# Coupled Codes for Multi-Physics Nuclear Reactor Simulation

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# Outline

- Background on Coupled Codes
  - Current Generation Methods (NRC):

    e.g. RELAP5-TRACE/PARCS + TRITON
  - Next Generation Methods (DOE):

    e.g. STAR-CD/DECART

- “Next” Next Generation Methods

# Research Group

Yunlin Xu, Post-Doc

Mikhail Kalugin, Post-Doc

Justin Thomas, PhD Student

Shaun Clarke, PhD Student

Volkan Seker, PhD Student

Emily Decaret, MS Student

Andrew Ward, MS Student

Jere Jenkins, MS Student

Brendan Kochunas, Undergrad

# Research Group Focus

- **U.S. NRC**
  - Reactor Physics Methods Development
    (LWR MOX, ESBWR, ACR-700, PBMR, PHWR)
  - Coupled Neutronics/Thermal-Hydraulic Code Development for Reactor Transient Simulation

- **U.S. DOE**
  - Coupled CFD/MOC (INERI/EPRI w/ ANL)
  - Advanced Fuel Cycle Initiative (UNERI)
  - Resonance Self-Shielding Methods (NEER w/ ORNL)

- **Other**
  - Homeland Security (DHS w/ ORNL)
  - Power Grid (NSF w/ CRI)

Purdue Advanced Reactor Core Simulator - Microsoft Internet Explorer provided by Purdue University

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Address https://engineering.purdue.edu/PARCS

Go

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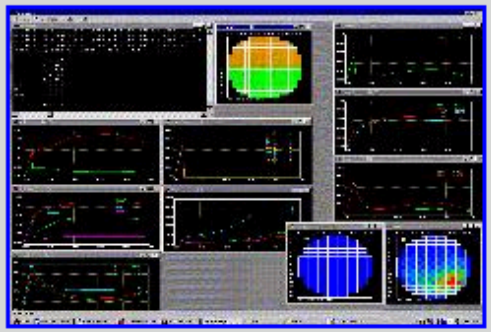
Purdue Advanced Reactor Core Simulator



## PARCS: Computer Code

- Manual
  - Theory
  - Users
  - Programmers
  - Software Quality Assurance
- Test Suite
- New Functionality
  - New Cross Section Model
  - Depletion Code System
  - Hexagonal Solution Model
- Support



## PARCS: Research Group

- Downar, Thomas J.
- Gan, Jun
- Kozlowski, Tomasz
- Lee, Deokjung
- Lee, Hyun Chul
- Miller, R. Matt
- Thomas, Justin
- Xu, Yunlin
- Zhaopeng, Zhong

- Alumni

Done Internet

# PARCS

## A Multidimensional Multigroup Reactor Kinetics Code Based on the Nonlinear Nodal Method

**Prepared for Release of PARCS / NRC-V2.7**

**Thomas J. Downar**

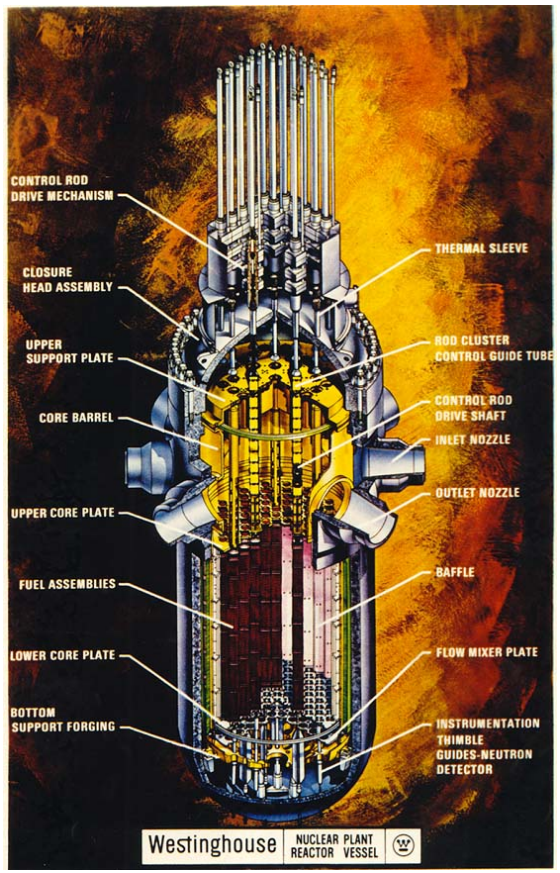
# Coupled Neutron / Nuclide and Temperature / Fluid Field Equations

Neutron Transport Equation (Boltzmann)

$$\frac{1}{v}\frac{\partial\phi}{\partial t}+\Omega\cdot\nabla\phi(r,E,\Omega,t)+\Sigma_t(r,E)\phi(r,E,\Omega,t)=\frac{1}{4\pi}S_f(r,E,t)$$
$$+\int_{\Omega}\int_{E'}\Sigma_s(r,E'\rightarrow E,\Omega'\rightarrow\Omega)\phi(r,E',\Omega,t)dE'd\Omega'$$

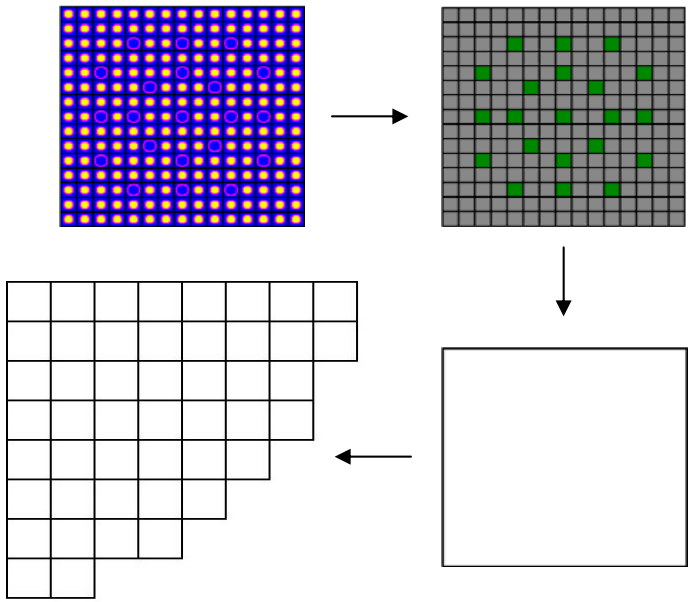
Nuclide Depletion Equation (Bateman)

$$\frac{dN_A(t)}{dt}=-(\sigma_A^a\phi+\lambda_A)N_A(t)+\sigma_C^\gamma\phi N_c(t)+\lambda_B N_B(t)$$

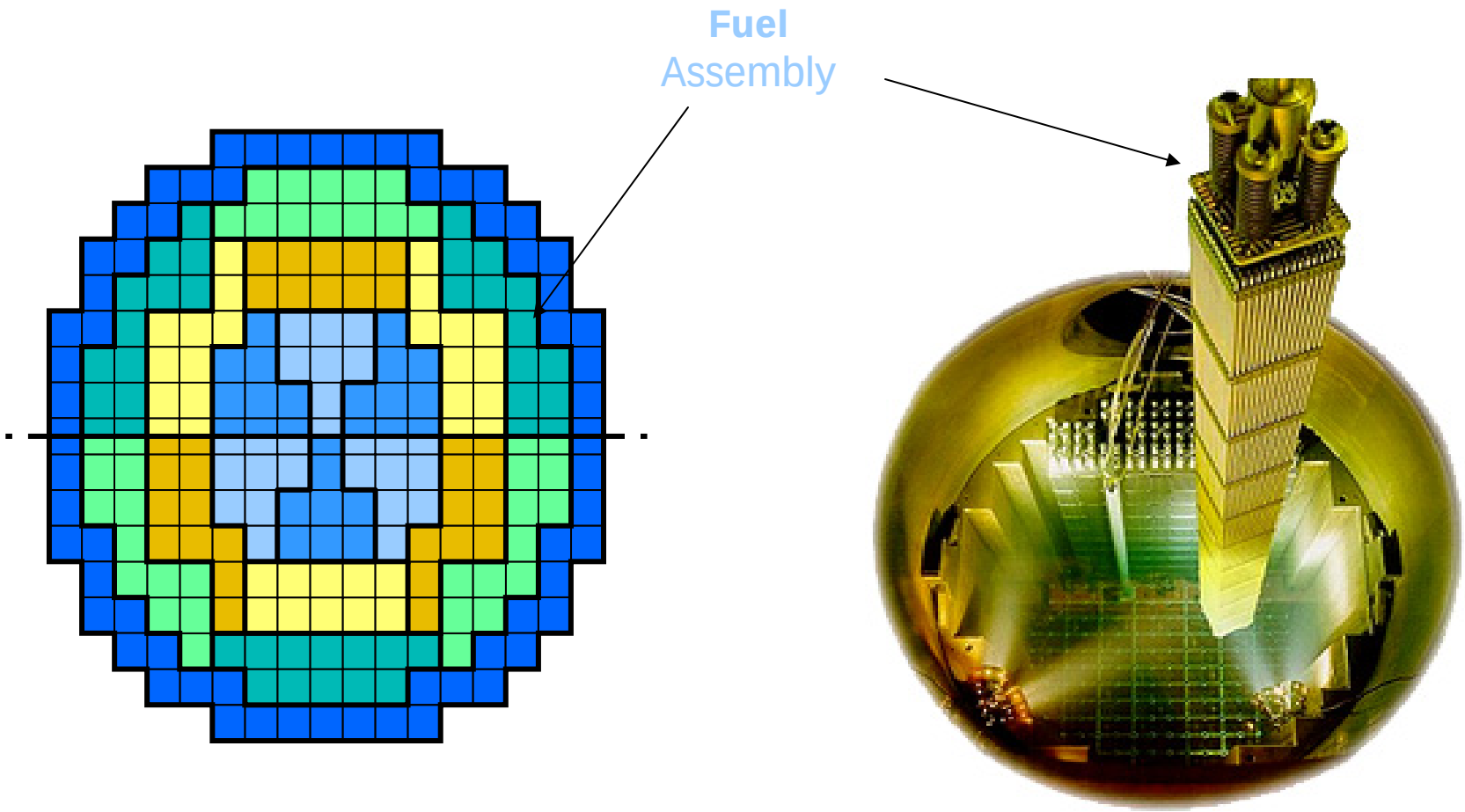


# Solving the Core Neutronics Problem

- "Conventional" Approach (TRITON/PARCS)
  - TRITON: Lattice Calculation Involving Homogenization and Group Condensation to Generate Few Group Xsecs
  - PARCS: Diffusion (P1) or SP3 Approximation for Core Calculation



# Core Neutronics Modeling



# Nodal Methods for Solving Reactor Neutronics

- 3D Neutron Diffusion Equation

$$-\left(\frac{\partial}{\partial x}D_k\frac{\partial}{\partial x}+\frac{\partial}{\partial y}D_k\frac{\partial}{\partial y}+\frac{\partial}{\partial z}D_k\frac{\partial}{\partial z}\right)\bar{\phi}_k+\Sigma_k\bar{\phi}_k=\frac{1}{k_{eff}}\nu\Sigma_{f,k}\bar{\phi}_k$$

- Transverse Integrated Equations

$$-\frac{\partial}{\partial z}D_{(i,j)}\frac{\partial}{\partial z}\phi_{(i,j)}+\Sigma_{(i,j)}\phi_{(i,j)}$$

$$=\frac{1}{k_{eff}}\nu\Sigma_{f,(i,j)}\phi_{(i,j)}-\frac{1}{h_{x,i}}\left(J_{x,(i+1,j)}-J_{x,(i,j)}\right)-\frac{1}{h_{y,j}}\left(J_{y,(i,j+1)}-J_{y,(i,j)}\right)$$

Where,

$$\phi_{(i,j)}=\frac{1}{h_{x,i}h_{y,j}}\int_{x_i}^{x_{i+1}}\int_{y_j}^{y_{j+1}}\phi(x,y,z)dydx$$

$$J_{x,(i,j)}=-\frac{1}{h_{y,j}}\int_{y_j}^{y_{j+1}}D\frac{\partial}{\partial x}\phi(x,y,z)\Big|_{x=x_i}dy$$

# Nodal Diffusion Methods

- The three, 1-D homogeneous equations are coupled through a “transverse leakage” source term.
- Nodal methods differ generally by the expansion used for the one-dimensional flux:
  - Analytic Nodal Method (ANM): analytic solution of the 1-D flux
  - Nodal Expansion Method (NEM): polynomial expansion ($4^{th}$ order) of the 1-D flux
- Various innovative “coarse mesh” acceleration methods (CMFD) are used to reduce the computational time

# PARCS Nodal Neutronics Methods: Solution Kernels

| Geometry Type | Kernel Name | Solution Method | Energy Treatment | Angle Treatment |
|---|---|---|---|---|
| **Cartesian 3D** | CMFD | FD | 2G | Diffusion |
| | ANM | nodal | 2G | Diffusion |
| | FMFD | FD | MG | SP3 |
| | NEMMG | nodal | MG | $SP_3$ |
| **Hexagonal 3D** | CMFD | FD | 2G | Diffusion |
| | TPEN | nodal | MG | Diffusion |
| **Cylindrical 3D** | CMFD | FD | 2G | Diffusion |
| | FMFD | FD | MG | Diffusion/ $SP_3$ |

CMFD = Coarse Mesh Finite Difference
ANM = Analytic Nodal Method
FMFD = Fine Mesh Finite Difference
NEMMG = Nodal Expansion Method

# Dehomogenization: Reconstructing Local Information from Nodal Solution

- PARCS Detector Model

$$LPRM_I(x,y,z) = \sum_g \sum_{j \in I} \phi_{g,j}^{global}(x,y)\phi_{g,j}^{local}(x,y)\sigma_{g,j}^{\det}(x,y)$$

Where j represents all nodes involves for Ith LPRM,

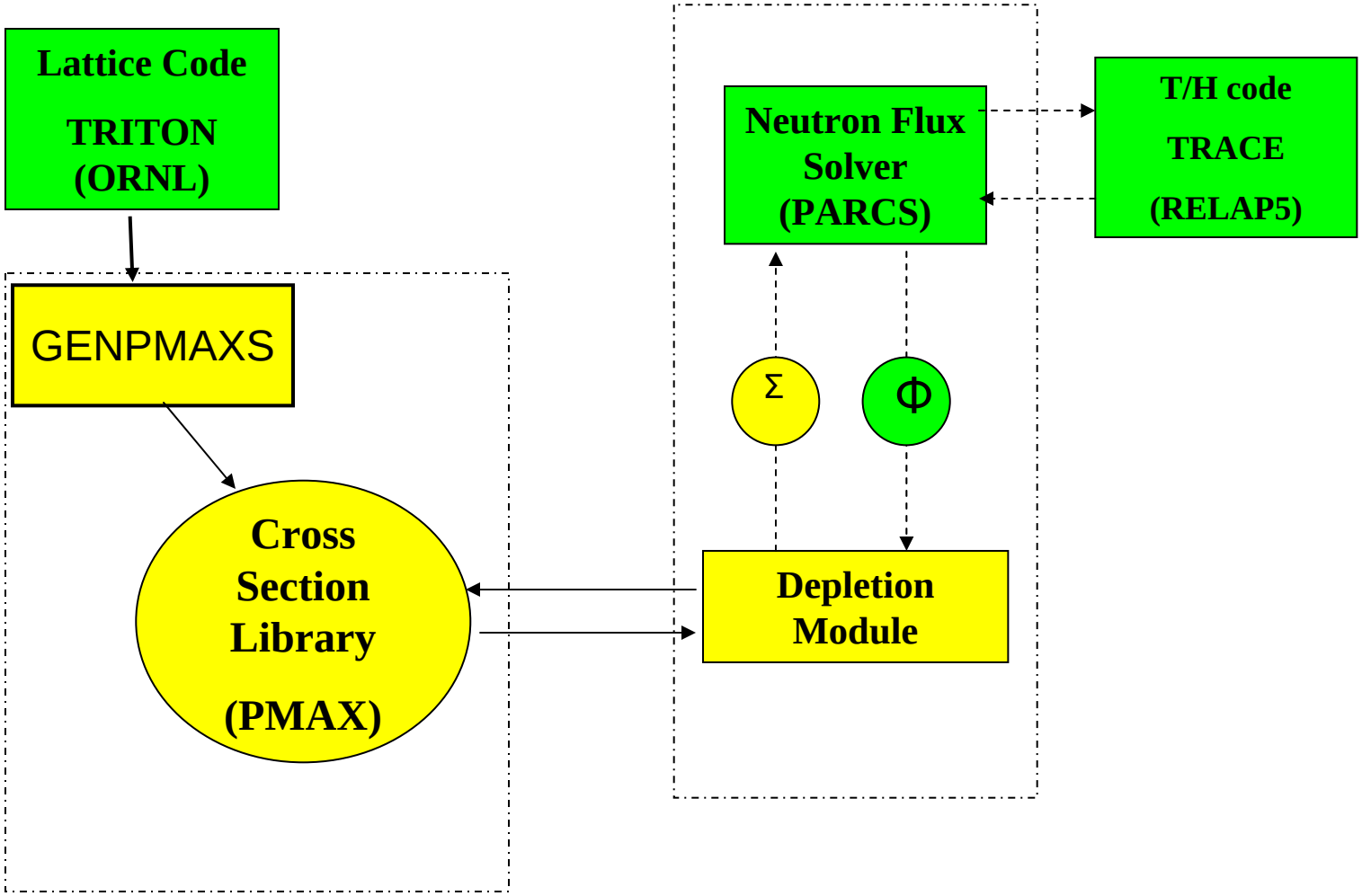
$\phi_{g,j}^{local}, \sigma_{g,j}^{\det}$ are provided from lattice calculation.

