ICENES 2007
03 - 08 June 2007
Istanbul - Turkey

REACTOR SIMULATIONS WITH COUPLED MONTE CARLO AND COMPUTATIONAL FLUID DYNAMICS

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June 5th, 2007

Outline

- Motivation
- McSTAR Code
- Cross-section update methods
- Tally Calculations
- Code Features
- Test Problems
- Results and Conclusions

Motivation

- To demonstrate the feasibility of coupling Monte Carlo with Computational Fluid Dynamics for reactor applications.

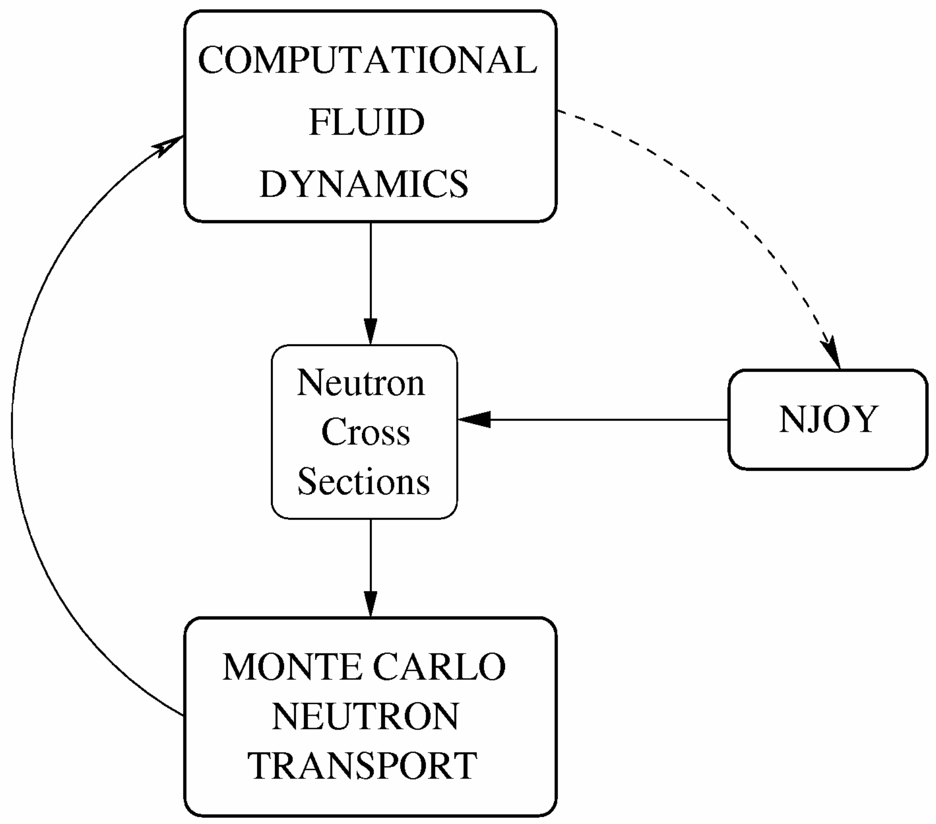
- To utilize Monte Carlo methods to validate the coupled deterministic neutron transport and CFD solutions

High-Fidelity Reactor Modeling

- Numerical Nuclear Reactor (NNR):
  - ANL/KAERI INERI 2001–04;
    - Whole-core discrete integral transport
    - Computational fluid dynamics
    - Structural thermo-mechanics
  - DeCART / STAR-CD Coupled Code
    - Neutronics: Integral Transport (MOC)
    - Thermalhydraulics: Computational Fluid Dynamics
- Previous Research on Monte Carlo w/ Feedback (McCARD – SNU; used to validate DeCART)

McSTAR

- Monte Carlo Neutron Transport : **MCNP5**
- Computational Fluid Dynamics : **STAR-CD**
- Cross Sections: **NJOY**



McSTAR's Principal Components

MCNP-5

- Eigenvalue calculation
- Power density through tallies
- Continuous energy neutron cross sections with thermal scattering data

NJOY

- Cross section generation at specific temperatures
- Thermal scattering data at specific temperatures

STAR-CD

- 3-D Thermal Hydraulics calculation.
- Employ user subroutines for data exchange

Challenges

- Cross-section update methods
- Tally calculations
  - Determining neutron histories necessary to achieve an acceptable standard deviation for each problem
  - Techniques to increase the accuracy but keep the computational burden reasonable
- Coupling efficiency and computation speed

Cross-section update methods

- Three possible methods:
  - **Method 1:** Running NJOY after each STAR-CD calculation to generate cross-section for any new temperatures obtained.
  - **Method 2:** Generating cross-section libraries with an increment of between 25K - 50K and interpolate data between.
  - **Method 3:** Generating cross section libraries with a smaller increment of temperature (e.g. 2-5K), and using the data generated closer to that temperature.

Method 1

- Most accurate of all three.
- If the number of nuclides and temperature range of the problem is small can be practically applied.
- For practical reactor applications;
  - Excessive amount of computation time is required.
    - For U-235 an NJOY99.161 run (BROADR + ACER) takes about 95 seconds on a 3Ghz P4 Linux computer.
  - May cause memory problems in the MCNP calculation.

