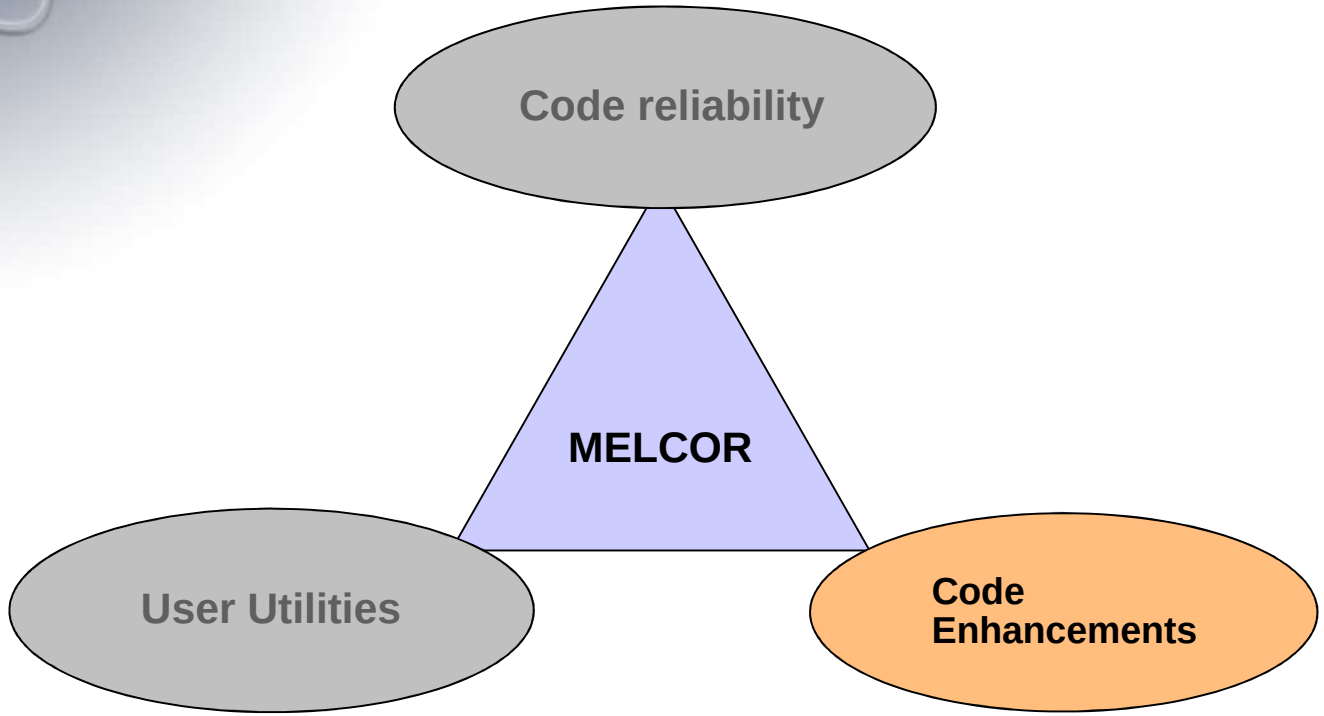
Legend

- 2.X deck runs to completion (rev 1743)
- 186 deck (containment only)
- Decks will not be available to users, only calculation description and results

Possibly in Vol III report

- **Separate Effects Tests**
  - AHMED
    - Hygroscopic model
  - BETHSY
    - RCS
  - CVTR
    - Containment Thermal Hydraulics
  - DEHBI
    - Containment Thermal Hydraulics
  - SURC
    - MCCI
  - FALCON 1
    - FP release & transport
  - FALCON 2
    - FP release & transport
  - FLECHT
    - Thermal Hydraulics (nat convection)
  - HDR V44 (ISP16)
    - Containment Thermal Hydraulics
  - HDR E11.2
    - Containment Thermal Hydraulics
  - LHF
    - Creep Failure of Vessel
  - MASCA deck
    - Molten pool modeling
  - NEPTUN
    - RCS
  - PBF
    - Core heatup, degradation & FP release
- **Plant Decks**
  - TMI-2 (build SNAP Model)
  - Grand Gulf SBO
  - Grand Gulf LBLOCA
  - Zion SBO (SNAP Model?)
  - FORSMARK-1 SBO (186 deck)
- Gedanken decks
- DOE LPF Benchmarks
- SFP validation deck