$\phi_{g,j}^{global}$ Will be obtained from flux reconstruction.

- PARCS utilizes Analytic Function Expansion Nodal Method (AFEN) for flux reconstruction, which involves analytic solution for 2-D diffusion solution in homogeneous media.

- Similar “reconstruction” is used to recover pin powers from nodal solution

# U.S. NRC Coupled Code System



# Coupling of Neutronics and Thermal-Hydraulics

- Neutron Cross Section Model

$$\Sigma(\alpha, Tf, Tm, Dm, Sb) = \Sigma^{r} + \alpha\Delta\Sigma^{cr} + \frac{\partial\Sigma}{\partial\sqrt{Tf}}\Delta\sqrt{Tf} + \frac{\partial\Sigma}{\partial Tm}\Delta Tm + \frac{\partial\Sigma}{\partial Dm}\Delta Dm + \frac{\partial\Sigma}{\partial Sb}\Delta Sb + \frac{\partial^2\Sigma}{\partial Dm^2}(\Delta Dm)^2$$

$$\Delta\Sigma^{cr} = \Delta\Sigma^{cr}(BU, HIS1, HIS2)$$

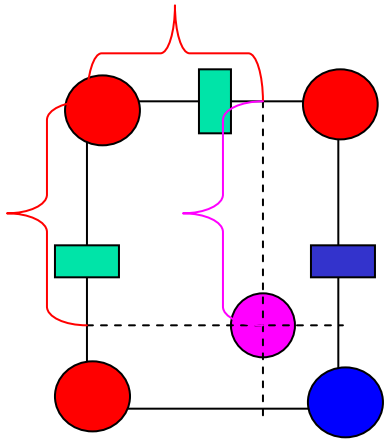
$$\frac{\partial\Sigma}{\partial Sb} = \frac{\partial\Sigma}{\partial Sb}(Sb, BU, HIS1, HIS2)$$

$$\frac{\partial\Sigma}{\partial\sqrt{Tf}} = \frac{\partial\Sigma}{\partial\sqrt{Tf}}(\sqrt{Tf}, BU, HIS1, HIS2)$$

$$\frac{\partial\Sigma}{\partial Tm} = \frac{\partial\Sigma}{\partial Tm}(Tm, BU, HIS1, HIS2)$$

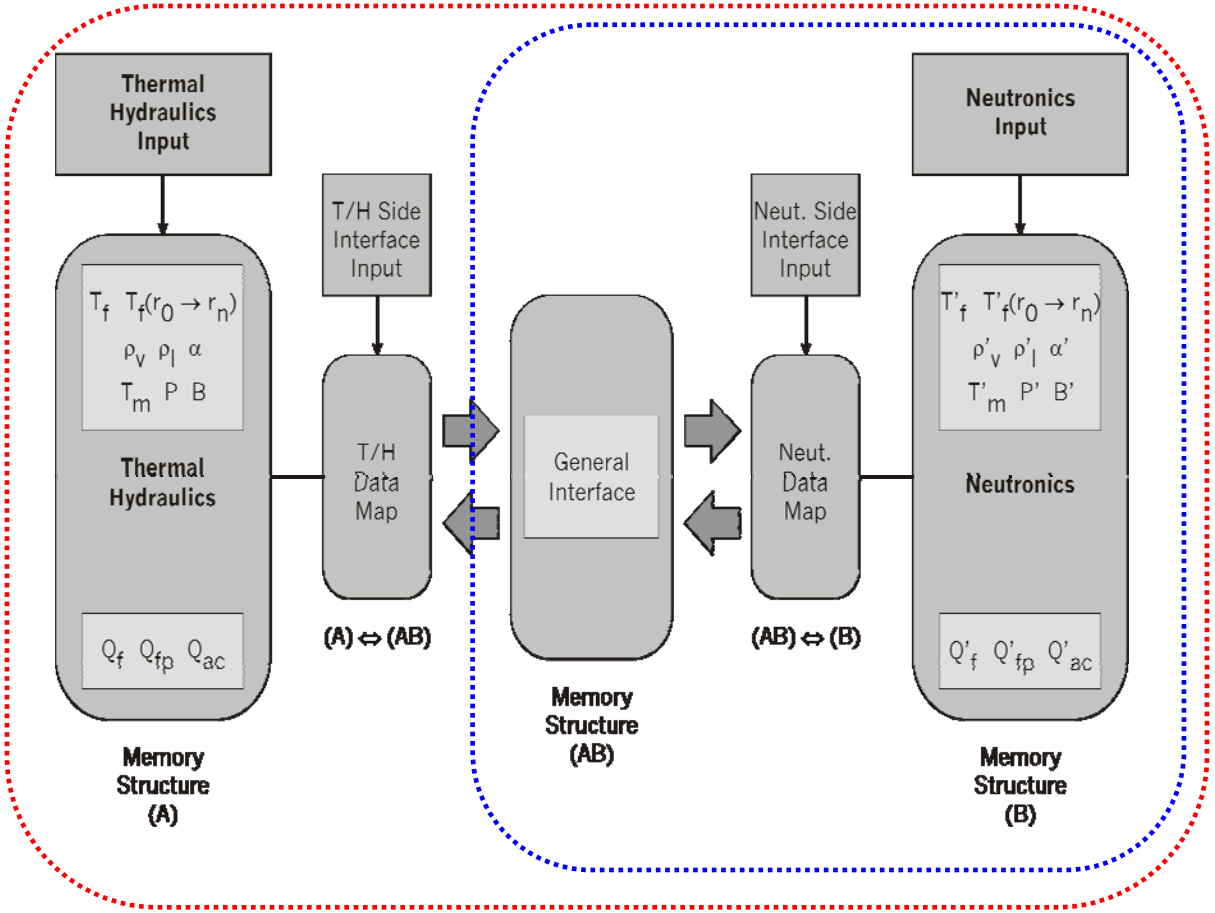
$$\frac{\partial\Sigma}{\partial Dm} = \frac{\partial\Sigma}{\partial Dm}(Dm, BU, HIS1, HIS2)$$

$$\frac{\partial^2\Sigma}{\partial Dm^2} = \frac{\partial^2\Sigma}{\partial Dm^2}(Dm, BU, HIS1, HIS2)$$



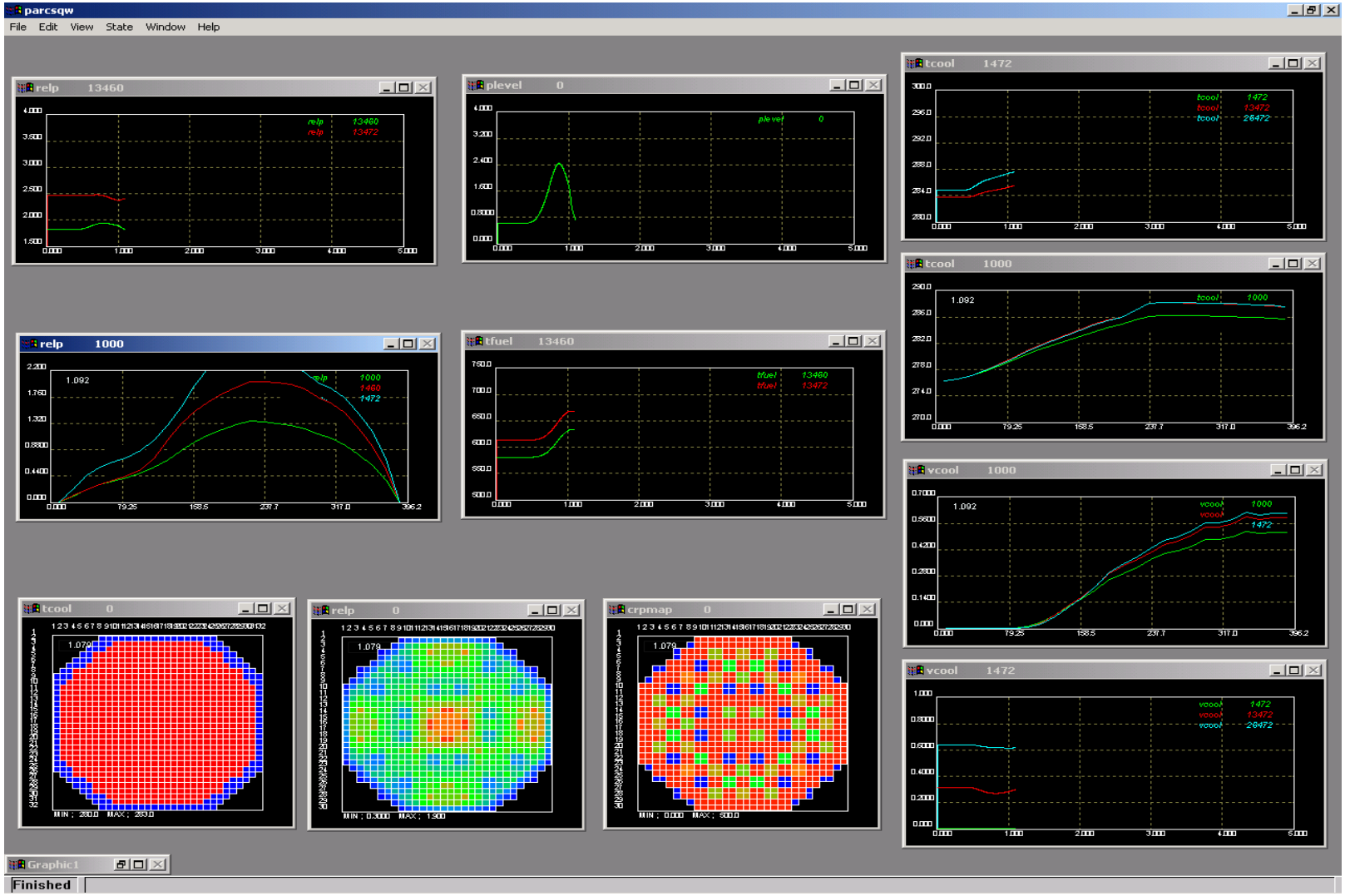
- Partials obtained by piecewise linear interpolation
- Burnup and burnup “history” dependence

# History of TRACE/RELAP5/PARCS Coupling




- 1998
  - PARCS / GI / RELAP
  - Parallel Virtual Machine
- 1999
  - PARCS / GI / TRAC-M
- 2000
  - Merging GI into PARCS
  - (Memory Copy instead of PVM)
  - Automatic Mapping for PARCS / TRAC-M
- 2004
  - Merging PARCS into TRACE
  - Static Linking Library
  - No PVM

# TRACE/PARCS GUI

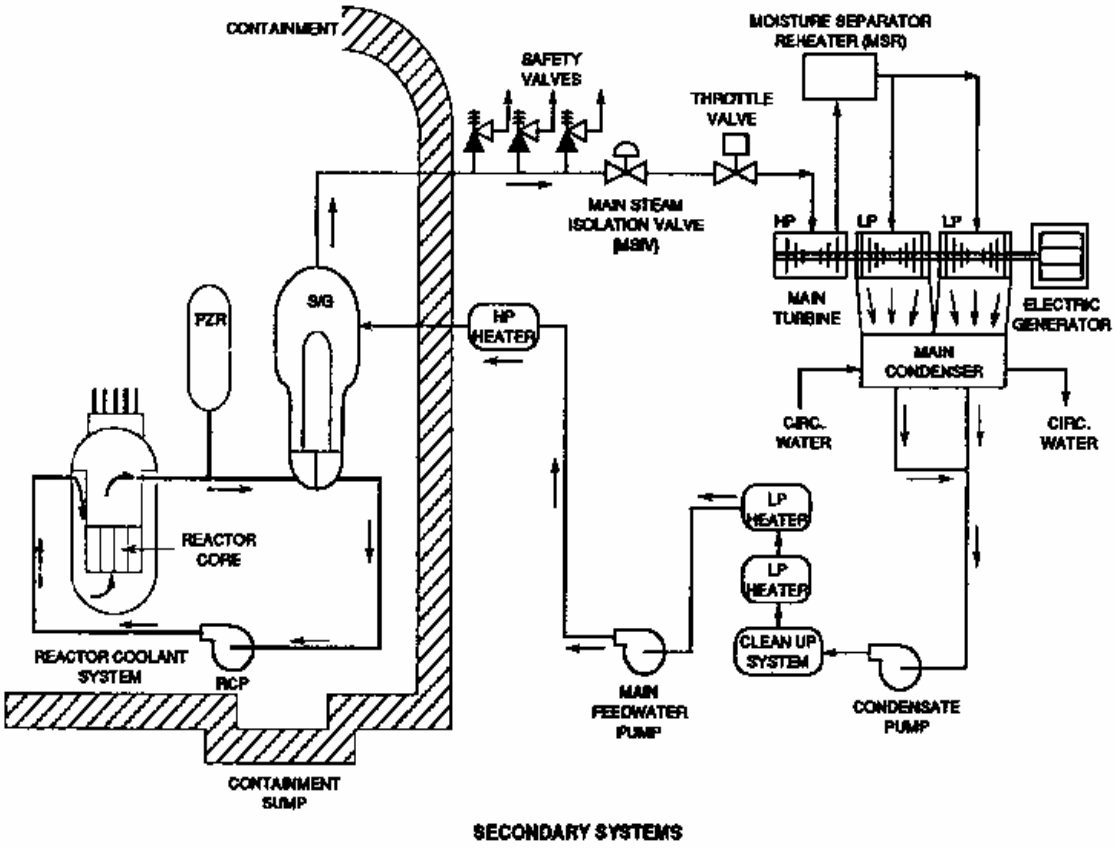


# NRC Coupled Code Assessment

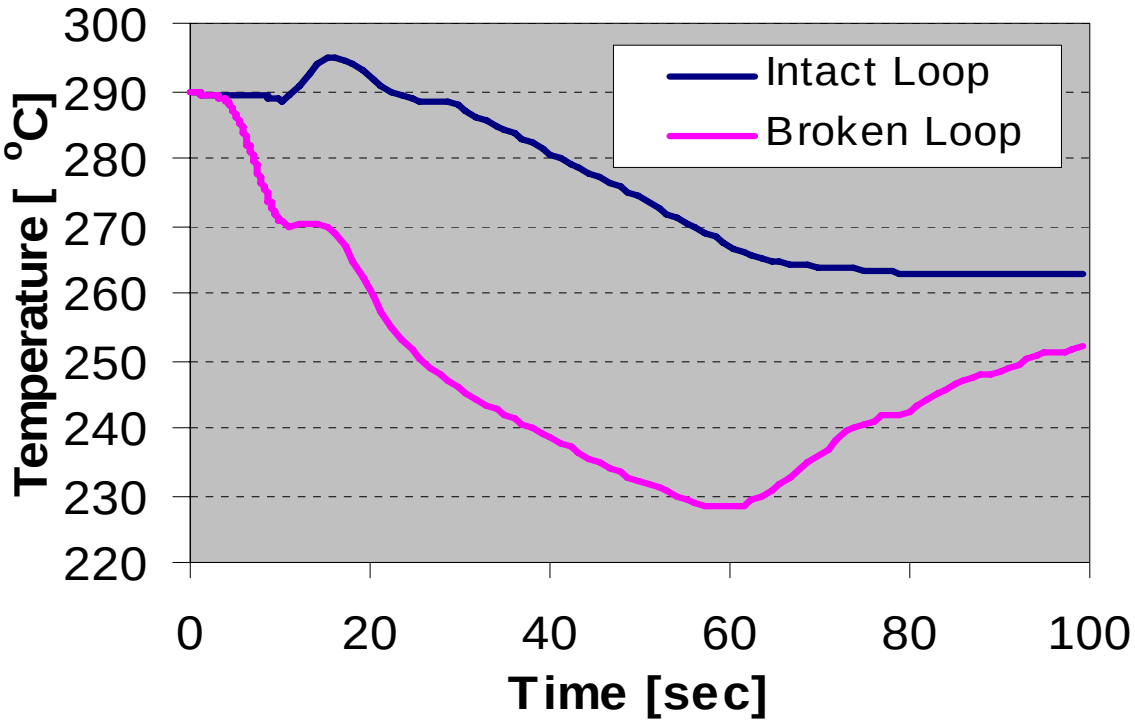
- Pressurized Water Reactor
  - Main Steam Line Break (i.e. plant uprates)
  - LOCA (e.g. David Besse)
- Boiling Water Reactor
  - Peach Bottom Depletion/Turbine Trip Test
  - Ringhalls Flow Instability
- Next Generation Reactors
  - ESBWR
  - Advanced CANDU (ACR-700)
  - PBMR