Method 2

- The only accuracy loss attributable to interpolation.

	325 K (NJOY)	325 K INT. (300-350K)	Deviation
k_{eff}	1.40974 (± 0.00043)	1.41008 (± 0.00044)	**34 pcm**
Cell flux	1.37933 (± 0.0003)	1.37929 (± 0.0003)	**0.00003**
ABS*F	3.67362e-03 (± 0.0006)	3.67648E-03 (± 0.0006)	**0.0008**
FIS*F	5.62964e-03 (± 0.0007)	5.63817E-03 (± 0.0007)	**0.0010**
NUF*F	1.38341e-02 (± 0.0007)	1.38548e-02 (± 0.0007)	**0.0010**

Method 3

- Most practical method (used in McCARD – SNU).
- Has an inherent error depending on the size of the temperature increment.
- Small increment sizes (1-2 K) causes memory problems in the MCNP calculation.

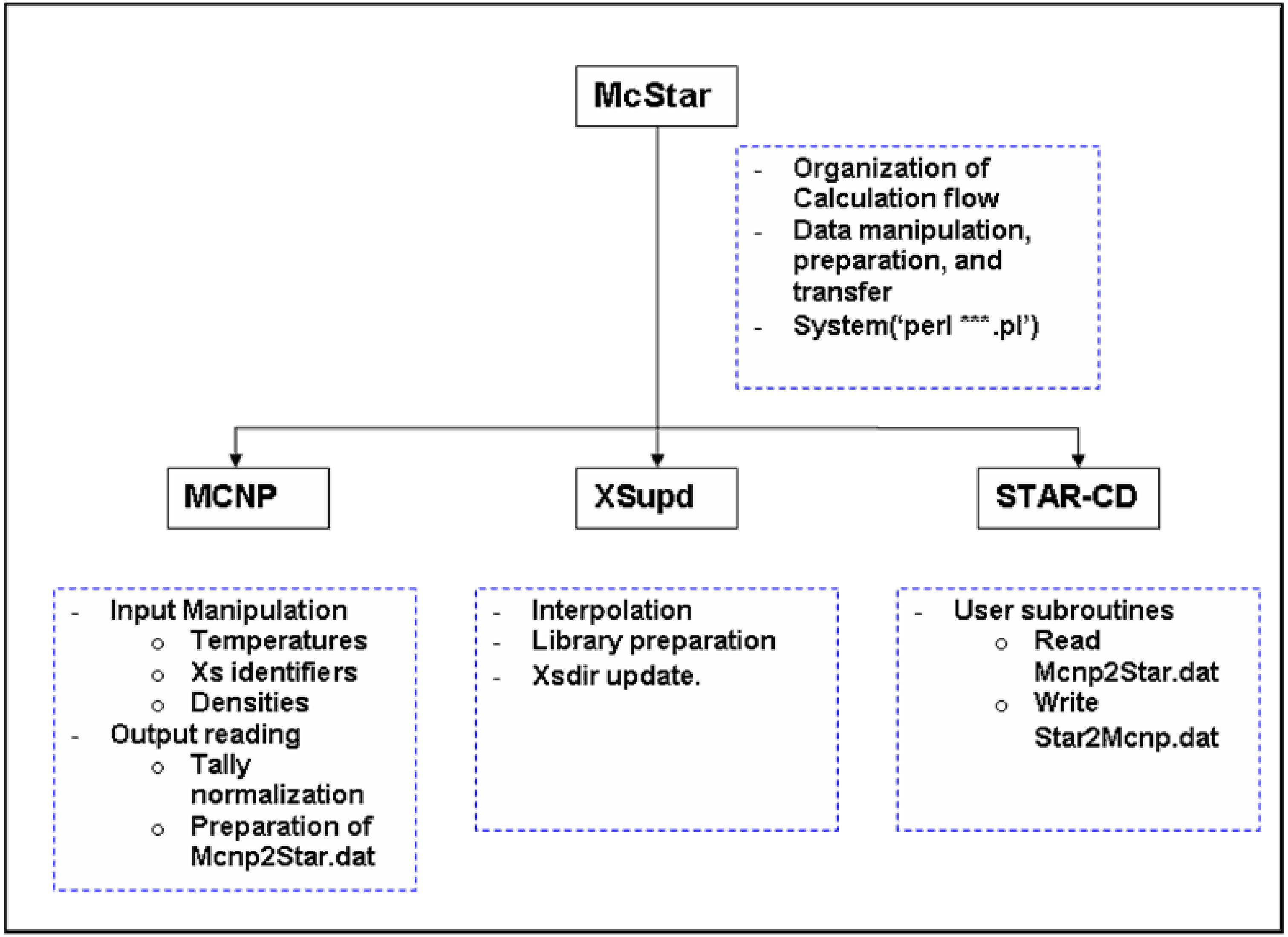
Tally calculations

- A detailed analysis should be done to determine the required number of histories for the problem.
- The use of pre-generated fission source distribution reduces the amount of necessary cycles.
- Methods to optimize the required number of histories and cycles is subject of ongoing research.