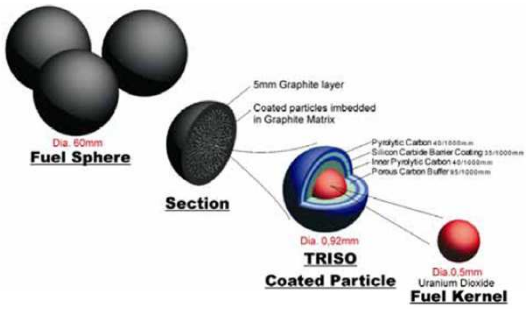
Code Development: Code Enhancements



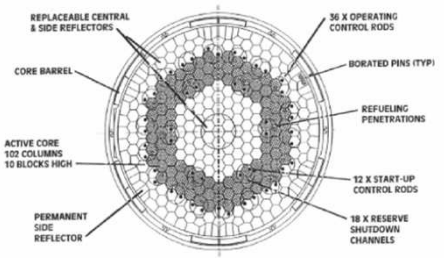
- **All new code development will be performed in MELCOR 2.1**
- **MELCOR 1.8.6 – Code Maintenance only**

Code Development
HTGR - COR Package Updates

- New reactor models (like present PWR, BWR)
- PBR (pebble bed)
  - New components
    - Pebble fuel
  - New heat transfer coefficients
  - Effective thermal conductivity
    - radiation/convection/conduction
  - Coolant friction loss



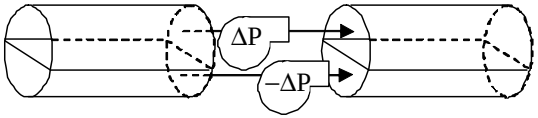
- PBR (prismatic)
  - New components
    - Reflectors
    - Hexagonal graphite blocks
  - cell-cell conductive/radiative heat transfer



- Graphite oxidation models
- On-going work
  - Fission product release and transport from HTGR fuel
  - Plant demonstration calculations

Counter-Current Stratified Flow Modeling

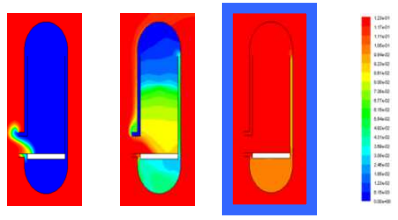
- **Counter-Current Stratified Flow Applications**
  - **Developed for HTGR air-ingress application**
  - **Modeling of natural circulation between the steam generator and the upper plenum of PWRs**
  - **Containment modeling**
- **Old concept used in MELCOR for many years**
  - **Split path in two to allow counter-current flow**
  - **Account for momentum exchange in flow equations**
    - **Implement as "pumps" with ΔP calculated from relative velocities**



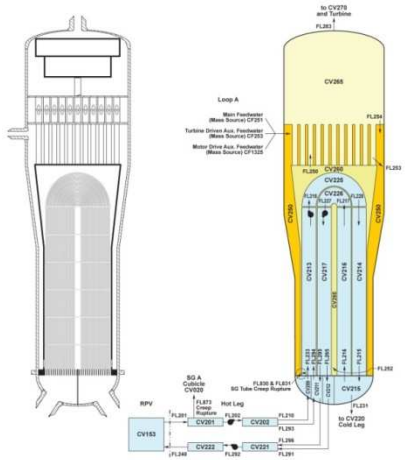
$$\Delta P = -\frac{2fL}{D_h}\bar{\rho}(v_1 - v_2)|v_1 - v_2| = -C\bar{\rho}(v_1 - v_2)|v_1 - v_2|$$

