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Radiation Transport on Unstructured Grids: the Long Journey Towards a Place in the Sun

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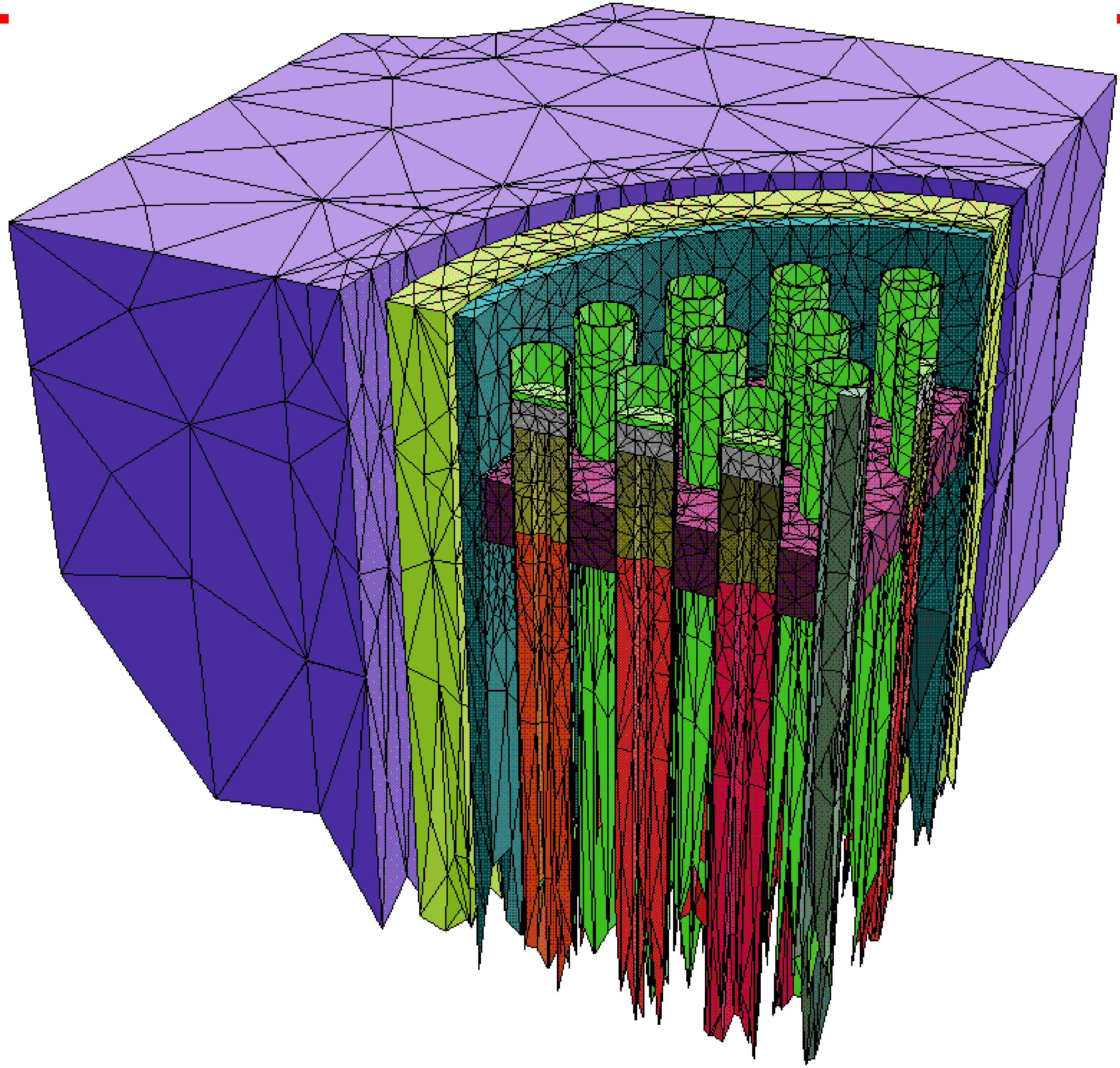
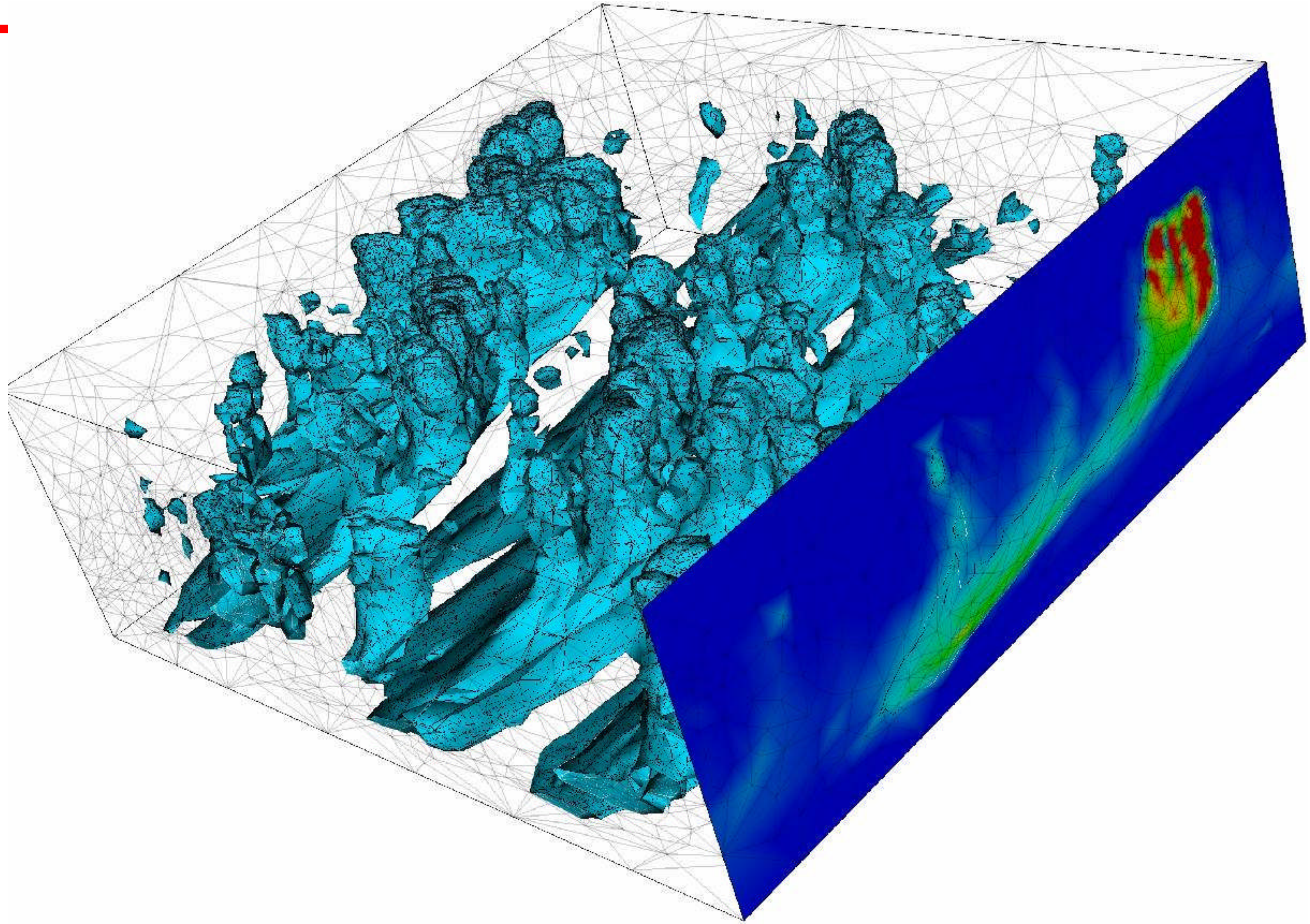
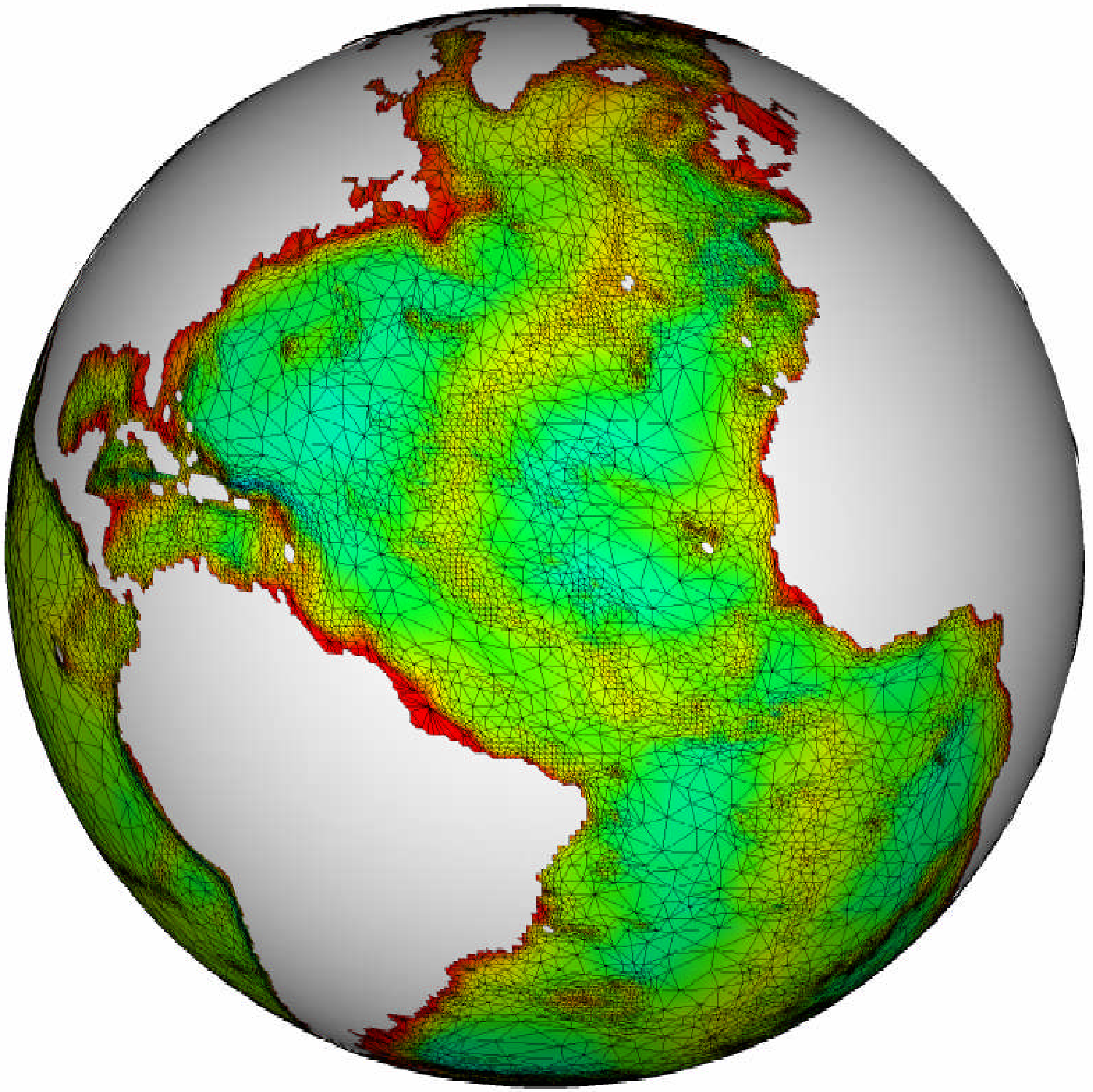
Advanced gas-cooled reactor model