# Nuclear Reactor Transient Analysis: Main Steam Line Break

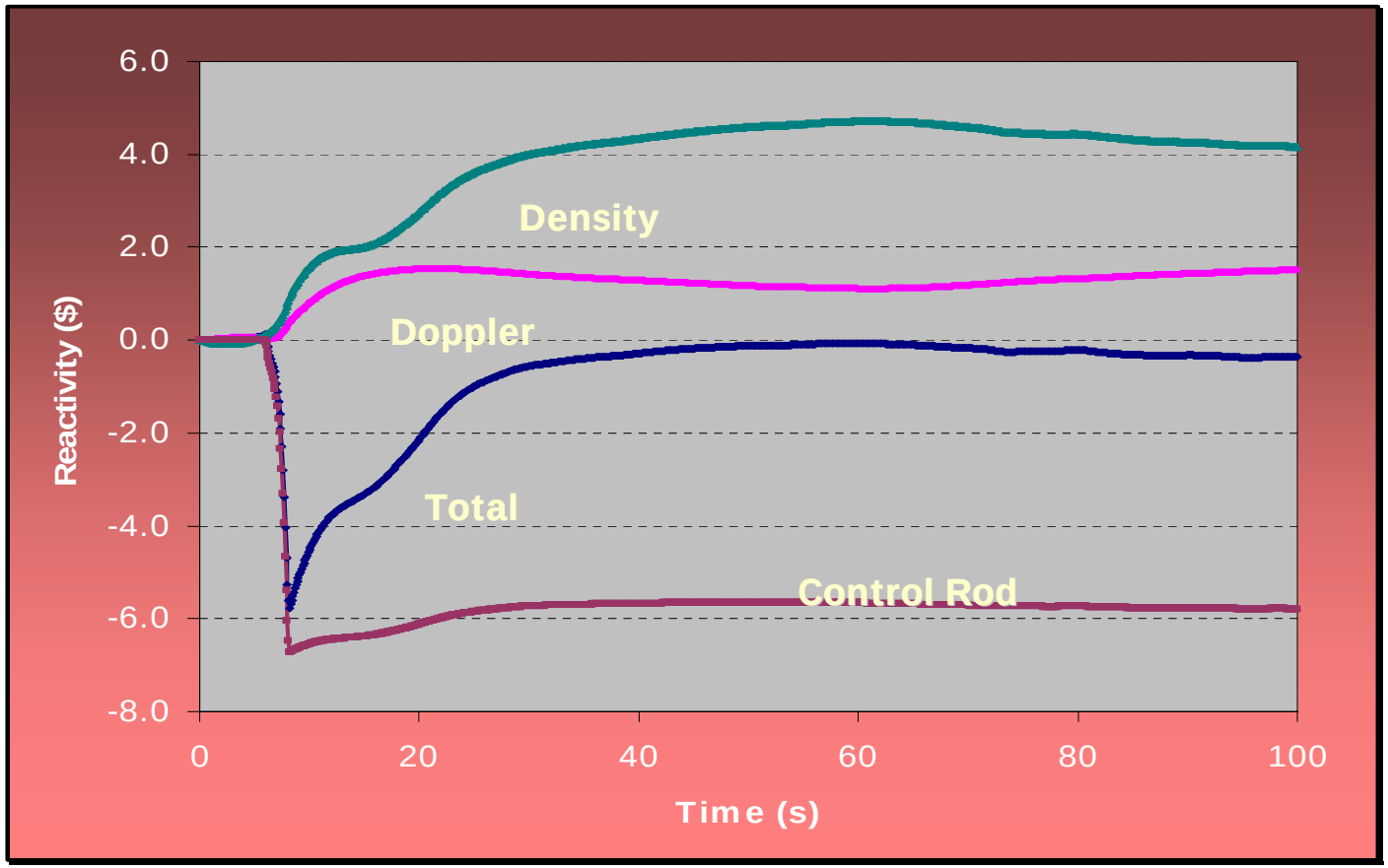
**PWR Plant Schematic**



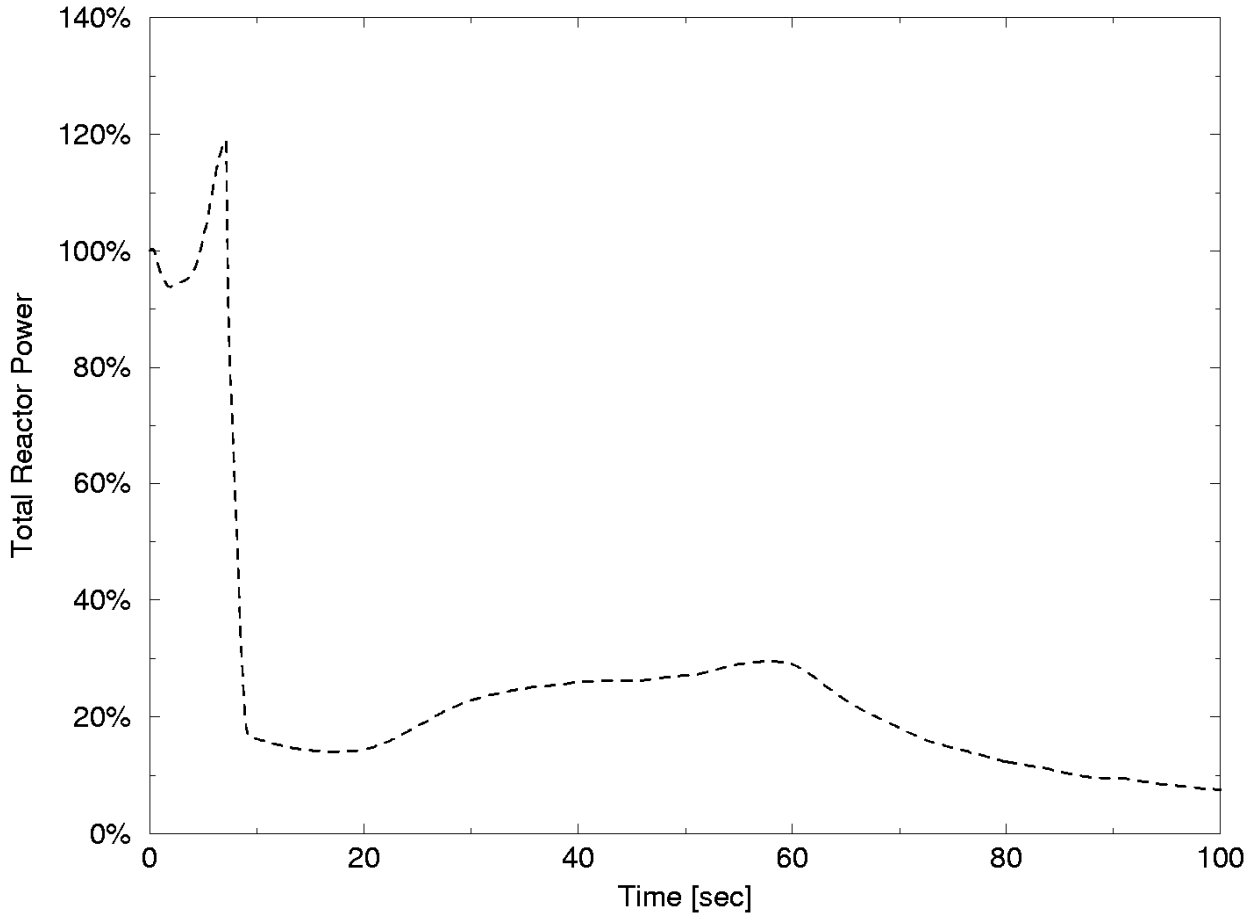
# Main Steam Line Break Transient: Core Coolant Temperature



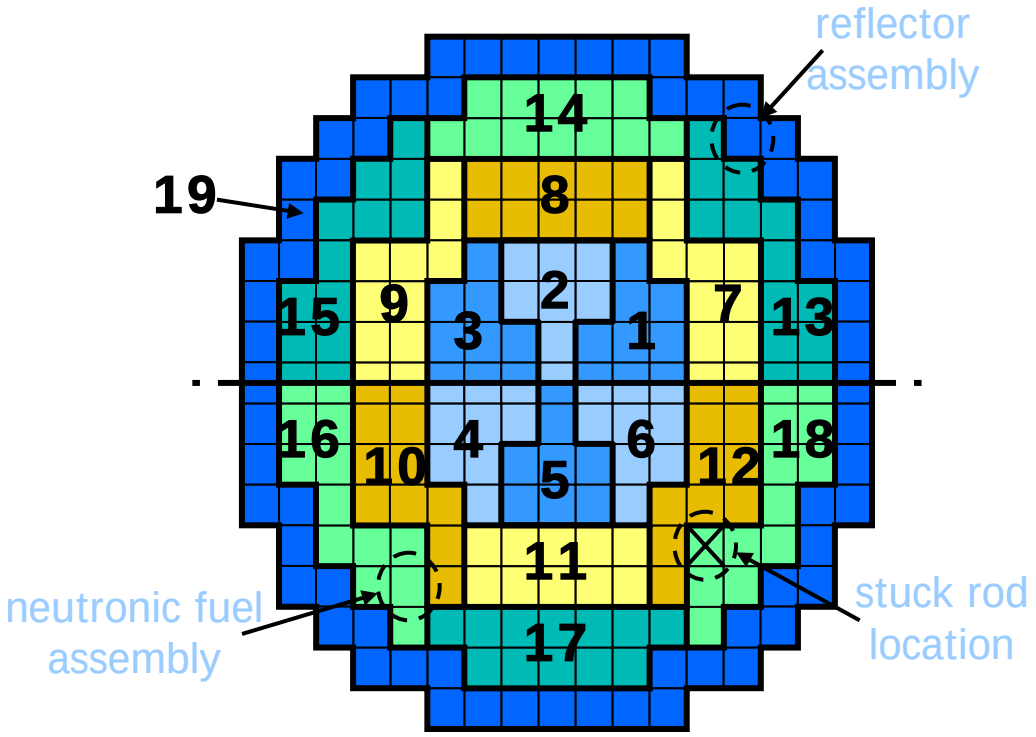
# MSLB: Reactivity Components



# Main Steam Line Break Analysis: Core Average Power (Point Kinetics)

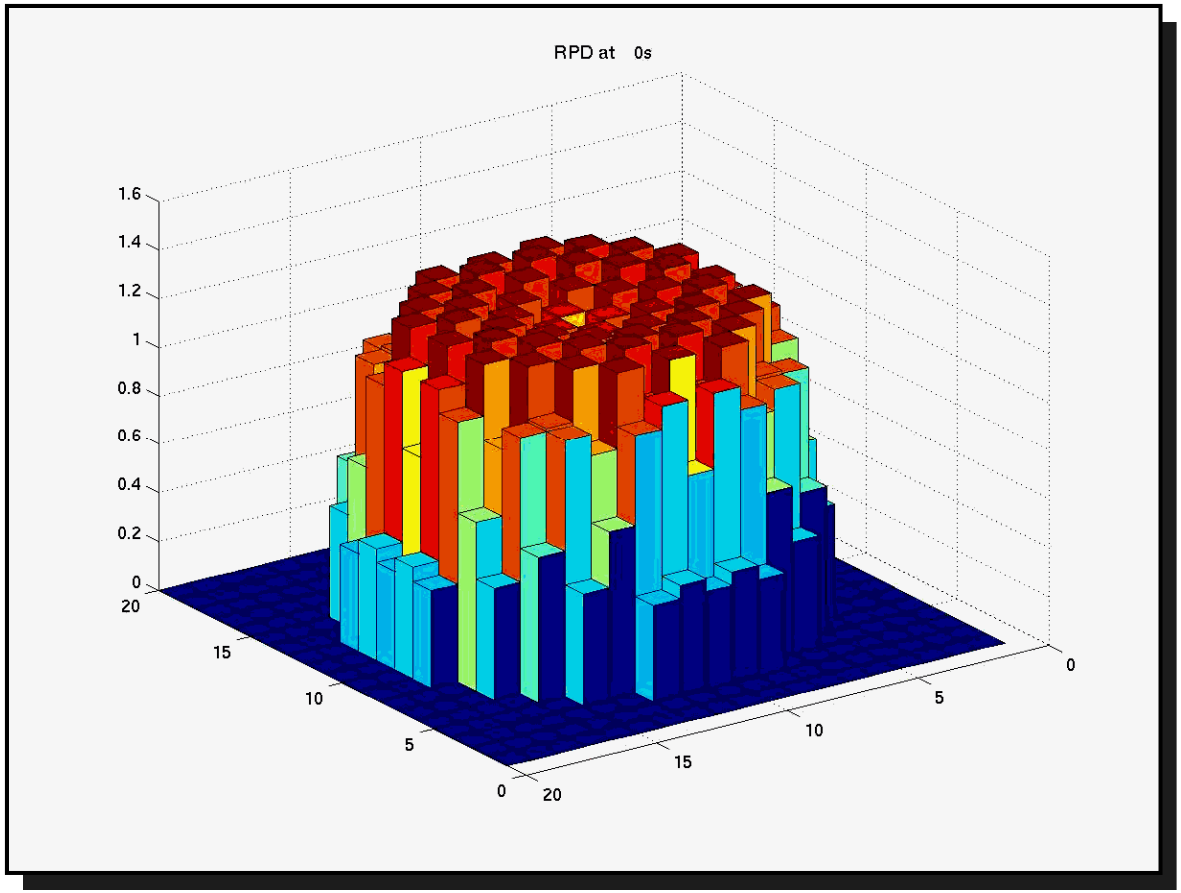


# Core Neutronics Model



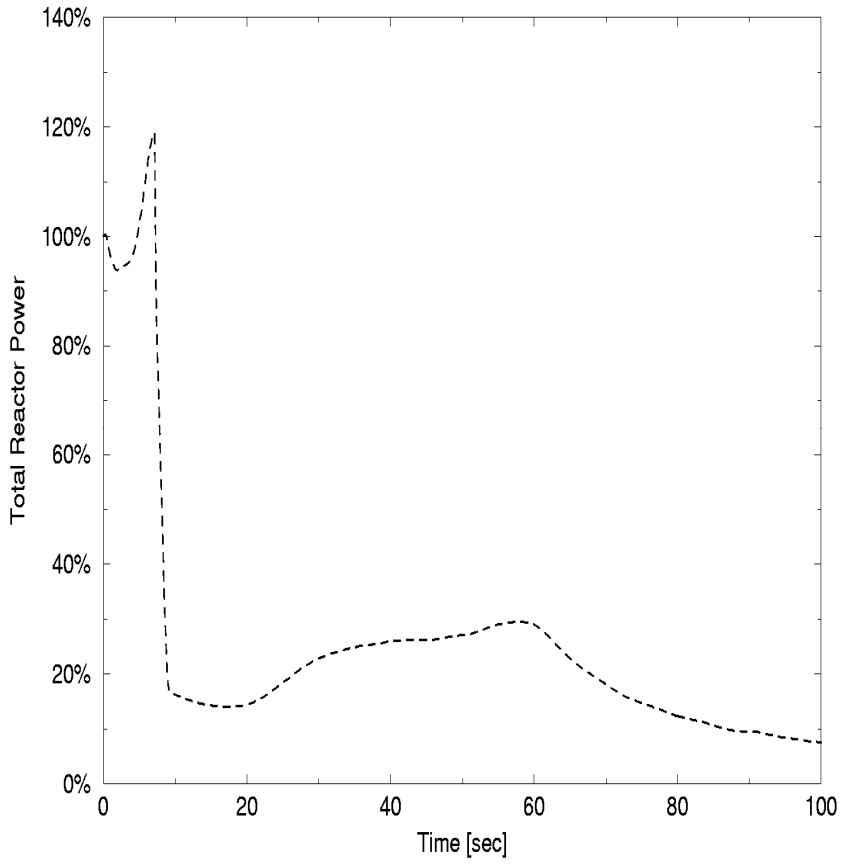
# Spatial Kinetics Analysis of Main Steam Line Break