Code Features

- McSTAR is written in FORTRAN90 program language.
- It utilizes two PERL scripts that executes MCNP and STAR-CD and performs some database operations before and after their execution.
- Other functions: Input manipulation, library generation, data exchange, mapping, etc..

Calculation Scheme

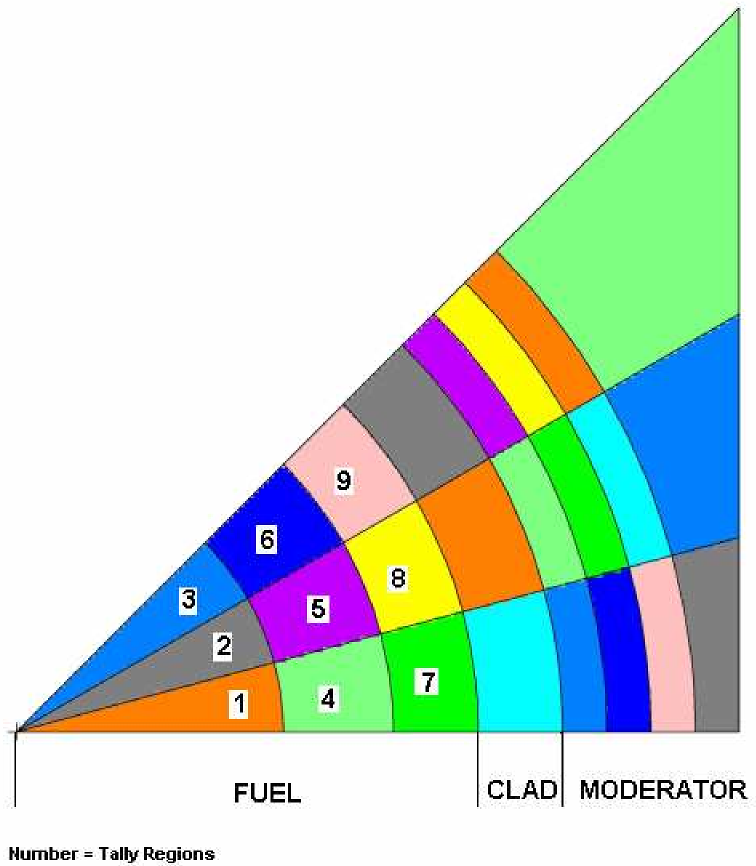


TEST PROBLEMS

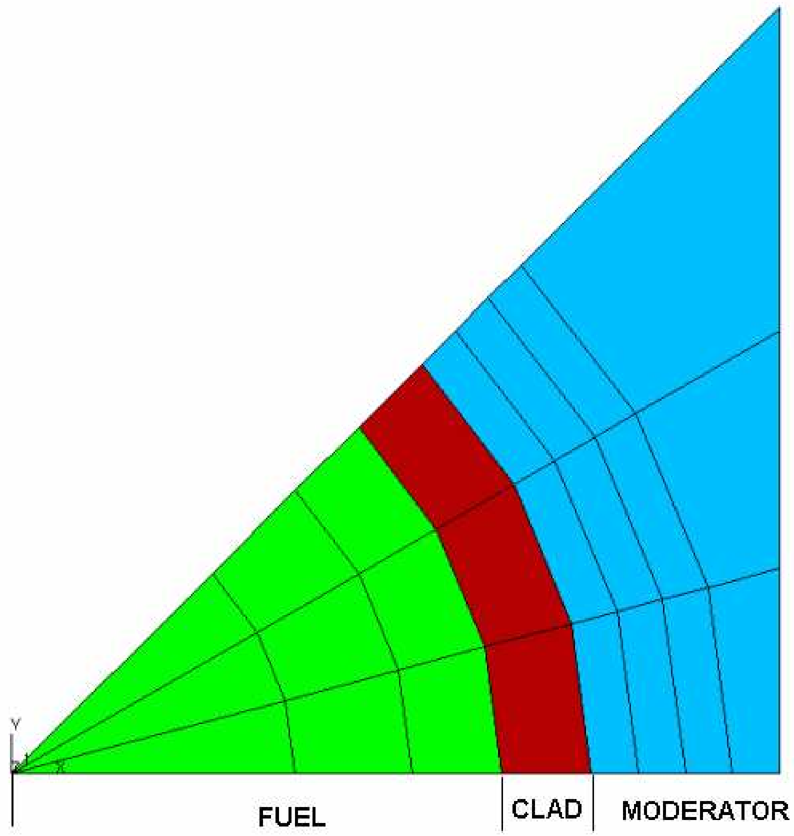
Problem 1: A 3D PWR Pin Cell

- pin-cell model includes a UO_2 fuel pin with the surrounding coolant and moderating water.
- 1/8th symmetric 3D model
- The active fuel is 200 cm in height and with 20 cm of water above and below the active fuel.
- The cladding is zircaloy and the moderator is liquid water.