Cloud field radiative transfer model



Global ocean circulation model



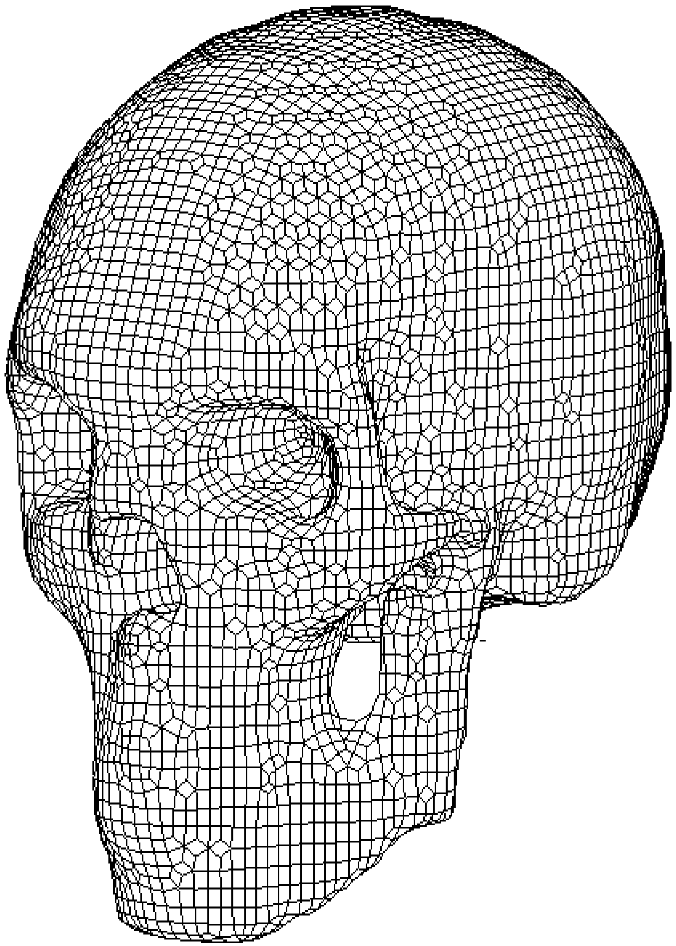
Preamble

- Duty of methods developers is to give back physics to physicists $\longrightarrow$ adaptive methods
- Emphasis now is on coupling of different physical phenomena
- Expectation from numerical simulations is not only to describe, but also help to prescribe and understand

Outline

- Background/motivation for unstructured RT methods
- The FE-P_N method
- Research issues
- Example of applications
- Solution adaptivity
- Summary

To be or not to be ….



a Legolander….

Motivation for Unstructured Grid RT Methods

- Monte Carlo is the reference method of solution for radiation transport and radiative transfer problems.

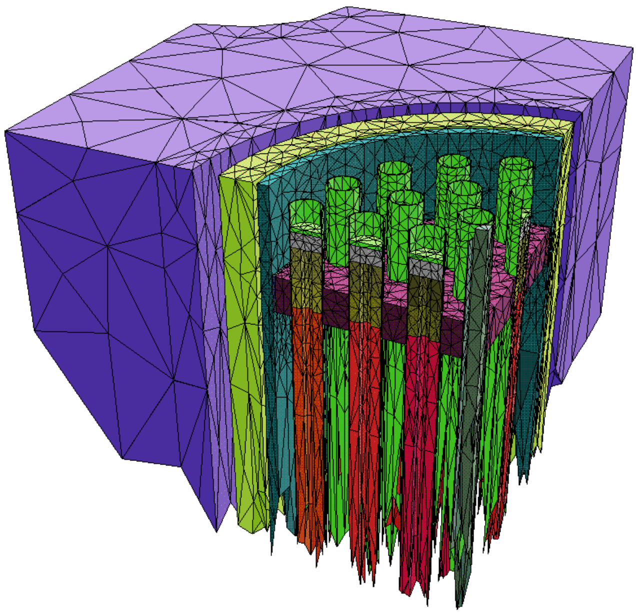
- It is conceptually simple and capable of handling geometrically complex problems. (No one gets fired for using MCNP… actually you get hired…)

Motivation for Unstructured Grid RT Methods

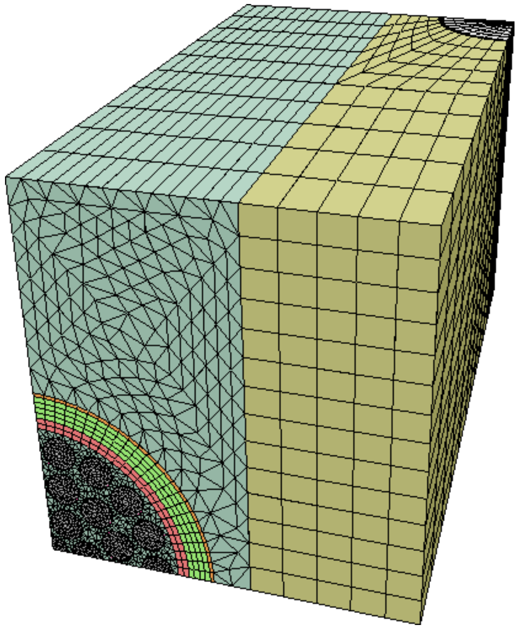
- There are drawbacks, however, with MC:
  - build-up of statistics can be very slow
  - user unfriendly results
  - lack detailed solution maps
  - poor multiphysics coupling

- Unstructured deterministic transport methods are potentially capable of alleviating (some of the) above drawbacks. However, methods are pitched here as complementary to MC

Unstructured Grid RT Methods – Complex Geometries



AGR fuel assembly



CANDU fuel assembly

ATR

Unstructured Grid Radiation Transport Methods - Status

- First-order form of radiation transport equation (ATILLA)
- Long- and Short Characteristics (HELIOS, DRAGON, NEWT)
- Second-order form of radiation transport equation (EVENT)

To do (20 years ago)

- 2D Meshing
- Multigroup anisotropic scattering
- In-core/out-of-core solver
- Vectorization

Computer HW background:

- 2Mwords (16Mbytes) RAM
- 100 Mflops

The Finite Element-Spherical Harmonics ($FE-P_N$) Method

- based on second-order form of transport equation

$$-\mathbf{\Omega}.\nabla\mathbf{G}\mathbf{\Omega}.\nabla\psi + \mathbf{C}\psi = \mathrm{S}^{+} - \mathbf{\Omega}.\nabla\mathbf{G}\mathrm{S}^{-}$$

- Ritz-Galerkin procedure using Finite Element Spherical Harmonics trial functions

$$\psi(\mathbf{r},\mathbf{\Omega}) = \sum_{e=1}^{E} \mathbf{B}^{eT}(\mathbf{r}) \otimes \mathbf{Q}^{T}(\mathbf{\Omega})\psi^{e}$$

$$\mathbf{Q}(\mathbf{\Omega})_{\ell m} = \sqrt{\frac{(2\ell+1)}{4\pi}(2-\delta_{\ell,0})\frac{(\ell-m)!}{(\ell+m)!}}\mathrm{P}_{\ell}^{m}(\mu)\begin{Bmatrix}\sin m\chi \\ \cos m\chi\end{Bmatrix}$$

The Finite-Element-Spherical Harmonics (FE-P_N) method

- FE-P_N characterized by explicit assembly and solution of coupled system of linear equations
- matrices are sparse, symmetric and positive definite
- scattering is treated implicitly
- no ray effects

FE-P$_N$ Equations

- Ritz-Galerkin procedure yields system of equations of the form:

$$A\psi = b \qquad A = \sum_{e=1}^{E} A^e$$

- The matrix A has a shell structure (for ℓ=0, 2, 4,…):

$$A = \begin{pmatrix} A_{11} & A_{12} & .. & A_{1N} \\ A_{21} & A_{22} & .. & A_{2N} \\ .. & .. & .. & .. \\ A_{N1} & A_{N2} & .. & A_{NN} \end{pmatrix} \qquad A_{ij} = \begin{pmatrix} a_{11} & a_{12} & .. & a_{1N} \\ a_{21} & a_{22} & .. & .. \\ .. & .. & .. & .. \\ a_{N1} & .. & .. & a_{NN} \end{pmatrix}$$

"Diffusion" matrix stencil

FE-P_N - Research issues

- fast solution strategies
  - algebraic and hierarchical solvers
  - angular and spatial domain decomposition methods

- ray-tracing for transparent/purely absorbing media

FE-P_N - Research issues (contd.)

