Enhancements to the Combinatorial Geometry Particle Tracker in the Mercury Monte Carlo Transport Code: Embedded Meshes and Domain Decomposition

Gregory Greenman, Matthew O'Brien and **Richard Procassini**
Lawrence Livermore National Laboratory

Kenneth Joy
University of California Davis

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Lawrence Livermore National Laboratory, P.O. Box 808, Livermore, CA 94551

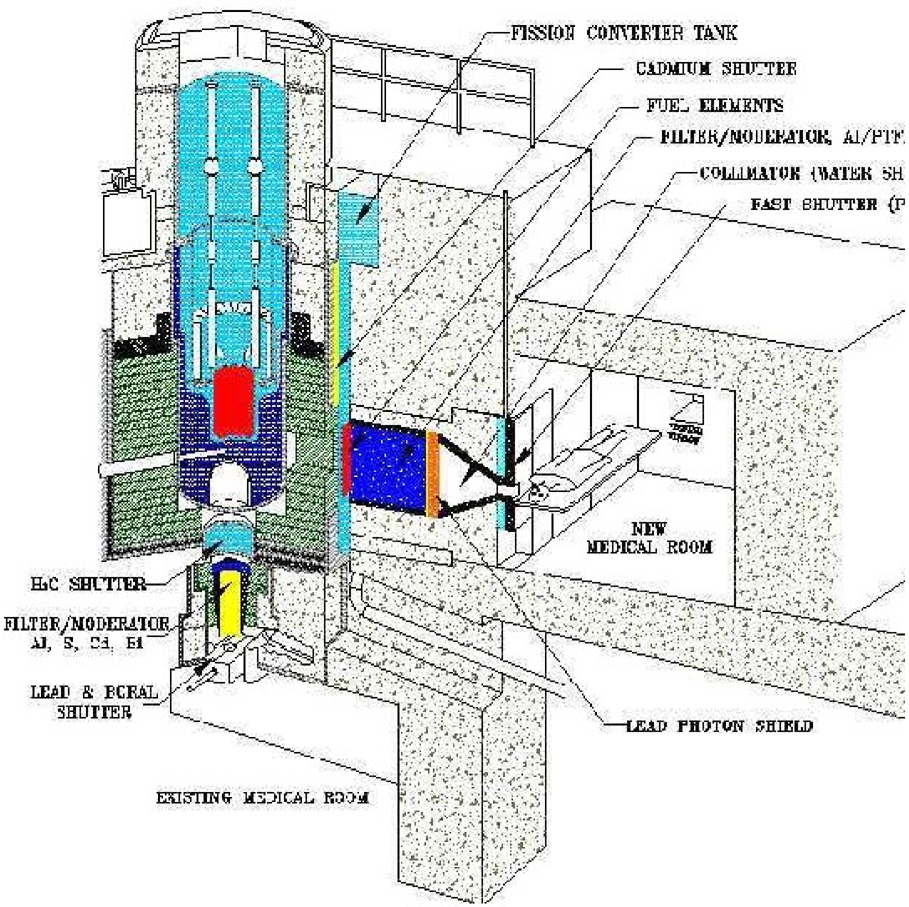
Motivation for Embedding Meshes within a Combinatorial Geometry

- In problems where the problem geometry contains large regions with homogeneous material properties, a combinatorial geometry (CG) representation is most useful for representing such a geometry.
- CG is not the most efficient when the problem geometry is highly heterogeneous. In these cases, a mesh representation is more appropriate.
- One may also wish to opt for a mesh representation when the transport problem in question is coupled to other physics, such as a thermal-hydraulics solver, which are usually mesh based.
- An optimal solution is a hybrid approach: use a CG representation in the regions with large volumes with homogeneous material properties, and a mesh representation where the flexibility of a mesh representation is required.
- One then needs to be able to “stitch” the two representations together wherever they meet and ensure the continuity of the transport solution across the boundaries of these regions.

