High-Fidelity NEWTRNX

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Reactor Analysis Group
Nuclear Science & Technology Division

Grand Challenge: FULLY-COUPLED NUCLEAR REACTOR SIMULATION

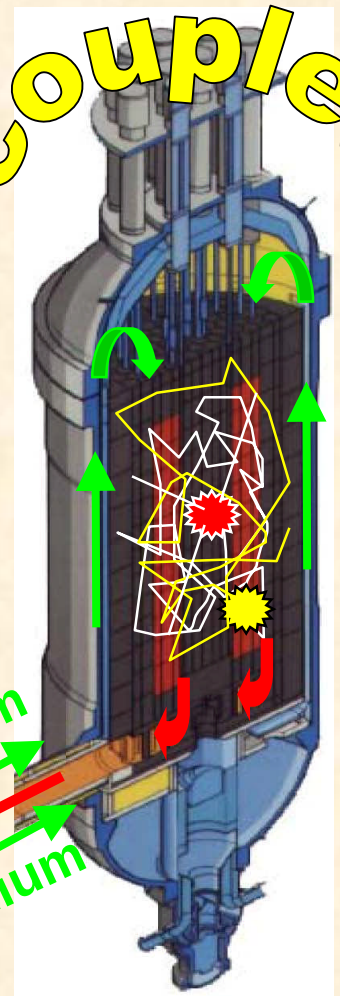
Heat Generation

6-D, quasi-static linear integral-PDE

Neutron Transport

Gamma Transport

10 orders of magnitude in neutron energy



Heat Transport

3-D, transient, compressible, turbulent, non-linear PDE

Conductive-Convective-Radiative-Heat Transfer

Fluid Dynamics

5 orders of magnitude in space

12 orders of magnitude in time

Current "coupled-physics" reactor simulation is very "coarse"

- Neutronics:
  - 3-Step approach of multi-level 'homogenization'
  - Fine-mesh solution must be 'reconstructed'
- Fluid-dynamics:
  - Single (few) channel reactor core
  - 1-D lumped fluid flow
- Heat transfer:
  - Coarse-mesh power distribution
  - Averaged heat transfer properties
- Coupling exists only on the coarsest mesh

Current reactor simulation is adequate for evolutionary improvements

- Empirical evidence
  - Test reactors and experiments operated for decades
  - 10,000+ reactor years of operation
  - Designs are static, operation has evolved
- Challenges remain for the current fleet
  - 90% voiding in BWRs
  - Crud buildup on cladding
  - Vibration / radiation effects in cladding and vessels
  - Advanced CANDU Reactor's "negative" void coefficient
  - Davis-Besse
  - Optimization = $$$

Novel reactor designs must compete with the present fleet

- Novel designs are not LWRs
  - Much higher temperatures
  - Fast and intermediate spectrum
  - Heavy actinide loading
  - "New" materials (graphite, salt, sodium, alloys, particle fuel)
- Licensing and safety assessment will be challenging
  - Less empirical data; much of which is insufficient
  - Few (if any) new test reactors will be built
  - Cost of even small-scale "nuclear" tests are astounding
  - Software was "biased" to fit the empirical evidence
- Economics has the final word
  - 90% capacity factor on day one
  - Must compete with optimized LWRs

Recent Advances in HPC Engineering

- Aerospace Industry
  - CFD + electronics
  - Great success for airplane and shuttle design
  - Wind tunnel testing now validates software accuracy
- Nuclear Weapons
  - Fission, fusion, chemistry, thermo-mechanics, …
  - How well do they predict past tests?
  - Could a revolutionary design be used without a test?
- Office of Science projects
  - Supernova, global warming, pharmaceuticals, etc.
- Where do nuclear reactors stand?
  - Harder than an airplane
  - Easier than a bomb
  - Empirical evidence must be used to validate the software

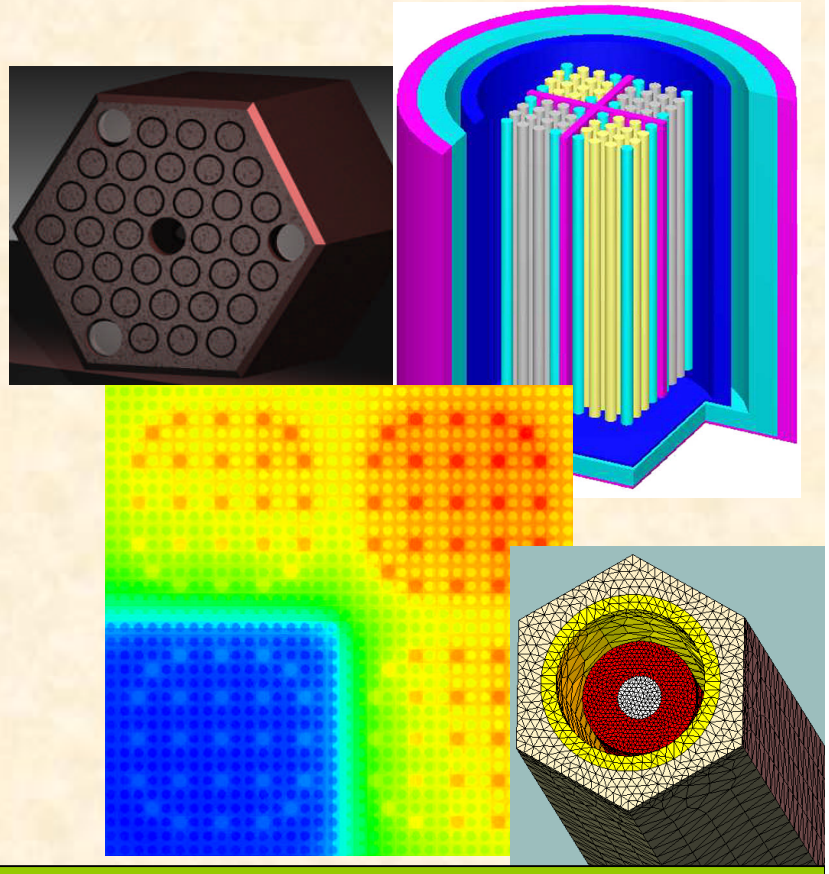
Recent Modeling & Simulation Findings for GNEP*

- **Current code base is inadequate**
  - Current nuclear industry code base is insufficiently predictive to guarantee meeting the ambitious GNEP technology goals
- **New codes can help in many areas**
  - Advanced M&S and HPC can improve designs of future reactors, reduce uncertainty in facilities development and construction costs, improve safety, and reduce development time of new fuels
- **Tough challenges remain**
  - Research challenges remain in developing and scaling multiphysics codes to the performance levels needed for fundamental studies, engr/design use
- **Must balance short and long term needs**
  - GNEP requires short term investment in existing nuclear energy codes and long term investment for the development of next-generation simulation codes
- **Nuclear community is "depleted", but US is up to the challenge**
  - US has the expertise to build the next-generation nuclear energy simulation codes, but not without a sustained software development activity
- **New codes can accelerate licensing process**
  - Creation of new physics-based high-fidelity simulation codes offers the possibility of accelerating the licensing process

*Joint DOE NE/ASCR Workshop for Simulation and Modeling for Advanced Nuclear Energy Systems