- adaptivity in space, angle and time
  - most accurate results with least computational effort
  - end-user transparency
- parallel processing

Motivation for Improved Solvers

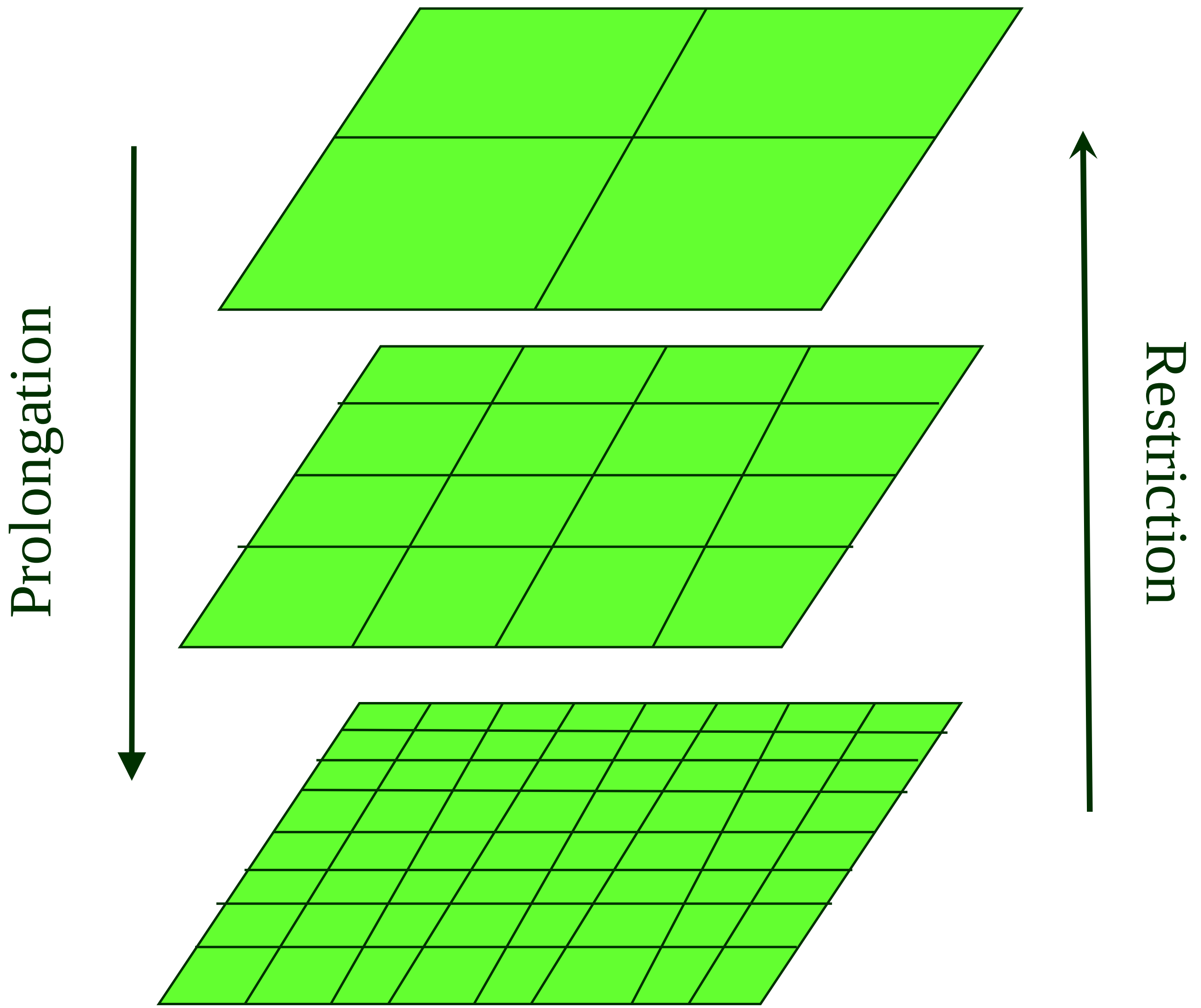
- Space+angle discretization gives rise to large systems of linear equations
- Multigrid/hierarchical solution methods have been shown to have optimal convergence properties (elliptical PDE's in space)
- FE-P_N framework specially suited for hierarchical solution methods in angle as well as space

Multilevel solution in space

- Geometric multigrid methods are very powerful techniques for the solution of linear systems of equations (hierarchy is given)

- Based on interplay between smoothing and coarse-grid correction

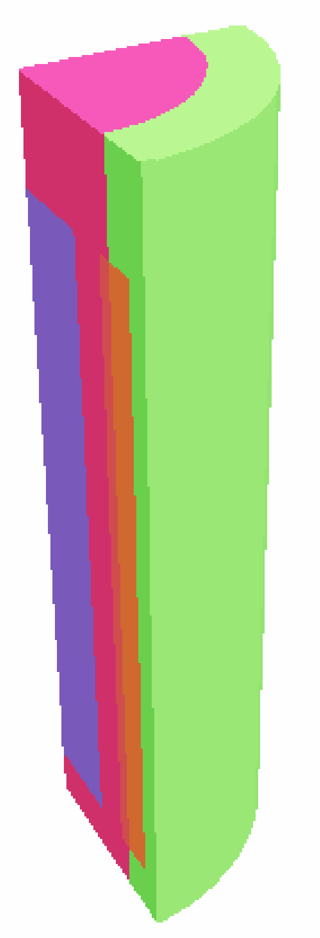
Multigrid method (for Legolanders)



Algebraic multilevel solution in space

- Unstructured grid methods require algebraic multilevel (AMG) methods
- Wholly based on matrix information (no hierarchy given)
- Automatically coarsen in directions which algebraically smooth error changes slowly

Test Problem 1



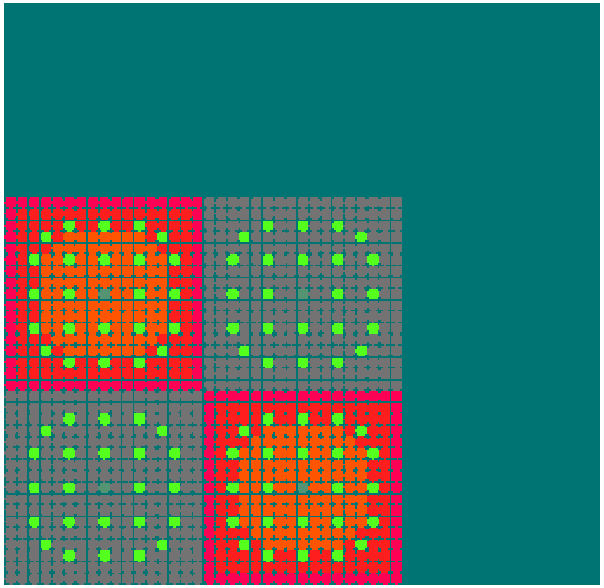
- TN-12 Shipping Cask benchmark problem.
- 22 groups, fixed source problem, with fission source.
- 3-dimensional, irregular grid. 12250 nodes in the system.
- Only P_1 approximation was tested.

Test Problem 1 results

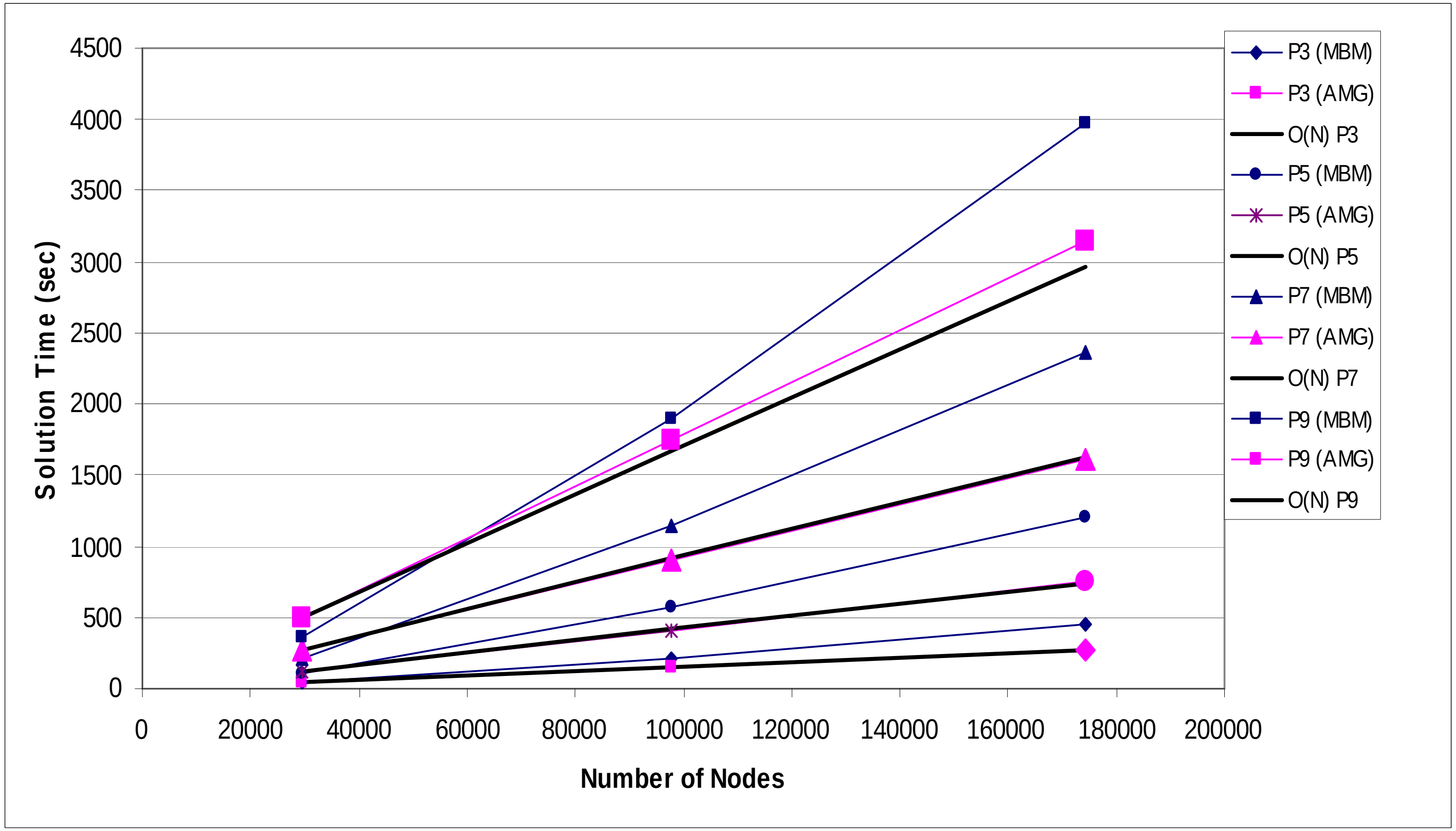
Method	# iterations	Solution time (sec)	Time per cycle (sec)
SSOR(1)/CG	20841	182.5	0.009
ILU(0)/CG	12524	110.6	0.009
AMG/CG	1686	57.7	0.034

Test problem 2

- 2D C5G7MOX benchmark problem
  - 4 fuel assemblies
  - Water moderator
  - 7 groups
  - Criticality problem



Solution time comparison for C5G7MOX test problem



AMG Findings (I)

- AMG/CG requires less number of iterations compared to both SSOR(1)/CG and ILU(0)/CG.
- AMG preconditioner is about 3-4 times computationally more expensive compared to ILU(0).
- AMG/CG reduces number of inner iterations 7-22 times compared to ILU(0)/CG
- If outer iterations exist (eigenvalue, upscatter, etc), AMG preconditioner becomes less effective. This is because preconditioning stage becomes prohibitively expensive compare to ILU(0) preconditioner.