Application of Embedded Mesh Technology

The MIT Reactor BNCT Radiotherapy Beamline

The MIT Radiotherapy Facility

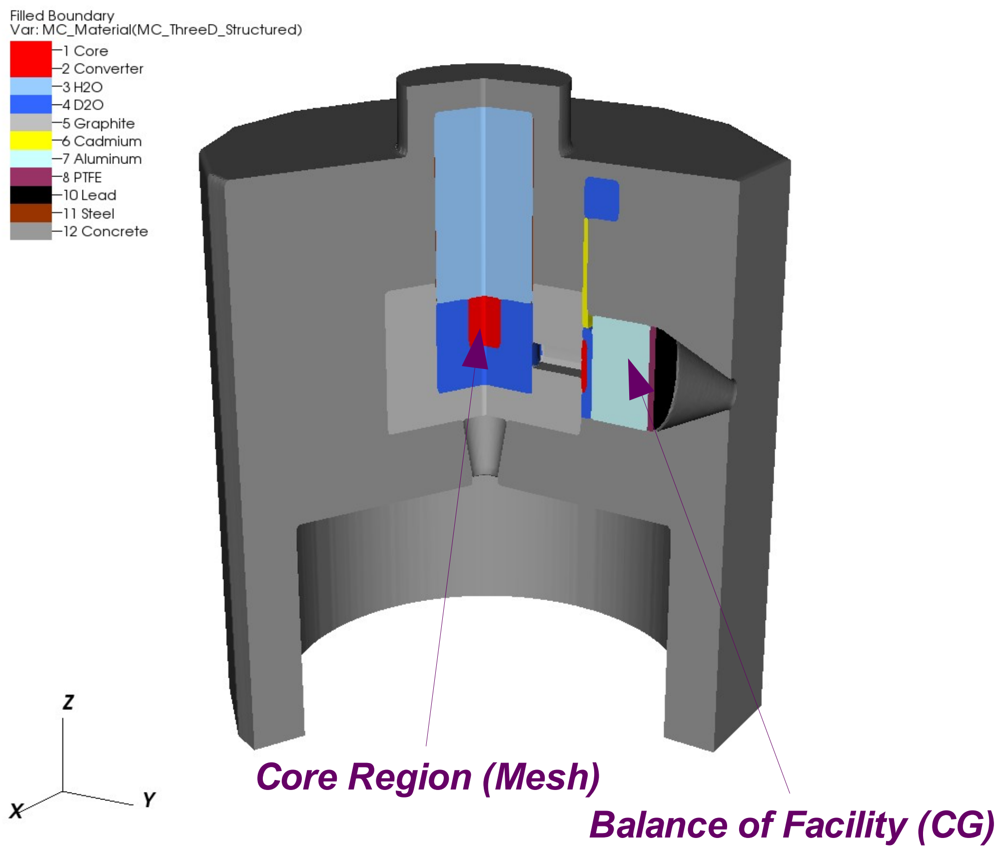


- The MIT radiotherapy facility [1], [2] couples the MIT reactor to a converter pile of spent fuel assemblies which produce an epithermal neutron spectrum.
- The epithermal neutron spectrum is used for boron neutron capture therapy (BNCT), since it provides a lower dose to the patient than would be received from thermal neutrons.
- Gammas are removed from the therapy beamline by a lead shield.

Application of Embedded Mesh Technology

The Mercury Model of the MIT Radiotherapy Facility

MIT Radiotherapy Facility (Mercury Model)