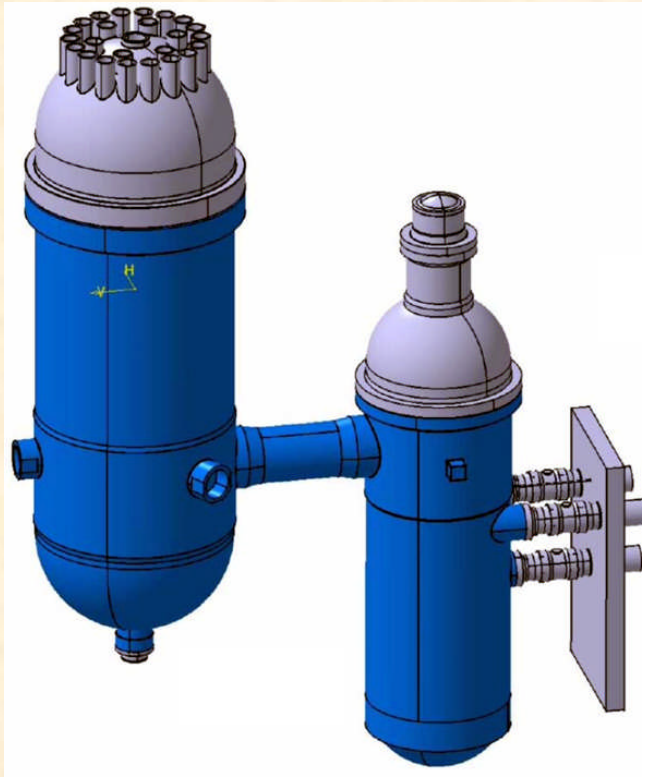
Predicting reactor safety and performance requires simulation

- **Severe Accidents**
  - **Experiments cannot be performed to assess safety**
- **Design-Basis Transients**
  - **Local effects on the cladding & fuel dominate safety-significant parameters**
  - **Instrumentation is not accurate for understanding local effects**
- **Performance**
  - **Large design margins provide room for computational/experimental error**
  - **Excellent LWR performance is based on decades of operation**



- **Predictive simulation is the only way to ensure the safety of advanced reactors without many costly experiments and decades of operation.**

CANS: Collaboration for Advanced Nuclear Simulation



- **Explore scientific phenomena**
  - **Complex interaction of nuclear, mechanical, chemical, and structural processes in fission reactors**
- **Simulate severe accidents**
  - **Multi-physics transients with advanced materials at high temperature and pressure in a changing radiation spectrum**
- **Optimize nuclear designs**
  - **Nuclear facilities are expensive: Cost and time**
  - **Radiation activation prevents retrofits**

Operate as a multi-laboratory, multi-university collaboration

ARGONNE NATIONAL LABORATORY · INL Idaho National Laboratory · Los Alamos NATIONAL LABORATORY · OAK RIDGE National Laboratory · THE UNIVERSITY OF ARIZONA · Columbia University · Georgia Tech · UT

Working <u>together</u> we can utilize <u>intellectual</u> and <u>financial</u> resources across institutions

- **Computer Science & Mathematics:**
  - Integrate scientific computing & mathematics tools from SciDAC
- **Heat Generation (Neutronics):**
  - Develop a high-fidelity nuclear reactor radiation transport solver for HPC systems
- **Heat Transfer & Fluid Dynamics:**
  - Multi-phase, non-isothermal CFD solver
  - Multi-material, chemically-reactive flow
- **Structural & Material Feedback:**
  - Fluid-structure interactions
  - Irradiation effects

In Progress

Future Work

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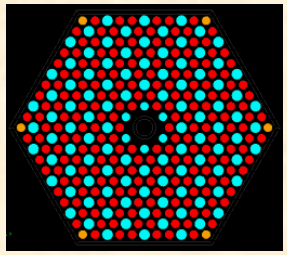
Fundamental Equations of Neutronics

- **Source-Driven Boltzmann Transport for Neutron/Gamma**
  - **Reactor kinetics (< 10 s time scales)**
  - **Source is delayed neutrons from previous times**
  - $$\vec{\Omega} \bullet \vec{\nabla}\psi + \left[\sum_i N_i \sigma_t^i\right]\psi(t) = S + \int_0^\infty dE' \int_0^{4\pi} d\Omega' \left[\sum_i N_i \sigma_s^i\right]\psi$$
- **Fundamental Mode Transport for Neutron/Gamma**
  - **Reactor depletion (> 10 s time scales)**
  - **Slow variation in time: delayed neutrons are approximated as prompt**
  - $$\vec{\Omega} \bullet \vec{\nabla}\psi + \left[\sum_i N_i \sigma_t^i + \alpha\right]\psi = \left(\frac{1}{k}\right)\int_0^\infty dE' \int_0^{4\pi} d\Omega' \left[\sum_i N_i \sigma_s^i\right]\psi$$
- **Bateman Equations for Isotopic Distribution**
  - **Source of delayed neutrons and depletion of fuel**
  - **Matrix exponential**
  - $$\frac{dN_i}{dt} = \sum_k \lambda_{ki} N_k(t) - \lambda_i N_i(t) + \int_0^\infty dE \left[\left\{\sum_j \sigma^{ji} N_j(t) - \sigma^i N_i(t)\right\} \int_{4\pi} d\Omega \psi\right]$$

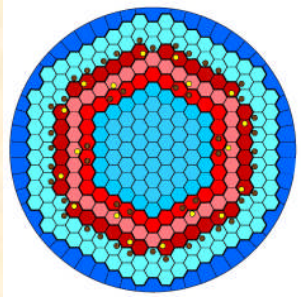
Current Neutronics methodology for a single state-point is a multi-step approach

1. **1-D Continuous-Energy Deterministic Transport**
   a. **Fission-source-driven transport on a spatial subset (particle or pincell) with approximate boundary conditions for space-angle dependent solution with complete point-wise energy resolution**
   b. **Weight point-wise cross sections with point-wise solution to create a spatially-homogenized multi-group data set (10^{1-2} energy groups)**

2. **2-D Multi-group Deterministic Transport**
   a. **Solve the k-eigenvalue transport on a larger spatial subset with approximate boundary conditions for space-angle dependent multi-group solution**
   b. **Weight the multi-group cross sections with multi-group solution to create a spatially homogenized few-group (2-10 groups) data set**