- **New approach where ΔP is "internalized"**
  - **We have coded an appropriate ΔP calculation**
    - **Specific input was added to couple two flow paths**
    - **Form of ΔP has been generalized to better match published correlations**
    - **Terms added directly to flow equations**
      - **Increased stability because of implicit numerics**

Snap Shots of Simulation (Air Mole Fraction) from "NRC/INL Meeting on Methods for VHTRs", E. Kim, C. Oh, R. Schultz, INL (2008)



1.0 sec **16.0 sec** **256.0 sec**

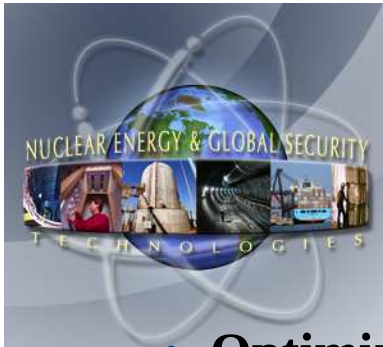


Ongoing or Recently Completed Code Model Development

- **Accumulator Model**
  - Replaces current control function approach to improve numerics and reduce errors and modeling effort of code user
- **Smart Restart Capability**
  - Allow user to change CF and TF parameters from the restart without adding new control or tabular functions.
- **Use a model to track activities.**
  - Existing MELCOR output doesn't allow tracking of radionuclides and user has to perform calculations to estimate activities.
- **Heat and Mass Transfer Correlations**
  - MELCOR code should be able to model the CONTAIN correlations by default
  - Modify the MELCOR film tracking model and default model parameters based on the CONTAIN parity
- **Engineered Safety Features (ESF) Enhancements**
  - heat exchanger models
  - fan cooler models
- **Improvement of SPARC Models**
  - Review the SPARC98 model for possible improvements over the earlier SPARC90 model
- **Improvement of VANESA Models**
  - improvements for ex-vessel fission product release. Specifically, the modeling of Ru and Mo)releases
- Others…

Code Optimization with Intel Compiler

- **O0 Early MELCOR 2.1 Release**
  - Disables all optimizations.
    This is the default if you specify -debug (with no keyword).
    Specifying this option causes certain -warn options to be ignored
- **O2 January 2010 MELCOR 2.1 Release**
  - Minimizes size; optimizes for speed, but disables some optimizations that increase code size for a small speed benefit; for the Itanium® compiler, -O1 turns off software pipelining to reduce code size. This option enables local optimizations within the source program unit, recognition of common subexpressions, and expansion of integer multiplication and division using shifts
- **O3 Possibly Future releases**
  - Maximize speed plus use higher-level optimizations; optimizations include loop transformation, software pipelining, and (IA-32 only) prefetching; this option may not improve performance for some programs. Specifying -O3 includes the optimizations performed by -O2. This option enables additional global optimizations that improve speed (at the cost of extra code size). These optimizations include:
    - o Loop unrolling, including instruction scheduling
    - o Code replication to eliminate branches
    - o Padding the size of certain power-of-two arrays to allow more efficient cache use.
- Qipo (Inter-procedural optimization)
  - IPO includes function-inlining to reduce function call overhead and improve data layout across functions. However, IPO can increase code size and compile time significantly



Optimization Studies

- **Optimization can lead to different results**
  - Uninitialized Variables (this is just one possible reason)
  - Can make it difficult to reproduce errors observed in the release version in the debugger
- Optimization Utility to test optimization of each file
  - Optimized and unoptimized versions of all object files are built
    - An entire module is tested for optimization first (optimized library is linked with debug library for all other modules)
    - A fast running test deck is run and the output is compared with the debug version for differences
  - If differences are observed, each file in the module is tested individually.
    - Testing of optimized files is performed in parallel
- Results indicate that only a few files cannot yet be optimized.
- Optimized executables are built with these files unoptimized
  - Give identical results to debug version !!!

