Enabling High-Fidelity Neutron Transport Simulations on Petascale Architectures

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Dinesh Kaushik
Micheal Smith
Allan Wollaber
Barry Smith
Andrew Siegel
Won Sik Yang

Argonne National Laboratory
Argonne, IL 60439
kaushik@mcs.anl.gov

Organization of the Presentation

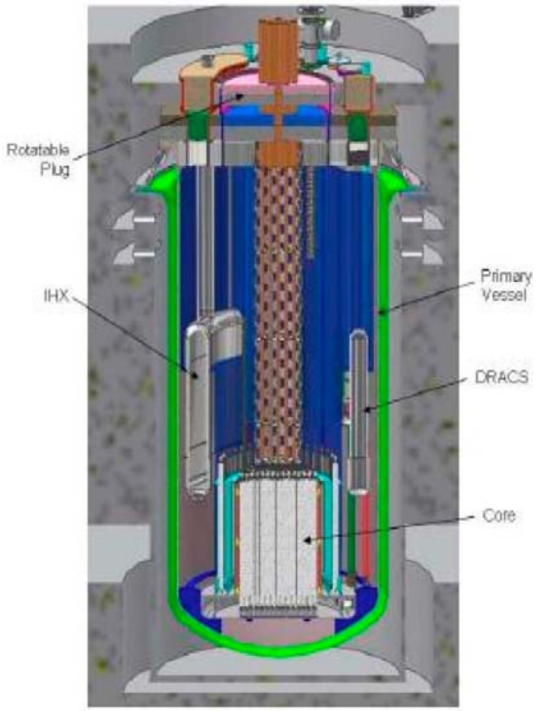
- Overview of SHARP Project at Argonne
- Computational issues for neutronics
- Full-core test problems
- Parallel performance of UNIC
- Summary

Nuclear Reactor Simulations

- Nuclear fission energy is key component of our current and future energy needs
- Urgent need to develop reactors that are
  - Safe
  - efficient
  - Affordable
- Modeling and simulation tools were simplified to match the available computing technology
  - designers relied on expensive and complicated experiments for satisfactory answers
- Advanced simulation can help in evaluating new designs with reduced dependence on experiments
- This work is supported by Nuclear Energy Advanced Modeling and Simulation (NEAMS) program of US Department of Energy

Case for Fast Reactor Simulations

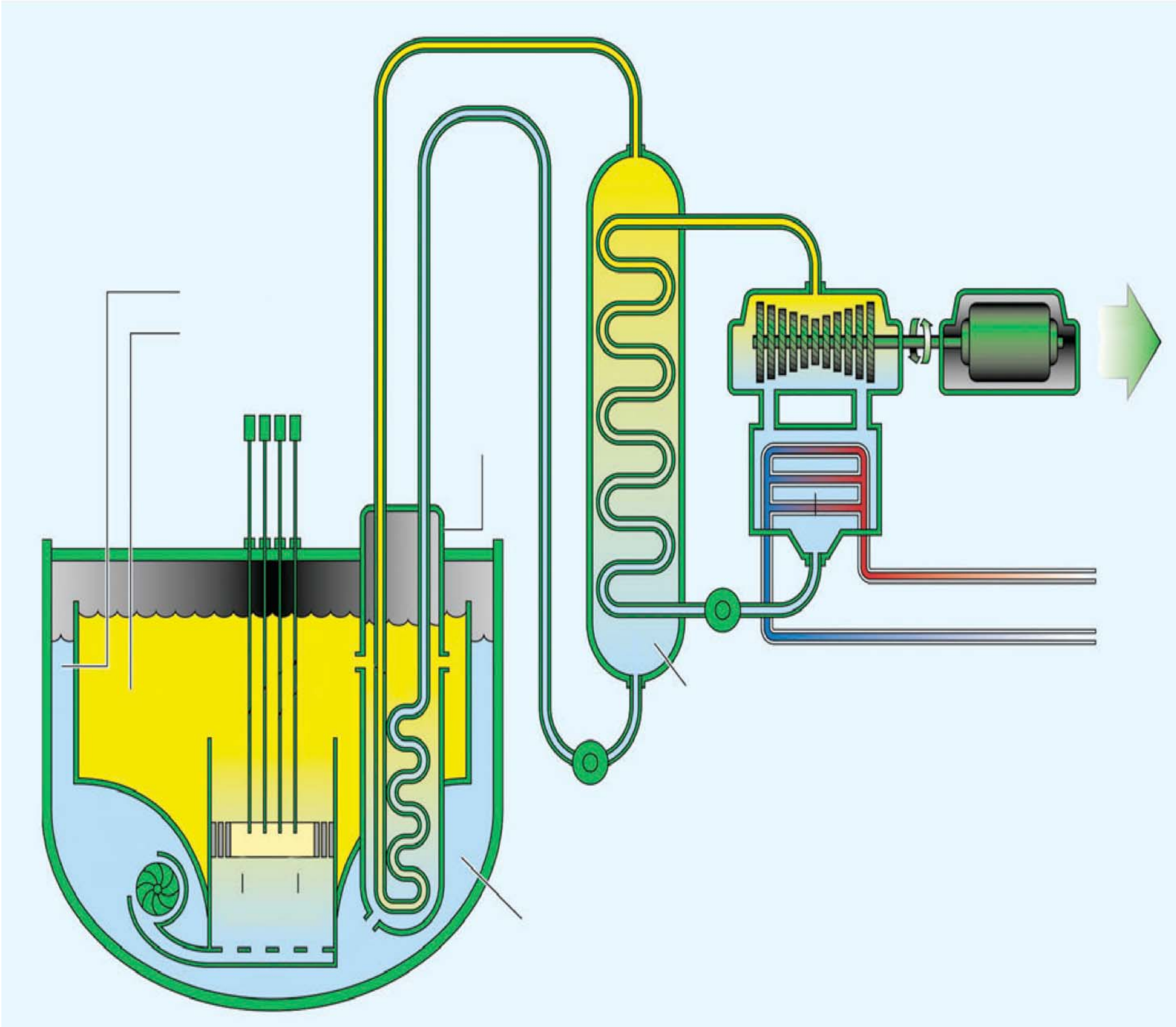
- High energy neutrons are used to convert uranium to plutonium
- Recycle the spent fuel from light water reactors (LWR)
  - Reducing heat load on storage because of lower concentration of transuranic elements
- Through high fidelity simulations,
  - Lower uncertainty margins of the new reactor designs
    - 1% improvement in daily power output translates to millions of dollars for utility companies
  - Global design optimization for enhanced safety and cost



