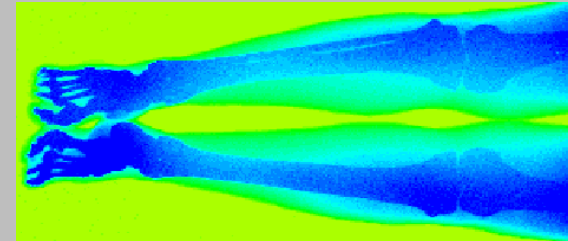
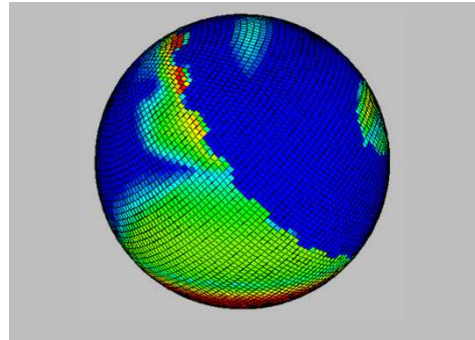
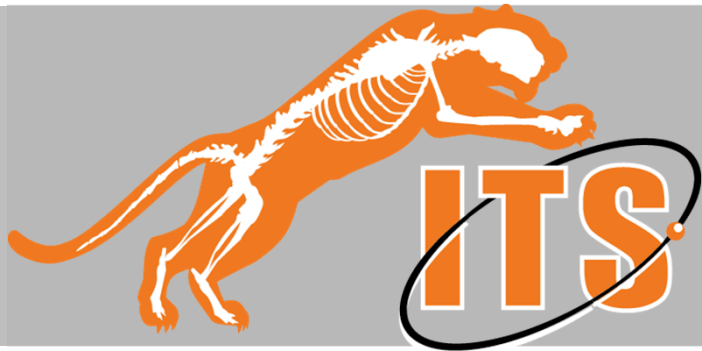


Exceptional service in the national interest



ITS Version 6.4: The Integrated TIGER Series

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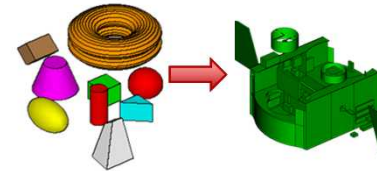
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Just What is ITS?

- A series of Monte Carlo Electron/Photon Radiation Transport Codes
 - Fully coupled
 - 1D (TIGER)
 - 2.5D (CYLTRAN, 2D geometry but 3D tracking)
 - 3D (ACCEPT – CG & CAD)
 - Continuous energy and multigroup versions
 - Adjoint capability (multigroup only)
- ITS has a long history
 - Member codes first released in mid 70's.
 - Integration was released in 1984.
 - Version 3 has been available through RSICC since 1992.
 - Later versions: 4, 5 had only very limited release.
 - Version 6 is now released through RSICC.

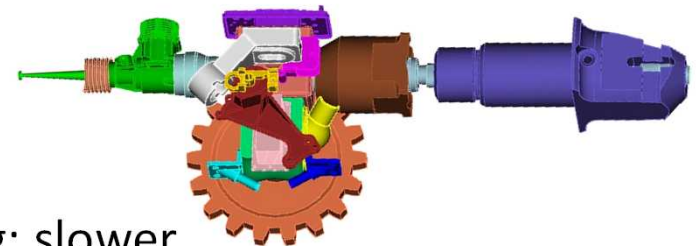
Multiple Geometry Formats

- Native combinatorial solid geometry
 - Boolean combinations of primitive bodies



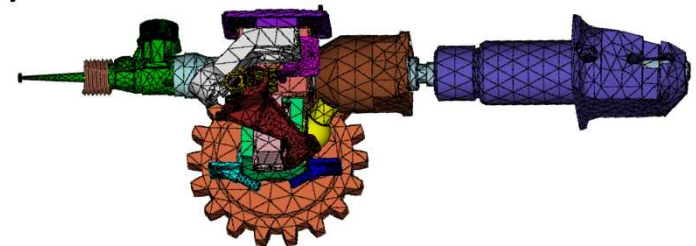
- CAD (ACIS® format)

- Can be as detailed as desired
- Separate ACIS® license is required
- ACIS® libraries not optimized for tracking: slower