Full Compiler/Linker Options Encoded in MELCOR

- **Compiler/Linker options printed in output and diagnostic file**
  - **Provides a QA check for reproducing results**

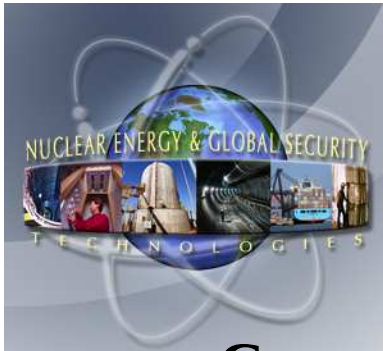
```
 Configuration information for MELGEN
 Subversion revision: 1951

 Compiler: IVF 11.1\065

 Compiler settings:
 /nologo /O3 /fpp /Qparallel  /DLICENSING_INACTIVE /DWINDOWS
/real_size:64 /Qaut
 o /align:rec8byte /Qtrapuv /module:'E:\CustomBuild\MELCOR_2x
\r1951\O2_CVF_IBRAE
 \modules' /traceback /fp:source /Qprec-div /Qprec-sqrt
/assume:protect-parens /
 assume:buffered_io /libs:static /threads /dbglibs /c
/assume:nocc_omp /QaxSSE4
 _2,SSE4_1,SSSE3,SSE3,SSE2,SSE
```

- **Is also accessible by running executable with command-line arguments**

  Melcor.exe -config



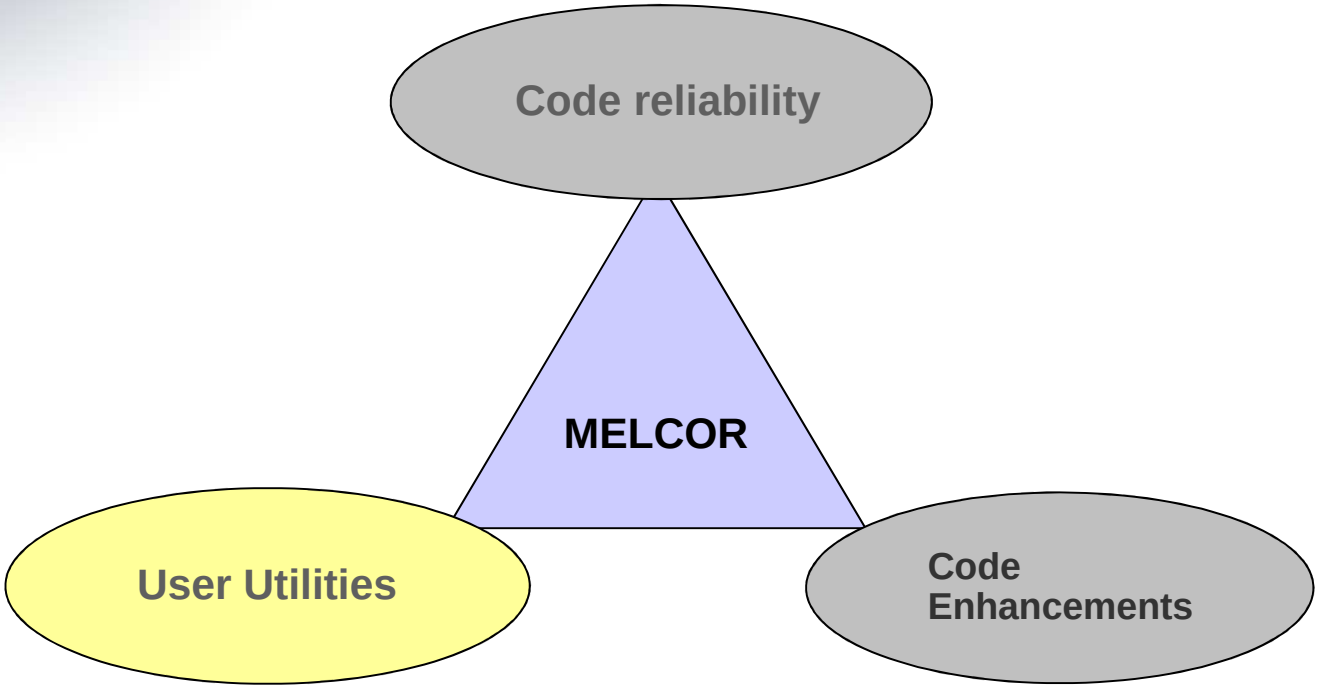
Auto Parallelization with Intel Compiler