MCNP and STAR-CD Models



MCNP MODEL

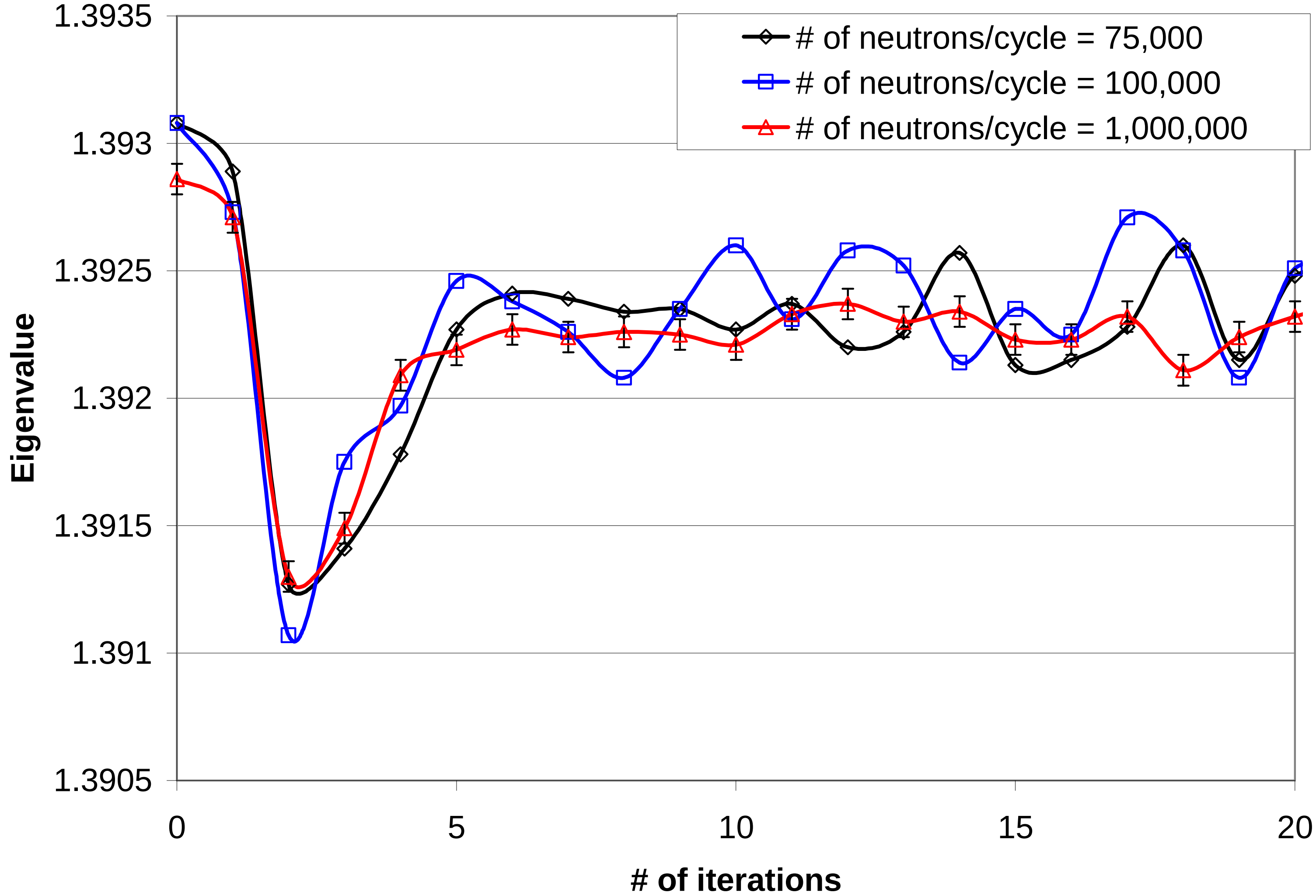


STAR-CD MODEL

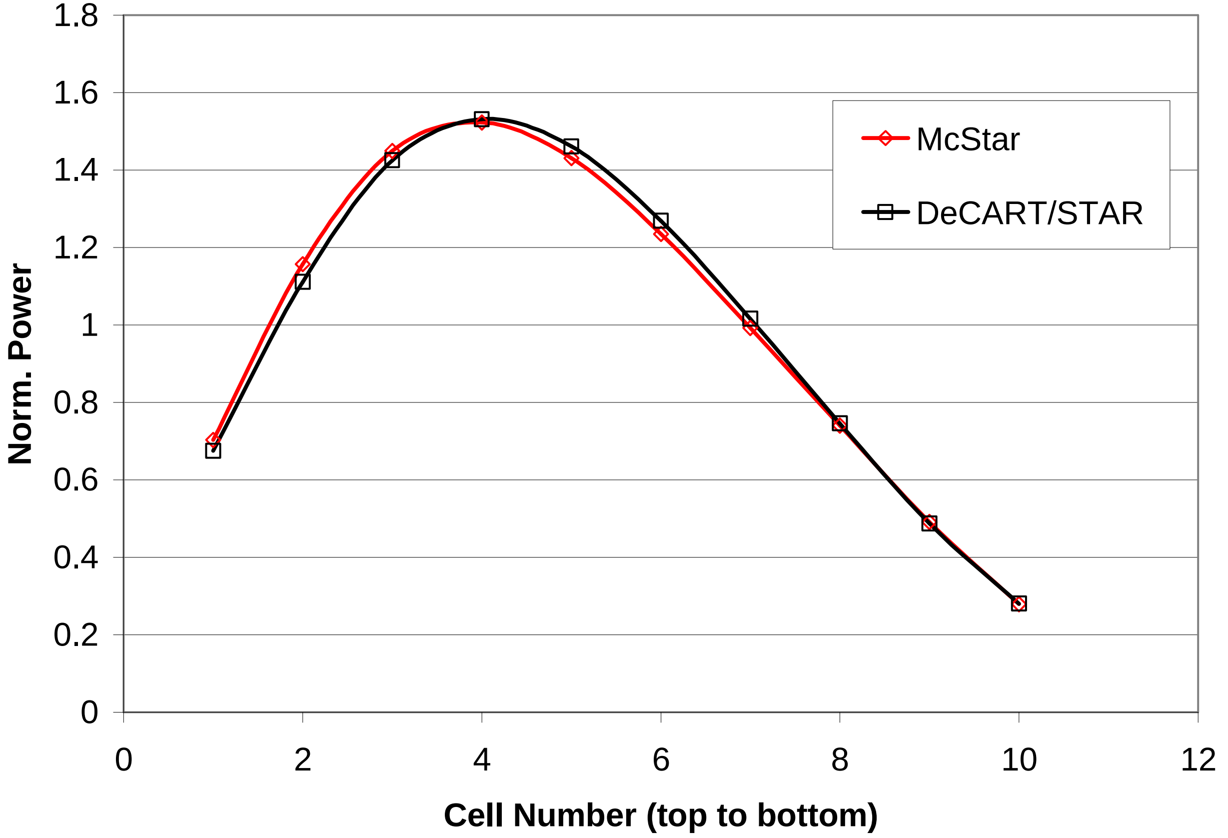
Cont…

- STAR-CD model consists of 24 radial cells, 9 of which are in the fuel region and 600 axial cells.
- Number of radial cells are consistent in the STAR-CD and MCNP models.