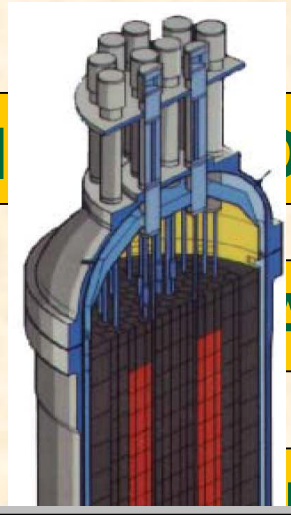


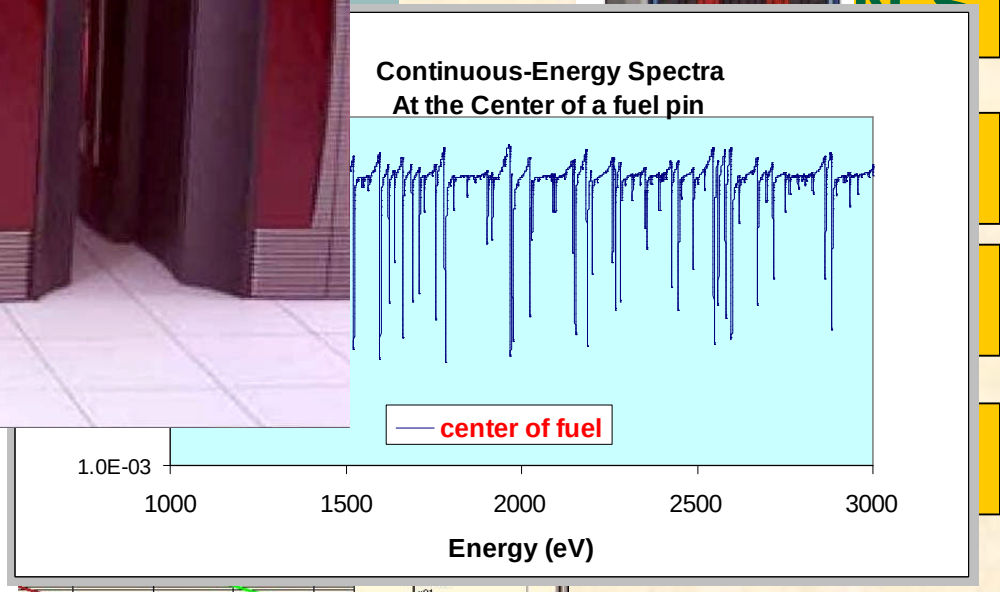
3. **3-D Few-group Coarse-Mesh Diffusion**
   a. **Solve the k-eigenvalue transport for the full spatial domain with accurate boundary conditions for the global coarse-mesh few-group solution**
   b. **'Reconstruct' global-fine-mesh solution by coupling magnitude of coarse-mesh solution (3) with shape-function from the two-levels of fine-mesh solution (1, 2).**

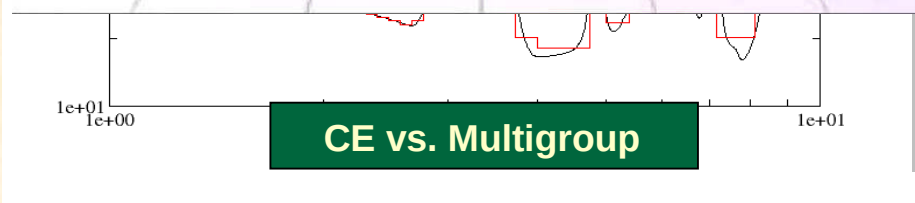


The ORNL LDRD will begin to remove these layers so that the software is available when computers catch up

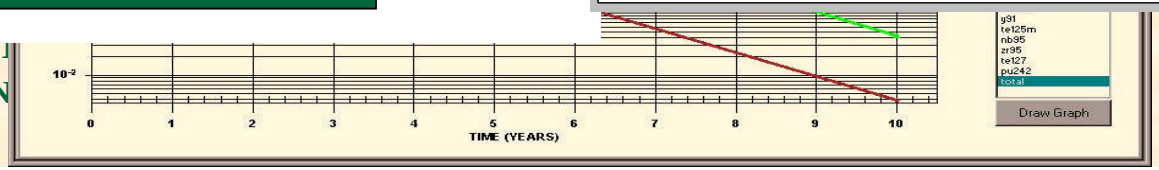
High-fidelity neutronics is dependent upon accurate data and boundary conditions