- **Compiler automatically parallelizes loops if**
  - **Number of iterations is known on entry to loop**
  - **No jumps into or out of loops**
  - **Loop iterations must be independent.**
  - **The compiler can only effectively analyze loops with simple structure**
  - **Inlining with Qipo can allow additional parallelization**
- **Qpar-threshold(n)**
  - **Threshold determines the likelihood that parallelization that a performance gain is possible by doing so (100 is conservative, i.e., 100% probability of performance improvement**
  - **Reducing threshold can lead to additional parallelization**

OpenMP and Solvers

- **OpenMP**
  - **When the compiler is unable to automatically parallelize complex loops that the programmer knows could safely be executed in parallel, OpenMP is the preferred solution. The programmer typically understands the code better than the compiler and can express parallelism at a coarser granularity. At this time, IBRAE has completed OpenMP parallelization of the CVH package.**
  - **Directives appear as comments unless enabled by compiler arguments**
- **Investigation of various flow solvers**
  - **Iterative Solvers (Current sparse matrix solver)**
  - **Direct Solvers (Pardiso, UMFPACK)**

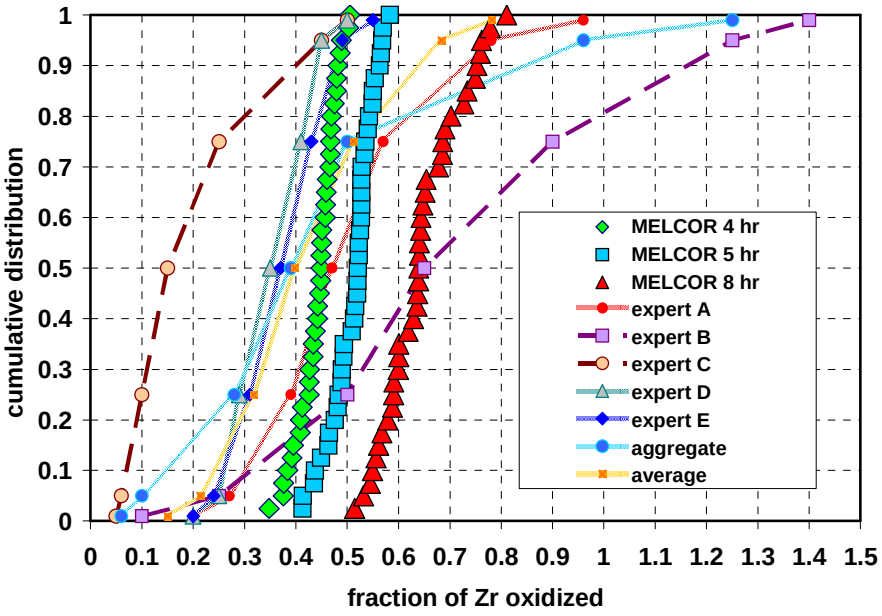
Code Development: User Utilities



Supporting Applications

- **SNAP**
  - **Symbolic Nuclear Analysis Package develped by API – MELCOR Plug-in**
- **PTFREAD**
  - **EXCEL add-in for generating plots, analyzing data, creating AVI's, generation of regression reports**
- **MELCOR 2.1 GUI & Converter**
  - **Utility for generating MELCOR 2.1 input decks and converting existing MELCOR 1.8.6 decks to new format**
- **Uncertainty Software**
  - **Suite of tools for running MELCOR in batch, Monte Carlo sampling of variables and analyzing statistics**

- ***Best Estimate with Uncertainty Quantification***
- ***Powerful tool for risk-informing regulations***