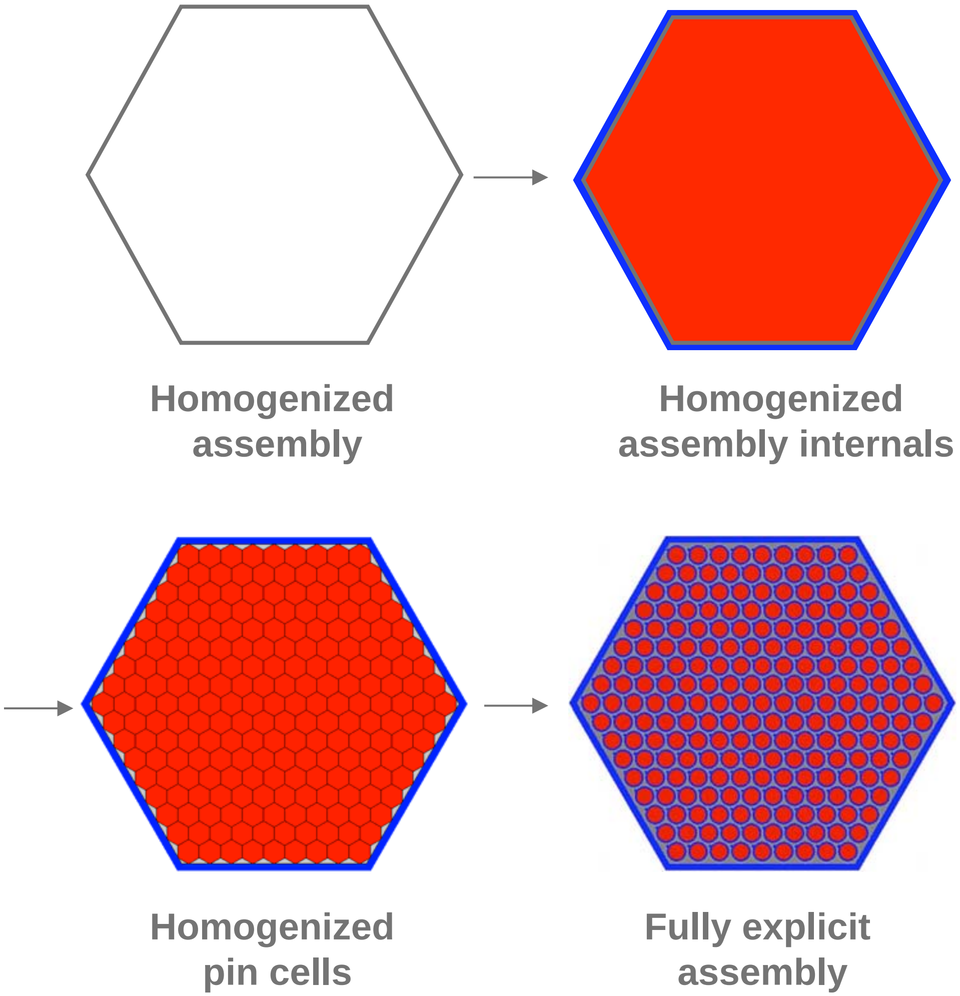
Simulation based High-efficiency Advanced Reactor Prototyping (SHARP)

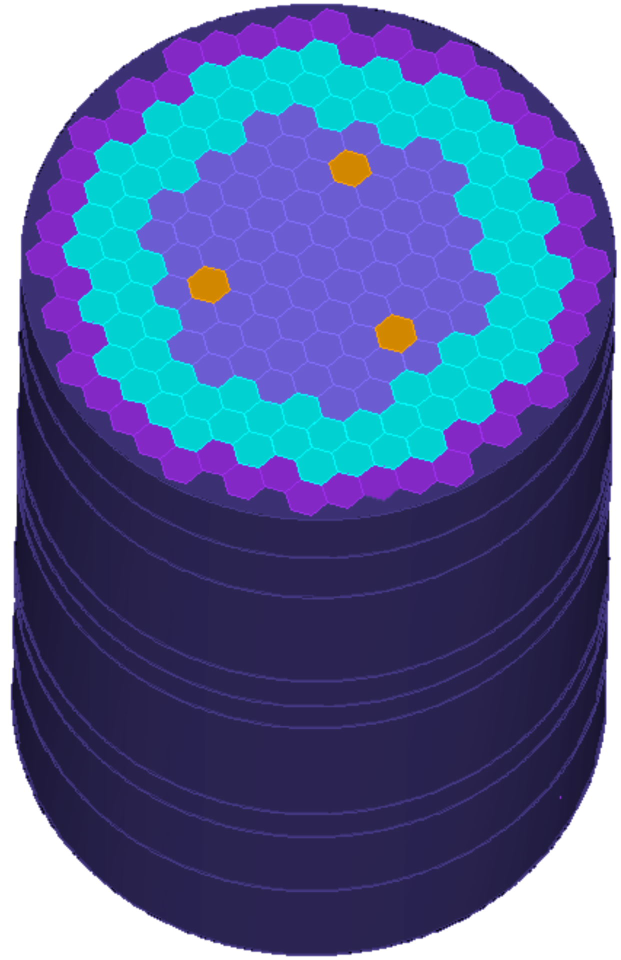
- A tight integration of multiphysics and multiscale modeling of physics phenomena based on a first principles approach
  - an integrated system of software tools
  - accurate description of
    - the overall nuclear plant behavior in a high fidelity way
    - coupling among the different phenomena taking place during reactor operation ranging from neutronics to fuel behavior, from thermal-hydraulics to structural mechanics
- Features
  - Ability to derive basic data and static and dynamic (operating conditions) properties from first principles based methodologies and fundamental experiments
  - to define and plug-in new and different combinations of physics-module implementations to study different phenomena,
  - define and combine different numerical techniques, configure the code easily to run on new platforms
  - develop new physics components without expert knowledge of the entire system.