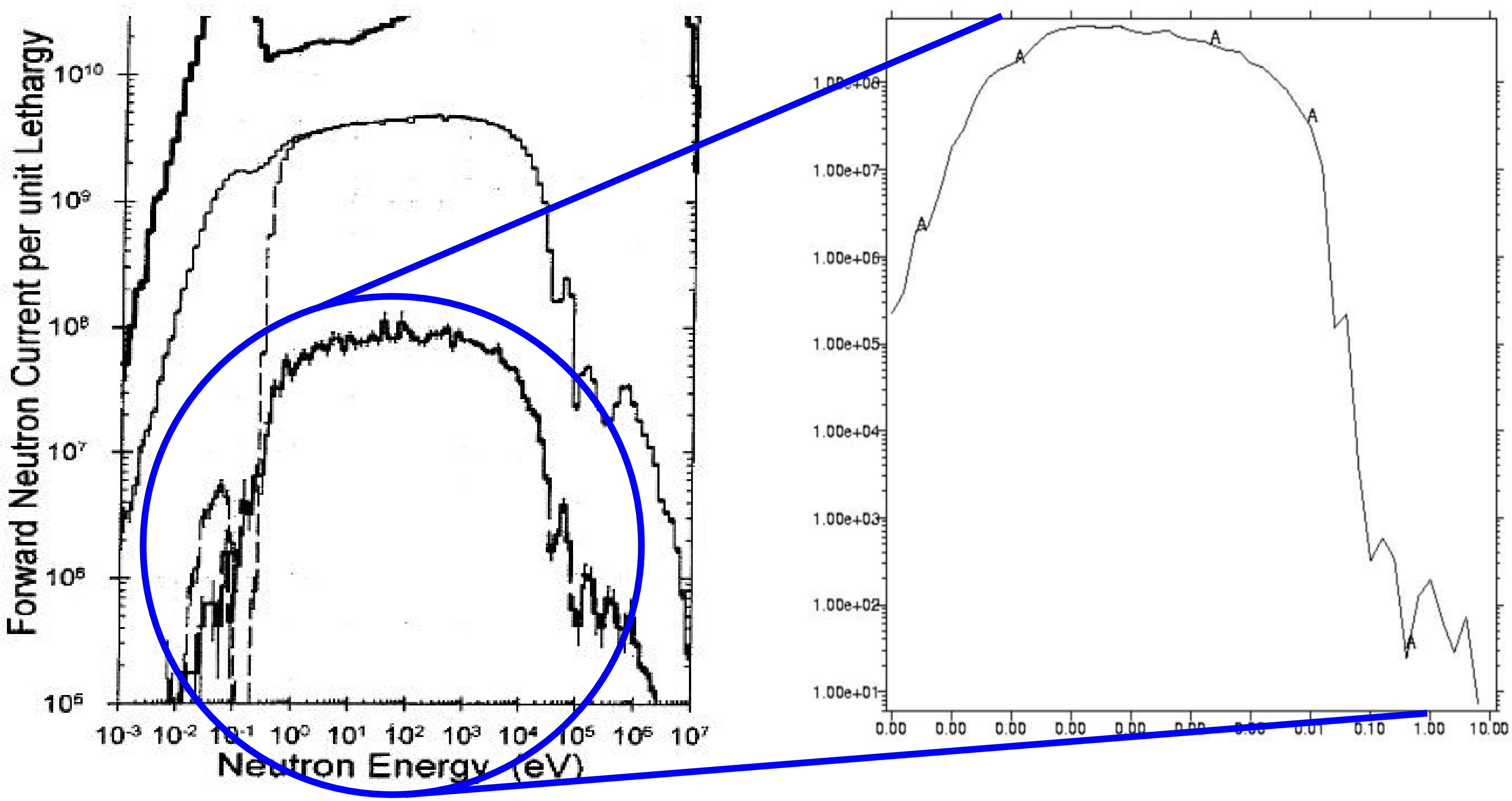


- The ***Mercury*** [3],[4] model of the MIT radiotherapy / BNCT facility:
  - ➔ Models the reactor core using a 3-D Cartesian mesh representation which permits coupled transport and thermal-hydraulics calculations
  - ➔ Models the balance of the facility with a CG representation to minimize the number of cells required

Application of Embedded Mesh Technology

Experimental vs Computed Therapy Spectrum

Experimental Spectrum ***Computed Spectrum***



Parallel Monte Carlo Transport Calculations Using Spatial Domain Decomposition

- In problems with large and complex geometries, the memory available to a single processor may be insufficient to store the entire geometry.
- In this case, the problem geometry can be spatially decomposed into domains, each of which has smaller memory requirements, that are assigned to several processors.
- Particles that are tracked to an inter-processor domain boundary must be communicated prior to completing its tracking.
- Domain decomposition of the problem geometry in Monte Carlo calculations has been used in mesh-based problems for more than a decade [5], but has not been applied to combinatorial-geometry-based problems until now.
- Determination of the cells that are assigned to each spatial domain requires knowledge of the cell connectivity.