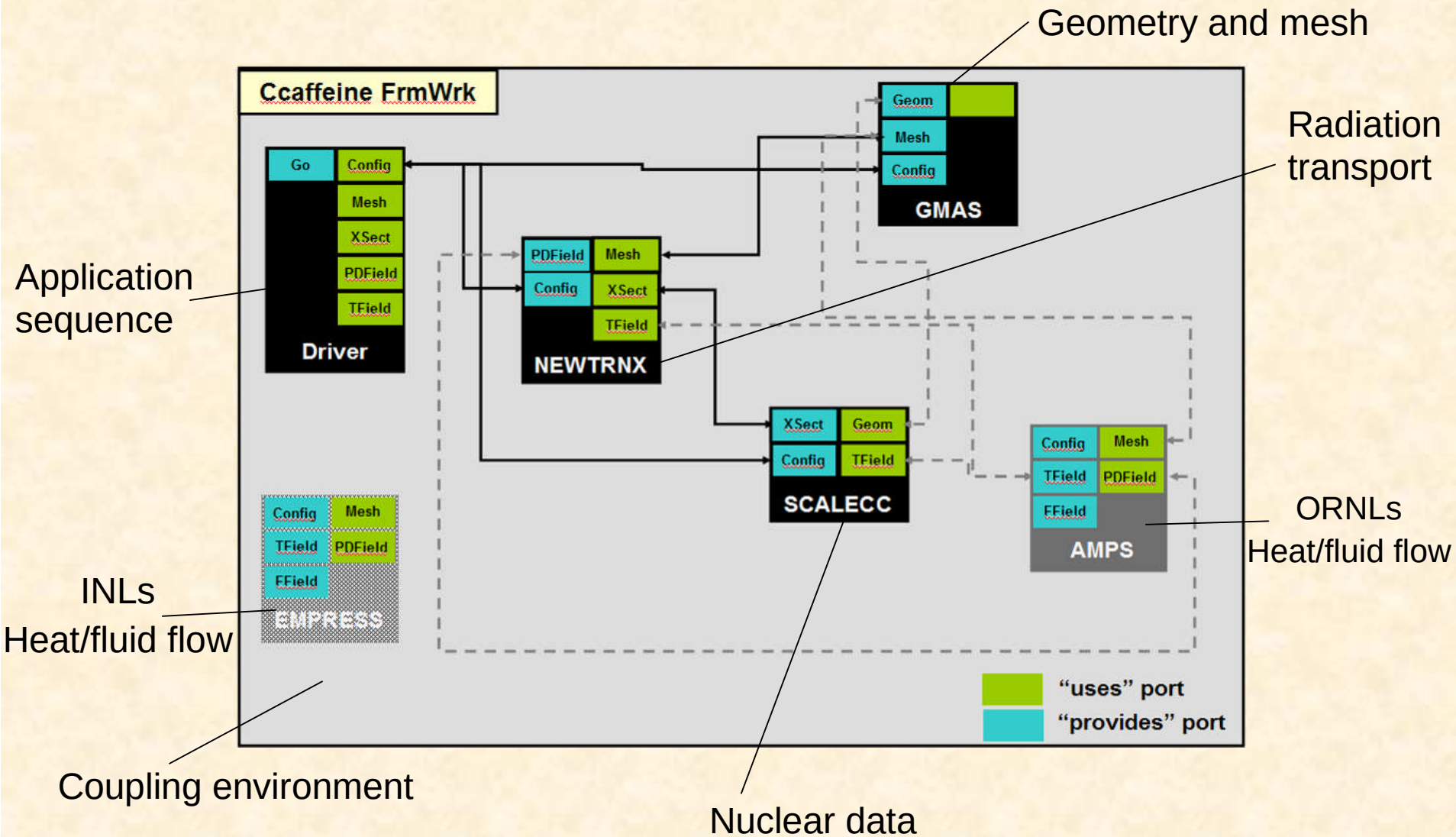




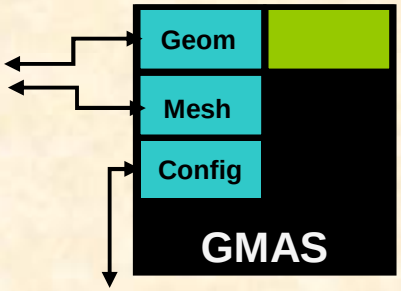
CE vs. Multigroup



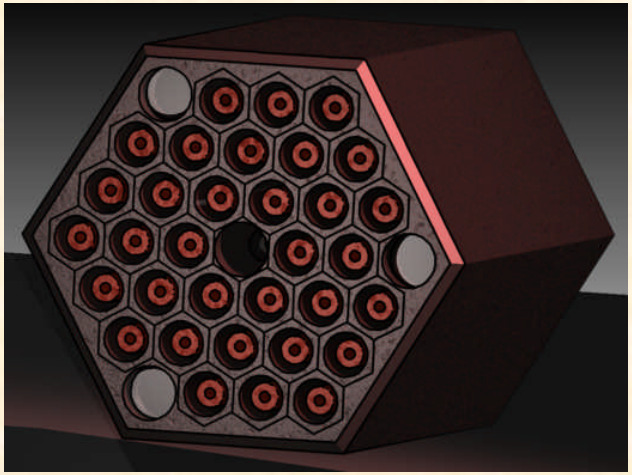
Common Component Integration



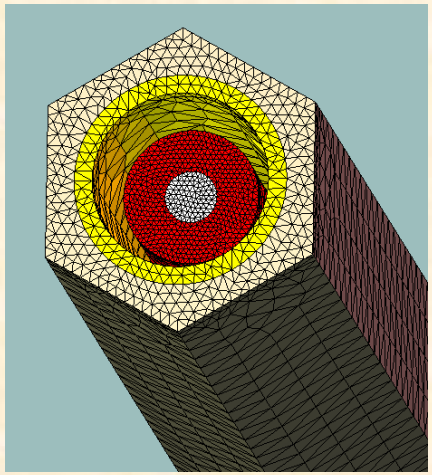
GMAS: Geometry and Mesh Adaptivity Server



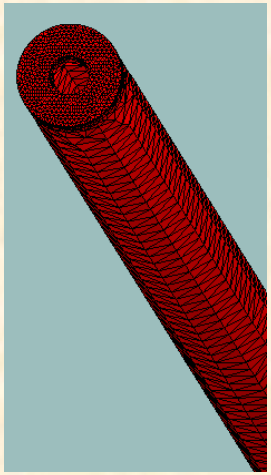
- Integration of SciDAC tools for geometry and meshing services in nuclear multi-physics
  - Geometry generation
  - Mesh data base generation
  - Partition and dynamic load balancing
  - Adaptive loop services



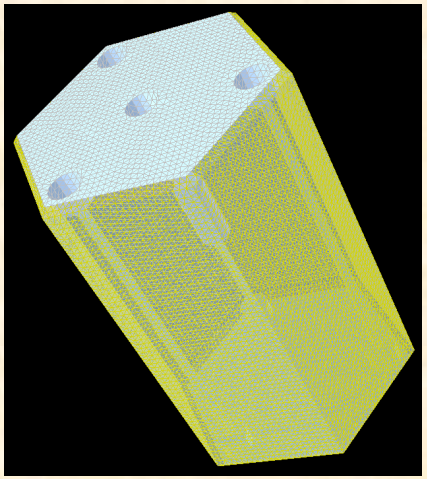
Fuel element assembly



Fuel channel



Fuel compact



Fuel block

- Research reactors = ~300 million mesh elements
- Production reactors = > one billion mesh elements

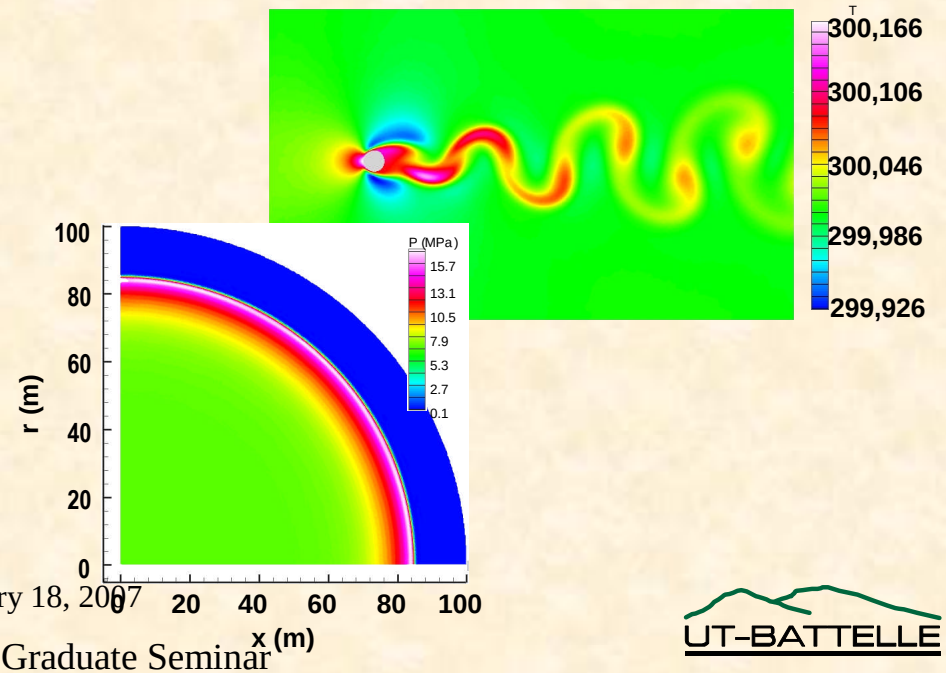
EMPRESS: All-speed CFD and conjugate heat transfer

Conjugate heat transfer

- Conduction and convection with all-speed computational fluid dynamics (CFD)
  - Three coupled, transient governing equations: Conservation of mass, momentum, and energy
  - Multi-scale simulation spans: 7 orders of magnitude in space, 10 orders in time
  - Solutions required for coupled equations, each with 10^{10} degrees of freedom per time-step
- Radiative heat transfer: Nonlinear Boltzmann transport and Planck emission
  - Coupled through quartic temperature dependence
  - Span similar orders of magnitude as convection
  - To be coupled with CFD and heat transfer
- High-fidelity distribution of heat generation

EMPRESS: Parallel CFD and conjugate heat transfer

- Development of advanced algorithms: Pressure-corrected implicit continuous Eulerian CFD
- Multi-laboratory code development
  - Idaho: CFD and non-linear coupling
  - Argonne: Numerical solvers/parallelization
  - Los Alamos: Radiative heat transfer