Schematic diagram of a fast reactor



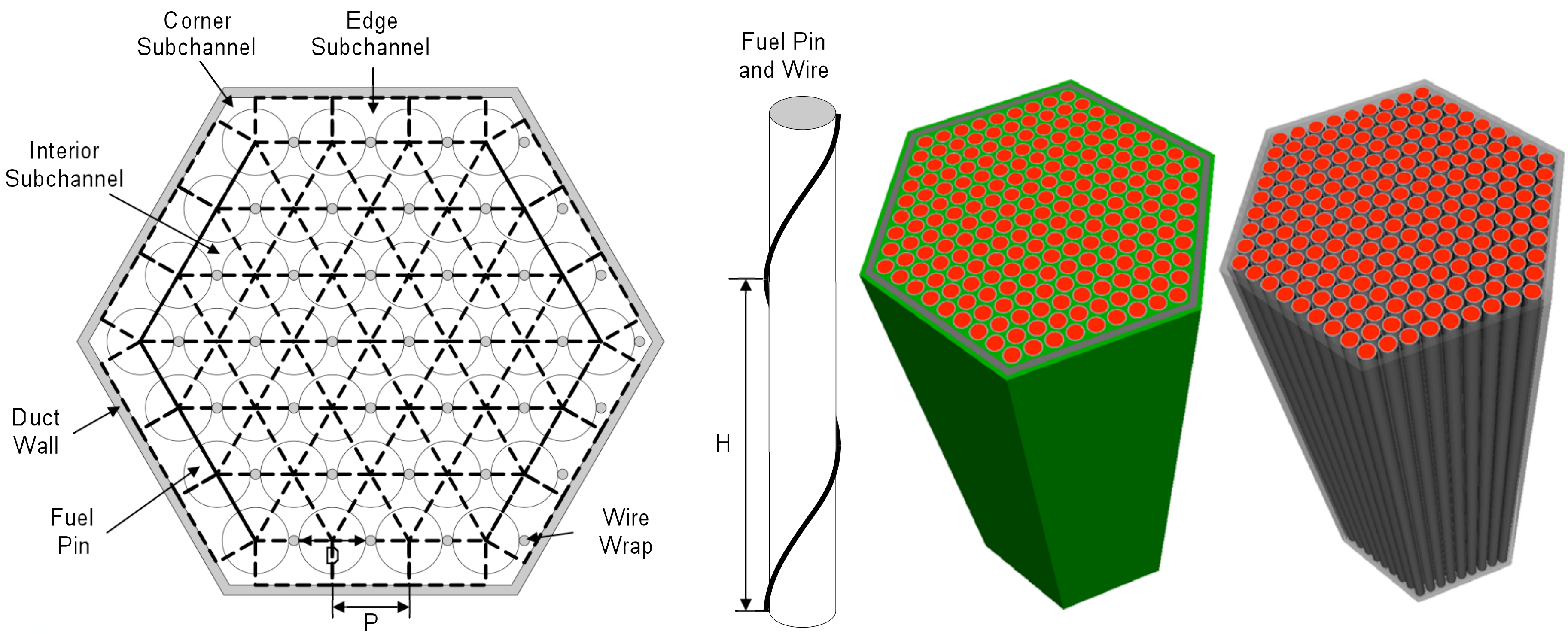
Homogenization at various levels





Fine Detail: Wire Wrapped Pins in Subassembly

- *Resolving wire wrap (diameter = 0.11 cm) leads to 10-100 billion element meshes and about 10^{15} degrees of freedom (DOF) for advanced burner test reactor (ABTR) core (2.3 m in diameter and 3.5 meter long)*



UNIC: Neutronics Module in SHARP

- A 3D unstructured deterministic neutron transport code
- solves
  - second order form of transport using FEM (PN2ND and SN2ND) and
  - first order form by method of characteristics (MOC)
- Parallel implementation using PETSc solvers

The Steady State Transport Equation (p46 in Lewis)

$$\hat{\Omega}\cdot\vec{\nabla}\psi(\vec{r},\hat{\Omega},E)+\Sigma_t(\vec{r},E)\psi(\vec{r},\hat{\Omega},E)=\int\int\Sigma_s(\vec{r},\hat{\Omega}'\rightarrow\hat{\Omega},E'\rightarrow E)\psi(\vec{r},\hat{\Omega}',E')d\Omega' dE'$$
$$+\frac{1}{k}\chi(\vec{r},E)\int\int\nu(\vec{r},E')\Sigma_f(\vec{r},E')\psi(\vec{r},\hat{\Omega}',E')d\Omega' dE'$$
$$+S(\vec{r},\hat{\Omega},E)$$

$\psi(\vec{r},\hat{\Omega},E)$	The neutron flux (neutron density multiplied by speed)
$\Sigma_t(\vec{r},E)$	The total probability of interaction in the domain
$\Sigma_s(\vec{r},\hat{\Omega}'\rightarrow\hat{\Omega},E'\rightarrow E)d\Omega dE$	The scattering transfer kernel
$\chi(\vec{r},E)\quad\nu(\vec{r},E)\quad\Sigma_f(\vec{r},E)$	The steady state multiplicative fission source
$S(r,\hat{\Omega},E)$	If a fixed source is present then k = 1
k	The multiplication eigenvalue

Solving the Eigenvalue Problem

$A\,x = \lambda\,x$ Cast the transport equation as a pseudo matrix-vector operation