Monte Carlo Spatial Domain Decomposition

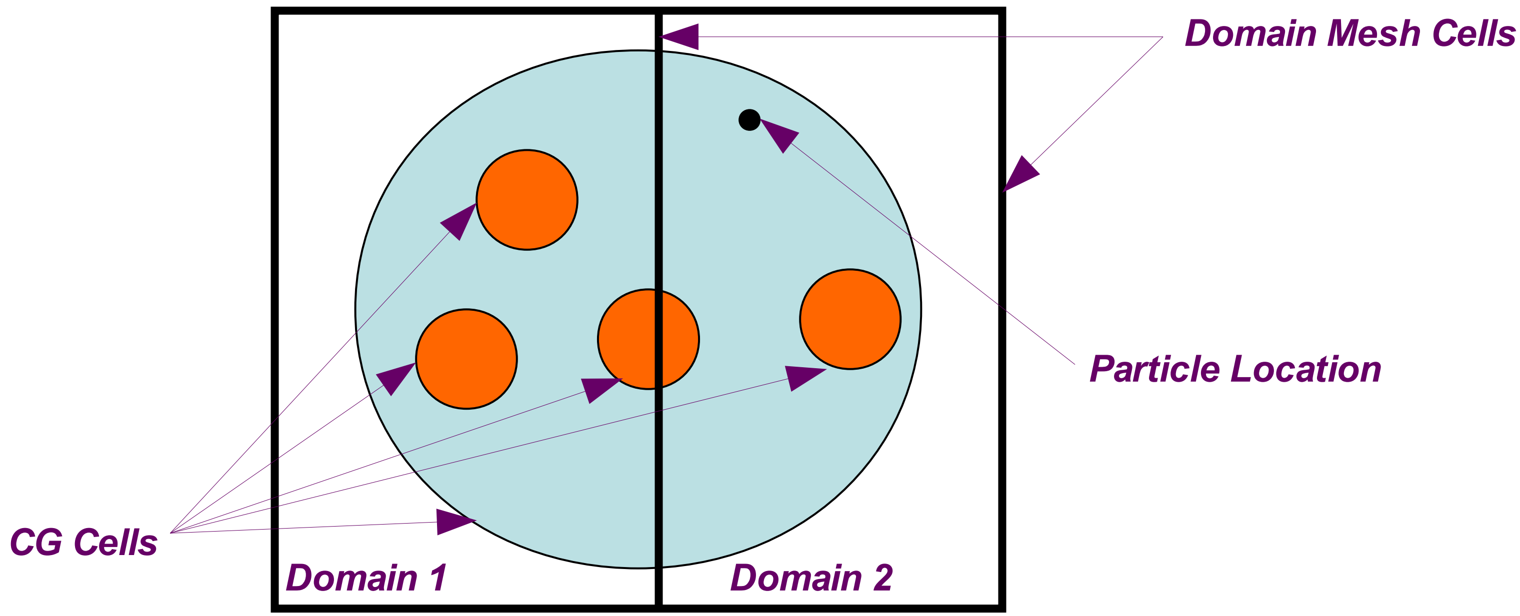
Mesh vs Combinatorial Geometry

- Differences in mesh and combinatorial geometry cell connectivities affect the decomposition strategies used in parallel Monte Carlo particle transport:
  - ➔ *Mesh Geometry:*
    - ✔ The cell connectivity is an integral part of the mesh description
    - ✔ When particles cross a cell facet, the cell connectivity is used to assign the particle's new cell and domain attributes
    - ✔ This connectivity is used to spatially decompose the mesh and determine the resulting communication patterns
  - ➔ *Combinatorial Geometry:*
    - ✔ Typically, the connectivity of cells in a CG is *not* known
    - ✔ When particles cross a cell surface, the cell that their coordinates reside in must be determined
    - ✔ Therefore, the connectivity of the CG cells has to be provided or derived