- for simplicity the number of axial cells was reduced to 12
- All the fuel cells in the MCNP model are tallied to extract the power density

Parametrics on # of histories



Results

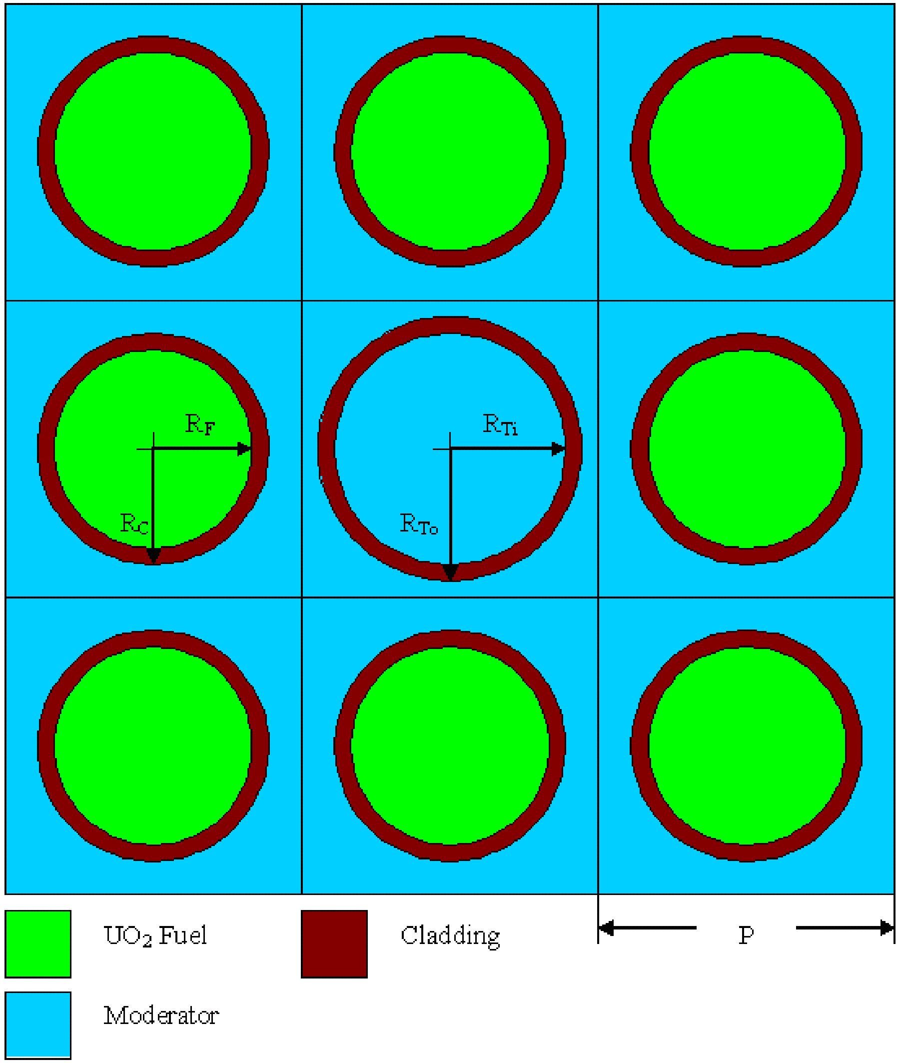


Codes	k_{eff}
McStar	1.39224 (±0.00006)
Decart/StarCD	1.39276 (+52 pcm)