AMG Findings (II)

- The scalability of the AMG preconditioner can be observed for the P_3, P_5, and P_7 cases and the solution time grows like $O(N^{\sim 1.04})$ for the P_9 case.

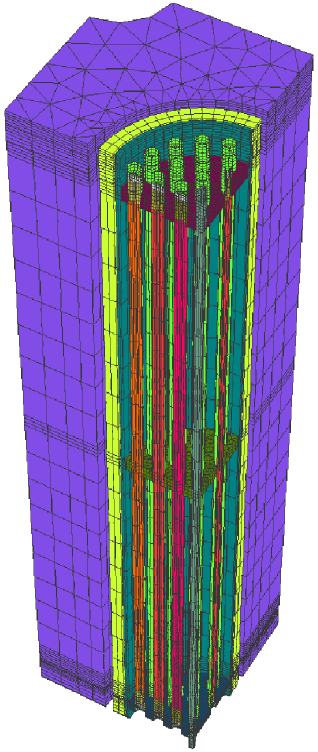
- The rate of the computational time grows like $O(N^{\sim 1.42})$ for the MBM preconditioner.

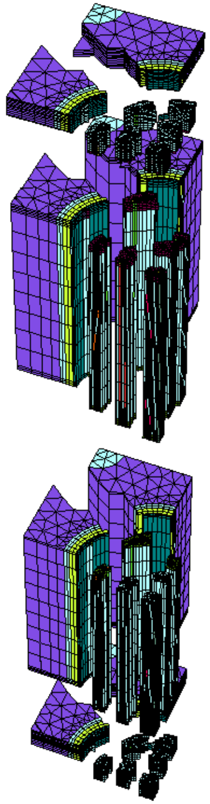
- This difference in the growth rate in the solution time indicates the advantage of the AMG preconditioner for the larger systems.

Parallel Processing

- Space+ angle discretization gives rise to large systems of linear equations
- Parallel processing has come to age
- FE-P_N framework specially suited for parallel domain decomposition methods

Domain Decomposition Example





3d AGR mesh decomposed into 32 subdomains

EVENT

➔ *Outgrowth of research into FE and P_N methods*

- 3D arbitrary geometry
- Arbitrary P_N approximations
- Multigroup anisotropic scatter
- Time-dependence

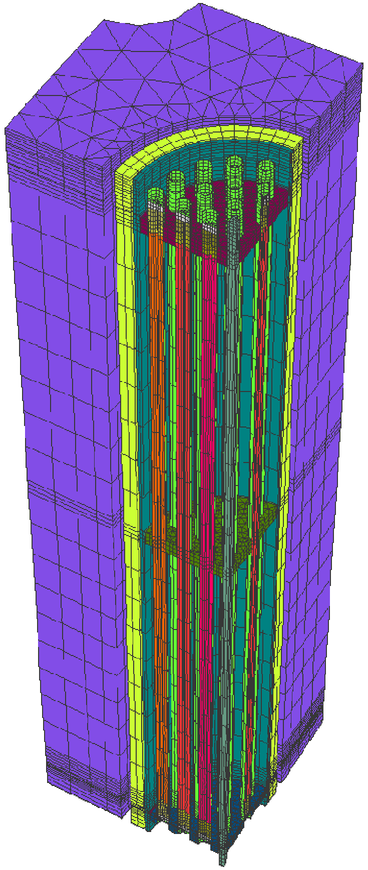
EVENT - Applications

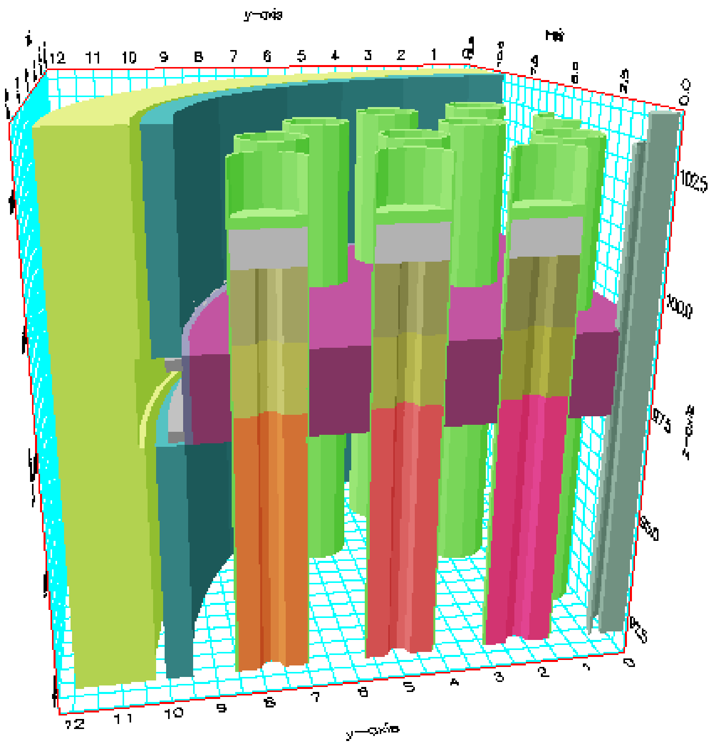
- shielding & criticality
- criticality assessment of fissile solutions
- near infrared optical tomography
- nuclear logging
- atmospheric & cloud physics
- medical dosimetry

Advanced Gas-Cooled Reactor (AGR) fuel assembly modelling

- Provide detailed flux distribution in fuel assembly
- Determination of K_{∞}
- Monte Carlo solution costly
- Characteristic methods not yet available/implemented in 3D

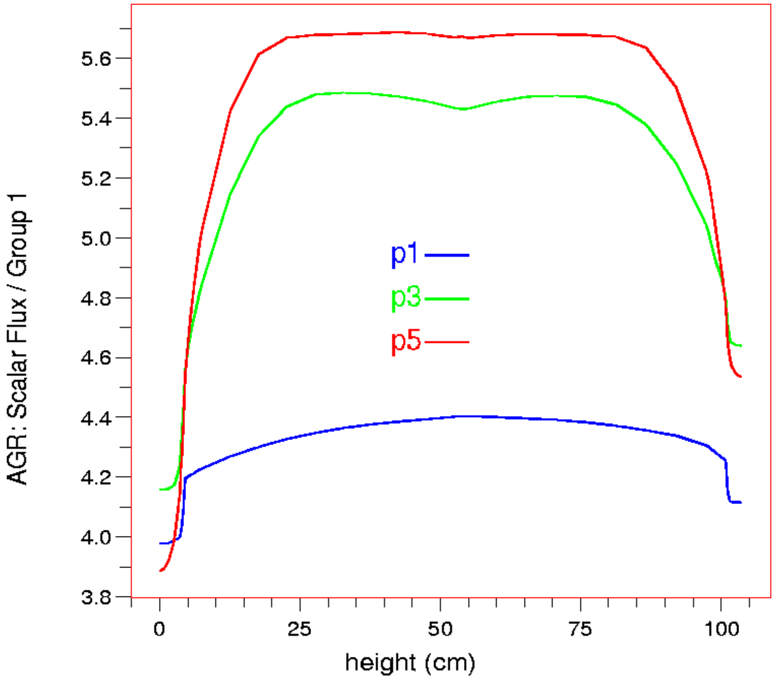
AGR Fuel Assembly

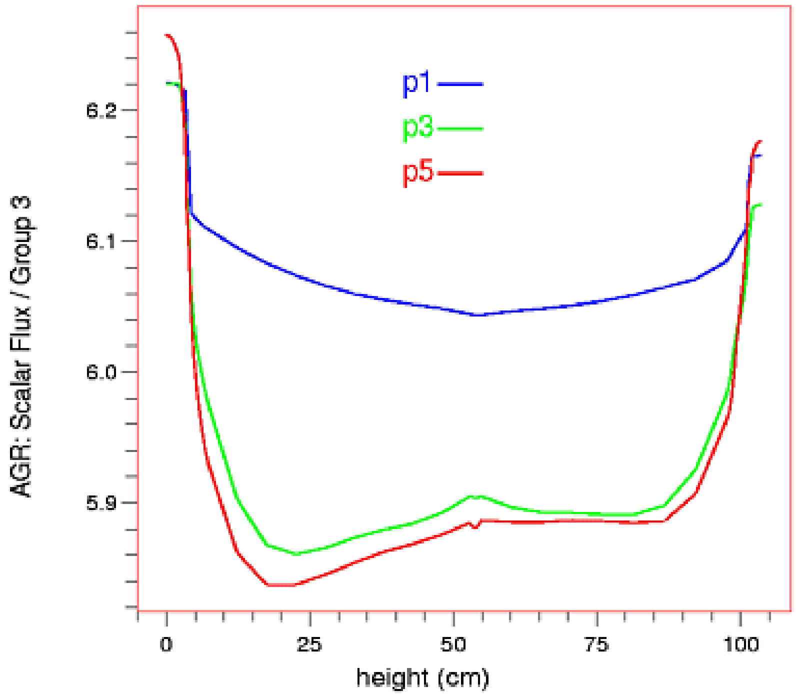




Top of central region of AGR element showing gadolinium rings (square x–s)

AGR Fuel Assembly results





Non-linear space-dependent kinetics

- Need for a fundamentally-based method
  - as a future resource for understanding complex criticality issues
  - to explore scenarios beyond range of experiment
- Emphasis on general geometry and multi-phase physics

Strategy for criticality modelling

- Coupled, transient neutronics/ hydrodynamics
- Allow geometrical flexibility through ‘finite element’ engineering modelling (*complex geometry*, *reflectors*, *liquid sloshing..)*
- As far as reasonably possible, fundamentally based modelling (*radiolytic gas equations linked with multi-phase equations involving pressure*)

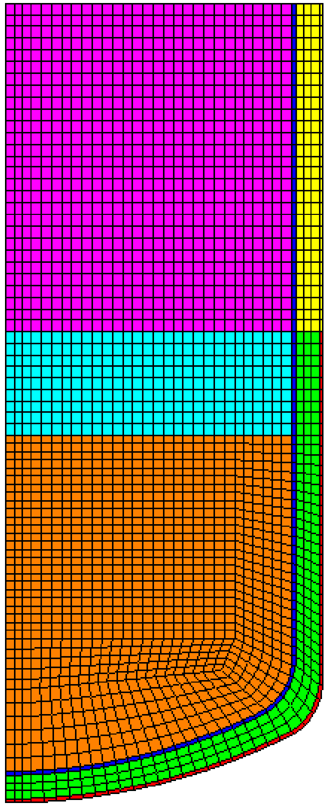
Modelling JCO Company Incident

- Used best available data
- Actual geometry including water jacket
- ‘Continuous filling’ while last beaker added
- multi-phase model for short times
- single phase model for longer criticality phase

JCO Accident scenario

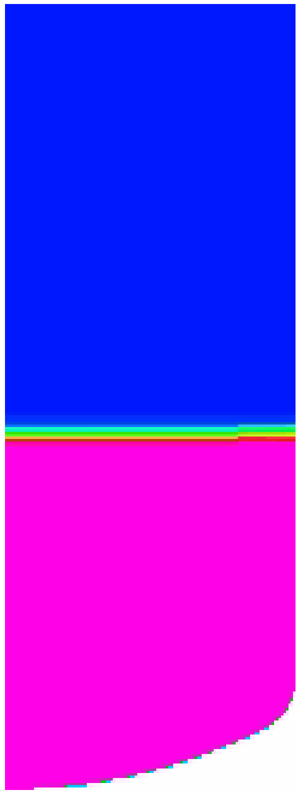
- Workers bypassed licensed fuel processing procedure
- Solution of Uranyl Nitrate with 18.8% enrichment (instead of expected 5%) carried in stainless steel buckets
- Total mass of uranium was 16kg (2.4kg limit)
- 7 batches of solution prepared, each batch divided into 2 beakers. Thus ‘intermittent’ continuous reactivity addition.