Monte Carlo Spatial Domain Decomposition

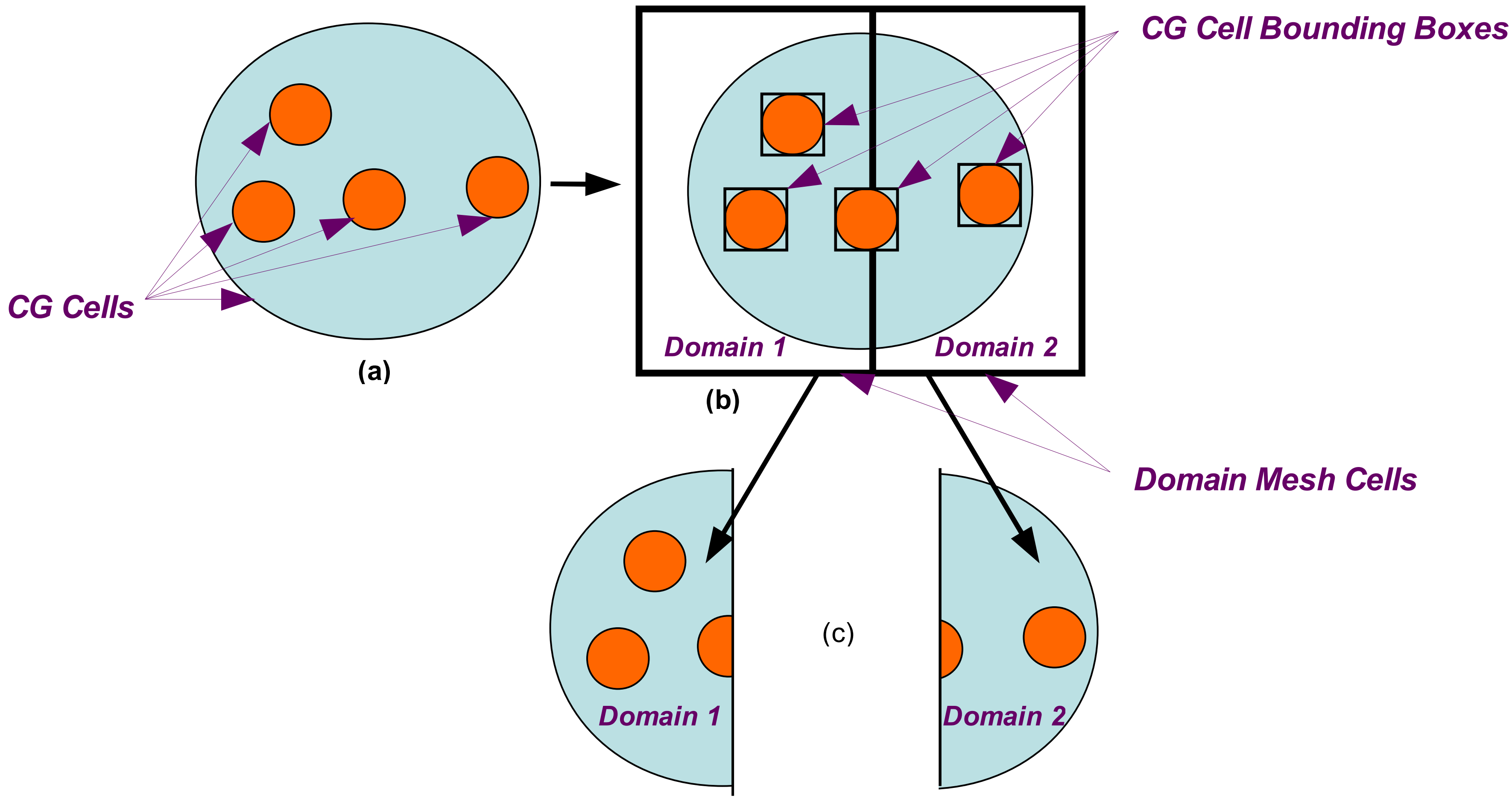
Combinatorial Geometry

- In the ***Mercury*** CG domain decomposition model:
  - ➔ Bounding boxes used to efficiently determine the CG cell connectivity based on the position of each cell
  - ➔ A domain mesh is overlaid on the CG in order to domain decompose the geometry