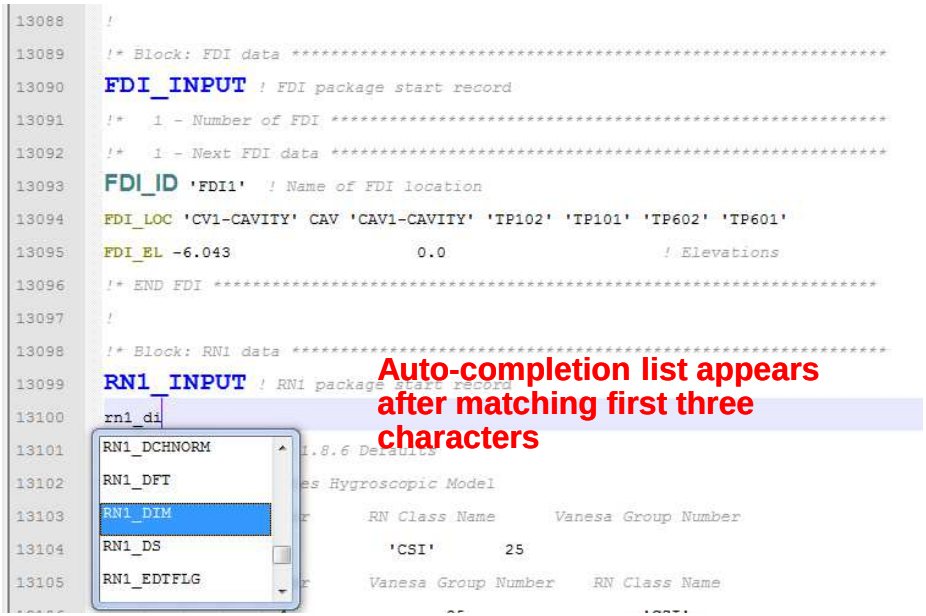


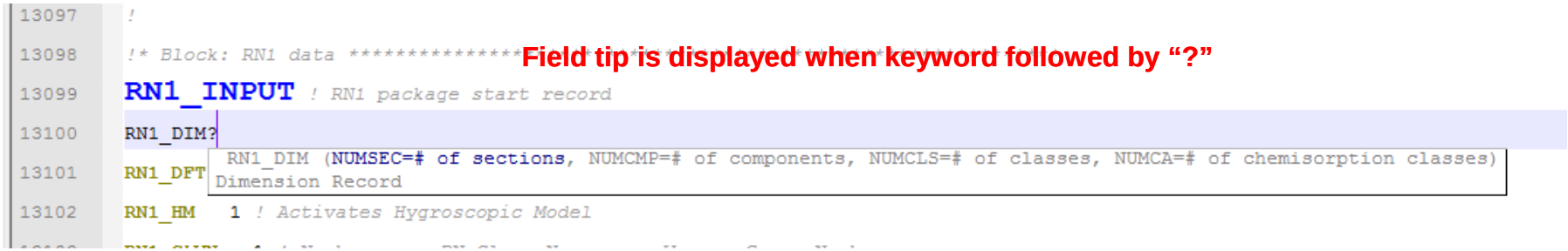
MELCOR 1.8.6 to 2.X Input Converter

- **Previous standalone converter will be phased out**
  - **Difficult to maintain and debug**
- **SNAP converter**
  - **Easier to maintain**
  - **Available to all MELCOR users**
  - **Extending converter so that it will be possible to convert from 2.x to 186 as well as from 186 to 2.x**
    - **Useful for users developing 2.x decks and comparing to 186**
    - **Recent bugs reported by users would be easier to identify by performing a "round-trip conversion" and testing because testing of the conversion is essentially performed with the same code version.**