## Initial Steady-State

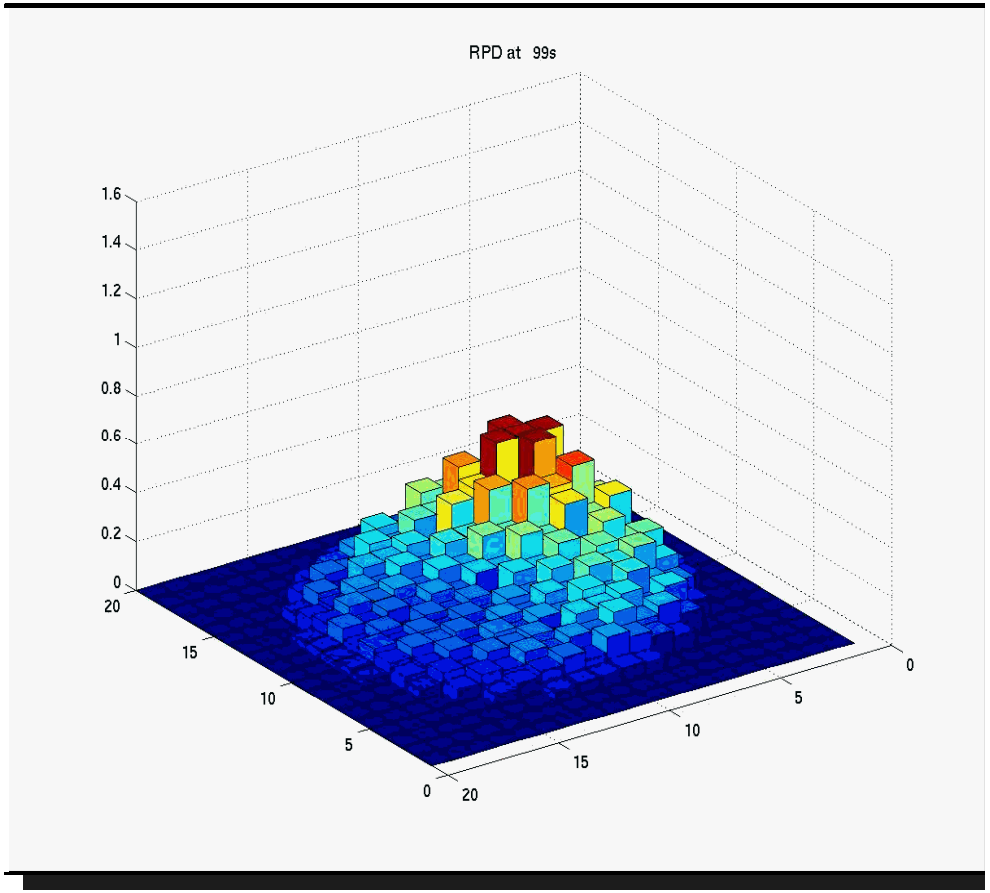


# MSLB Transient Analysis

## Core Average Power



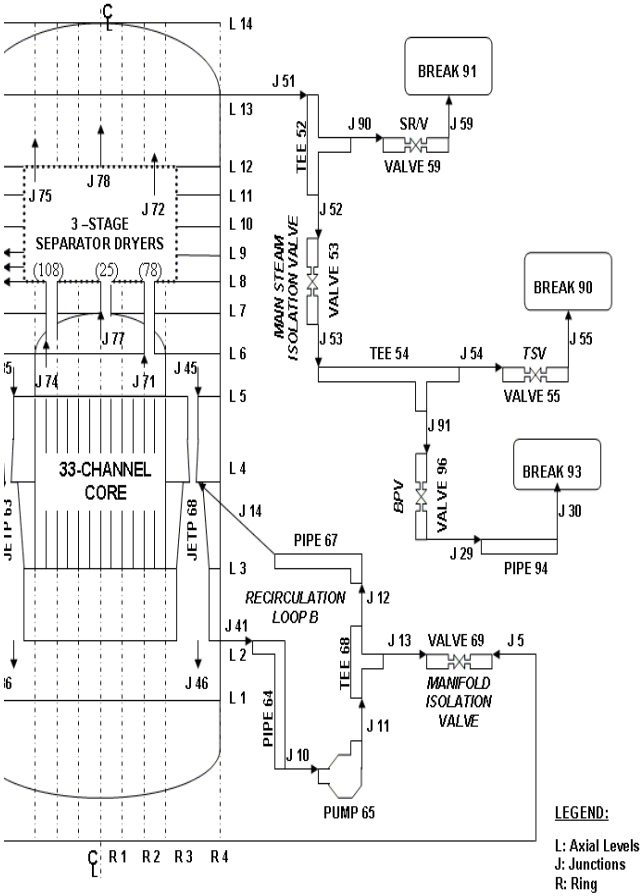

## Core Radial Power

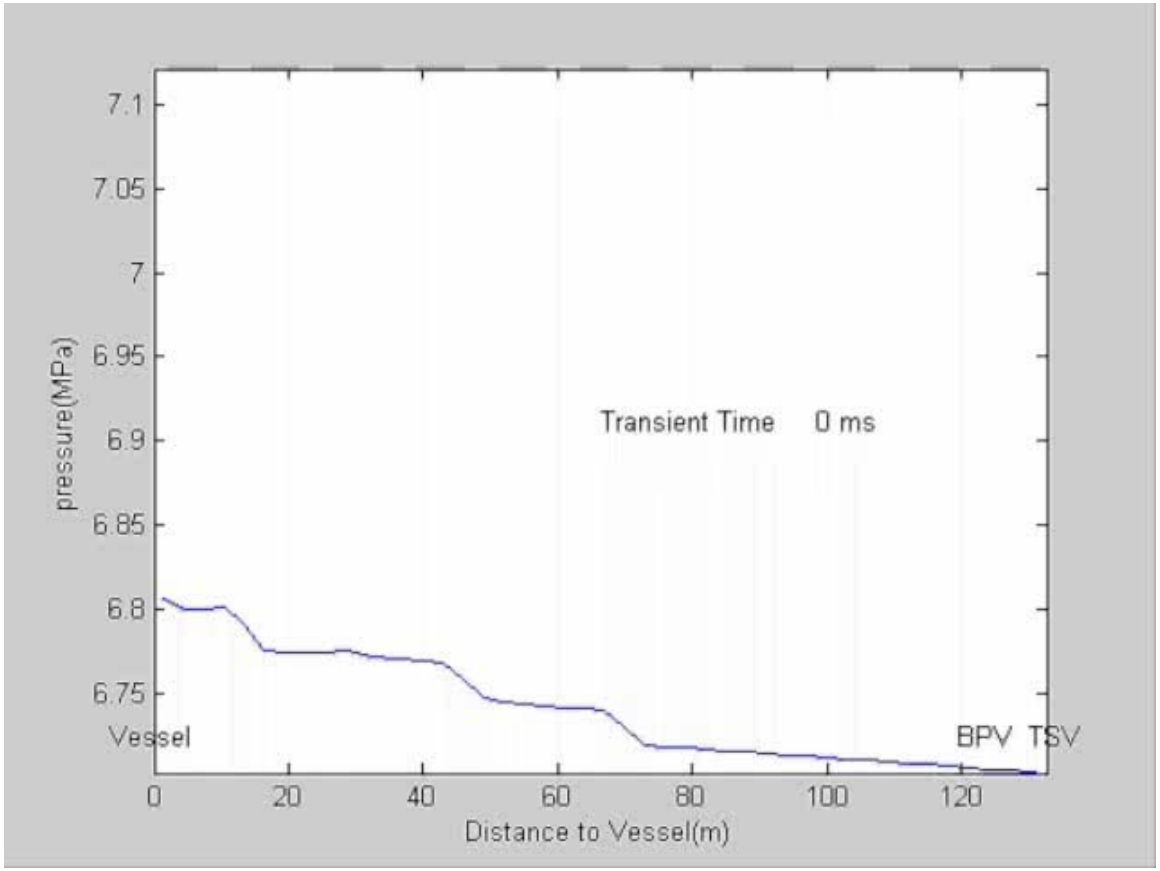


# BWR Assessment I:
# Peach Bottom Turbine Trip Transient

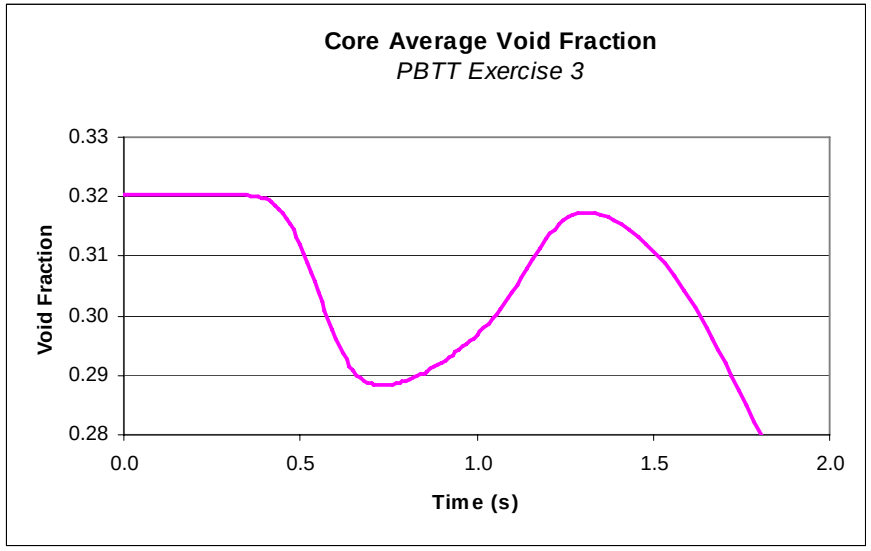
- Sudden Closure of the Turbine Stop Valve (TSV)
- The Pressure Oscillation Generated in the Main Steam Piping Propagates With Relatively Little Attenuation Into the Reactor Core
- The Core Pressure Induced Oscillations Result in Dramatic Changes in the Core Void Distribution and Fluid Flow
- The Magnitude of the Neutron Flux/Power Increase is Strongly Affected by the Initial Rate of Pressure Rise Caused by the Pressure Oscillation and has a Strong Spatial Variation

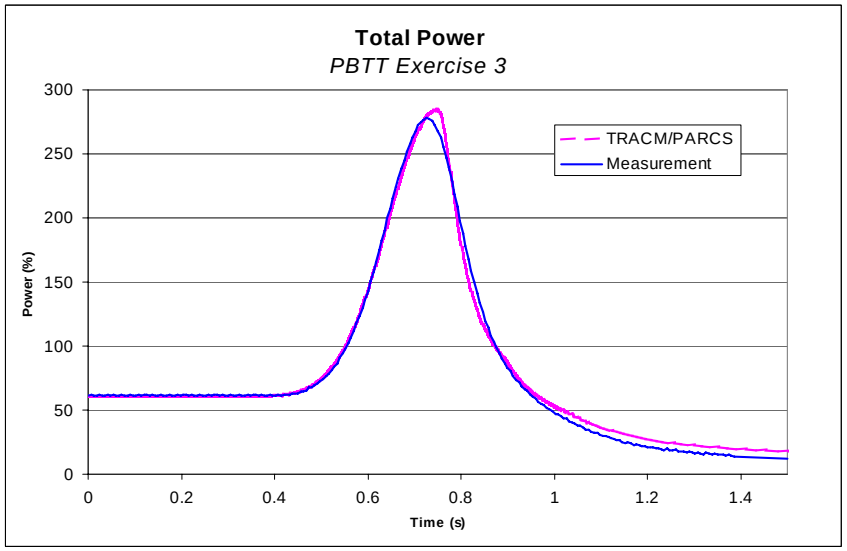
# Pressure Wave After Turbine Trip



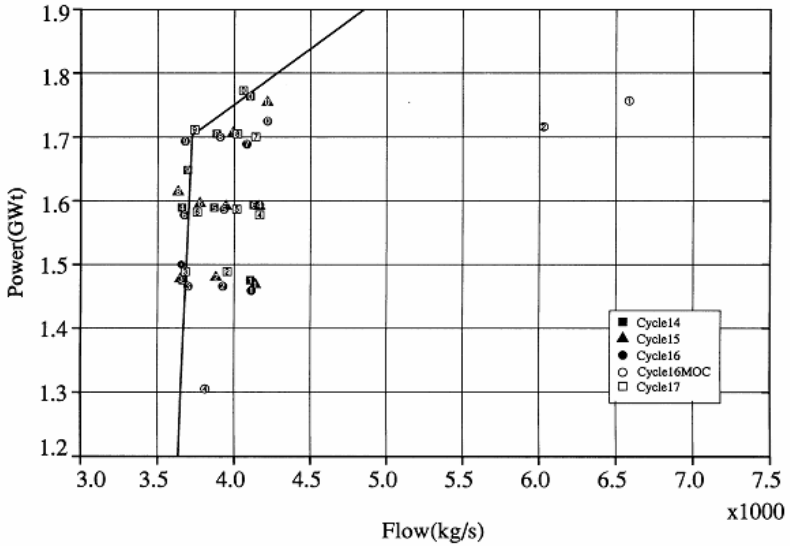



# Core Void / Power During Transient



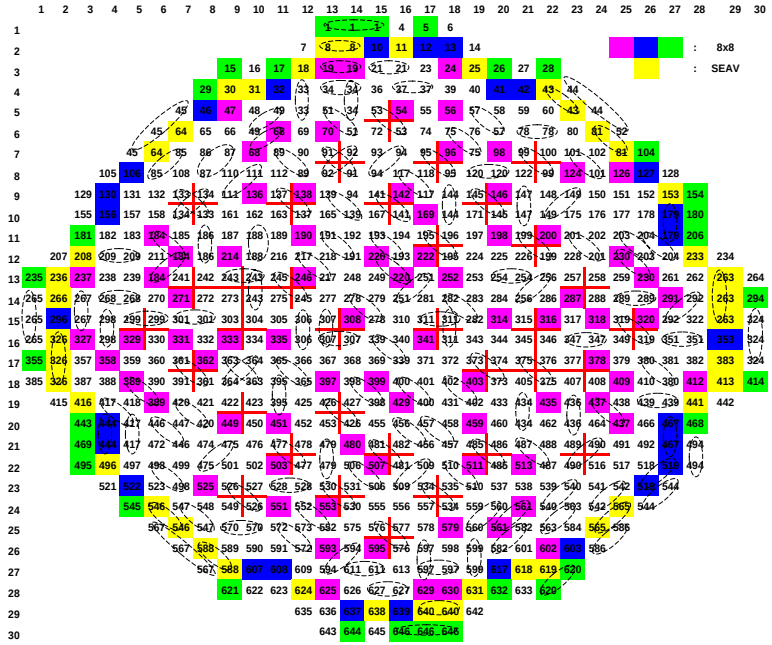



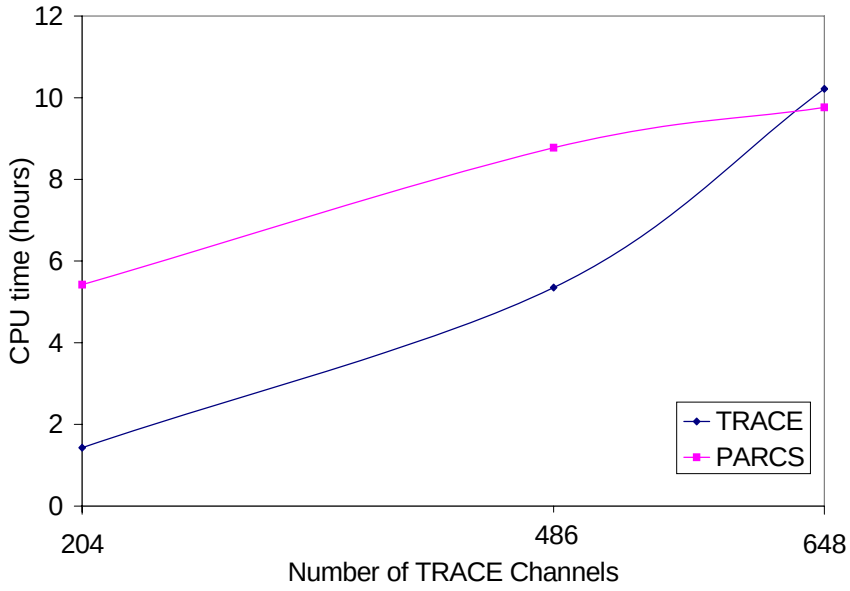
# BWR Assessment II: Ringhalls OECD/NEA Stability Benchmark




| Case | Power % | Flow Kg/s | Global D.R. | Global Freq (hz) | Regional D.R. | Reg. Freq (hz) |
|---|---|---|---|---|---|---|
| 9 | 72.6 | 3694 | 0.80 | 0.56 | **0.99** | 0.54 |
| 10 | 77.7 | 4104 | **0.71** | 0.50 | 0.63 | 0.49 |