Geometry of JCO accident



RZ geometry finite-element mesh of the precipitation vessel

Simulation of JCO Accident



Animation of a step reactivity transient (of 2$)

JCO Simulation - Continuous Filling

Fission Rate for $0.375/s reactivity insertion

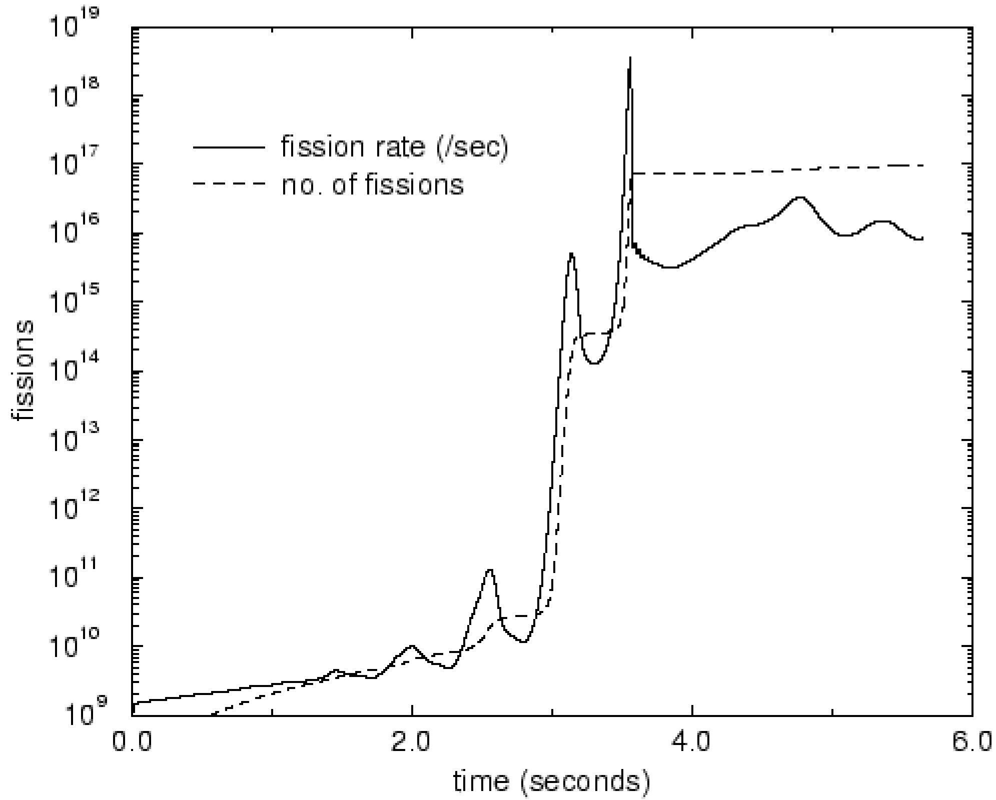
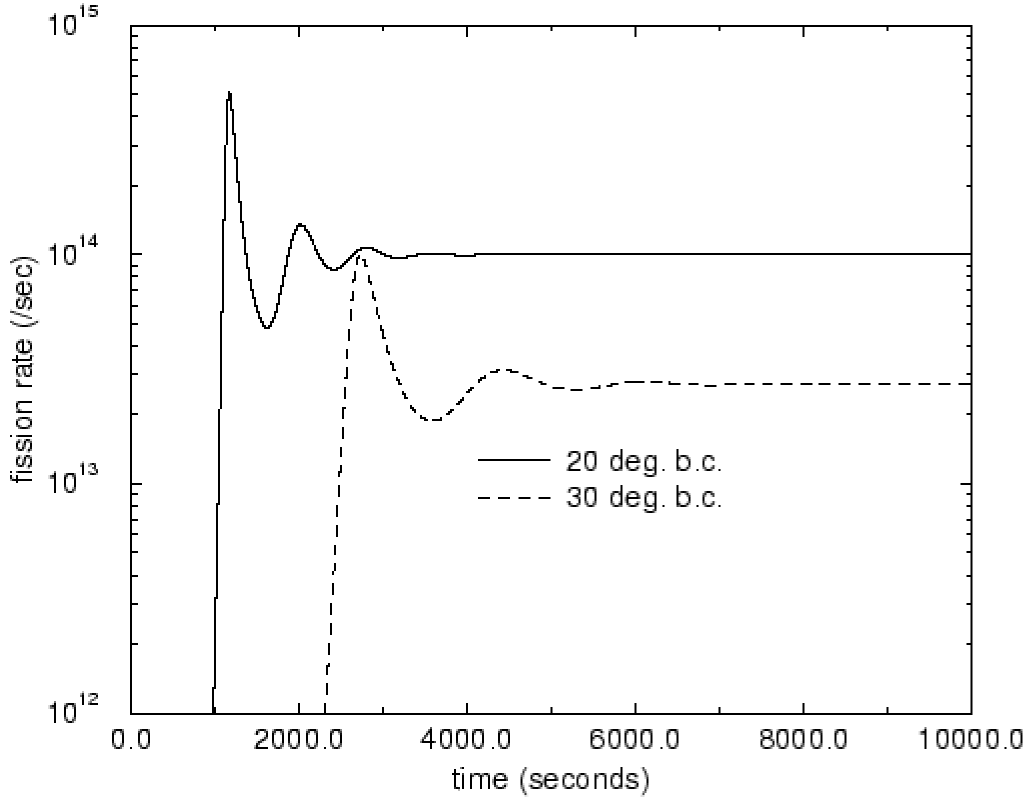


Illustration re. recovery from accident

- In uranium systems the negative feedback from temperature means that ‘steady state’ fission power is sensitive to heat removal rate
- Calculations performed with two different temperature boundary conditions for precipitation tank show different power levels

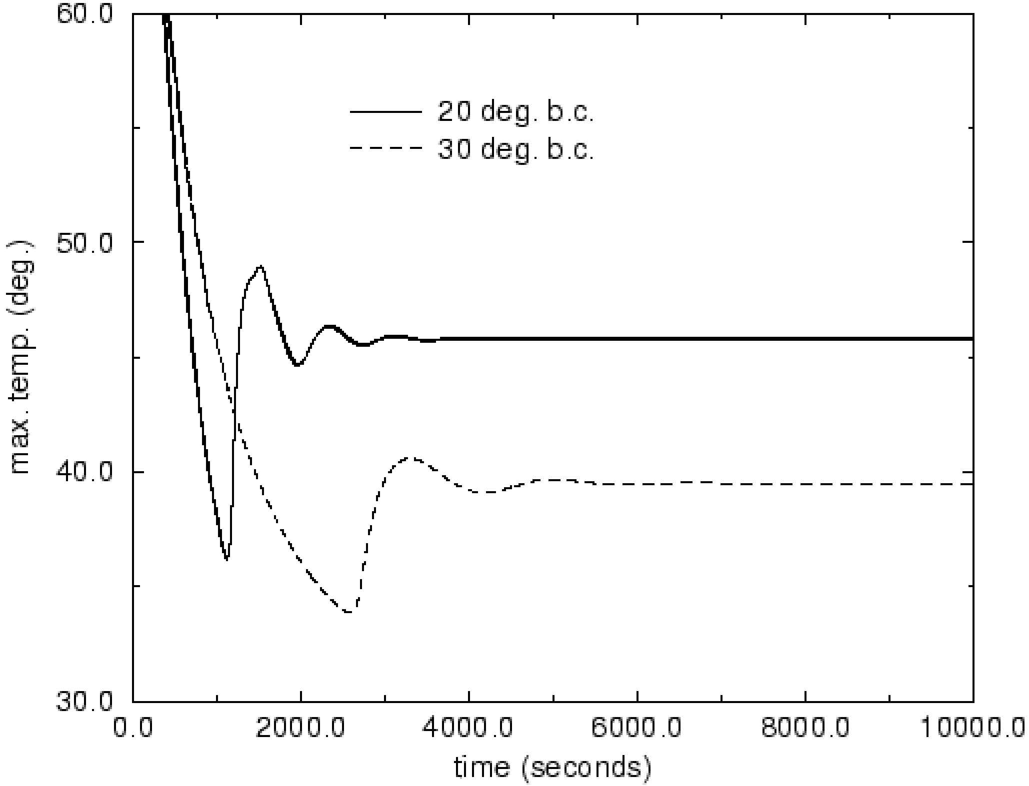
JCO Simulation - Prolonged Transient

Fission rate for two different water jacket temperatures



JCO Simulation - Prolonged Transient

Maximum temperature of liquid in vessel for two different water jacket temperatures



Solution resolution

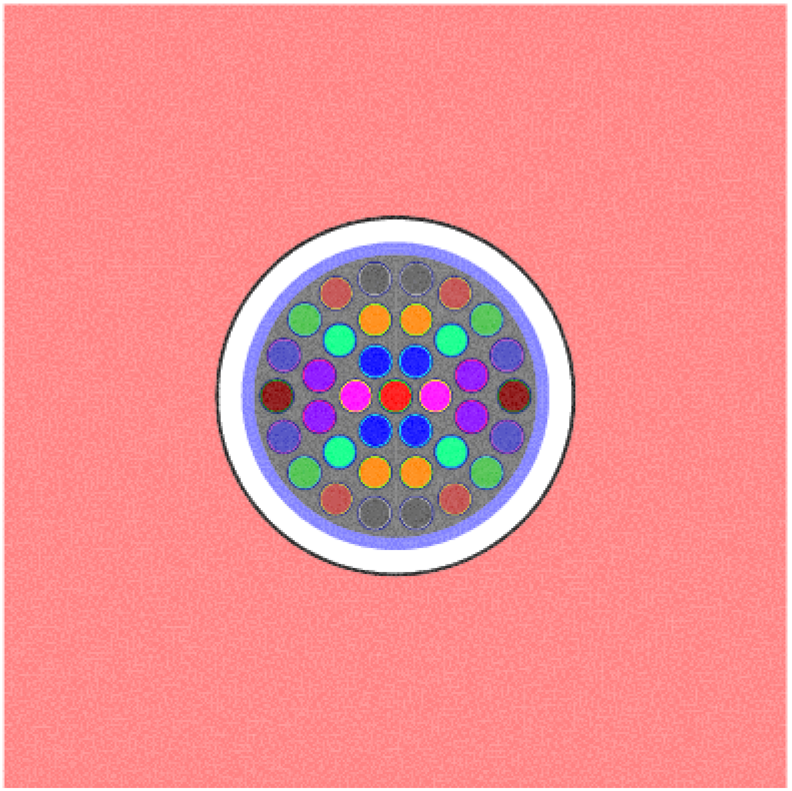
Q: what is the necessary time, energy, space-angle resolution for a problem?