Notepad++ MELCOR 2.1 Language

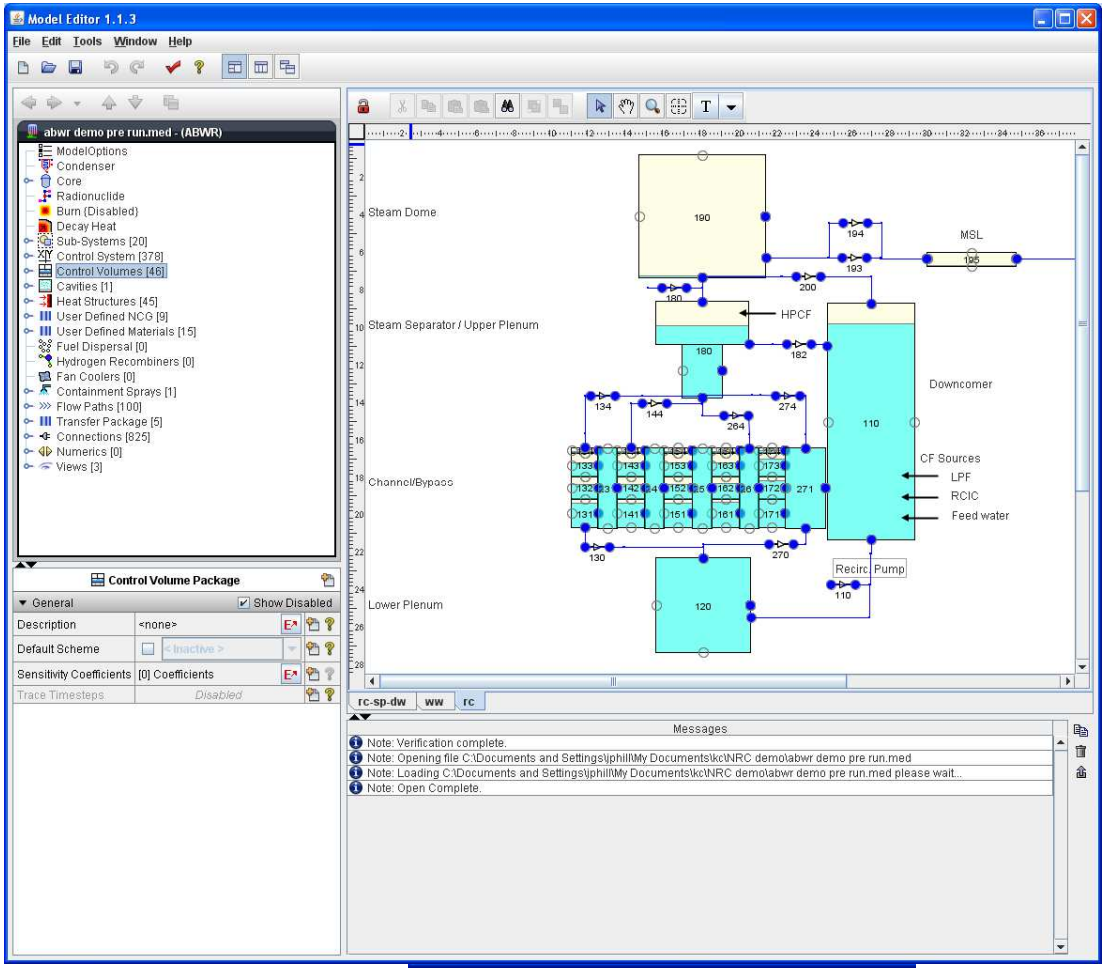
- **Recognition of MELCOR record identifiers**
- **Style applied to various levels of MELCOR records (comments are gray italics)**
- **Auto-completion of record identifiers**
- **Field tips are provided for record fields**
- **Can be updated by user**
- **Can be downloaded from download manager with a readme file for installation**