# TRACE/PARCS CPU Requirements* vrs Number of TRACE CHANs



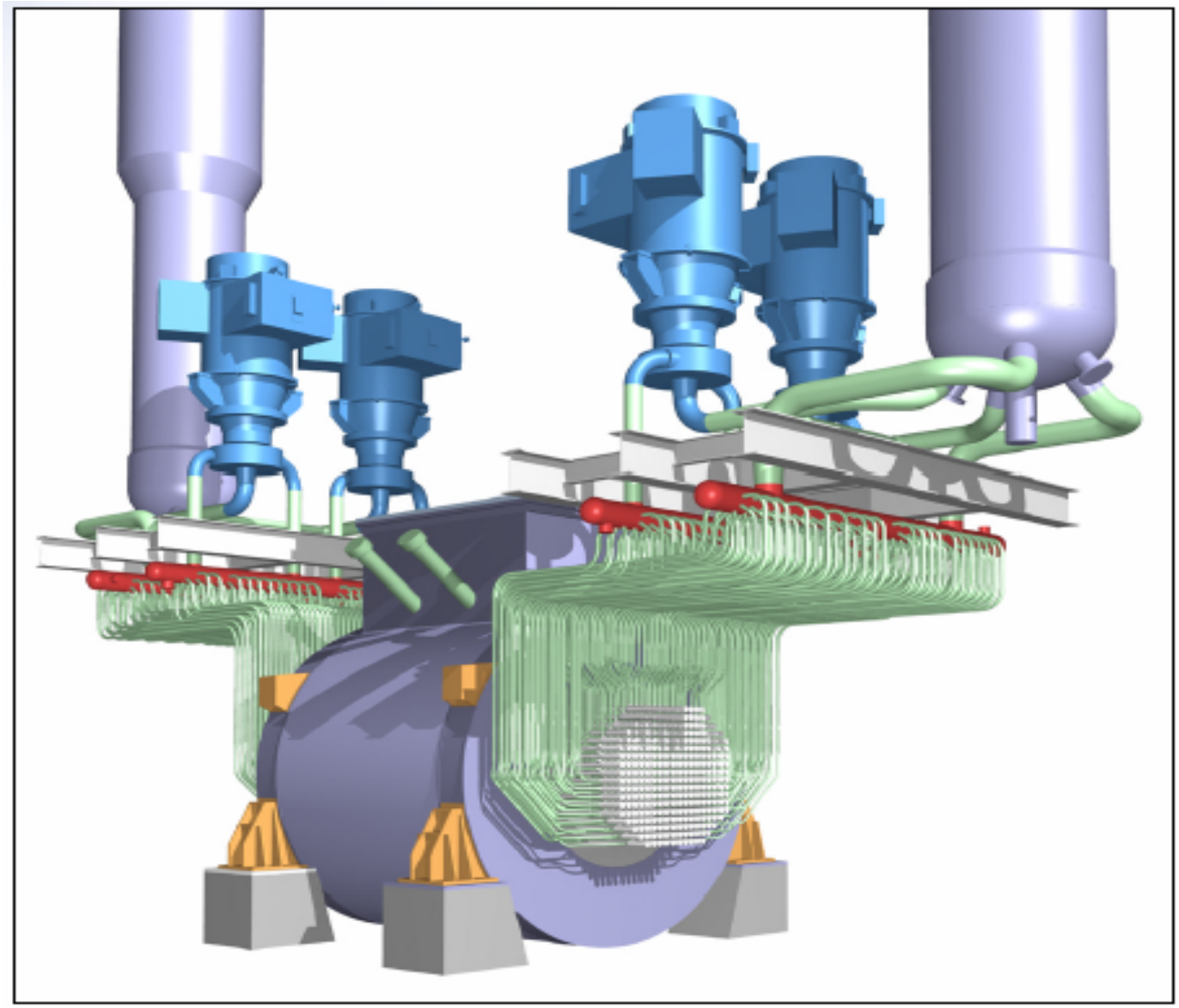



- TRACE/PARCS Problem size
  - Core TH ->684 x 27= 18468 TRACE cells
  - Core Neutronics->684 x 27=18468 PARCS nodes
- **~2 hours on 2 GHz machine for initialization ☹**

# Advanced Reactors

- Recent emphasis has been on addressing GENIII+/GENIV licensing concerns:
  - ESBWR
  - ACR-700
  - HTR
- Neutronics methods for MOX fuel analysis as part of the LWR PU Disposition program

# Advanced CANDU Reactor



# PEBBLE BED MODULAR REACTOR

## THE OECD/NEA PBMR COUPLED KINETICS CORE THERMAL-HYDRAULICS BENCHMARK TEST PROBLEMS

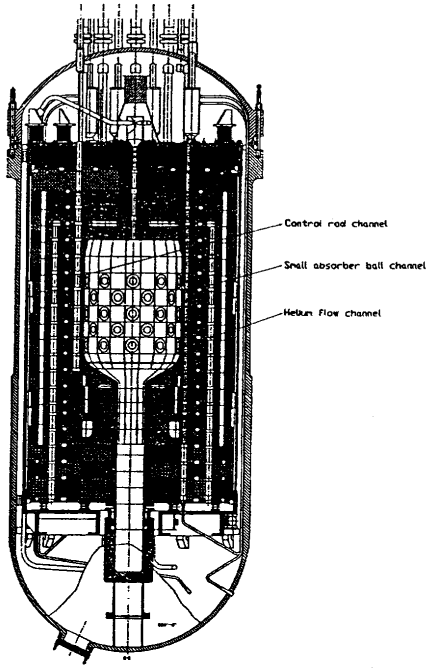

Frederik Reitsma PBMR Ltd, South Africa

Gerhard Strydom [1], Han de Haas [2], Kostadin Ivanov [3], Bismark Tyobeka [3], Ramatsemela Mphahlele [3*], **Tom Downar [4], Volkan Seker** [4], Hans D Gougar [5], D F Da Cruz [2]

[1] Reactor Analysis Group, PBMR (Pty) Ltd, South Africa
[2] Fuel, Actinides & Isotopes Group, NRG, The Netherlands
[3] Nuclear Engineering Program, Penn State University, USA
[4] Nuclear Engineering Department, Purdue University, USA
[5] Fission & Fusion Systems, INEEL, USA
[*] National Nuclear Regulator, Centurion, South Africa



The Second Topical Meeting on High Temperature Reactor 2004
September 22-24, 2004
Beijing, China

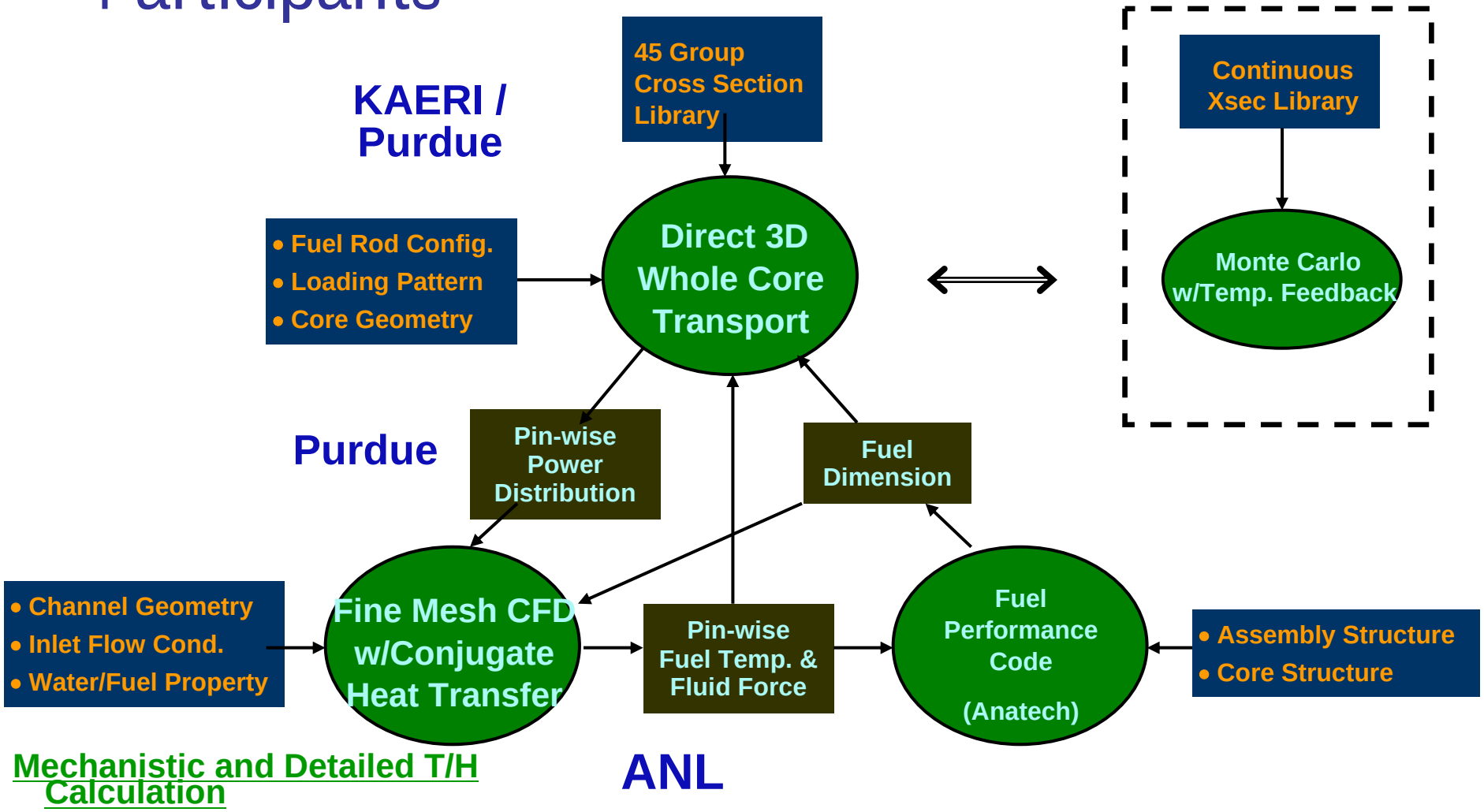
# Next Generation Coupled Code Methods

## The Numerical Nuclear Reactor (DOE INERI 2001-04) (EPRI/DOE 2005-2007)

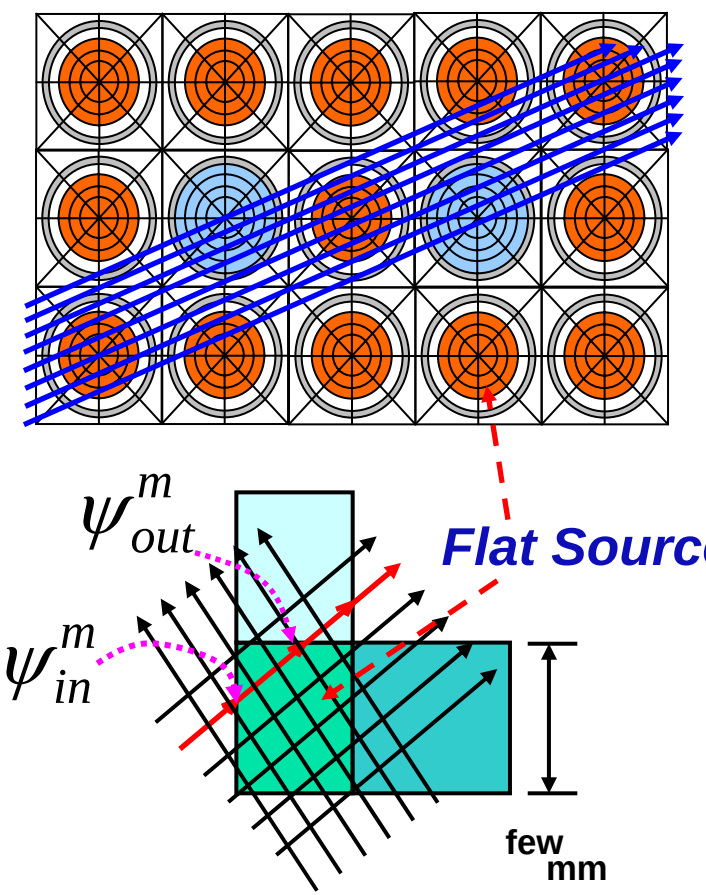
- Goal
  - Develop a *Numerical Nuclear Reactor* which performs detailed, first-principle based simulation of the multi-physics phenomena occurring in nuclear reactors

- Objectives
  - Provide a fully integrated, high-fidelity simulation capability that can be used for the analysis of light water reactors and advanced reactors
  - Exploit high performance computers and elaborated models to complement experimental verification when designing a new system

# Numerical Reactor Elements and Participants



# Ray Tracing and Method of Characteristics




*(s = segment length)*

**Neutron Balance along Ray**

$$\frac{d\psi(\xi)}{d\xi} + \Sigma\psi(\xi) = q \;; \quad \psi(0) = \psi_{\text{in}}$$

**Assume Constant Xsec and Flat Source within a Micro Region**

$$\psi^m_{out} = \psi^m_{in} e^{-\Sigma s} + \frac{q}{\Sigma}\left(1 - e^{-\Sigma s}\right)$$

$$\overline{\psi}_m = \frac{\psi^m_{in} - \psi^m_{out}}{\Sigma s} + \frac{q}{\Sigma}$$

**Segment Average Angular Flux**

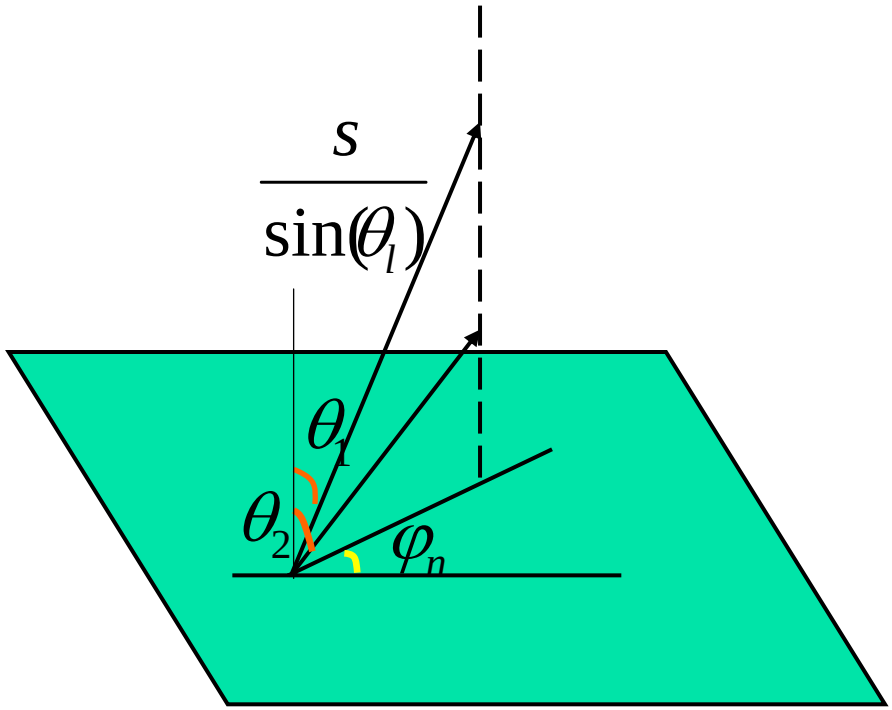
$$\phi = \sum_m \omega_m \overline{\psi}_m$$