- Facet-based geometry representation

- Cubit facet format
- Use Cubit to surface mesh and export

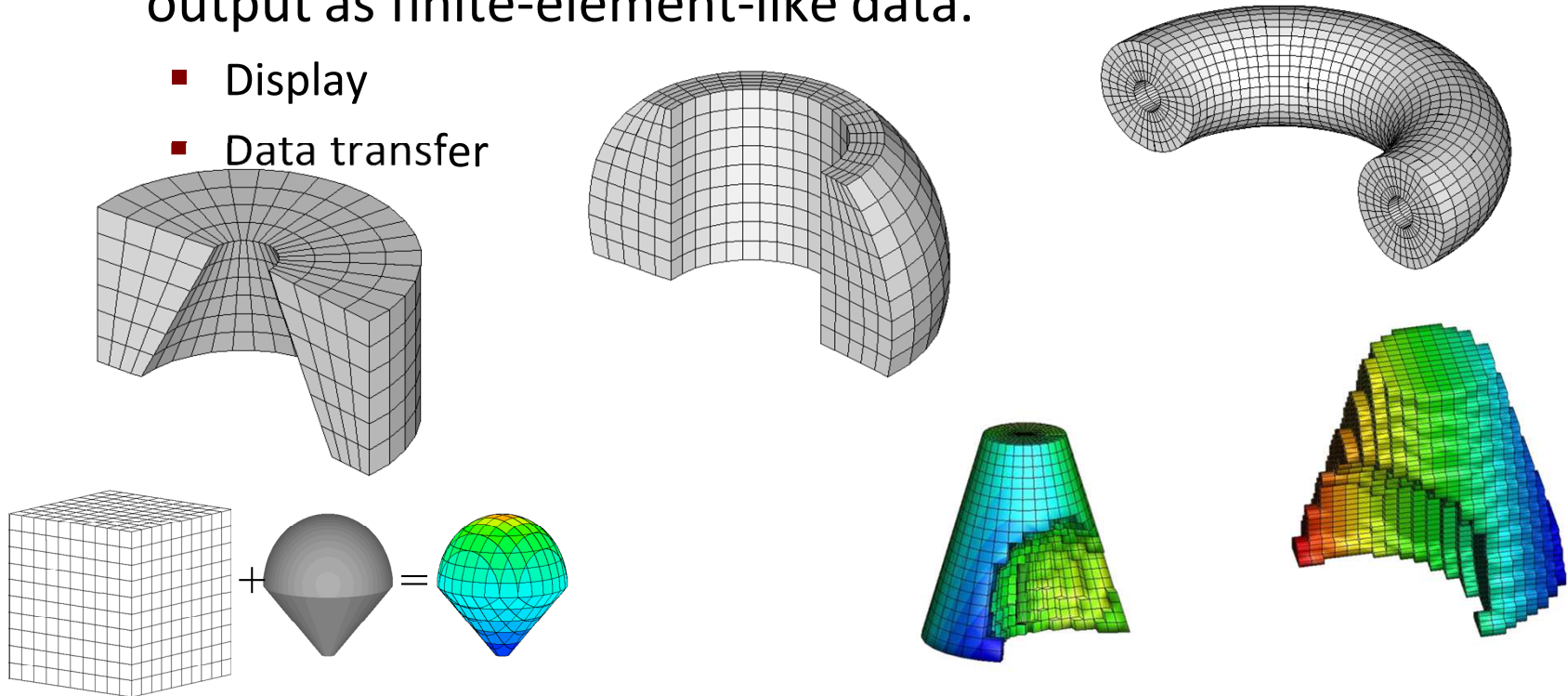


- Any combination of the three formats can be used in a single calculation.