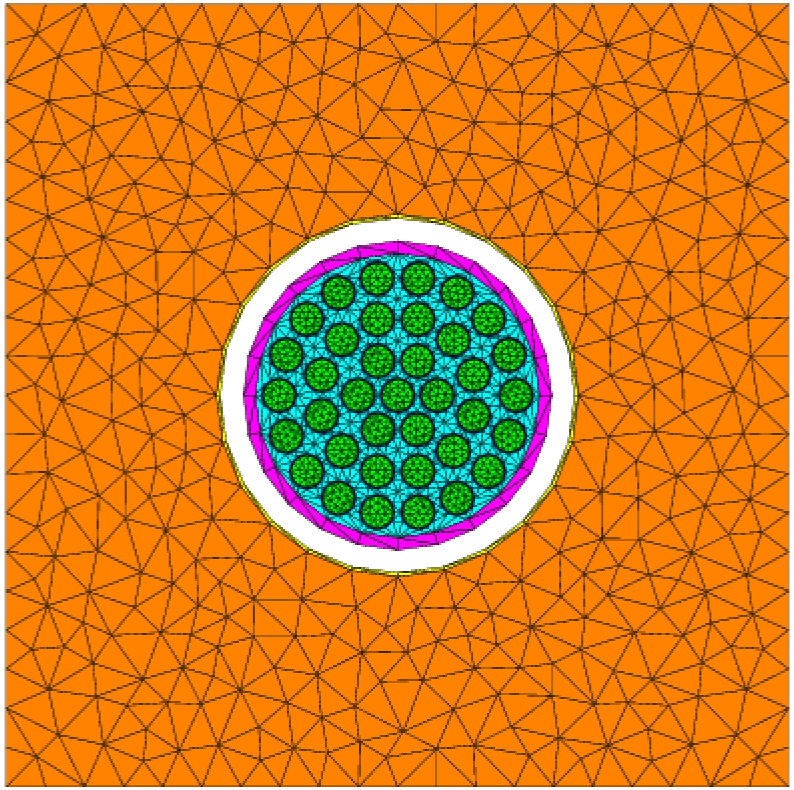
A: we don't know – let the method, not the practitioner decide

No tool is so clever that it cannot be used by an idiot **(Confucius)**

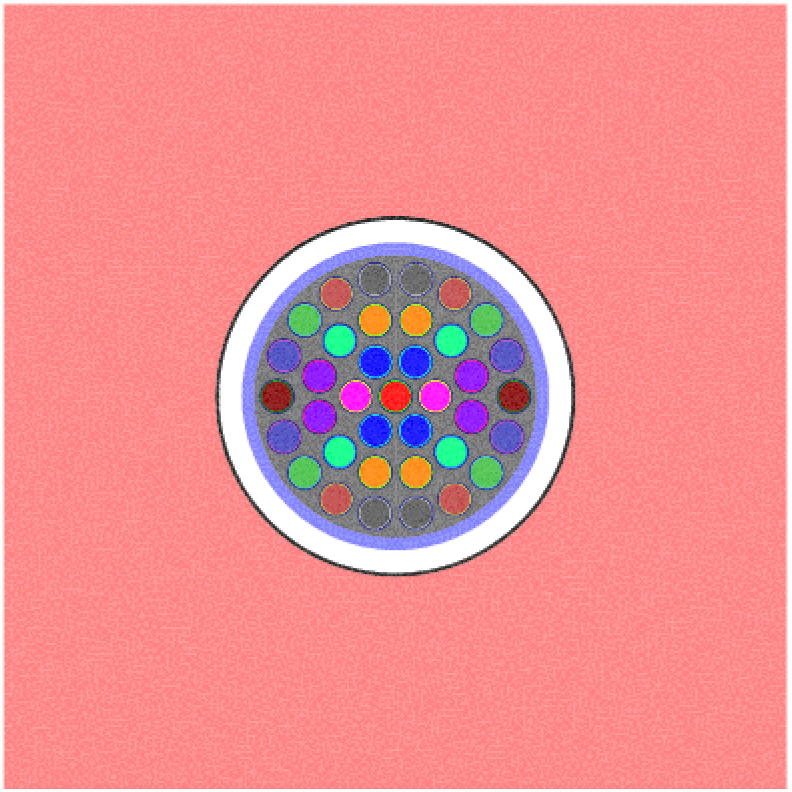
(However, this is easier said than done…)