Monte Carlo Spatial Domain Decomposition
Combinatorial Geometry

Spatial Domain Decomposition of a Combinatorial Geometry



Domain-Decomposed CG Monte Carlo

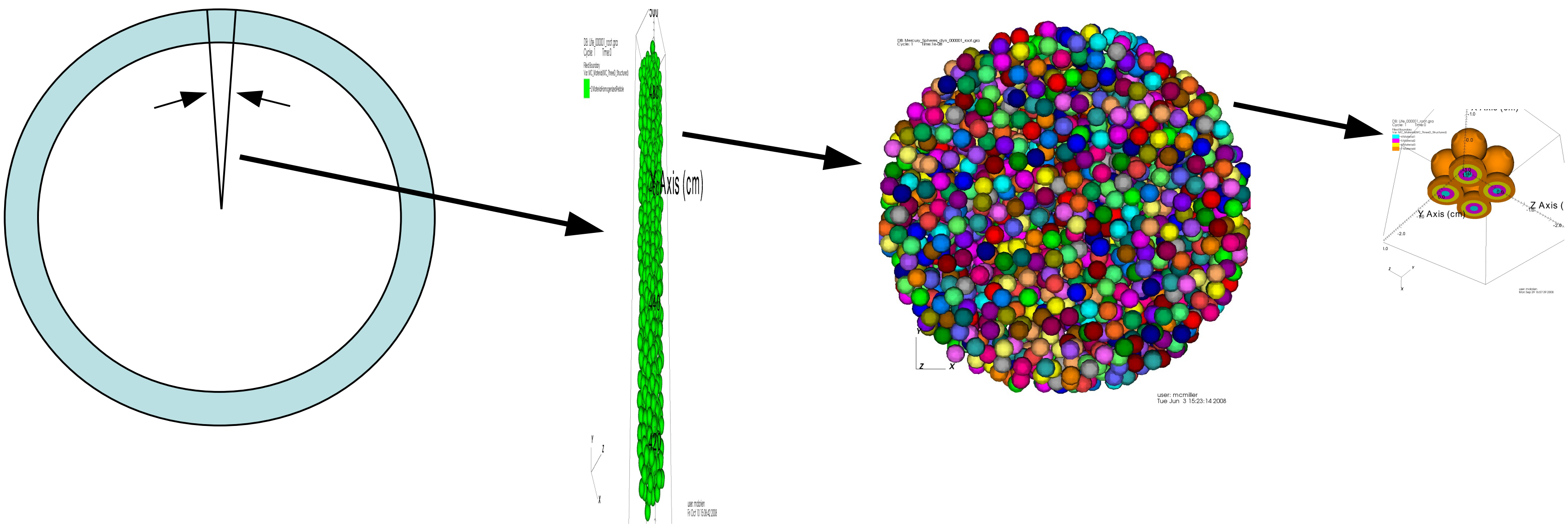
Neutron Transport in the LIFE Engine

- The Laser Inertial Fusion-Fission Energy (LIFE) [6] engine is a concept for a spent-nuclear-fuel isotope transmutation device:
  - ➔ Isotope transmutation is driven by high-energy neutrons obtained from a burning inertial confinement fusion (ICF) capsule
  - ➔ The fission fuel in the LIFE engines is contained within a flowing bed of millions of pebbles, each of which is comprised of thousands of TRISO pellets
- The LIFE engine exemplifies a large-scale, complex problem that is requires spatial decomposition of the problem geometry:
  - ➔ A 1º x 1º solid angle representation of the fuel pebble bed requires in excess of 5.6 million CG cells
  - ➔ The full 4π problem requires billions of CG cells
  - ➔ A 175 group calculation of this "small" portion of the LIFE facility requires in excess of 36 Gb of memory
- Parallel *k* eigenvalue calculations of this 5.6 million cell problem have been successfully performed using the ***Mercury*** Monte Carlo code.

Domain-Decomposed CG Monte Carlo

Neutron Transport in the LIFE Engine

Hierarchical Nature of the LIFE Engine Neutron Transport Model



(a)
LIFE Target Chamber
1° x 1° Solid-Angle
Wedge

(b)
569 Fuel Pebbles

(c)
2445 TRISO Pellets
per Fuel Pebble

(d)
4 Layers
per TRISO Pellet

*569 Pebbles * 2445 Pellets/Pebble * 4 Layers/Pellet = 5.6 x 10^6 CG Cells!*

Domain-Decomposed CG Monte Carlo

Neutron Transport in a Single LIFE Fuel Pebble

- Parallel *k* eigenvalue calculations of a LIFE fuel pebble containing 2445 homogenized TRISO pellets were performed using spatial domain decomposition for various numbers of domains and processors.
- Decomposition of the problem geometry into domains:
  - ➔ Reduces the number of CG cells per domain reduces the number of facet crossing calculations on each domain and the run time *(Even on 1 processor!)*
  - ➔ Results in superlinear parallel speedup *(Compare 1 domain, 1 processor to 8 domains, 8 processors → A speedup of 42.4!)*

Time Required to Complete a k Eigenvalue Calculation in the Homogenized-TRISO LIFE Fuel Pebble for Various Domain and Processor Configurations

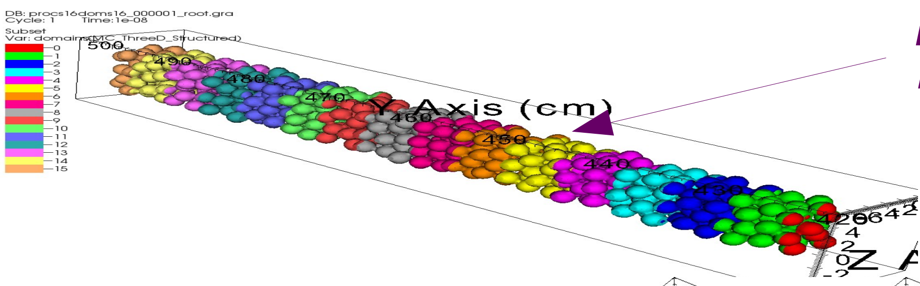
Time Required to Complete k Eigenvalue Calculation (sec)					
	1 processor	***2 processors***	***4 processors***	***8 processors***	***16 processors***
1 domain	**848**	**427**	**226**	**131**	**74**
2 domains	**736**	**235**	**148**	**82**	**52**
4 domains	**668**	**190**	**65**	**34**	**20**
8 domains	**659**	**162**	**57**	**20**	**12**
16 domains	**686**	**214**	**113**	**32**	**12**
64 domains	**732**	**207**	**116**	**37**	**18**

Dynamic Load Balancing in Parallel CG Monte Carlo Transport Simulations

- The dynamic load balancing capability that had been previously developed in ***Mercury*** [5] is independent of the underlying cell geometry: both mesh-based and CG-based geometries.
- When the number of processors is greater than the number of domains, the code assigns multiple processors to track particles on a given domain.
- The particle workload is shared evenly among the processors that are working on a particular domain by varying the number of processors assigned to it.
- This hybrid domain-decomposition *(spatial parallelism)* and domain-replication *(particle parallelism)* model has provided additional parallel speedups on mesh-based problems in the past.
- Neutron transport in the 1º x 1º solid-angle wedge version of the LIFE engine has been modeled using this capability.
- For this time dependent source calculation, each fuel pebble homogenizes all of the TRISO pellets into a single sphere.
- Dynamic load balancing provides an additional speedup of 1.4 on this problem.