Problem 2: A 3x3 Array of PWR pins

- 8 fuel UO2 fuel pins and a guide tube in the center
- 200 cm active fuel height
- 20 cm water reflector at the top and bottom
- Cladding: Zircaloy
- Moderator: Liquid water

Geometry of Problem 2

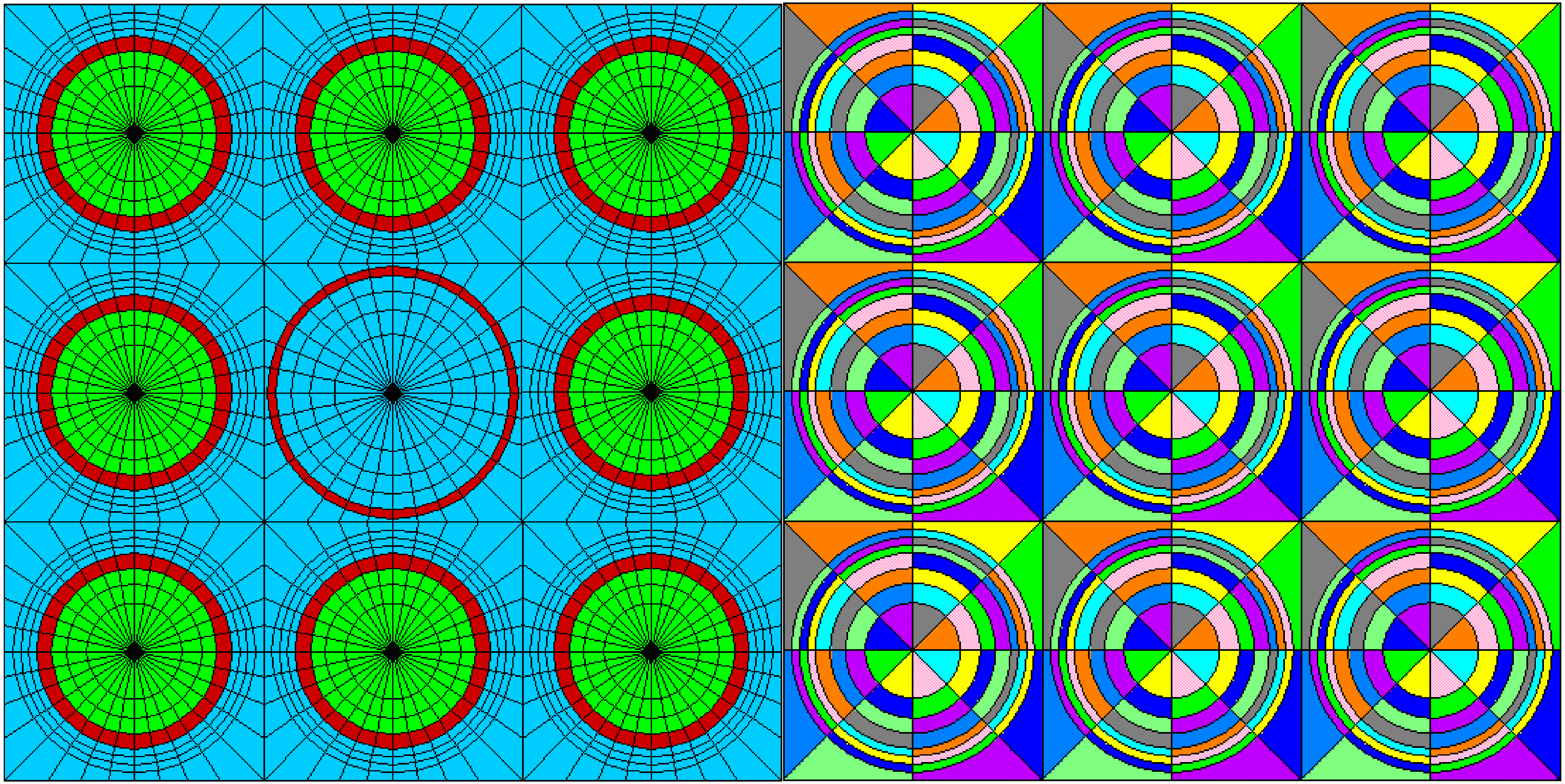


R_F	Fuel pellet radius	0.4025 cm
R_C	Cladding outer radius	0.4759 cm
R_{Ti}	Guide tube inner radius	0.5709 cm
R_{To}	Guide tube outer radius	0.6130 cm
P	Cell pitch	1.2600 cm