T = streaming/collision/scattering F = fission

$$\psi = \left[\psi_1(\vec{r},\hat{\Omega}) \quad \psi_2(\vec{r},\hat{\Omega}) \quad \cdots \quad \psi_G(\vec{r},\hat{\Omega}) \right]^T$$

$$T\psi = \hat{\Omega}\cdot\vec{\nabla}\psi_g(\vec{r},\hat{\Omega}) + \Sigma_{t,g}(\vec{r})\psi_g(\vec{r},\hat{\Omega}) - \sum_{g'=1}^{G}\int \Sigma_{s,g'\to g}(\vec{r},\hat{\Omega}'\to\hat{\Omega})\psi_{g'}(\vec{r},\hat{\Omega}')d\Omega'$$

$$F\psi = \chi_g(\vec{r})\sum_{g'=1}^{G}\int \nu_{g'}(\vec{r})\Sigma_{f,g'}(\vec{r})\psi_{g'}(\vec{r},\hat{\Omega}')d\Omega'$$

$$T\psi = \frac{1}{k}F\psi$$

Standard eigenvalue notation:

$$A\,x = \lambda\,x$$

$$A = T^{-1}F$$

$$x = \psi$$

$$\lambda = k$$

k-Eigenvalue Power Iteration

Begin Outer Iteration

Begin Loop over energy groups

Begin Scattering iteration for the within-group scattering system

Begin Conjugate gradient over the whole space-angle system

Obtain group scattering+fission+fixed sources

Solve a symmetric positive definite linear system for flux

(preconditioned conjugate gradient)

End Conjugate gradient over the whole space-angle system

End Scattering iteration for the within-group scattering system

End Loop over energy groups

Check for convergence in eigenvalue, angular flux, and sources

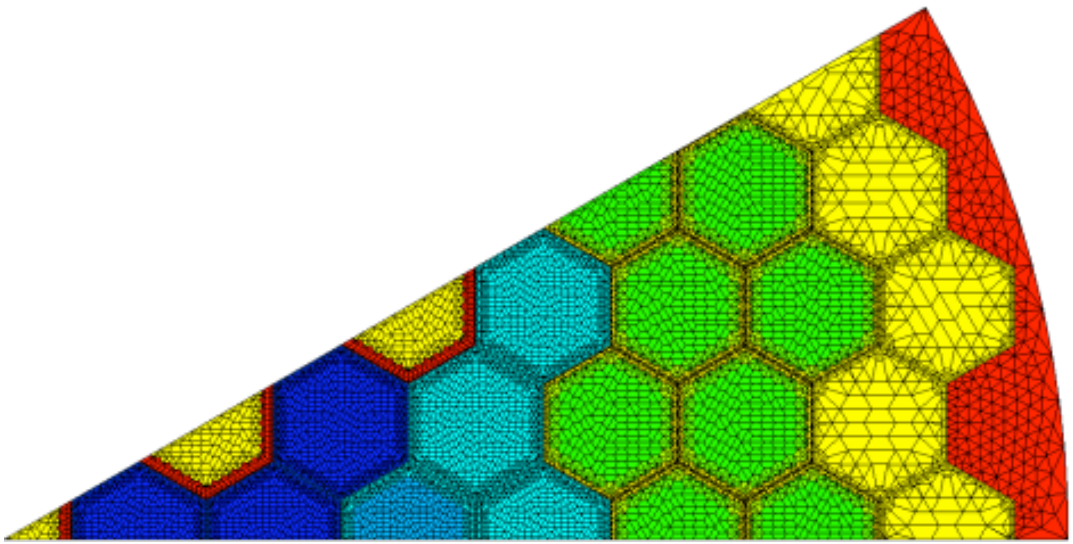
End Outer Iteration

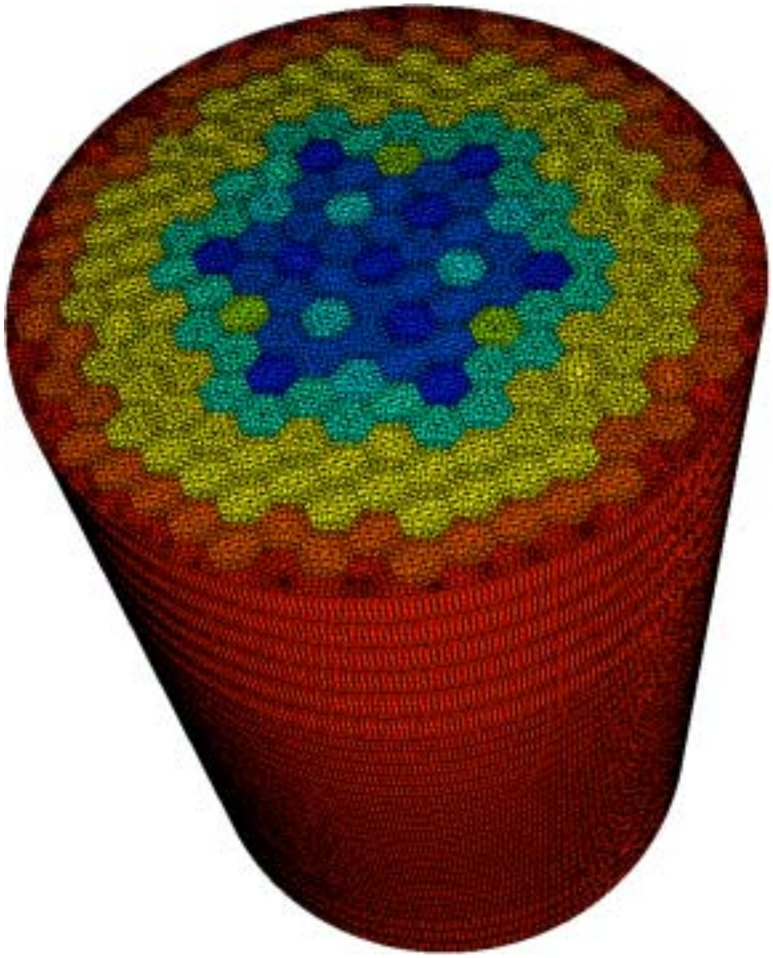
Features of Second Order Form Solutions in UNIC