Dynamic Load Balancing in Parallel CG Monte Carlo Transport Simulations

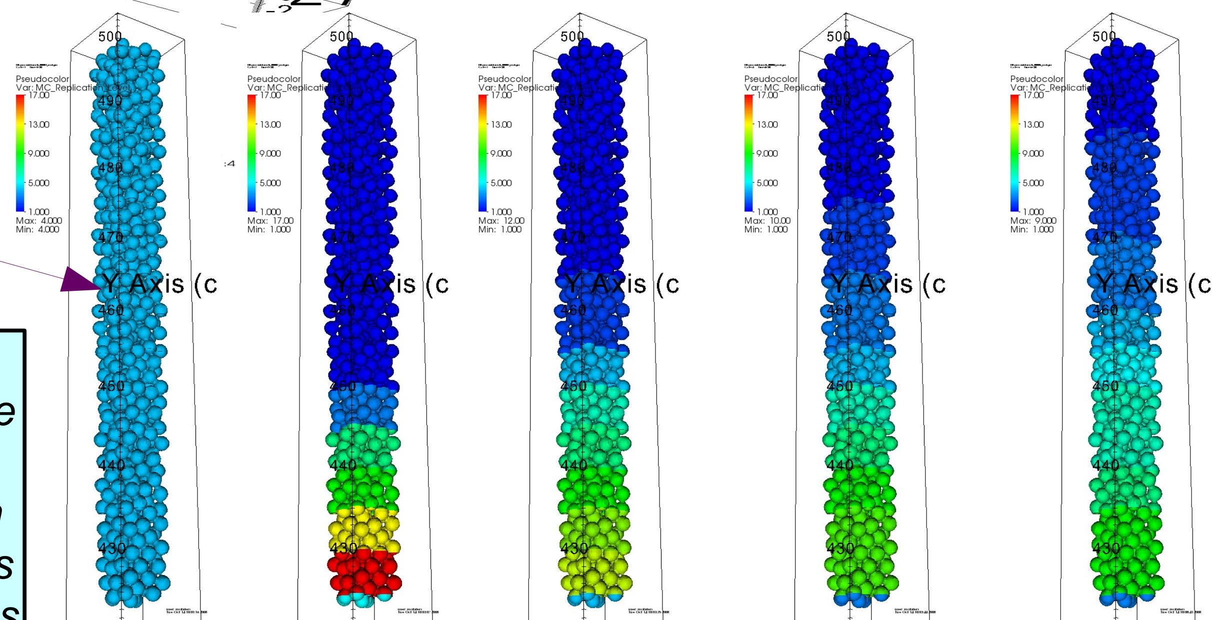
Dynamic Load Balancing in Action



Fuel Pebbles Color Coded by Initial Processor Assignment

Dynamic Load Balancing Yields an Additional Speedup of 1.4!

Fuel Pebbles Color Coded by the Number of Processors Assigned to the Domain



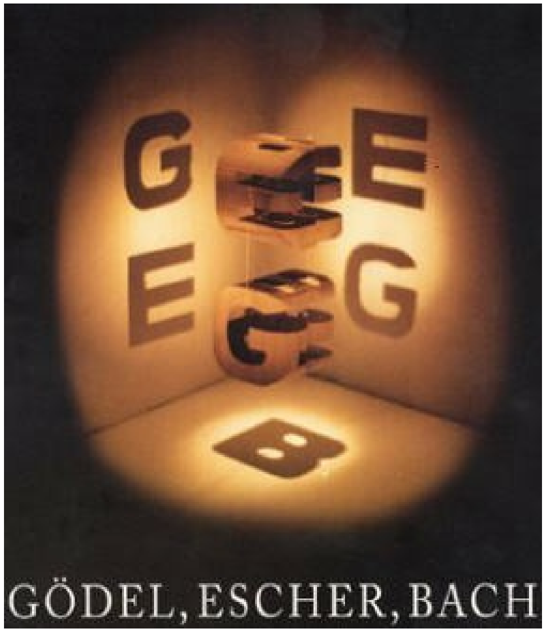
Cycle 0 ***Cycle 1*** ***Cycle 2*** ***Cycle 3*** ***Cycle 4***

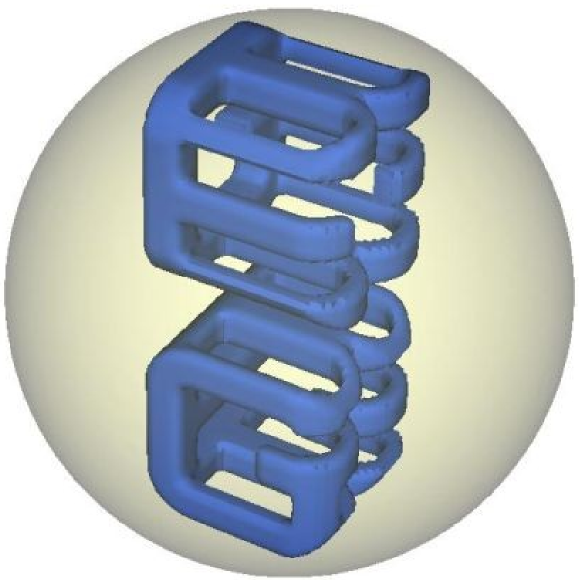
Neutrons are injected at the bottom of the pebble bed at the start of Cycle 0. As neutrons transport up the pebble bed in time, the number of processors assigned to each domain varies with the particle workload.