EMPRESS:
CFD + Conjugate Heat Transfer

- **The macroscopic cross section …**

$$\Sigma = \sum_{isotopes} \sigma_i N_i$$

- **Depends on the temperature of the material …**

$$\sigma_i \propto \sqrt{Temperature}$$

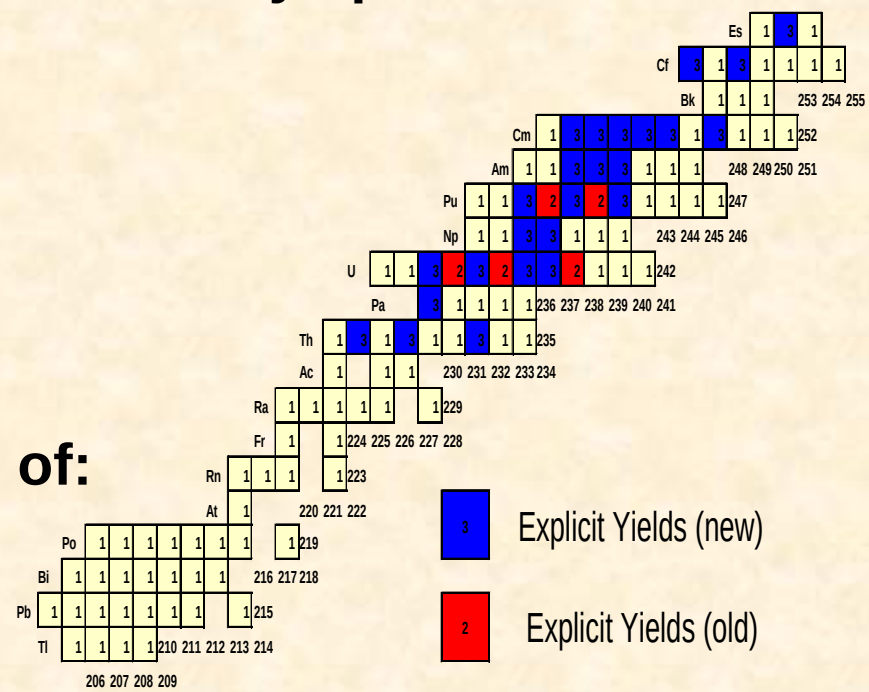
- **And the density of the material …**

$$N_i \propto Density$$

- **So we better use a high-fidelity CFD + CHT solver.**

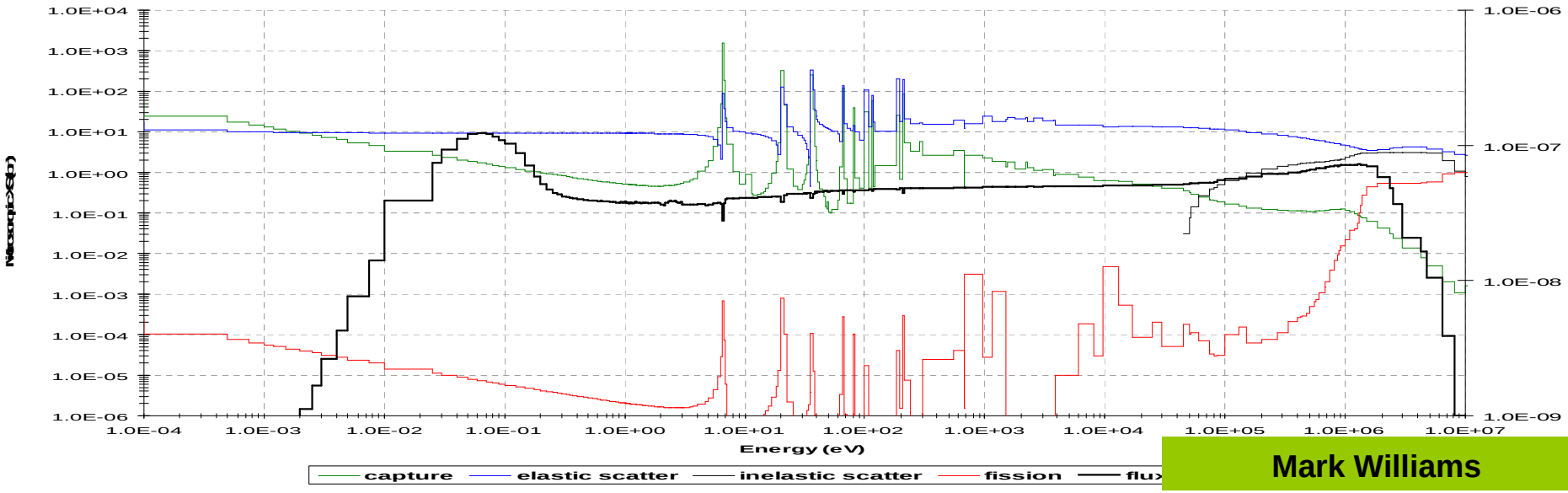
ORIGEN-S:
Isotopics and delayed neutrons

- **Solving:**
  - $$\frac{dN_i}{dt} = \sum_k \lambda_{ki} N_k(t) - \lambda_i N_i(t) + \int_0^\infty dE \left[\left\{ \sum_j \sigma^{ji} N_j(t) - \sigma^i N_i(t) \right\} \int_{4\pi} d\Omega \psi \right]$$
- **With the Matrix Exponential Method for every space/material**
  - $$\overline{N(t)} = \overline{\overline{A(t)}}\,\overline{N(0)}$$
- **For real nuclear energy systems**
  - **~1600 individual isotopes**
  - **From ENDF, ENSDF, JEF, FENDL, etc.**
- **To provide time/space distribution of:**
  - **Isotopes during operation and transient**
  - **Delayed radiation (n, gamma, etc)**
    - **With energy dependence of radiation**