- PN2ND and SN2ND solvers have been developed to solve the steady-state, second-order, even-parity neutron transport equation
  - PN2ND: Spherical harmonic method in 1D, 2D and 3D geometries with FE mixed mesh capabilities
  - SN2ND: Discrete ordinates in 2D and 3D geometries with FE mixed mesh capabilities
- These second order methods have been implemented on large scale parallel machines
  - Linear tetrahedral and quadratic hexahedral elements
  - Fixed source and eigenvalue problems
  - Arbitrarily oriented reflective and vacuum boundary conditions
  - PETSc solvers are utilized to solve within-group equations
    - Conjugate gradient method with SSOR and
    - ICCgives better flop rates but requires more memory (not used)
  - Synthetic diffusion acceleration for within-group scattering iteration
  - Inverse Power iteration method for eigenvalue problem
  - MeTiS is employed for mesh partitioning

ABTR Whole-Core Calculations

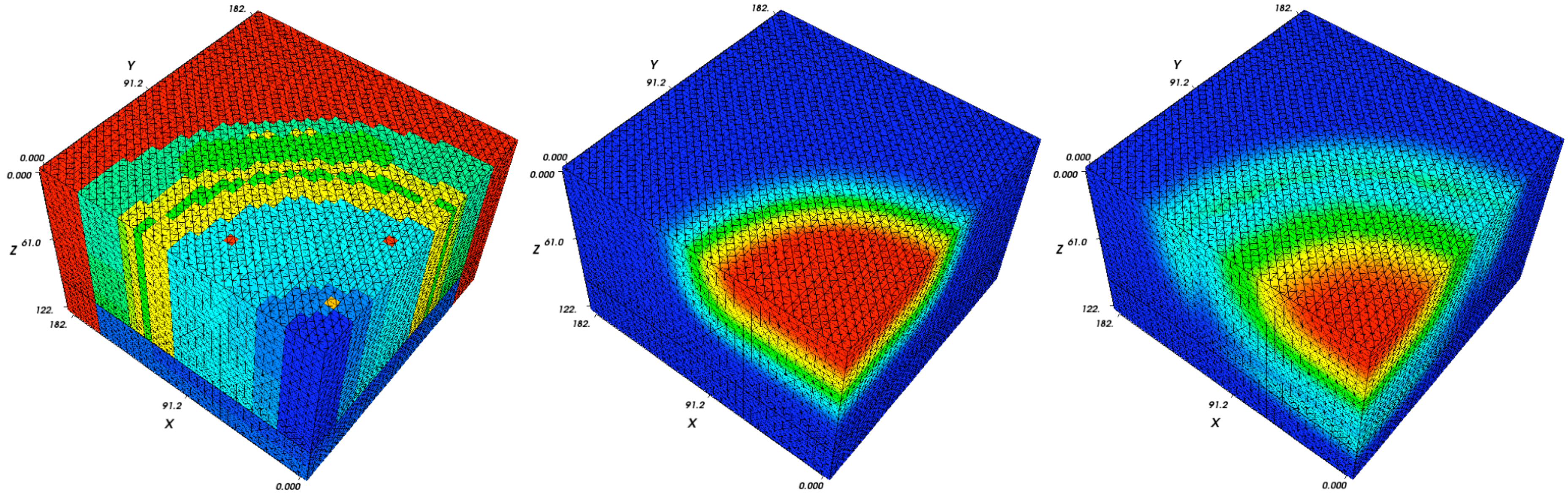
Angular Directions	Spatial Mesh Approximation				
	78243	113873	461219	671219	785801
32	-241	-233	-69	-64	-59
50	-220	-210	-47	-40	-37
72	-225	-217	-51		
98	-216	-207	-43		
288	-216				