**Scalar Flux**

# Ray Tracing Computational Rqmts (2D)

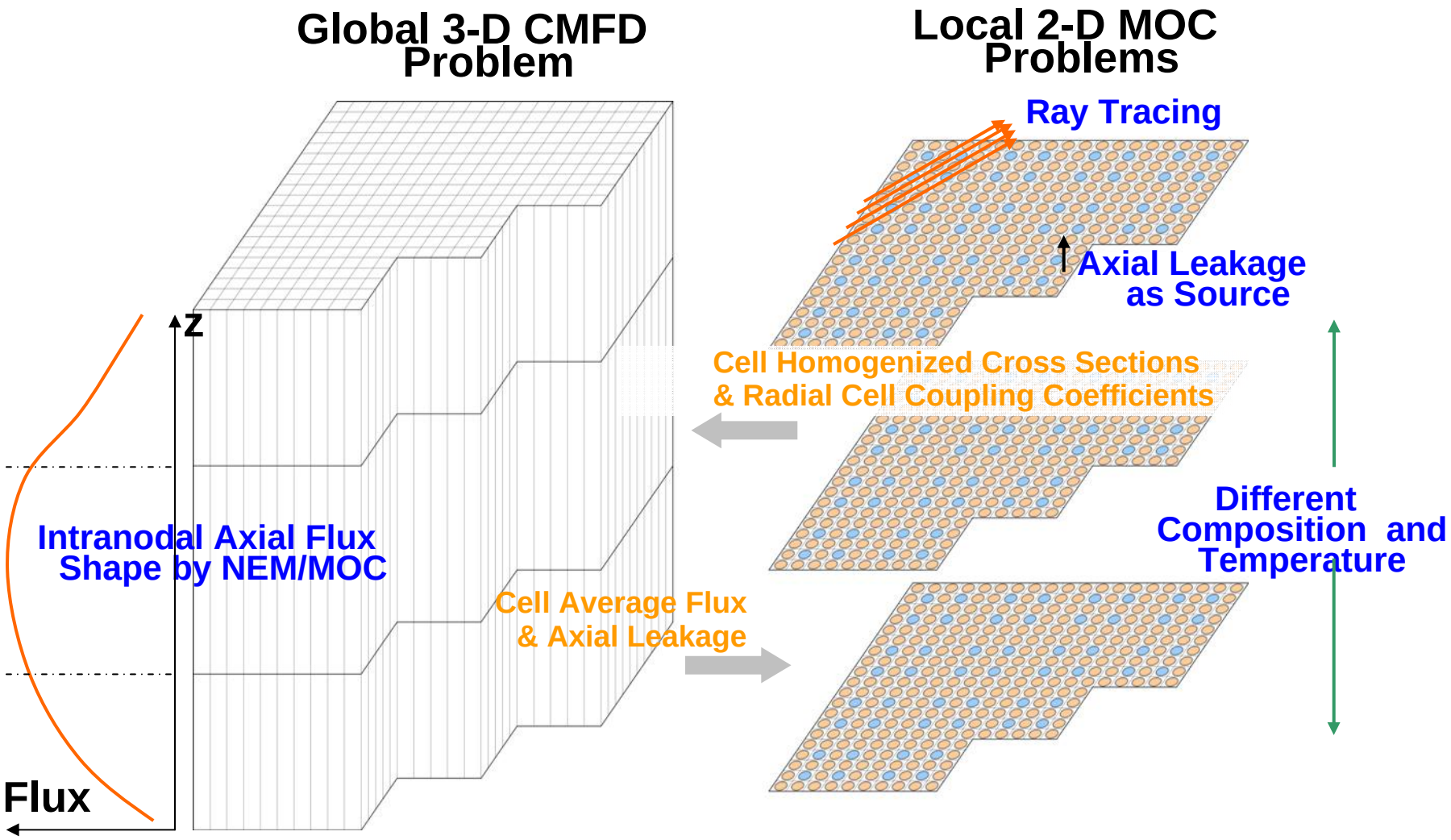
$$\psi_{out}^{m,g} = \psi_{in}^{m,g} \exp\left(-\frac{\Sigma_g s}{\sin\theta_l}\right) + \frac{q_g}{\Sigma_g}\left[1 - \exp\left(-\frac{\Sigma_g s}{\sin\theta_l}\right)\right]$$

**Typical Ray Tracing Parameters and Execution Requirements for a Quarter Core Problem**

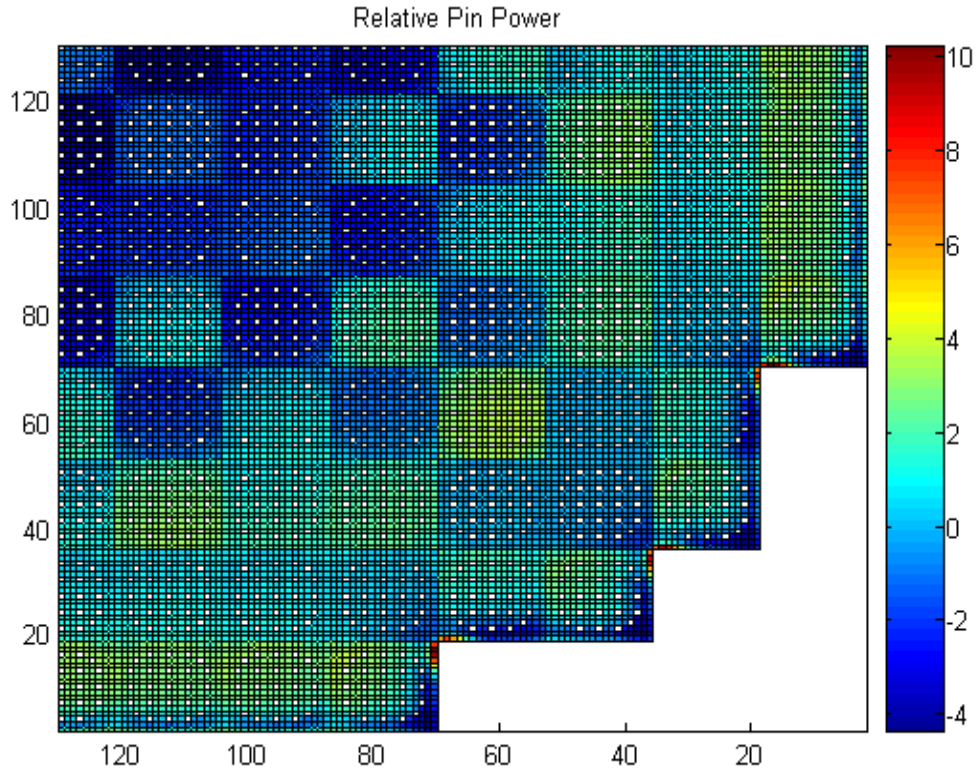



| Parameter | Value |
|---|---|
| # of Azimuthal/Polar Angles (per 90 Degrees) | 8/4 |
| Ray Spacing | 0.2 mm |
| Number of Regions per Cell | ~50 |
| Number of Cells | ~10000 |
| Total Number of Regions | 500000 |
| Total Number of Rays | ~120000 |
| Number of Energy Groups | 45 |
| Number of Planes | 12 |
| Number of Ray Tracing Sweeps | ~10 |
| Memory Required | ~9 GBytes |
| Run Time (1 CPU) | ~24 hours |

# Planar MOC Solution Based 3-D CMFD



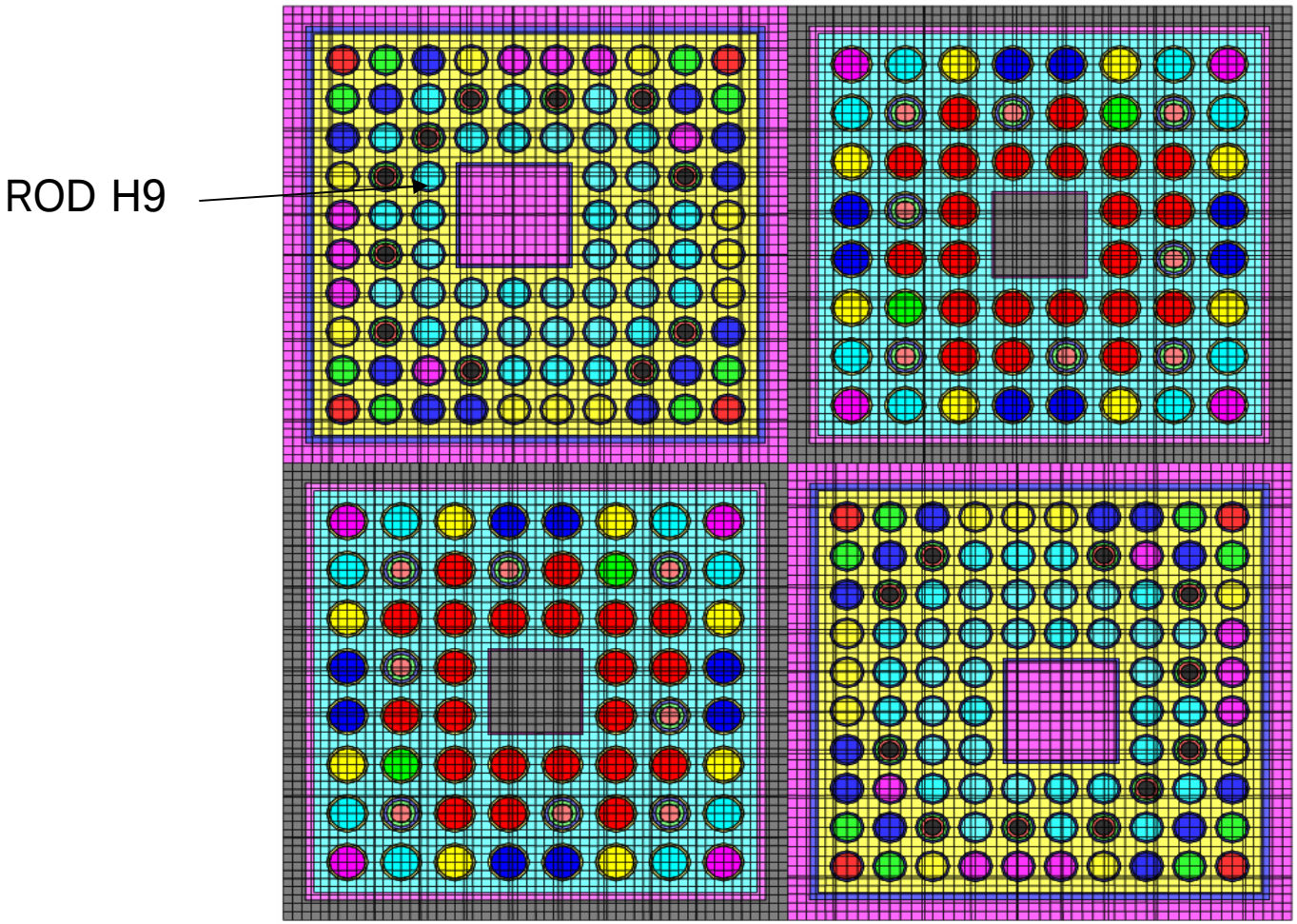
# PWR Comparison of PARCS vs. DeCART (ARO-HZP)




**Relative Axially Integrated Pin Power Difference between PARCS and DeCART**

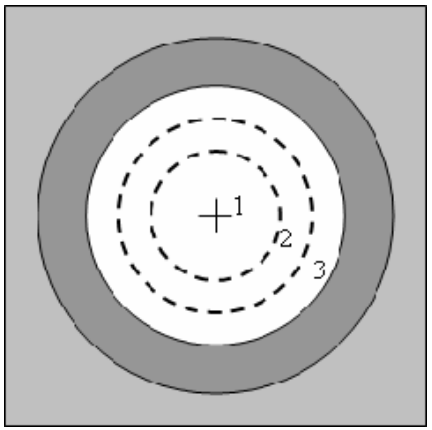
**(PARCS - DeCART) / DeCART x 100%**

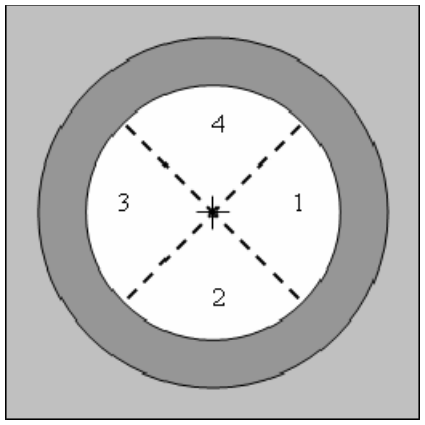
# BWR Applications:
# 2x2 Assembly Benchmark



# Comparison w/ Monte Carlo

| | Radial Division | | |
|---|---|---|---|
| Azimuthal Division | 1 | 2 | 3 |
| 1 | 0.99 (-0.32%) | 1.05 (0.25%) | 1.11 (-0.87%) |
| 2 | 1.00 (-0.73%) | 1.06 (0.89%) | 1.13 (-0.42%) |
| 3 | 0.93 (0.81%) | 0.94 (0.91%) | 0.97 (-0.24%) |
| 4 | 0.93 (-0.01%) | 0.93 (0.41%) | 0.95 (-0.50%) |



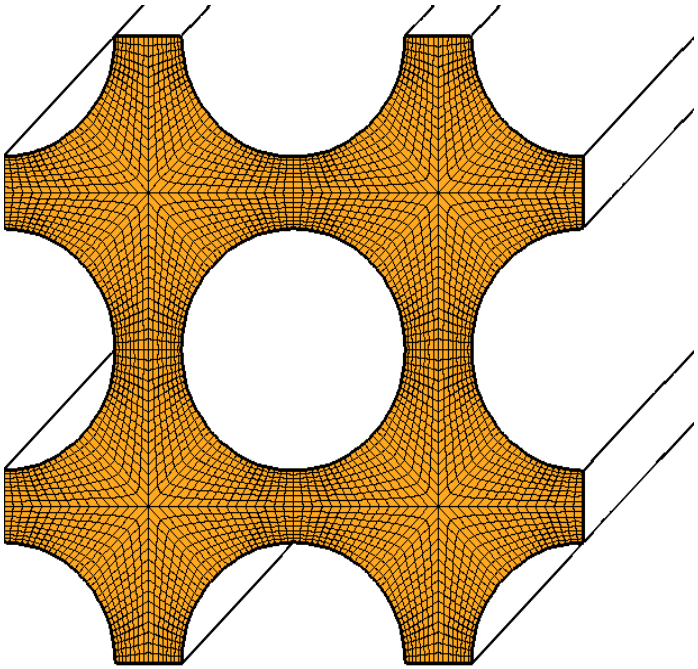
# Example of CRUD on BWR Fuel Rods

**Proceedings of the 2004 International Meeting on LWR Fuel Performance,
Orlando, Florida, September 19-22, 2004,
Paper 1016."Fuel Failures During Cycle 11 at River Bend", Edward Ruzauskas,
AREVA, Framatome ANP, Inc., David L Smith, Entergy Operations**