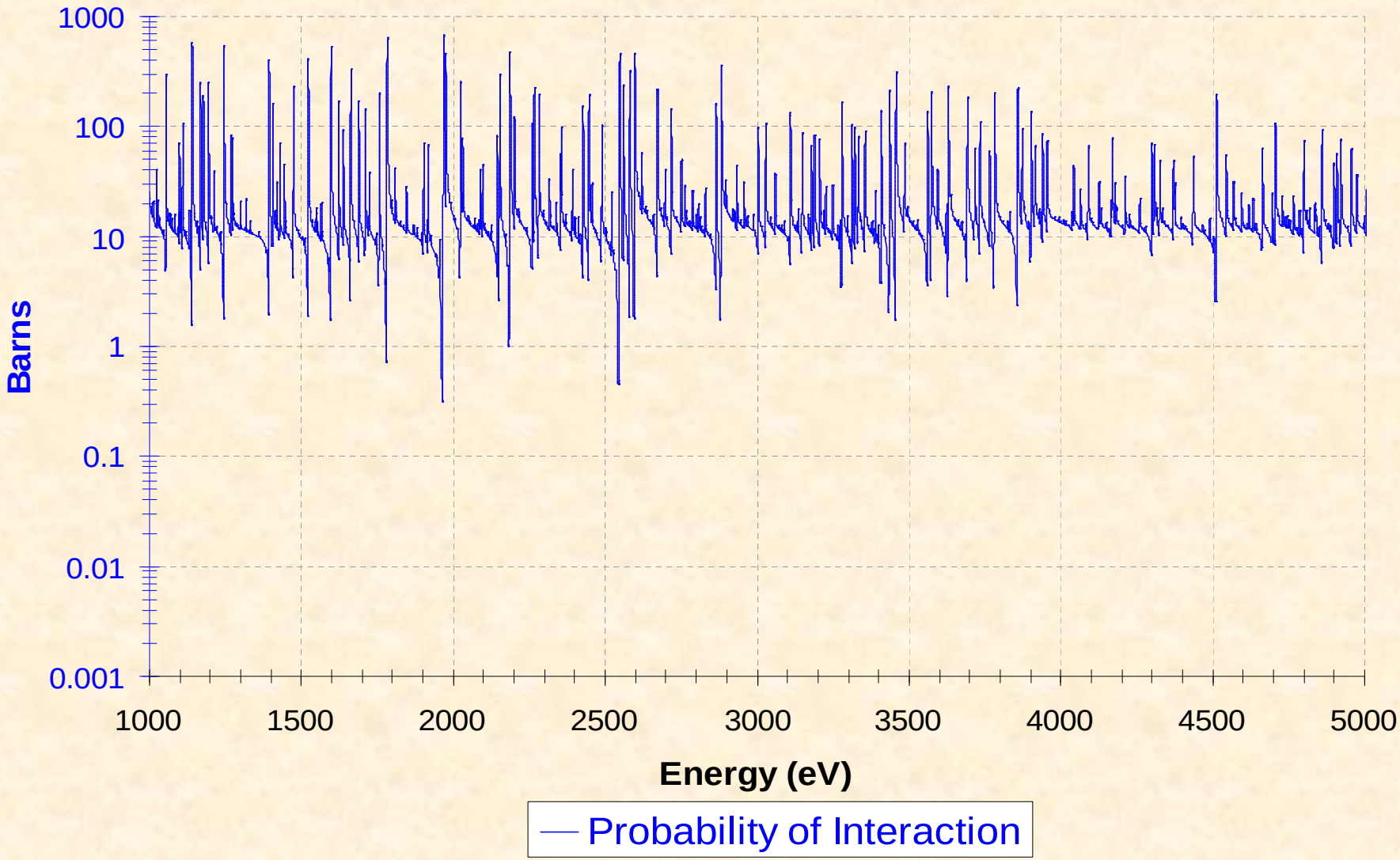
SCALECC: SCALE Component Container

- A foundation of accurate nuclear data
  - Direct link to AMPX processed Evaluated Nuclear Data Files
  - Automated processing for temperature/geometry effects
- SCALECC is a module for parallel computing
  - Driver main replaced with module, some I/O removed
  - Additional work that is in the near future:
    - Continued removal of I/O
    - Continued removal of mains to link as subroutines/modules

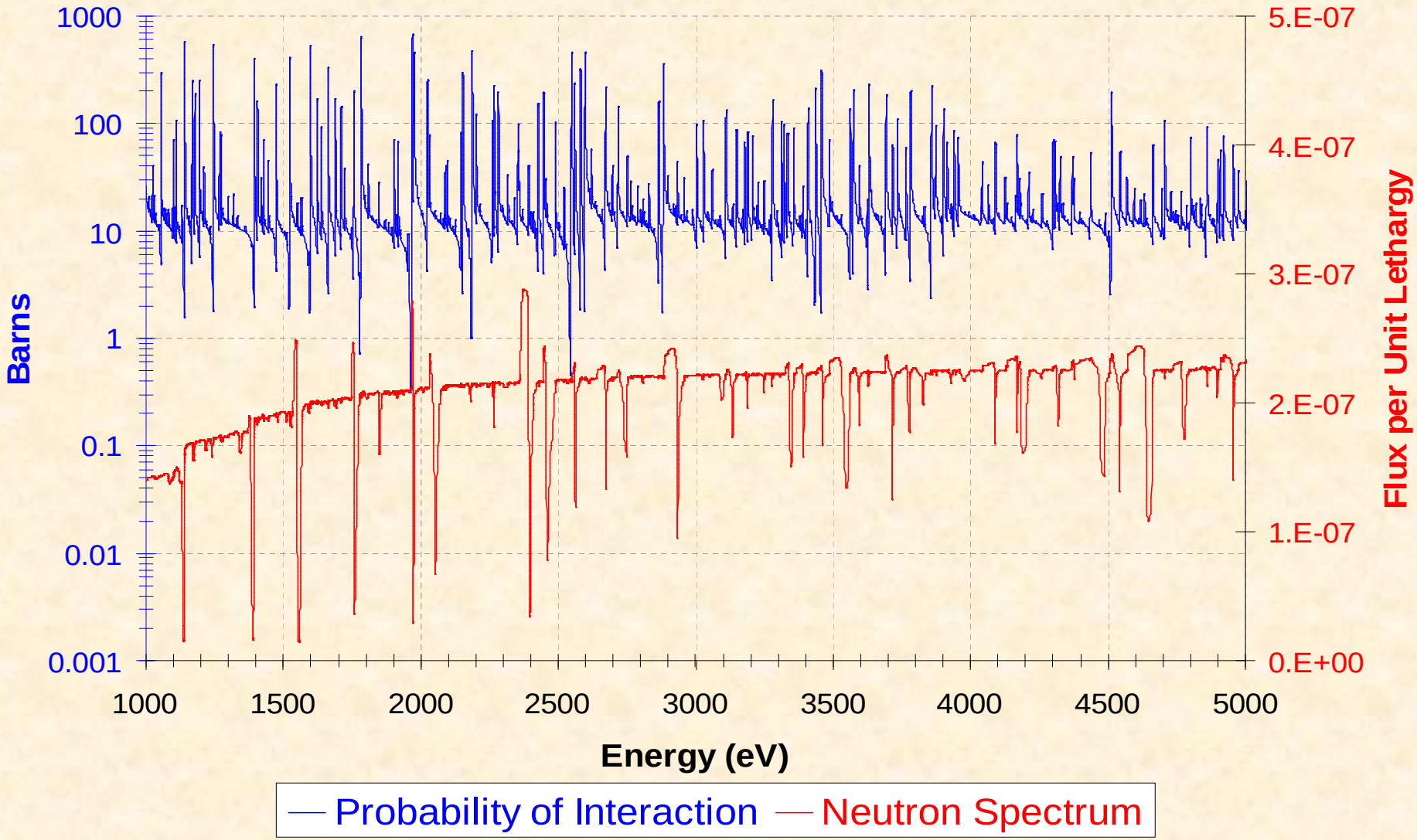


Mark Williams

Fine Energy Resolution of the Data for only 6 of 238 Groups for a Given Temperature and a Single Isotope



The Fine Energy Resolution of the Solution is the Weighting Function to Create a "Multi-Group Cross Section Set"



Only now we can start talking about solving the transport equation.

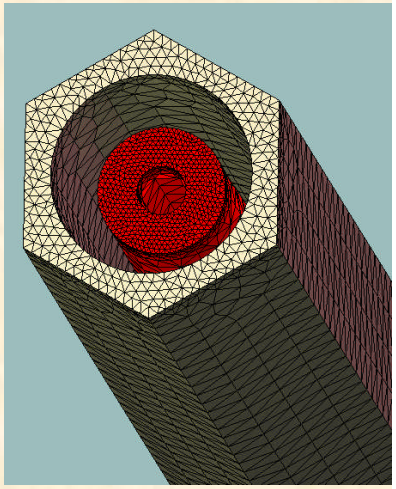
$$\overrightarrow{\Omega}_m \bullet \vec{\nabla}\psi + \left[\Sigma_{g,t}^{total} + \alpha\right]\psi_{m,g,t} = \sum_{g'}\left[\int_0^{4\pi} d\Omega'\ \Sigma_{g'\to g,t}^{m'\to m}\psi_{m',g',t}\right]$$

$$+ S_{g,t} + \left(\frac{1}{k}\right)\chi_g \sum_{g'}\left[\Sigma_{g',t}^{fission}\int_0^{4\pi} d\Omega'\psi_{m',g',t}\right]$$