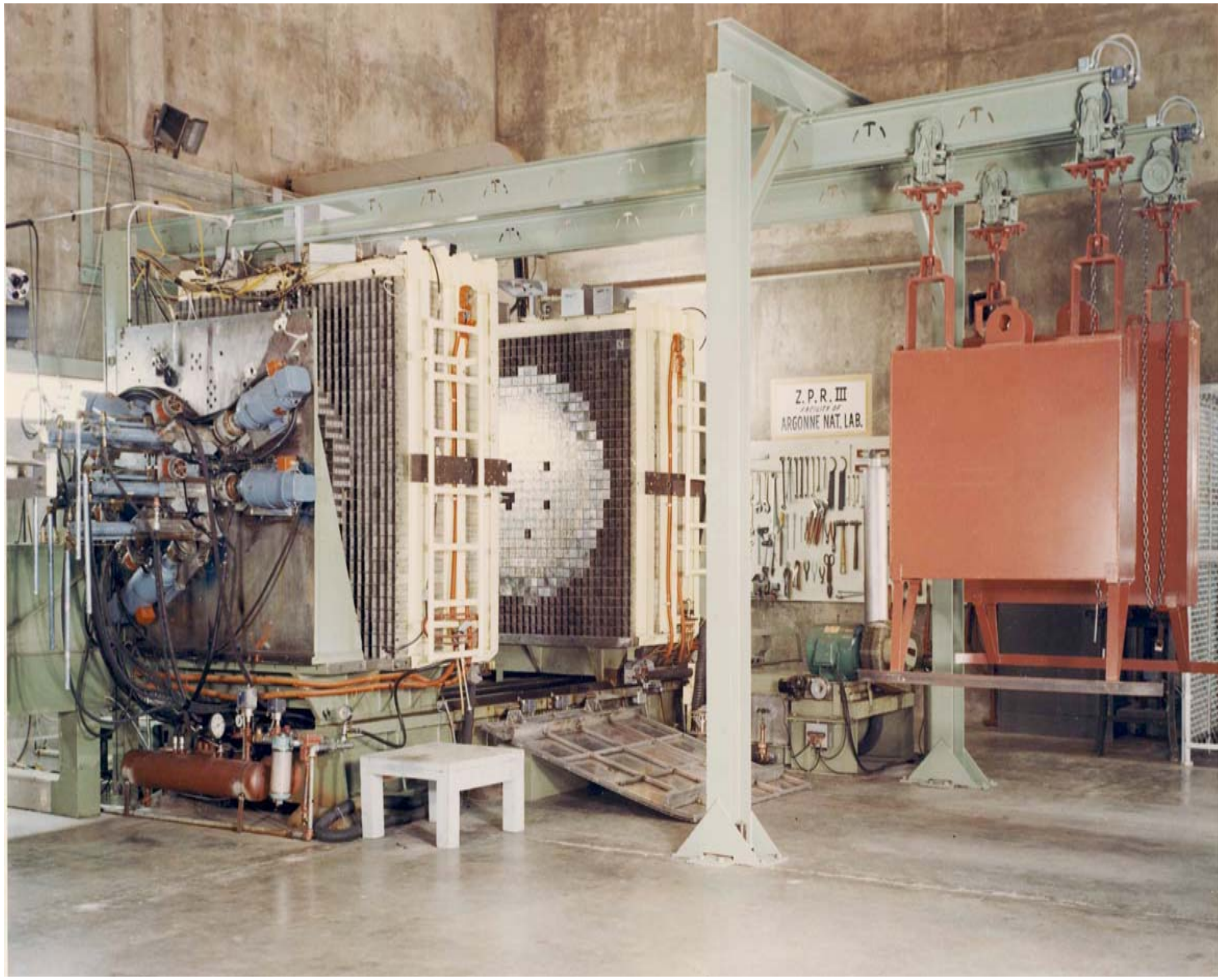


ZPPR-15 Critical Experiments

Flux expansion order	Scattering order	Eigenvalue
P_1	P_1	0.99258
P_3	P_3	0.99640
P_5	P_3	0.99651
Monte Carlo (VIM)		0.99616±0.00010



Computational Mesh and Example Flux Solutions of ZPPR-15 Critical Experiment

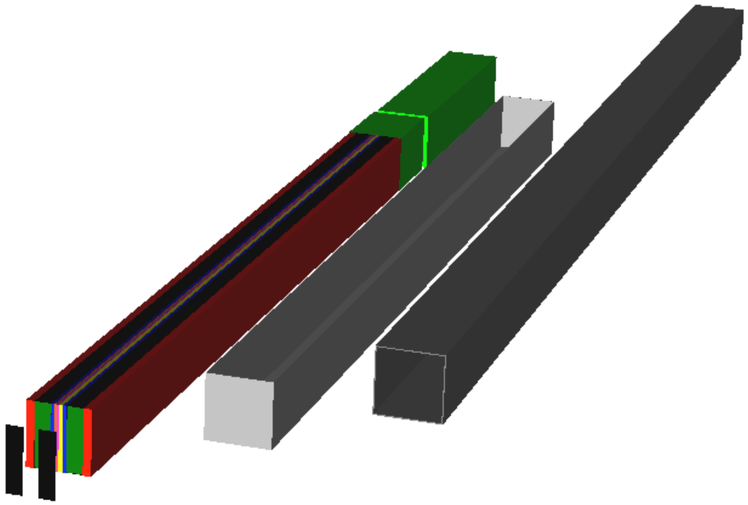


ZPR-3

Over a period of 30 years more than a hundred Zero Power Reactor (ZPR) critical assemblies were constructed at Argonne National Laboratory.

ZPR-3, ZPR-6, ZPR-9 and ZPPR, were all separate fast critical assembly facilities with each machine being used for thousands of individual experiments