STAR-CD and MCNP Models

- STAR-CD
  - 600 axial planes, 32 azimuthals, 8 radial rings (6 rings in the guide tube)
    - **1344000** CFD cells
- MCNP
  - 12 axial planes, 8 azimuthal, 8 radial rings (6 rings in the guide tube)
    - **6720** MCNP cells (**1920** Tally regions)

STAR-CD   MCNP



RESULTS

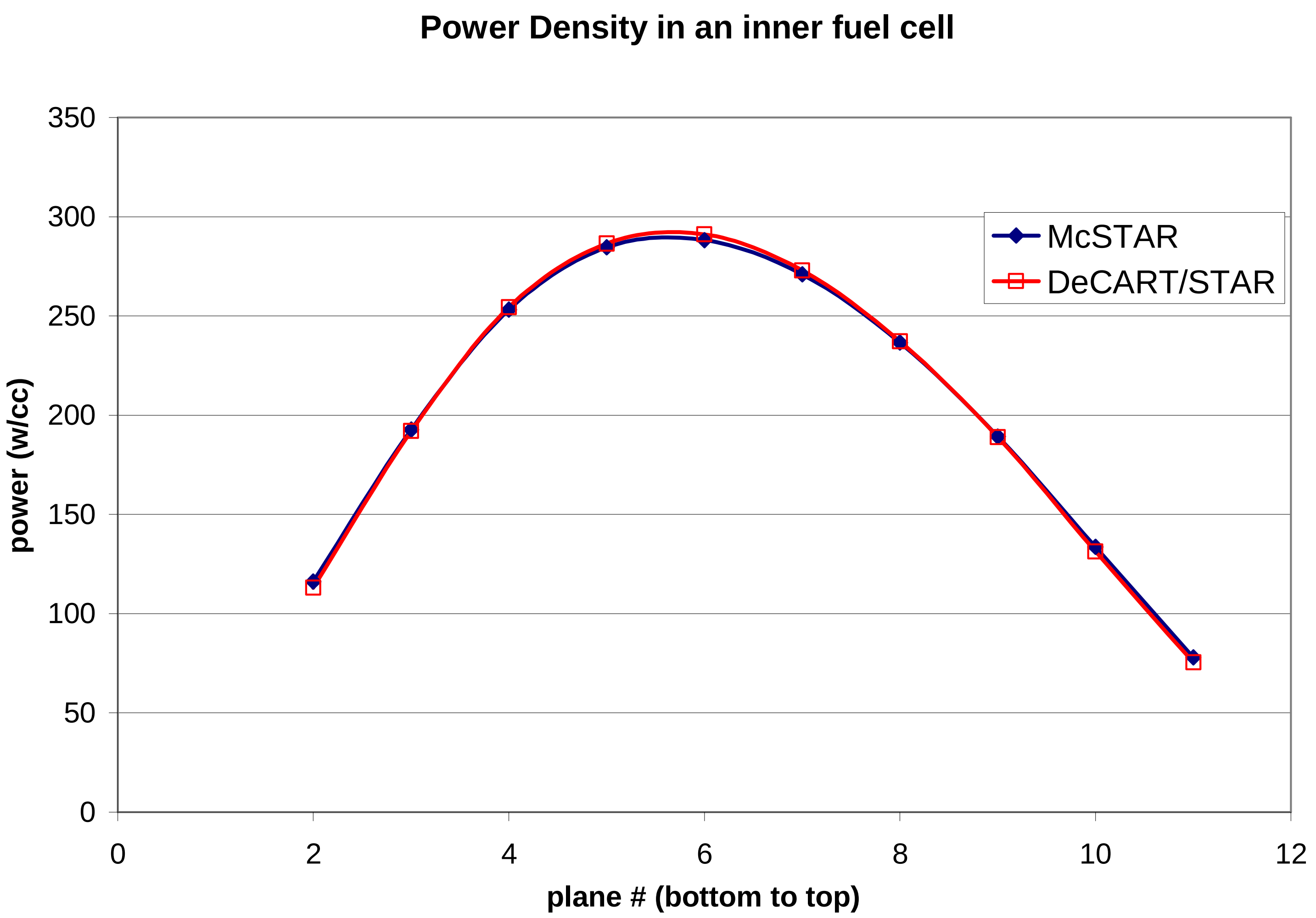
Eigenvalues at fixed temperature

CODE	**k_{eff} (3x3 pins) @300C**
MCNP	1.42852 (±0.00006)
DeCART	1.42778 (-74 pcm)