- **Caveats:**
  - **Without all of the previous pieces, the solution to this problem is useless.**
  - **There is no need to converge this problem to a much higher fidelity than that of the data (10^{-4} at best).**
- **For a full reactor, this problem is large:**
  - **$10^{8\text{-}12}$ in space, $10^{2\text{-}5}$ in direction, $10^{1\text{-}4}$ in energy**
  - **Increasing fidelity in a single dimension requires increasing in others**
- **Solving this problem requires lots of memory:**
  - **You cannot (and do not need to) store the entire matrix: $10^{11\text{-}21}$ unknowns**
  - **Store the RHS and LHS differently:**
    - **Angle: store low-order spherical harmonics ($P_{3\text{-}5}$)**
    - **Space: low-order spatial moments or combine elements (polyhedral RHS mesh)**

NEWTRNX: development of a robust, efficient NEUTRAL-PARTICLE TRANSPORT ALGORITHM

- 3-D Slice-Balance Approach – based on 2-D Version in SCALE
  - Spatial Mesh:
    - Present: Unstructured tetrahedral mesh
    - Future: Unstructured polyhedra mesh (2007+)
  - Particle Direction: Discrete-ordinate directions
  - Neutron Energy:
    - Present: Multi-group approximation
    - Future: Point-wise (continuous-energy) (2007+)
- Accuracy and efficiency is in progress
  - Matching KENO (Monte Carlo transport in SCALE) for simple problems
  - Initial acceleration using Krylov sub-space solver
  - Execution with up to 10^9 degrees of freedom



$$\frac{1}{v}\frac{\partial \psi}{\partial t} + \vec{\Omega} \bullet \vec{\nabla}\psi + \Sigma_t \psi = S_{ext} + \int_0^{\infty} dE' \int_0^{4\pi} d\Omega' \left[\Sigma_s + F\right]\psi$$

MOC and Slice-Balance solve the RHS and LHS on independent mesh.

- **The LHS is solved on an angle-dependent fine-mesh:**
  - $\overline{\Omega_m} \bullet \overline{\nabla}\psi_m + \Sigma\left(\overline{r}, E\right)\psi_m\left(\overline{r}, E\right) = q_m\left(\overline{r}, E\right)$

$$\overline{\overline{L_m}}\,\overline{\psi_m} = \overline{q_m}$$

- **The RHS is solved on an angle-independent coarse-mesh:**
  - $Q_m\left(\vec{r}, E\right) = \int_0^\infty dE' \int_{4\pi} d\Omega_n \; \sigma_{E'\to E}^{n\to m} \; \Psi_n\left(\vec{r}, E'\right)$

$$\overline{Q} = \overline{\overline{S}}\,\overline{\Psi_m}$$

- **Prolongation and restriction operators relate the two equations:**
  - $q_m\left(\overline{r}, E\right) \approx Q_m\left(\overline{r}, E\right)$
  - $\Psi_m\left(\overline{r}, E\right) \approx \psi_m\left(\overline{r}, E\right)$

$$\overline{q_m} = \overline{\overline{P}}\,\overline{Q_m}$$

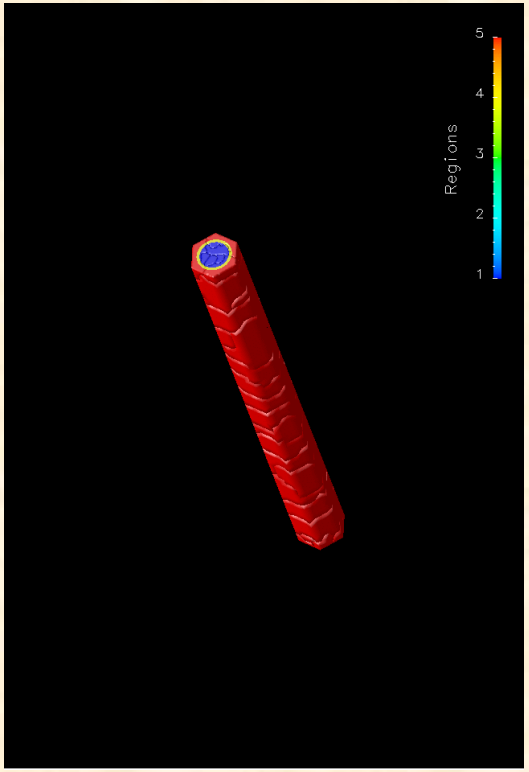
$$\overline{\Psi_m} = \overline{\overline{R}}\,\overline{\psi_m}$$

- **Fine-mesh accuracy with Coarse-mesh memory**
  - **Angular moments are smooth spatially**
  - **Spatial moments can account for spatial distribution**

NEWTRNX: Scalable transport for nuclear reactor simulation

- **Memory and computation decomposition**
  - **Spatial domain decomposition**
    - **Executed on up to 128 processors**
    - **Efficient terascale scaling expected for full reactor systems**
  - **Phase-space decomposition**
    - **Required for petascale, sub-set of full reactor, or other systems**

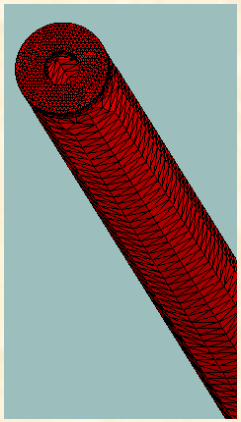
- **Asynchronous MPI communication**
  - **Well-suited for weakly-dependent domains**
  - **Provides a level of built-in load balancing**



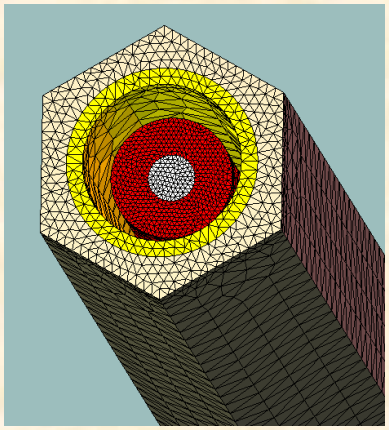
$$\vec{\Omega} \bullet \vec{\nabla}\psi + \Sigma_t \psi - \int_0^{\infty} dE' \int_0^{4\pi} d\Omega' \ \Sigma_s \psi = \lambda \int_0^{\infty} dE' \int_0^{4\pi} d\Omega' \ F\psi$$

Comparison with KENO

- **Infinite homogeneous medium**
  - **Identical cross sections**
  - **Identical solution**
- **HTTR fuel compact**
  - **44 or 238 groups – vacuum boundaries**
  - **Isotropic scattering, 2400 ordinates**
  - **keff:**
    - **KENO: 0.001564 (σ =0.03%)**
    - **NEWTRNX: 0.001567 (err =0.02%)**
- **HTTR fuel channel**
  - **44 or 238 groups – mirror boundaries**
  - **P_2 scattering, 144 ordinates**
  - **keff:**
    - **KENO: 1.1093 (σ =0.03%)**
    - **NEWTRNX: 1.1037 (err=0.03%)**



Fuel compact



Fuel channel

HPC Tools Have a Lot to Offer

- Performance analysis
- Visualization
- Mathematics libraries
- Parallel communication routines
- Domain decomposition
- Load balancing