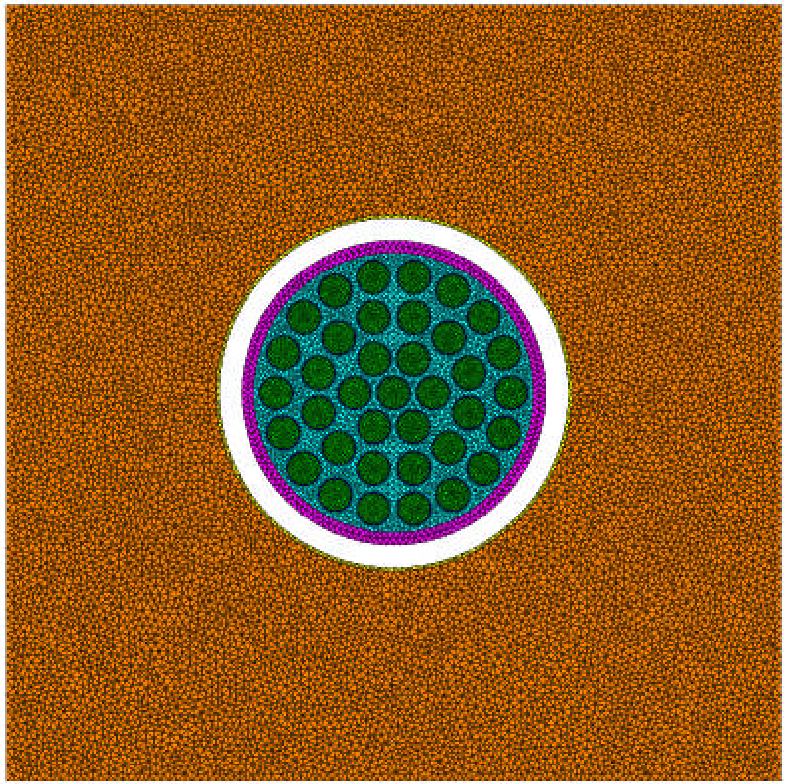
2D Cross Section of Candu Fuel Assembly



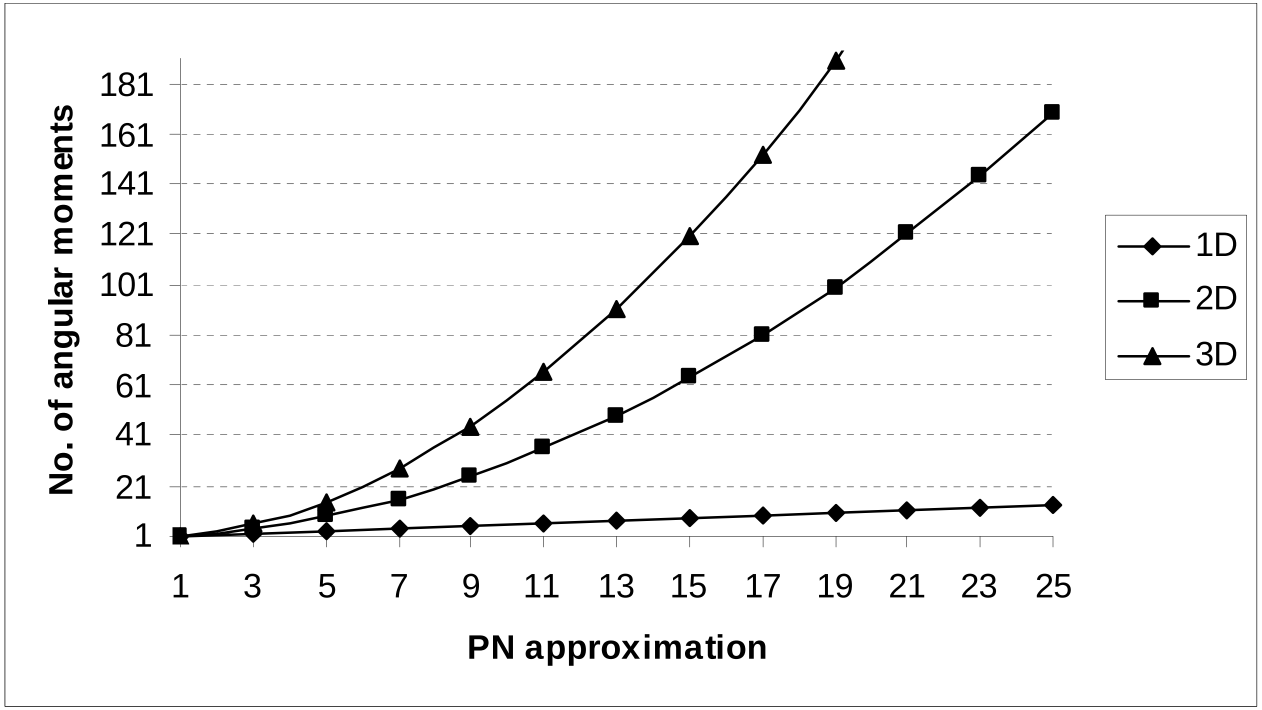


2D Candu fuel assembly – spatially refined mesh

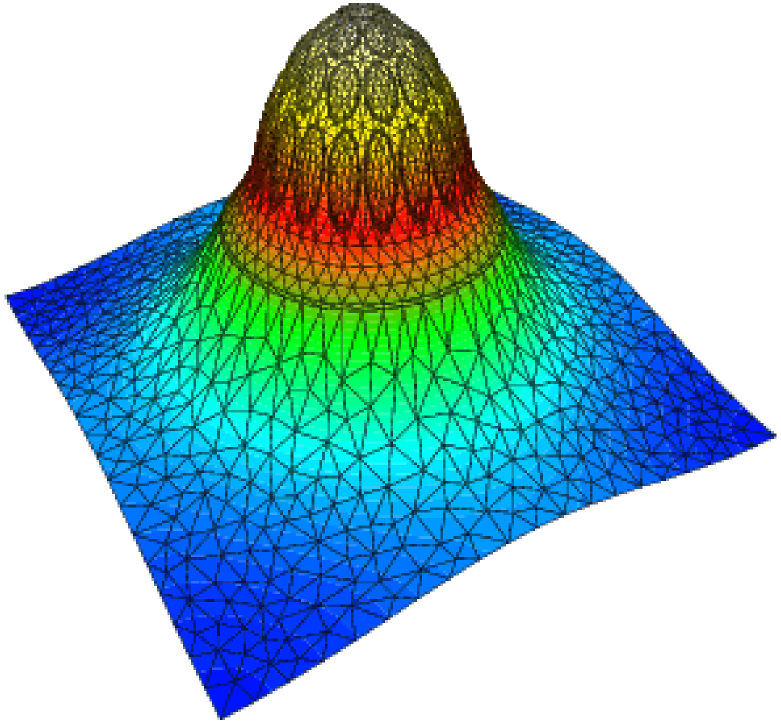




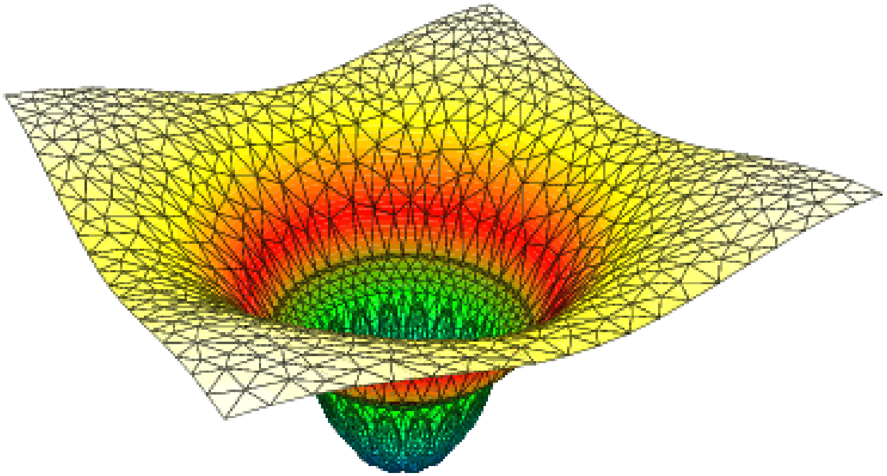
Refinement of Angular Resolution



Contrasting physics with energy



Group 1



Group 2

Adaptive Strategy

1. Discretization of system of equations
2. Solution of discretized system of equations
3. Measure of the discretization error
4. Refinement/creation of new discrete system

A Posteriori Error Measurement

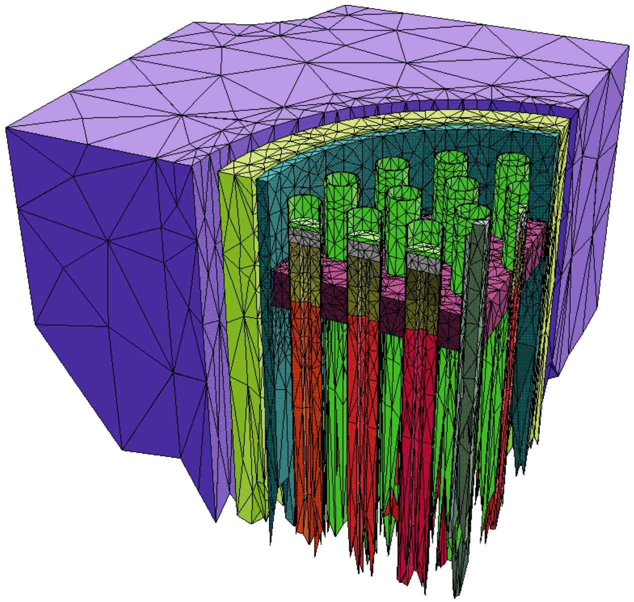
- A posteriori error measurement provides information where the discretization needs to be altered (refinement or coarsening) to achieve desired accuracy.
- Two basic strategies to compute posteriori error measure.
  - Derivative recovery error estimator (gradient or Hessian)
  - Residual based error estimator

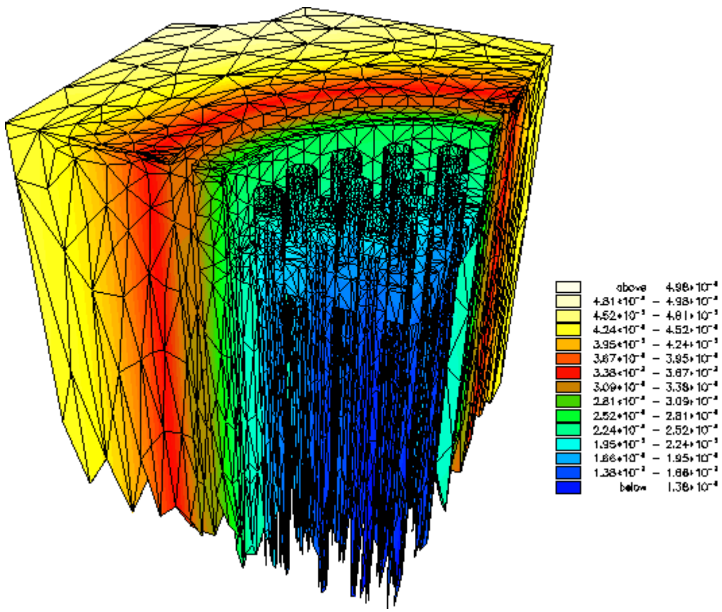
Solution spatial self-adaptivity

- Allows effort to be concentrated where and when it is needed
- Governed by appropriate error measure
- Mesh should coarsen as well as refine
- Geometry must be preserved

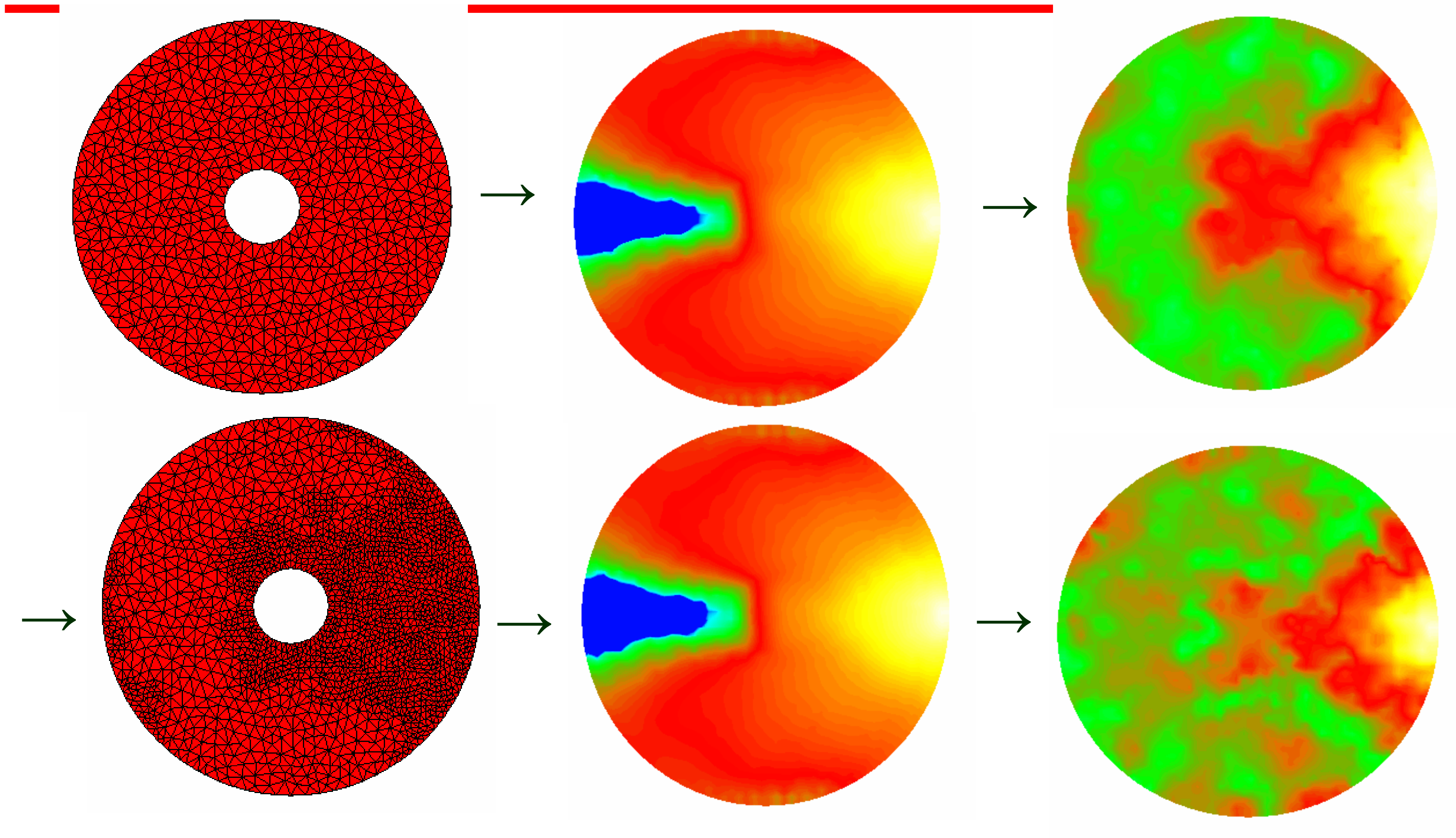
Spatial adaptivity for AGR problem

Mesh adapted to predefined pitch and mesh adapted to error measure based on thermal flux