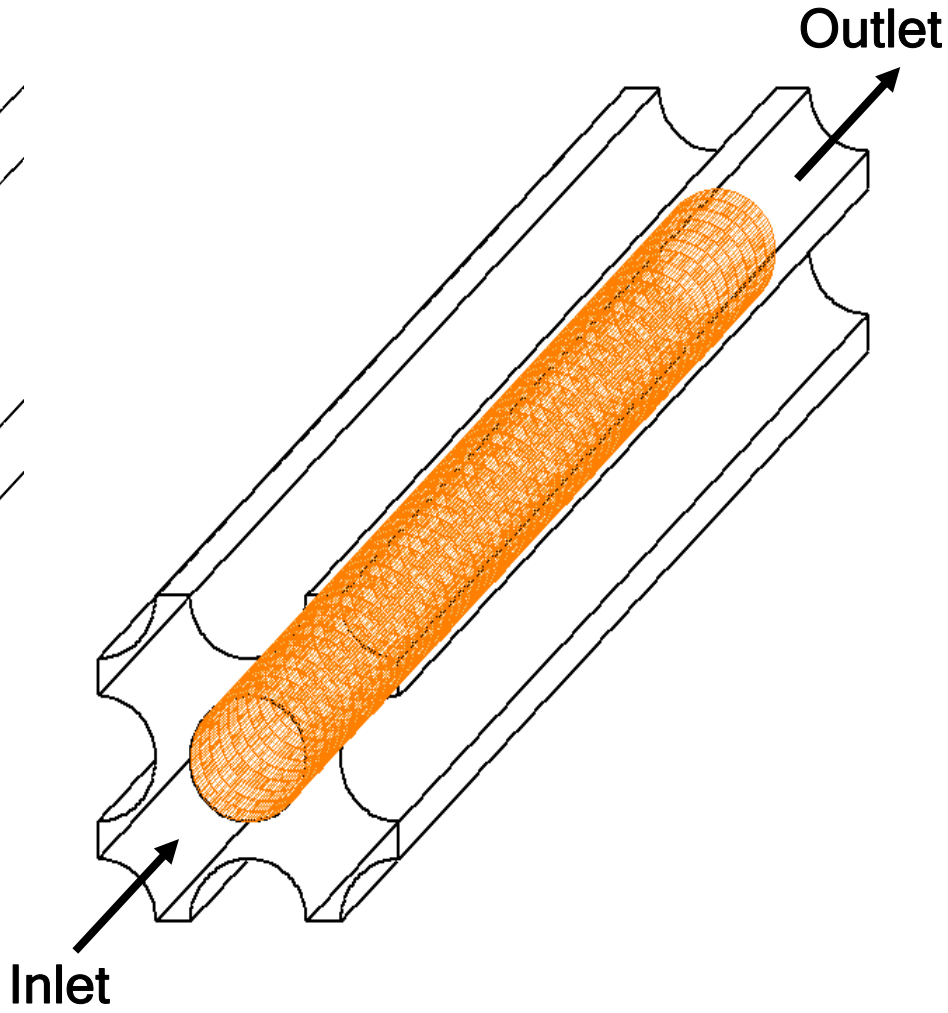
# Thermal-Hydraulics: CFD Code STAR-CD

- Commercial code developed by CD-Adapco.
- Finite-volume based code for the solution of pressure, 3-D momentum, enthalpy, and turbulence equations over an arbitrary mesh.
- Capabilities required for this project:
  - Conjugate heat transfer
  - Transient analysis
  - Multi-phase models
  - Moving boundary and FSI
  - Parallel computing

# CFD Modeling of a Fuel Channel

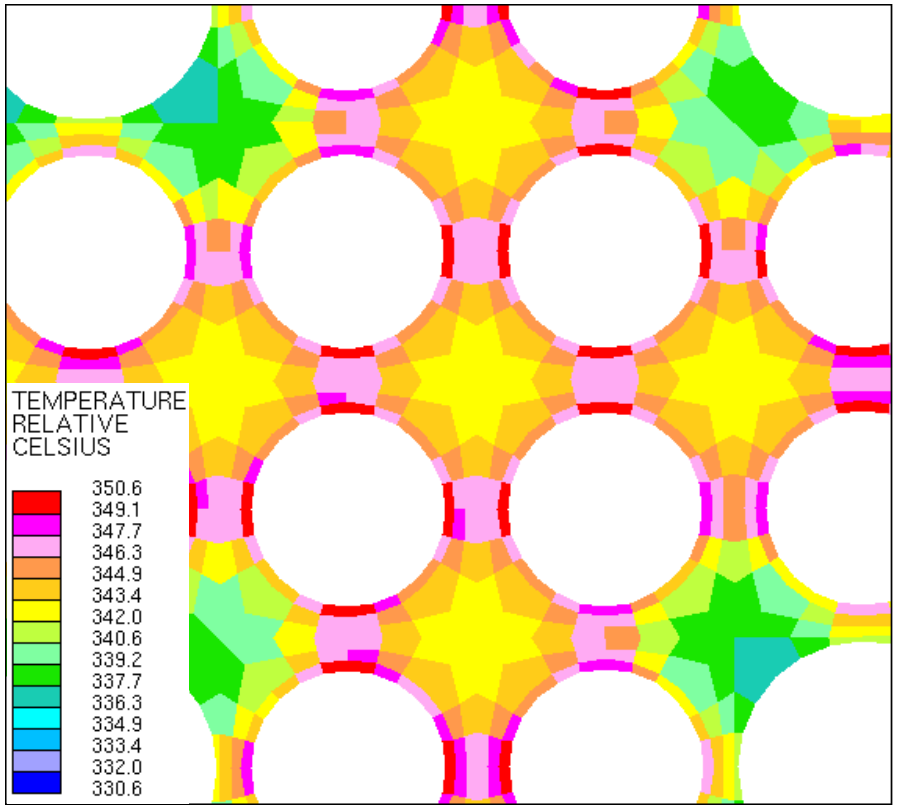


Total 192000 cells

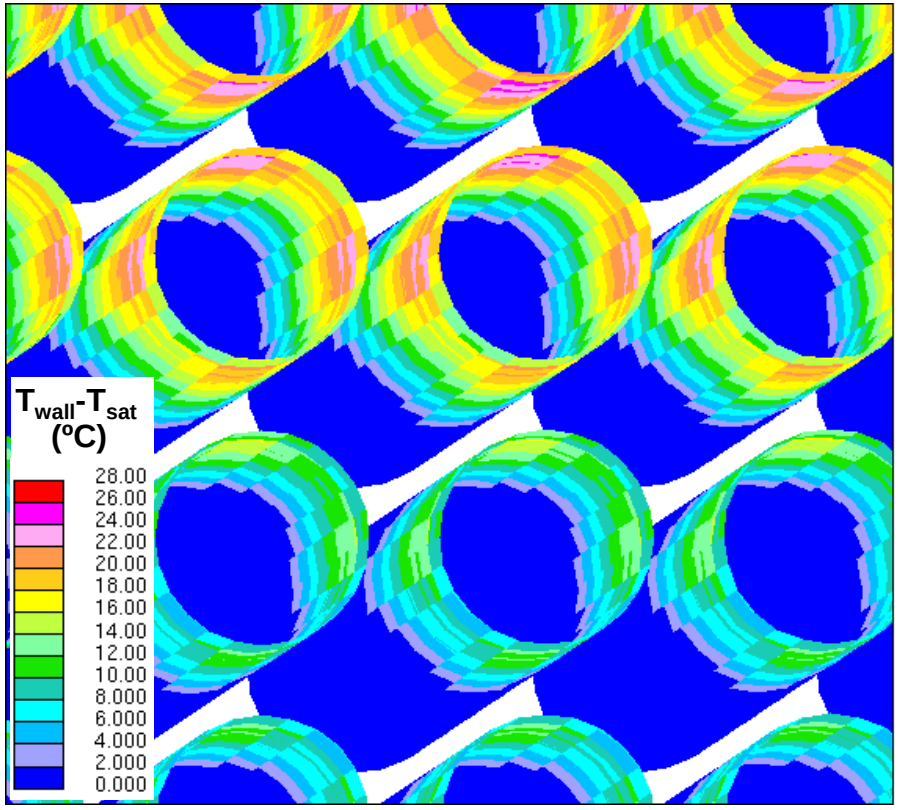


# Catawba PWR Results

**Coolant temperatures at core outlet**

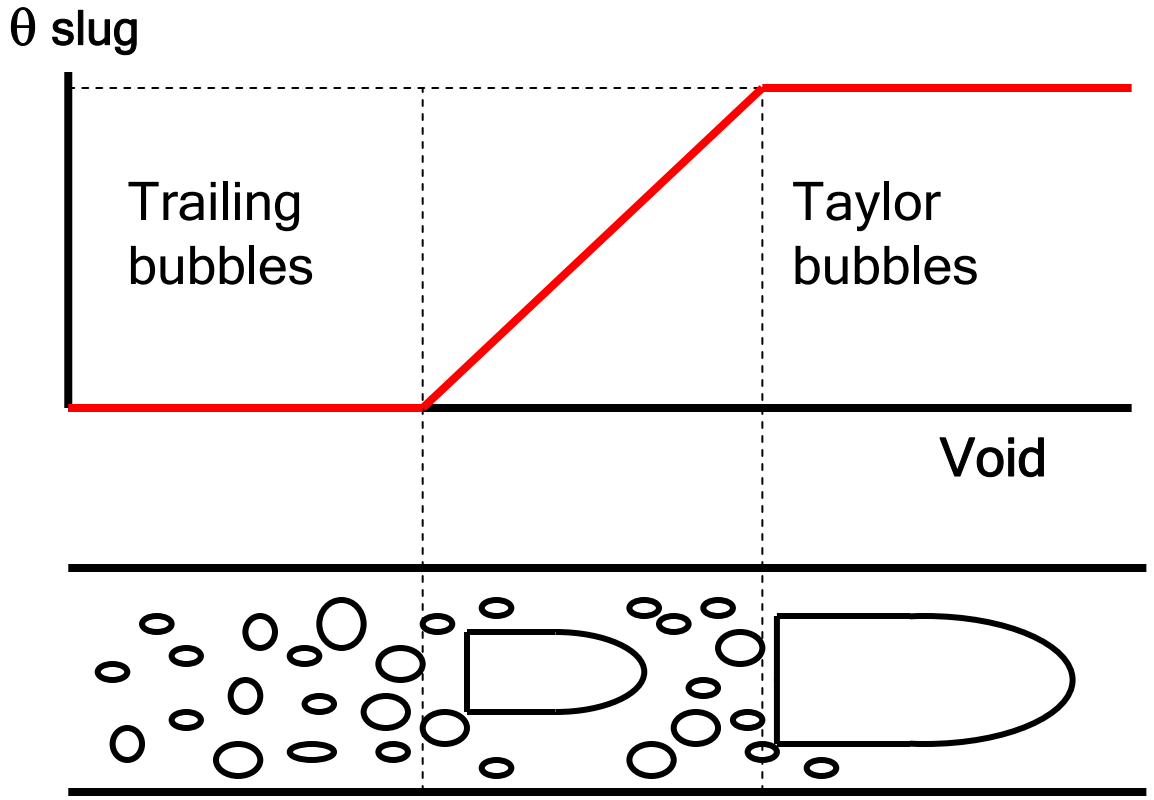



**Cladding outer surface temperatures at assembly interface**



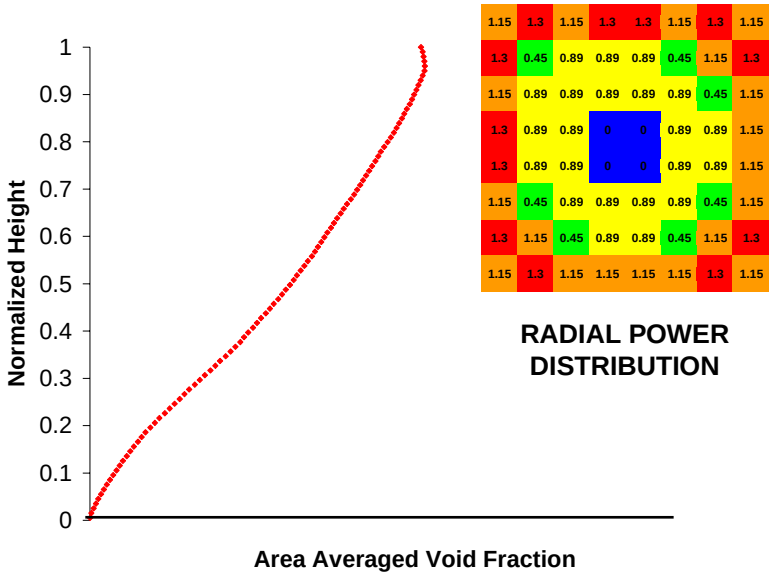
# STAR-CD 2-Phase Flow Model

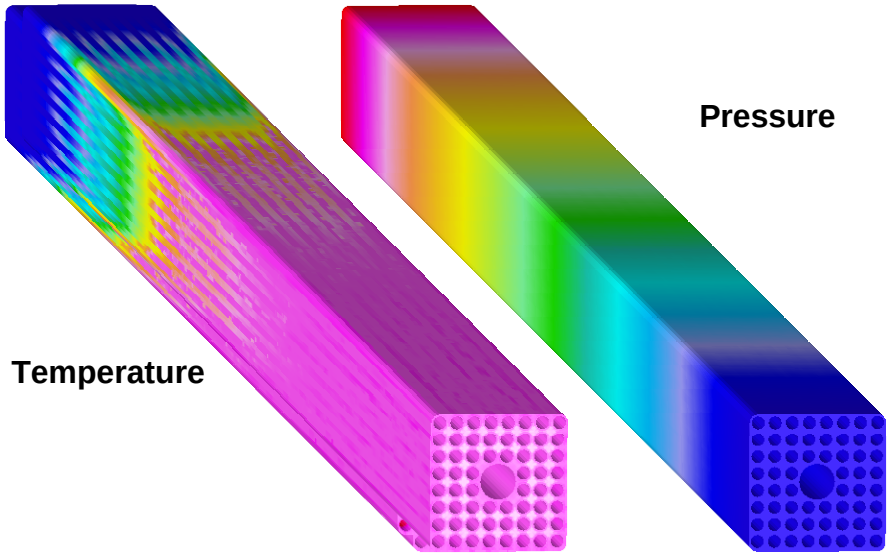
- Regime variable within liquid-continuous region.
- Used to calculate effective length scales and drag coefficient for mixed Taylor and trailing bubbles.

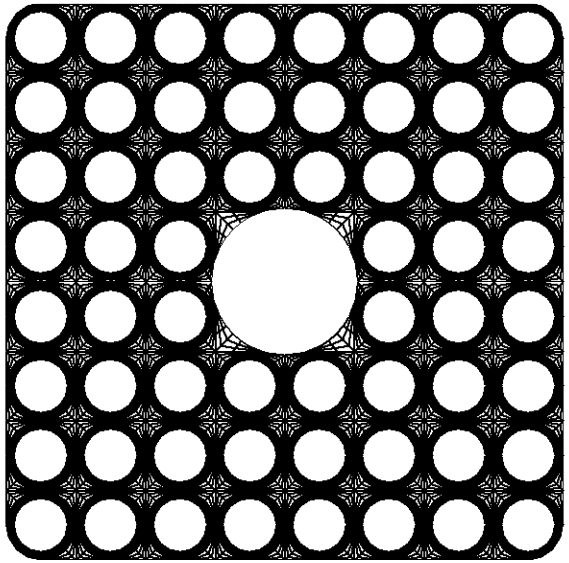


# Two-Phase CFD Simulations
# OECD-NEA/US-NRC NUPEC BFBT Benchmark

- Benchmark based on NUPEC BWR Full-size Fine-mesh Bundle Tests (BFBT)
  - Full-height, heated 8 pin by 8 pin assembly tests
  - Distributed radial profile
  - Temperature, pressure and detailed void distribution measurements