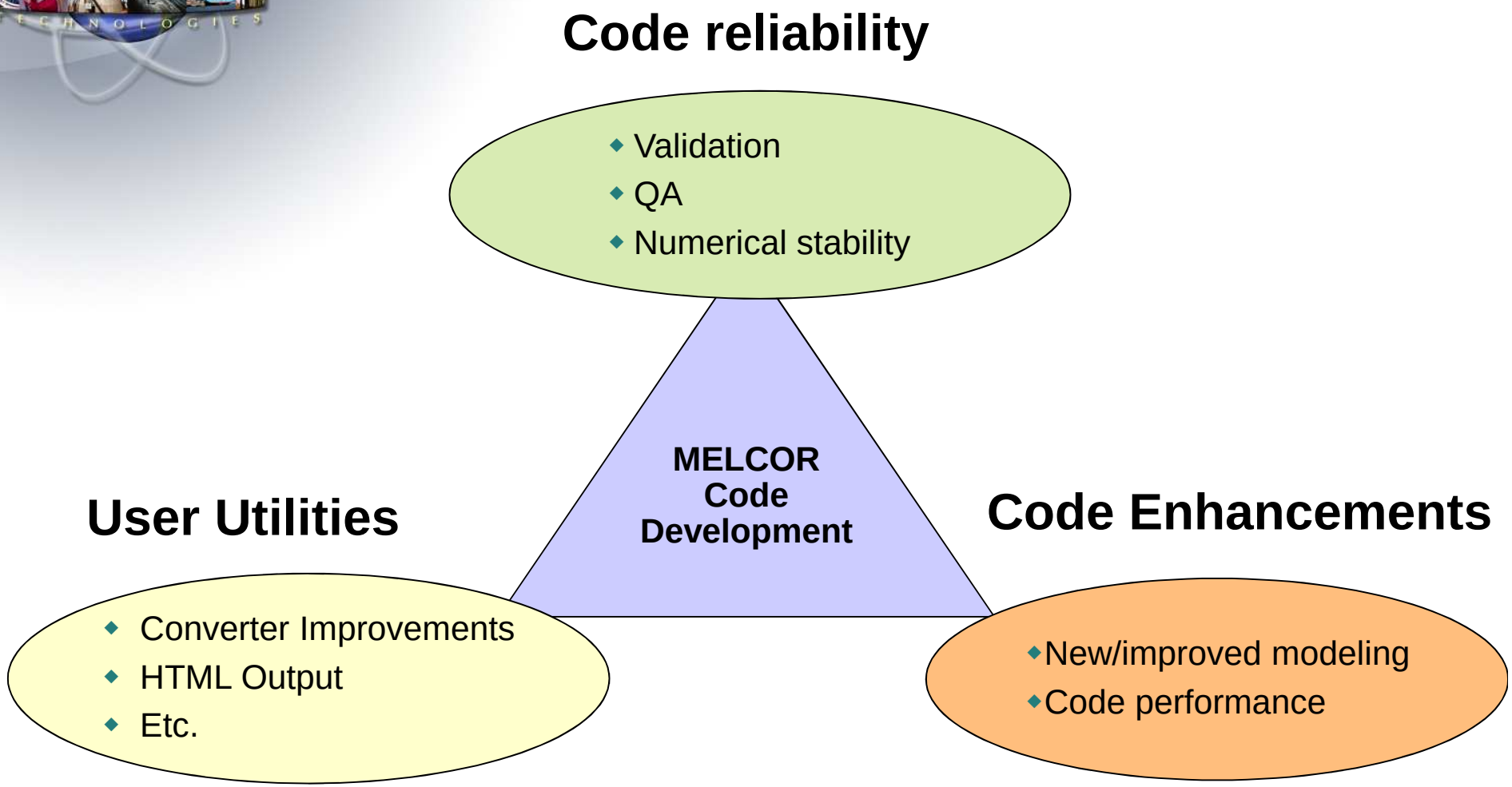


SNAP Development

- **MELCOR 2.1 Plugin**
  - **Version 1.0.0 - Released 7/17/09**
  - **Will convert a 1.8.6 input deck to 2.x**
  - **Sandia is working with SNAP developers to recommend enhancements for MELCOR plug-in**
- **A future workshop will focus on the use of SNAP**
- **Model Editor -Components**
  - **Tree Structure organization**
  - **Arranged according to MELCOR package**
  - **ASCII view of object available**
  - **DIFF capability for components**
- **Object Properties Window**
  - **User Aids**
    - **User Guide Information**
    - **Field units**
  - **Tabular input**
    - **Can paste data from spreadsheet**
- **Views**
  - **Trend plots**
  - **Custom animations**
  - **Others**



Summary


Code reliability
Validation
QA
Numerical stability
MELCOR Code Development
User Utilities
Converter Improvements
HTML Output
Etc.
Code Enhancements
New/improved modeling
Code performance