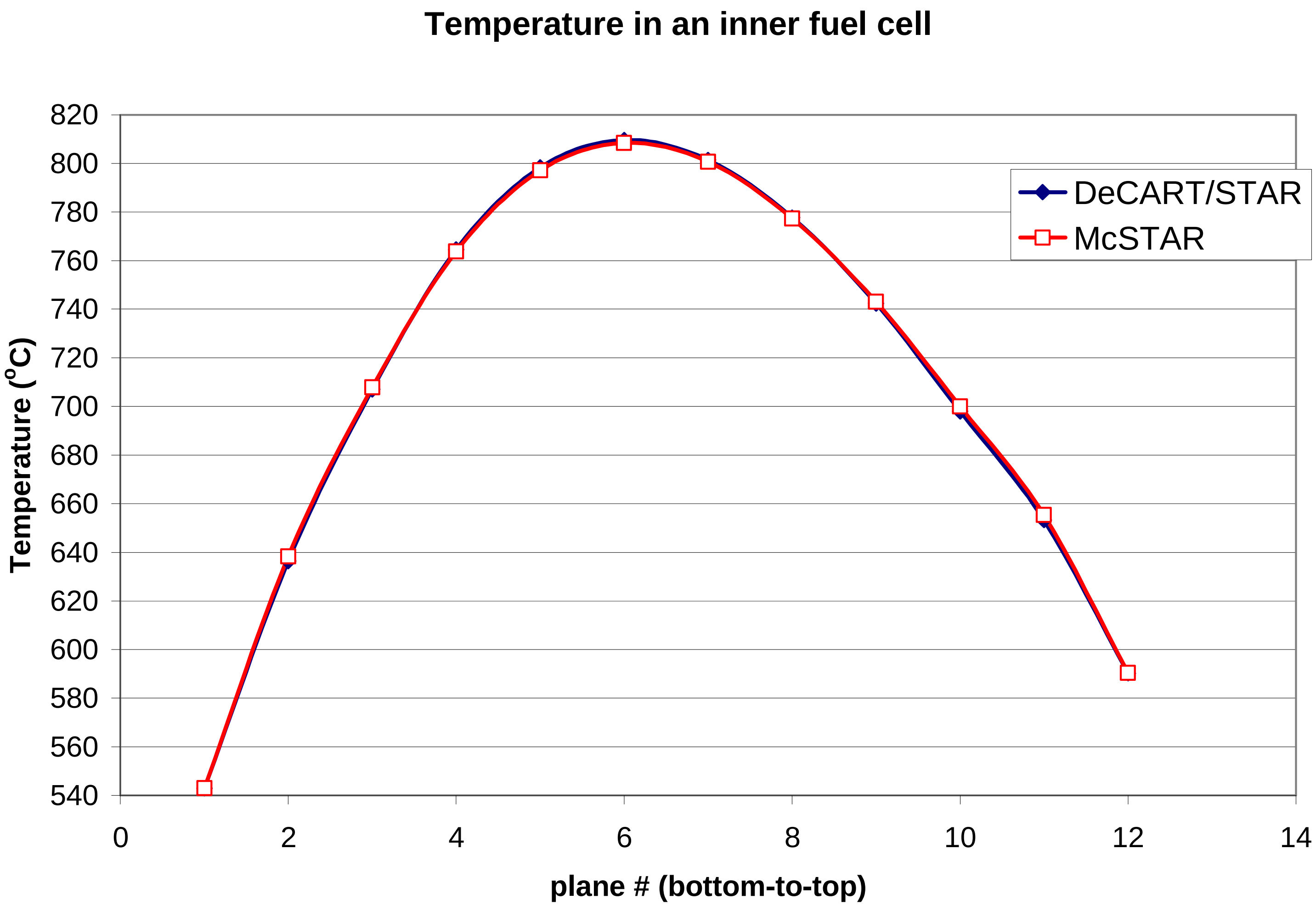
Eigenvalue comparison for Problem-2

CODE	**k_{eff} (3x3 pins)**
McStar	1.41555 (±0.00006)
DeCART/STAR -CD	1.41489 (-66 pcm)

Cont … (Results)



Cont … (Results)



Some Remarks

- The difference in eigenvalues is consistent with those obtained at constant temperature

- The maximum power density difference between MCNP and DeCART at constant temperature is about **3.2%** which is similar to the accuracy of the power density with a variable temperature which is about **4%**

Calculation Run-Time

- Problem 1:
  - MCNP: 1M histories
  - a total run time of 28 hours was required on 30 nodes with 3.4 GHz Pentium 4 processors on the ANL *Reserv* linux cluster

- Problem 2:
  - MCNP
    - 500000 n's per cycle, 250 cycle (50 inactive + 200 active), 100M histories
  - STAR-CD
    - Convergence criterion = 10^{-5}
  - The total runtime for 12 iterations was about 100 hours 30 compute nodes of Purdue University's *Hamlet* linux cluster 3Ghz Pentium 4 processors with 2 GB memory

Conclusions

- A methodology was developed to couple the Monte Carlo code MCNP5 to the Computational Fluid Dynamics code STAR-CD.
- The preliminary results for two simple PWR test problems demonstrate the feasibility of coupling Monte Carlo to CFD.
- Preliminary validation of the cross section update methodology was performed to assess the accuracy of the 5K increment tables for these problems.

Cont … (Conclusions)

- The principal role for Monte Carlo based coupled methods will be as an audit tool for specific problems

- McSTAR is now being applied to advanced BWR fuel assemblies with strong axial heterogeneities to verify the accuracy of the 2D/1D solution methods in DeCART