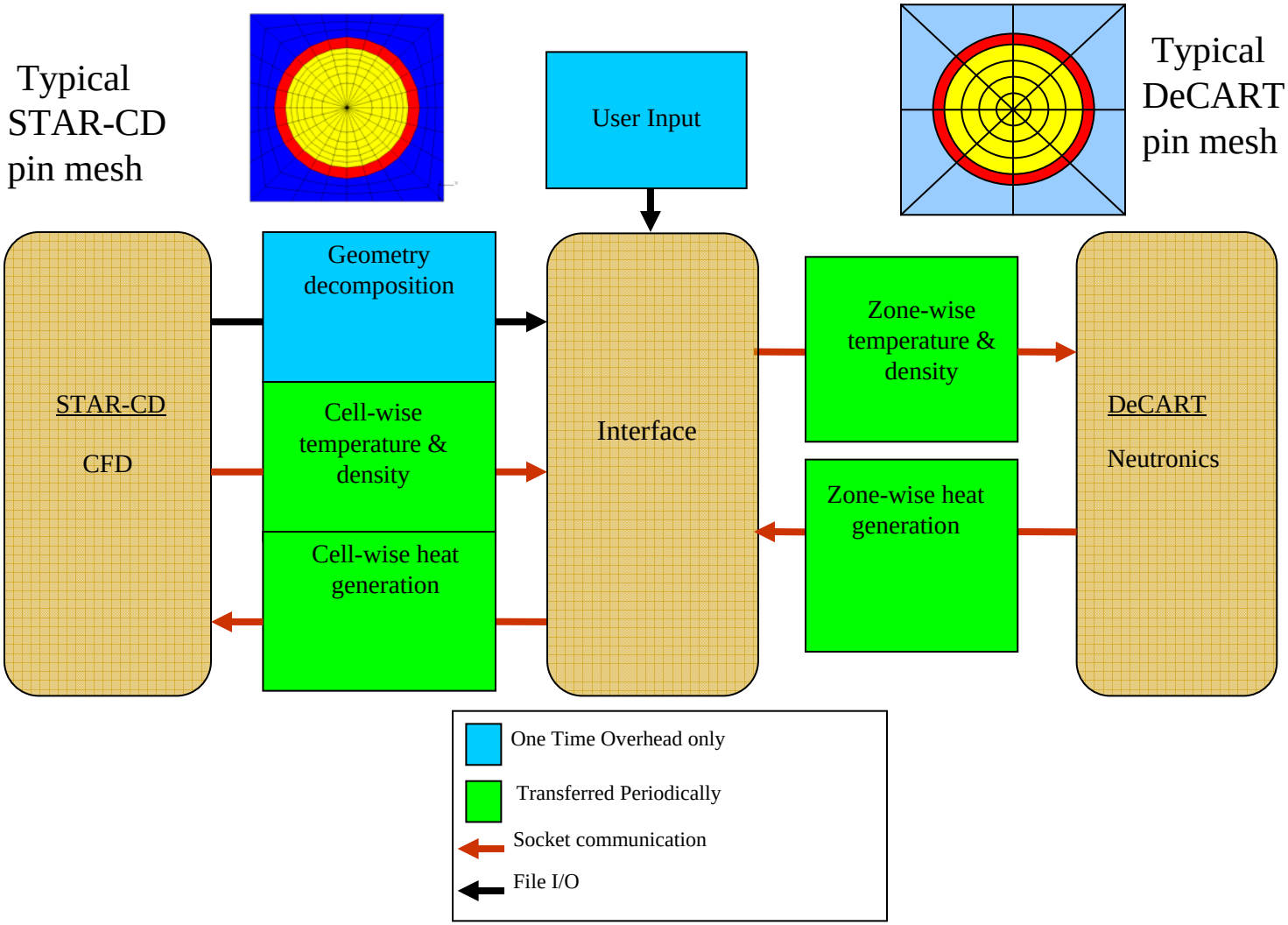



# Summary of 2-phase CFD Research

- Assembly level two-phase boiling with STAR-CD bubbly flow model (Completed)
- Extended flow regime models in STAR-CD (Ongoing)
- Experimental Validation of the STAR-CD two-phase boiling models (Ongoing)
- Coupled Code Applications under BWR Operating Conditions (Initiated)

# Coupling Mechanics: Interface Design

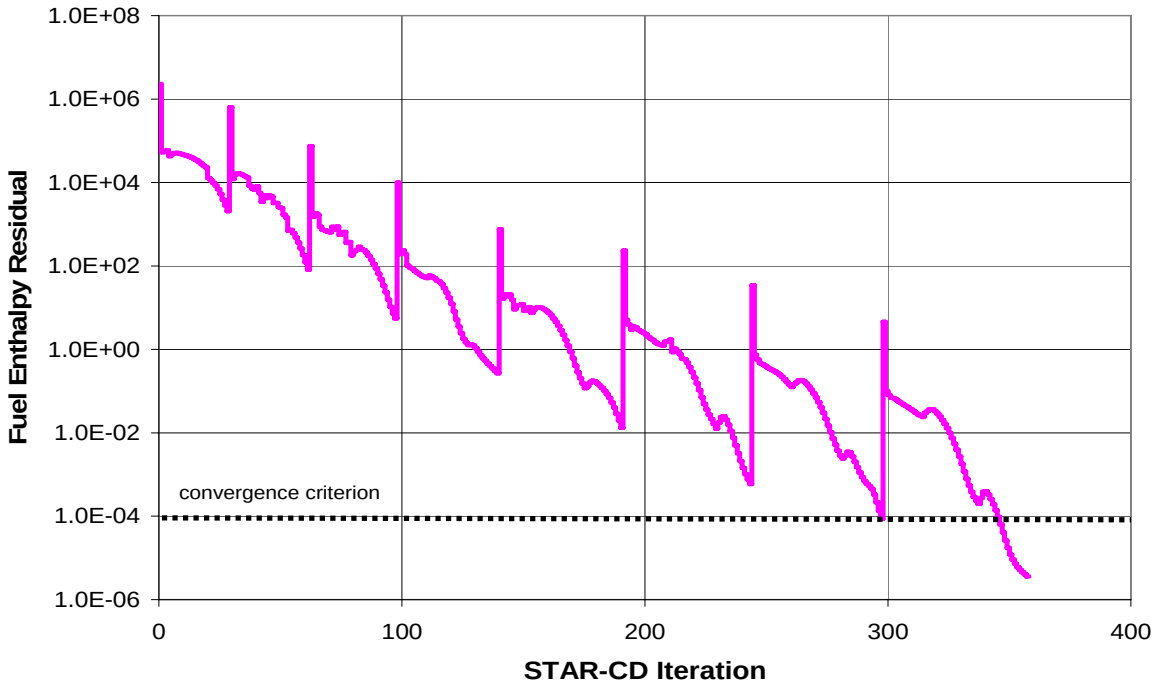


# Convergence of Coupled Calculations

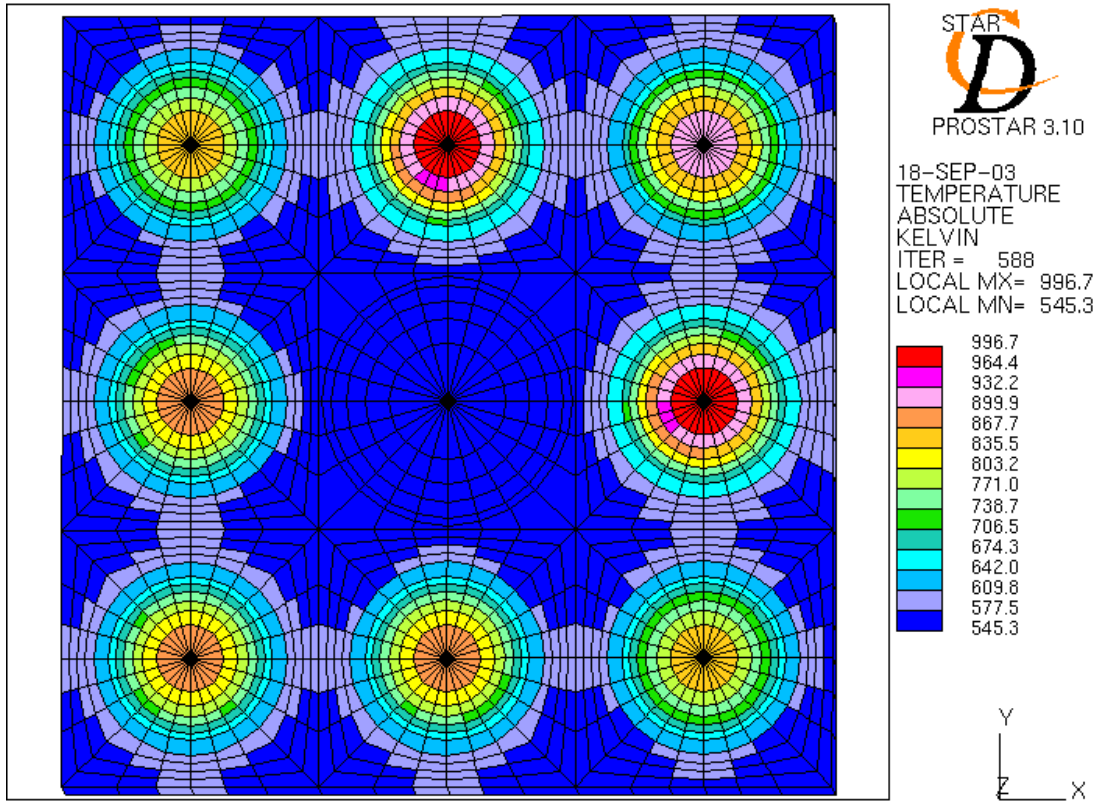
- **Two important convergence criteria tracked:**
  - **DeCART side: change in the power distribution between consecutive data exchanges:**

$$\|q\| = \max_{izone} \left\{ \frac{\left| q_{izone}^{k} - q_{izone}^{k-1} \right|}{q_{izone}^{k}} \right\}$$

  - **STAR-CD side: fuel enthalpy residual, computed internally each CFD iteration**



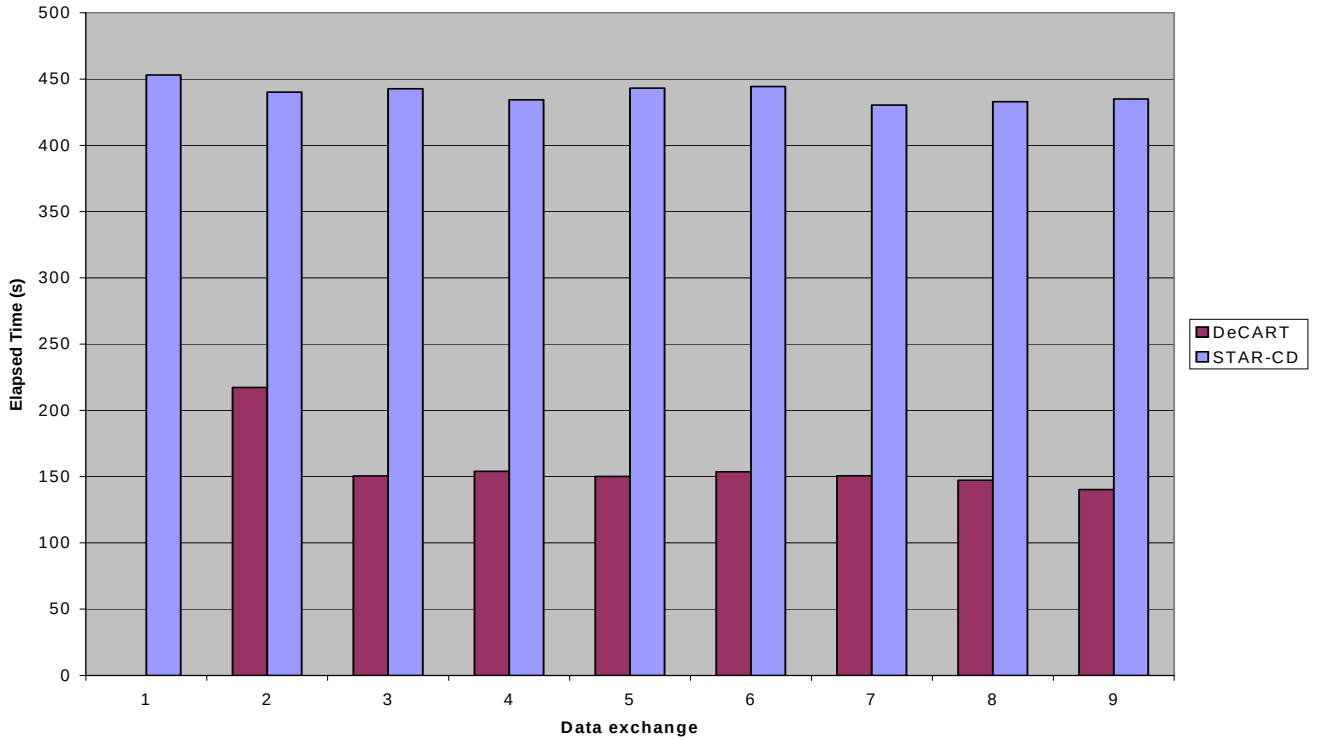
# 3 x 3 Pin Array Model: Results




**Midplane Temperature Distribution**

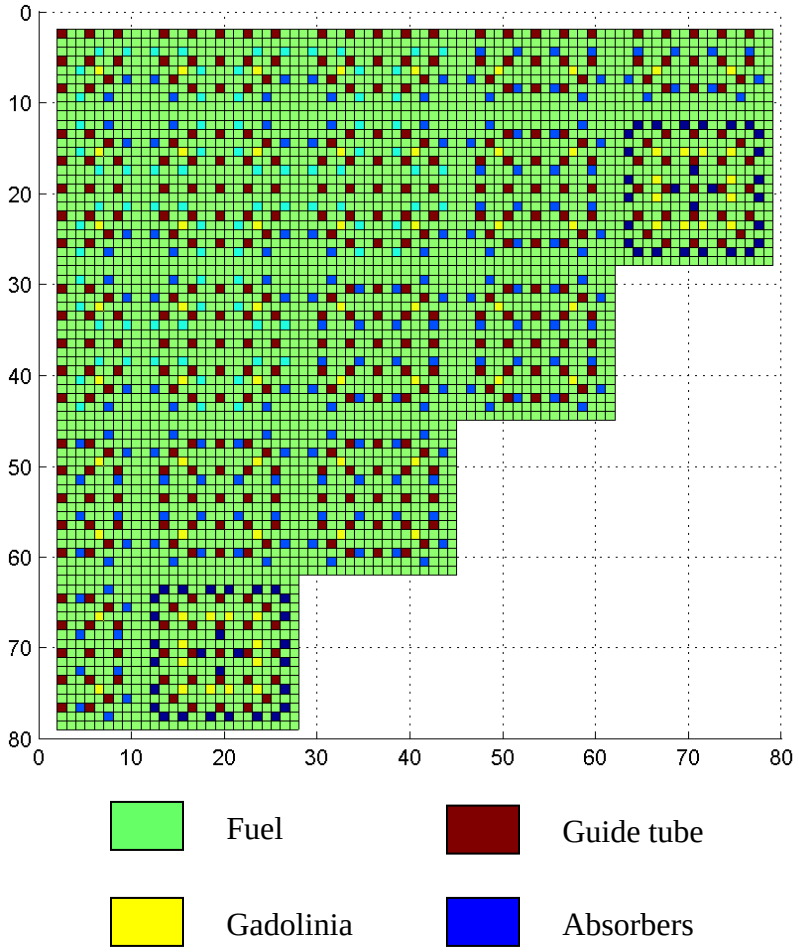
# Test Problem Timing

- STAR-CD:
  - 24 processors
  - ~207,000 mesh/processor
  - Manual decomposition (4 x 6)
- DeCART:
  - 12 processors
  - ~13,000 mesh/processor



# Coupled DeCART/STAR-CD

- 3D Model of Small PWR
- DeCART discretization: (1/4 core)
  - 3½ million flat flux regions in DeCART
  - 45 energy groups
  - 8 azimuthal & 4 polar angles in 90°.
- 70 million cells in STAR-CD (uses 1/8 core segment).



# Small LWR Core Calculation

- Coupled DeCART/STAR-CD calculations have been performed on the ANL Beowulf cluster *jazz:*
  - **24 processors for DeCART** (10 million flat flux regions)
  - **104 processors for STAR-CD** (70 million CFD cells).
  - 1 processor for the external interface.

- Steady-state calculations required **~5-6 hours** (not yet optimized)

# Summary of NNR Research

- The Numerical Nuclear Reactor (NNR) provides an integrated, high fidelity analysis capability for PWR applications
  - Verification and validation of phenomenological modules was successful
  - Computational burden is high and needs to be reduced
    - Parallel computing
    - More sophisticated coupling: Matrix-Free Newton Krylov
  - Extensions of NNR models and methods are now underway for application to BWRs
- The Numerical Nuclear Reactor code system forms a foundation for adding important phenomenology to the analytical tool
- **EPRI currently supporting application to important practical issues for LWR operation (e.g. crud deposition analysis)**

# The “Next” Next Generation*

- Neutronics
  - 3D Transport (Kevin Clarno et al)
  - 3D MCNP + Massively Parallel computing ☺
- Thermal-Hydraulics
  - Interfacial Area Transport (e.g. explicit modeling of bubble-bubble interactions)
- The “Grandest Nuclear Challenge”
  - Improved Nuclear Fuel Performance Modeling
  - Coupling to of Neutronics/TH to Fuel Performance Code

* >3-5 years

Thanks for you attention!

# Questions?