ZPR Test Problem



Single ZPR Drawer

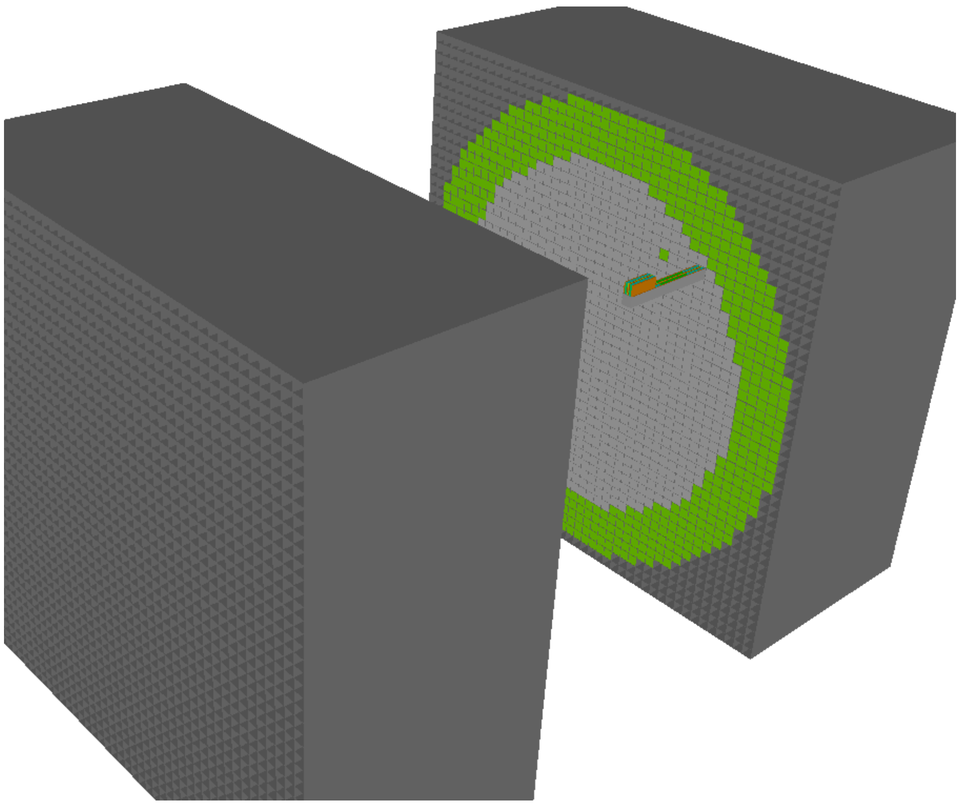


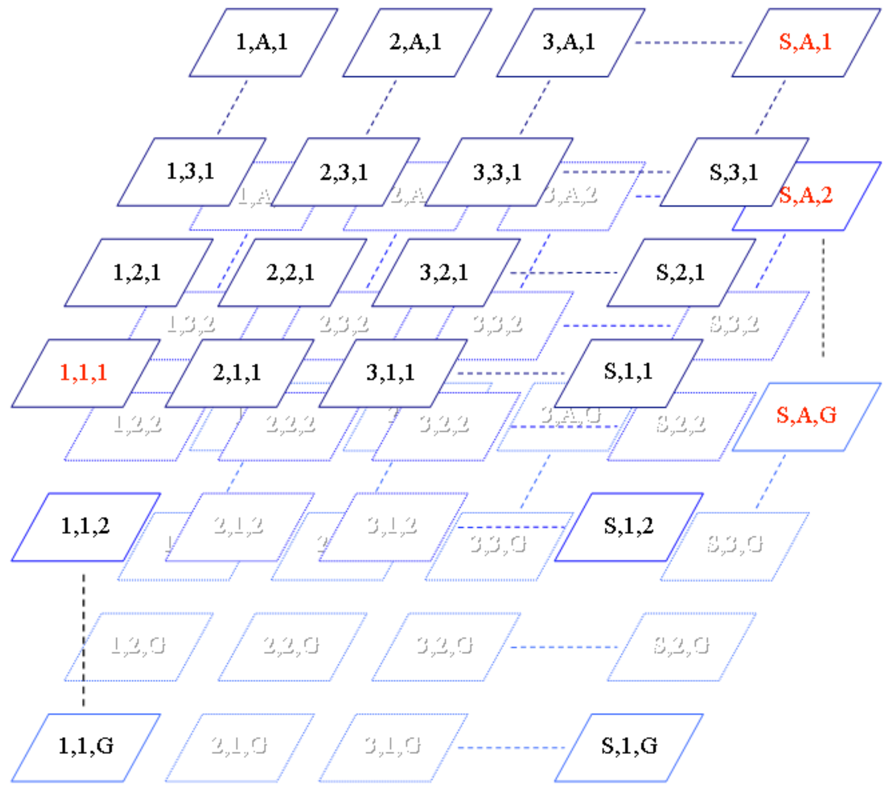
Plate by Plate ZPR Geometry

A ZPR calculation is the first step to full core heterogeneous reactor calculations

- Up to 50 million vertices (~equivalent to 200 million PARTISN finite difference cells)
- 100+ angles with P_5 anisotropic scattering
- 100 energy groups
- No thermal-hydraulics considerations (i.e. clean comparison, MCNP/VIM solvable)

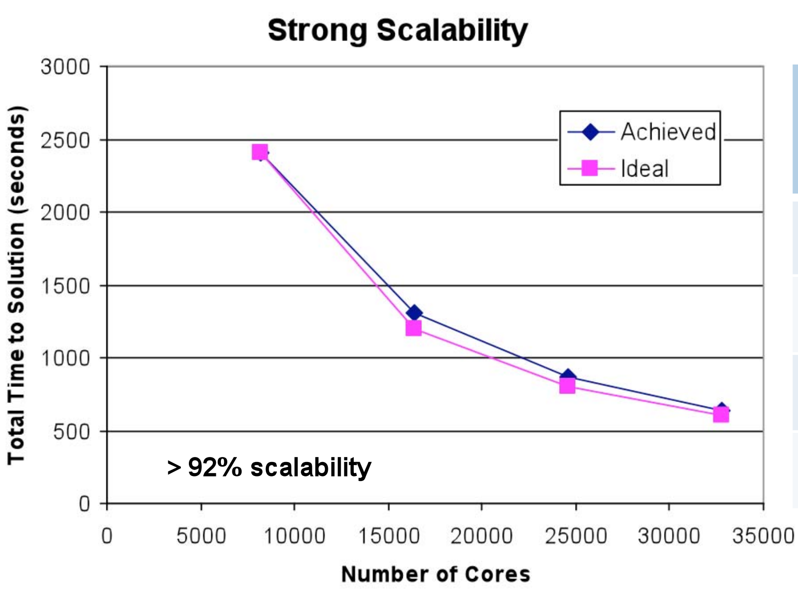
Parallelism in Space, Angle, and Energy

- Hierarchical Partitioning by using MPI communicators
- Parallelization in every dimension is important (to avoid per-core memory limit)
- User defined MPI communicators are not always optimized for mapping to cores



Performance on Blue Gene/P – Strong Scaling

- 9 energy groups
- Mesh (simplified geometry)
  - 15 million vertices and 1.8 million hexahedral quadratic elements
  - Spread over 4,096 processor cores (virtual node mode)
  - 4 angles per processor-core



Total Cores	Vertices/ Process	Total Time (seconds)	Parallel Efficiency
8,192	7,324	2,402	100%
16,384	3,662	1,312	92%
24,576	2,441	873	92%
32,768	1,831	637	94%

Performance on Blue Gene/P – Weak Scaling
ANL: 40 racks (163,840 cores); JSC: 72 racks (294,912 cores)

- Weak scaling important for scoping studies
- 9 energy groups
- Mesh
  - 7 million vertices and 1.7 million hexahedral quadratic elements
  - Spread over 4,096 processor cores (virtual node mode)
  - 2 angles per processor-core

Total Cores	4π Angles	Total Time (seconds)	Weak Scaling
32,768	32	579	100%
73,728	72	572	101%
131,072	128	581	100%
163,840	160	691	84%
294,912	288	763	76%