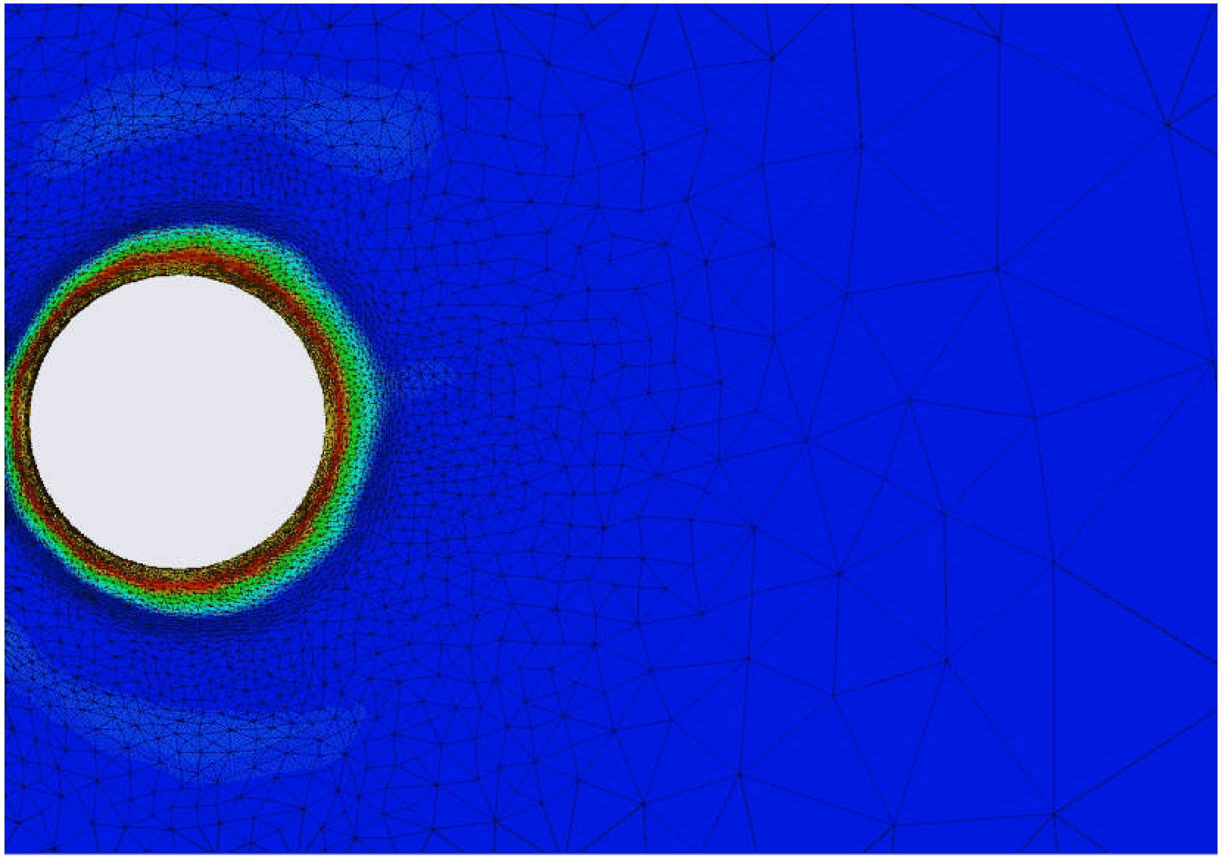




Numerical Example (photon propagation)



Adaptivity on unstructured meshes



Angular Adaptivity

- The degree of anisotropy in angular flux varies widely with space and energy groups.
- Highly-anisotropic angular flux region may be largely localized.
- Uniform refinement is not computationally efficient.
- Local refinement of angular expansion is more desirable.

FE-P$_N$ Equations

- Ritz-Galerkin procedure yields system of equations of the form:

$$A\psi = b \qquad A = \sum_{e=1}^{E} A^e$$

- The matrix A has a shell structure (for ℓ=0, 2, 4,…):

$$A = \begin{pmatrix} A_{11} & A_{12} & .. & A_{1N} \\ A_{21} & A_{22} & .. & A_{2N} \\ .. & .. & .. & .. \\ A_{N1} & A_{N2} & .. & A_{NN} \end{pmatrix} \qquad A_{ij} = \begin{pmatrix} a_{11} & a_{12} & .. & a_{1N} \\ a_{21} & a_{22} & .. & .. \\ .. & .. & .. & .. \\ a_{N1} & .. & .. & a_{NN} \end{pmatrix}$$

"Diffusion" matrix stencil

Angular Adaptivity

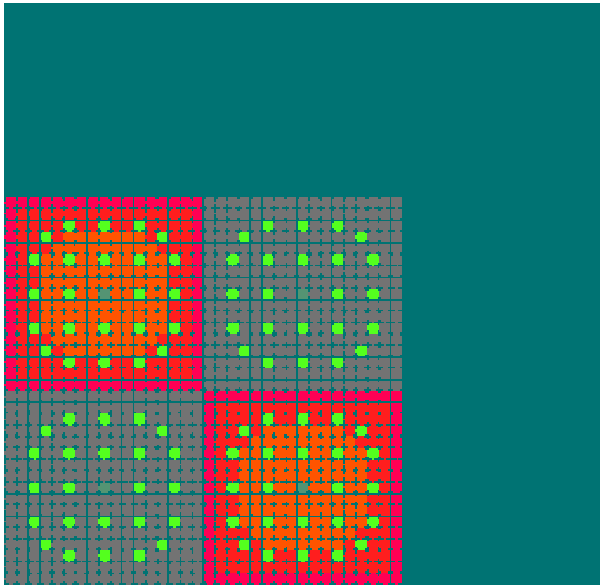
- Variable angular resolution can be achieved by truncating the angular expansions nodal-wise.

- The hierarchical nature of spherical harmonics expansion allows addition of higher moments shell without changing the existing matrix.

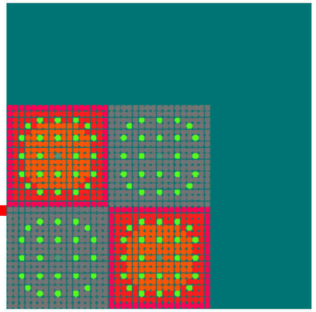
- Error can be estimated by computing residual of new system with old solution.

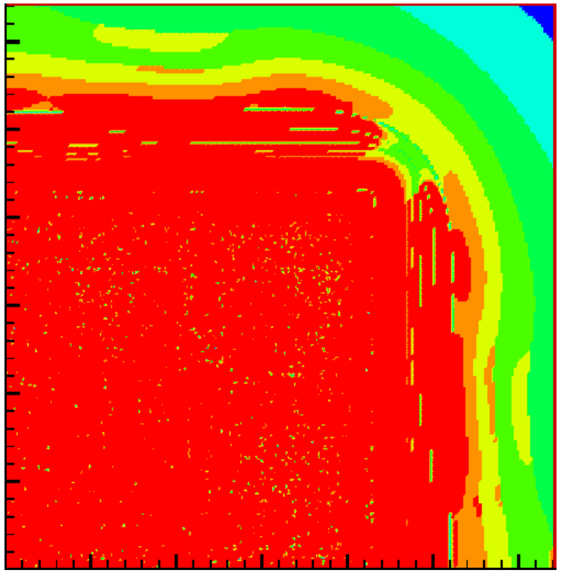
Example (nuclear reactor lattice)

- 2D C5G7MOX benchmark problem
  - 4 fuel assemblies
  - Water moderator
  - 7 groups
  - Criticality problem

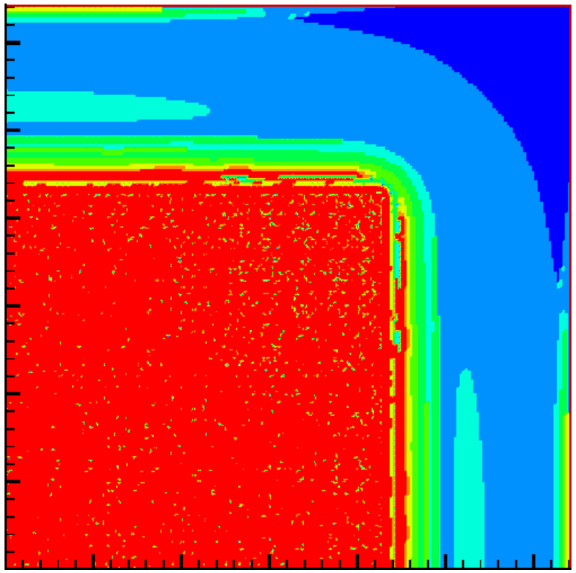


Numerical Example (P_{15} approximation)

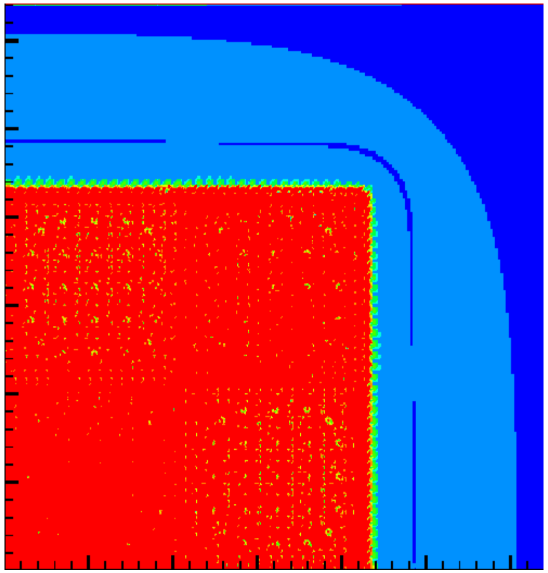




Group 1



Group 4



Group 7

Adaptivity in angle

- Has to operate in conjunction with spatial adaptivity
- Has also to work in conjunction with preconditioning strategy

Summary

- Unstructured radiation transport methods are gradually coming to the fore
- Complex geometry modelling capability relatively more sophisticated than Monte Carlo
- Flexible and versatile formulations enable linkage and reapplication to other physics

The Challenges

- Optimization problems in nuclear engineering and medical physics
  - Thousands of realizations?
- Inverse (data assimilation) problems
  - What mesh?
  - What angular resolution?

To do (after 20 years)

- 3D Geometry and Meshing interfacing
- Space-angle adaptivity
  - Error measures
  - Parallel processing
- Solution acceleration→multigrid fomulations
- Higher-order discretization methods
- Multiphysics interfacing