- Don't reinvent the wheel
- But it might take an expert to use them correctly…

Conclusions and Present Status

- **GMAS: Geometry and Mesh Adaptivity Server**
  - **Utilizing HPC tools from the Office of Science's SciDAC program**
  - **Off-line CAD (Solid Works) to Mesh (Solid Works / GRUMPP / CUBIT)**
  - **On-line decomposition of the spatial domain (Metis)**
  - **Future: incorporation of Zoltan load balancing**
- **SCALECC: SCALE Component Container**
  - **On-line execution of cross section processing sequence**
  - **Including double-heterogeneity effects with CENTRM**
  - **Currently only scalar execution**
  - **Future: coarse-grained parallelization, less I/O**
- **NEWTRNX: 3-D Neutral-Particle Transport**
  - **3-D slice-balance on a tetrahedral mesh**
  - **Executed on 128 processors for 3 billion degrees of freedom**
  - **Replicating KENO solutions for simple problems**
  - **Future:**
    - **Incorporate preconditioners (TSA, CMR) and Krylov solvers**
    - **Add arbitrary polyhedral mesh & solver with linear characteristics**

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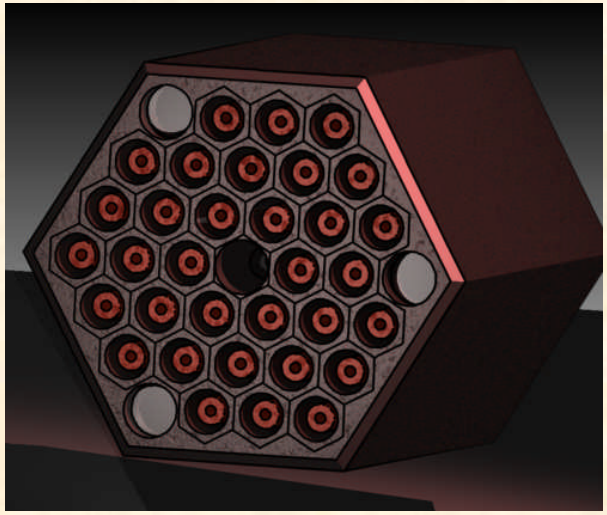
Backup Slides

Driver Sequence: HTTR

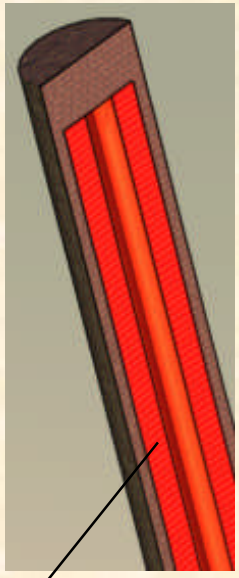
- **Controls execution flow for a given application**
  - **Operating HTTR (High-Temperature Test Reactor) facility in Japan**
  - **Well documented and benchmarked (IAEA-2003)**
  - **Our demonstration case for independent and coupled-physics simulation**



CAD model of an HTTR fuel element

Axial slice of fuel element

Fuel channel



Fuel rod

heated by fission

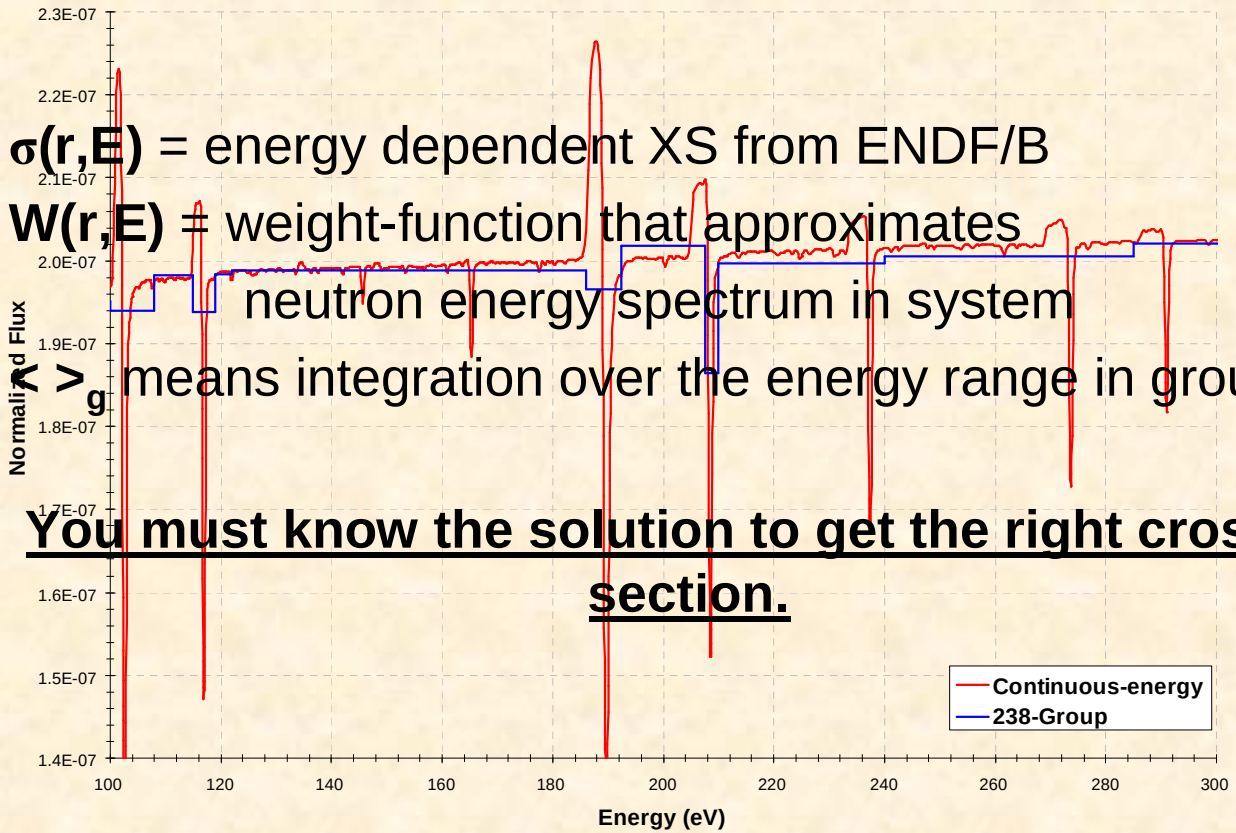
Common Component Architecture allows diversity to interrelate

- Diverse physics applications
  - Modularized coding simplifies complexity of system models
- Code development within a multi-institution team
  - Allows developers with diverse backgrounds to work remotely on large, complex codes
- Coupling of independent physics codes
  - Relevant applications use many codes, which were not originally intended to interoperate
  - Codes must maintain a stand-alone capability
- Language interoperability
  - Presently we utilize C, C++, and F90 languages
  - Multiple languages within a code
  - Multiple codes each with a different language

- SciDAC CCTTS – Center for Component Technology and Terascale Software
  - Software engineering and integration (www.cca-forum.org)

We need continuous energy transport when simple weighting functions fail.

$$\sigma_g(r) = \frac{\langle \sigma(\mathrm{r,E}) W(\mathrm{r,E}) \rangle_g}{\langle W(\mathrm{r,E}) \rangle_g}$$



- **σ(r,E)** = energy dependent XS from ENDF/B
- **W(r,E)** = weight-function that approximates neutron energy spectrum in system
- **$\langle\ \rangle_g$** means integration over the energy range in group 'g'

<u>You must know the solution to get the right cross section.</u>