Performance on XT5

Recently upgraded hex-core system, 2.6 GHz, 225K total cores

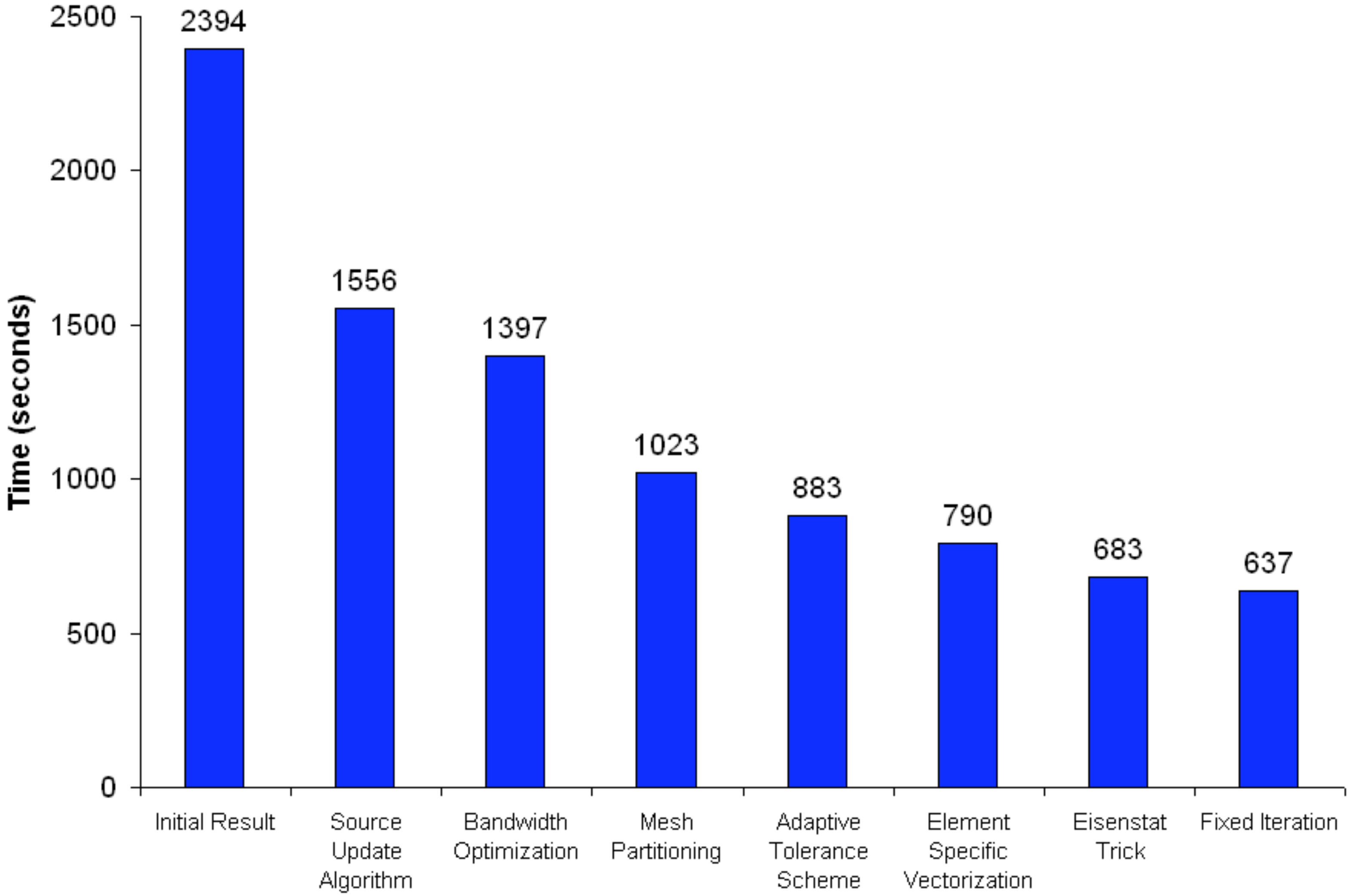
- 33 energy groups
- Mesh (real experimental geometry)
  - 10 million vertices and 2.4 million hexahedral quadratic elements
  - Spread over 2,064 processor cores
  - 2 angles per processor-core

Total Cores	4π Angles	Total Time (seconds)	Weak Scaling
16,512	32	1891	100%
37,152	72	1901	99%
66,048	128	1829	103%
103,200	200	2050	92%
148,608	288	2298	82%
222,912	432	2517	75%

Performance Optimizations

- Reordering for better cache reuse
- Unrolled loops for specific element types (better vectorization)
- Weighted partitioning for load balance in mesh partitioning
- Fixed iteration scheme for load balance across angular systems
- Eisenstat's Trick (lower flop rate but better execution time)

Performance Optimizations –
Execution Time Reduced by a Factor of 4 on 16,384 Cores



Assessing the Single Core Performance

- Execution time was optimized (often) at the cost of flops (likely unnecessary)
- Sparse matrix vector multiplication (BLAS Level 2) operation is the main kernel
  - Performance is memory bandwidth limited (little data reuse)
  - High ratio of load/store to instructions/floating-point ops
  - Flops not the right metric
  - Inadequate memory bandwidth on both architectures

Stream Benchmark on Cray XT5 and BlueGene/P (MB/s for the Triad Operation)

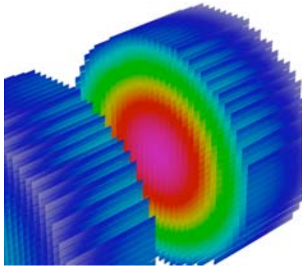
Threads per Node	Cray XT5		BlueGene/P	
	Total	Per Core	Total	Per Core
1	8448	8448	2266	2266
2	10112	5056	4529	2264
4	10715	2679	8903	2226
6	10482	1747	-	-

Ideal Sparse Matrix-Vector Performance

Required: 6 bytes/flop

Machine	Peak MFlop/s per core	Bandwidth (GB/s)		Ideal MFlop/s
		Required	Measured	
Blue Gene/P	3,400	20.4	2.2	367
XT5	10,400	62.4	1.7	292

Summary



- UNIC provides reactor designers a scalable and flexible simulation tool that has the potential to transform the reactor analysis field by exploiting supercomputing with far reaching consequences on reactor development cost and safety.
- We were able to resolve the complex geometric features of the full ZPR core geometry for the first time.
- UNIC scales well on the two largest machines:
  - 76% on 294,942 cores of Blue Gene/P (ANL& JSC, Jugene is the largest in core count)
  - 75% on 222, 912 cores of XT5 (ORNL, #1 in TOP500)
  - Uses up to 500 billion degrees of freedom
- No other code in the field (deterministic neutron transport) has scaled to this level or solved full core-sized problems with this fidelity.
- Computational challenges need to be tackled at the modeling, algorithmic, and architectural levels for future machines with millions of cores.

Acknowledgements

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