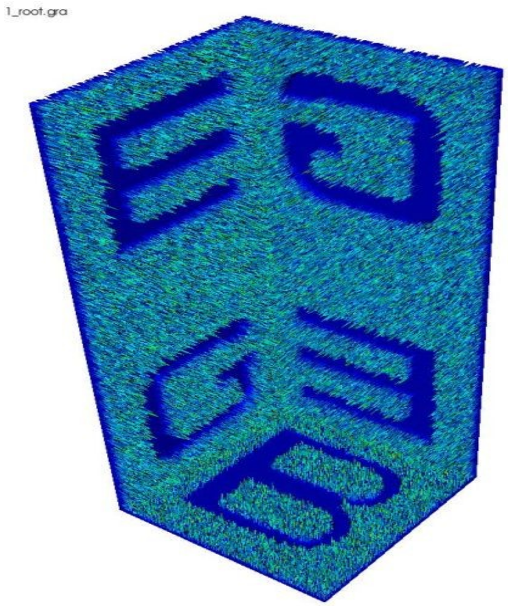
Combinatorial Geometry Definition Using Logical Aggregation of Surfaces

New Feature!

- The CG cell definition syntax in ***Mercury*** has been extended with the ability to define cells via logical aggregation of surfaces:
  - ➔ Only the "implicit *AND*" logical aggregation operation had been supported
  - ➔ Supported logical aggregation operations now also include *"AND"* ('&&' / intersection), *"OR"* ('||' / union) and *"NOT"* ('!' / negation)







Summary and Conclusions

- A hybrid particle tracker has been implemented in the ***Mercury*** Monte Carlo code. This method, in which a mesh region is embedded within a CG region, permits:
  - ➔ Efficient calculations of problems which contain both large-scale heterogeneous (mesh) regions and homogeneous (CG) regions
  - ➔ Simulation of particle transport in both the mesh-based and CG-based regions, while other physics (thermal-hydraulics, structural mechanics, etc) is also run on the mesh
- The MIT radiotherapy facility was modeled via the hybrid particle tracker, where the reactor core was modeled by a mesh region and the balance of the facility was modeled with a CG region.
- A new feature in ***Mercury*** is the ability to define CG cells via logical aggregation of surfaces:
  - ➔ Using *'AND'*, *'OR'* and *'NOT'* operators
  - ➔ Greatly simplifying the definition of complex geometries with the "cell bloat" that results from the sole use of "implicit *ANDs*"

Summary and Conclusions *(continued)*

- The combinatorial geometry (CG) particle tracker in ***Mercury*** has been extended to support both particle parallelism (via domain replication) and spatial parallelism (via domain decomposition):
  - ➔ Problems of very large geometric complexity can now be run, which, due to the large memory requirements of the CG, could not be solved through particle parallelism alone
  - ➔ Both CG cells and particles are decomposed across processors using a bounding box algorithm
  - ➔ Particles are communicated to an adjacent processor when they track to an interprocessor boundary
- *k* eigenvalue calculations of a single, TRISO-pellet-loaded fuel pebble from the LIFE engine has shown that:
  - ➔ Domain-decomposed CG particle transport can run faster than use of particle parallelism (“embarrassing parallelism”) alone
  - ➔ A domain-decomposed calculation with 8 domains / processors produced a superlinear speedup of 32.95 relative to the serial calculation.

Summary and Conclusions *(continued)*

- Parallel *k* eigenvalue calculations of a "small" 1° by 1° wedge of the LIFE engine has also been achieved:
  - ➔ The wedge is comprised of 5.6 million CG cells
  - ➔ Serial memory requirements for the geometry alone would have been > 36Gb
- The use of both domain decomposition (spatial parallelism) and domain replication (particle parallelism) in a time dependent version of the problem was studied. Enabling dynamic domain replication:
  - ➔ Means the system is able to better balance the load over multiple cycles
  - ➔ Resulted in a speedup of 1.4 over the static assignment of processors to domains

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[3] R. J. Procassini, et al., "*Mercury User Guide (Version c.2)*", Lawrence Livermore National Laboratory, Report UCRL-TM-204296, Revision 1 (2008).

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