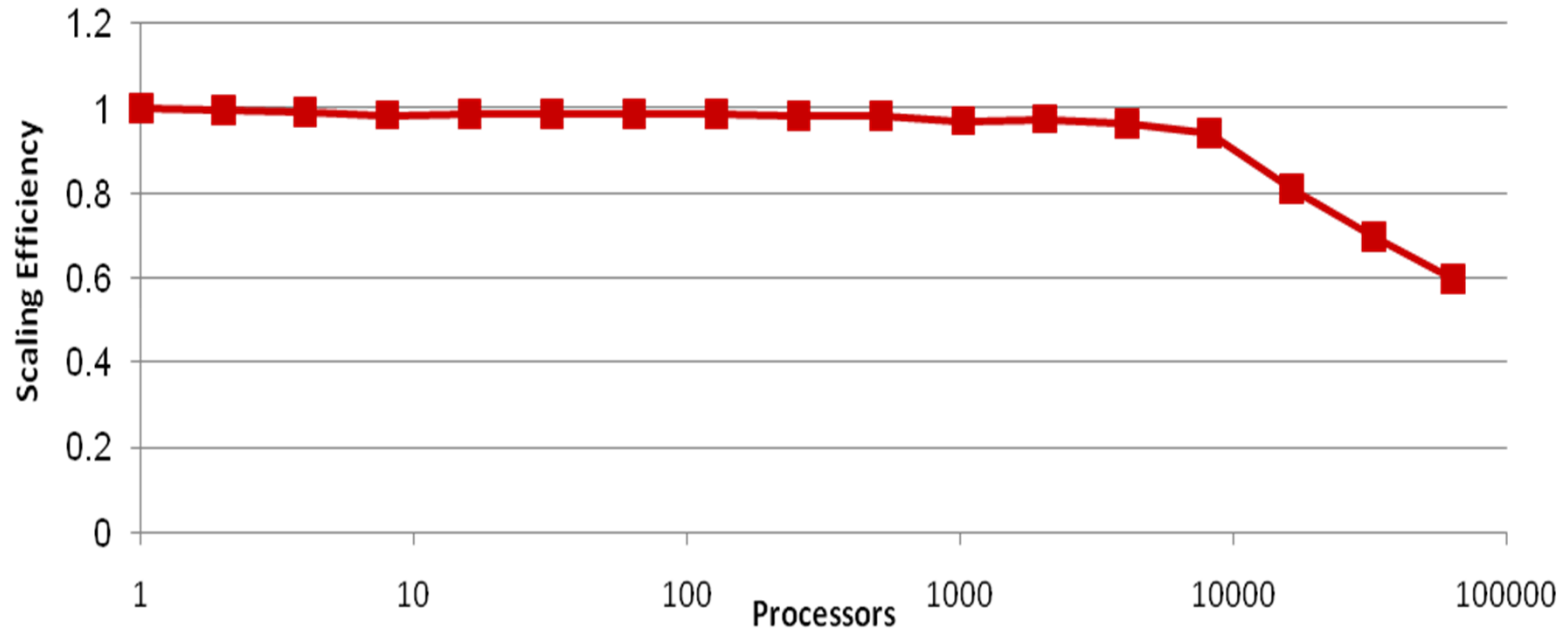
Automatic Subzoning

- There are about a dozen subzoning structures that can be overlaid on our geometry representations for volume tallies.
- Energy and charge deposition in these subzones can be output as finite-element-like data.

- Display
- Data transfer



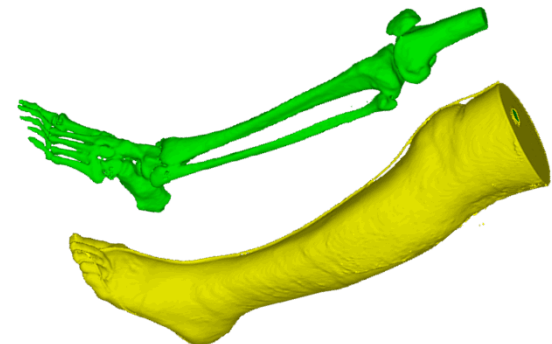
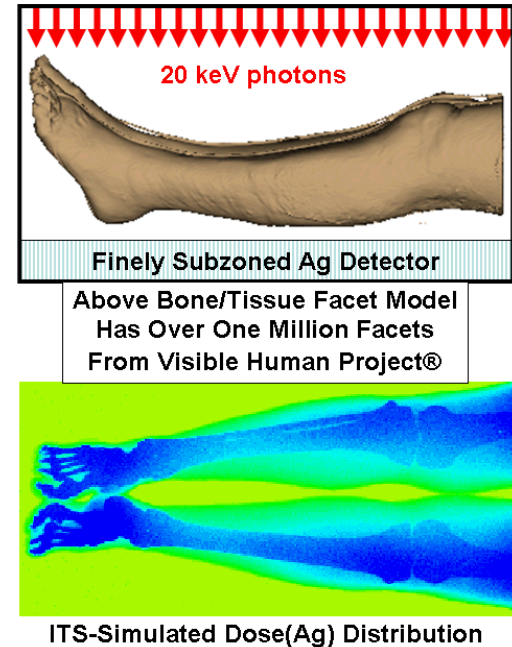
ITS is Massively Parallel



- Above scaling for CAD photon transport calculation on Cielo (LANL ASC machine)
- Loss of efficiency is primarily due to increasing MPI communication costs relative to the computational work (This was a short-running calculation)
- Production (long-running) calculation machine utilization efficiency:
 - 94.4% (91.4 – 95.9) for static load balancing option
 - 96.9% for static load balancing with master idle
 - 96.8% (93.7 – 98.6) for dynamic load balancing

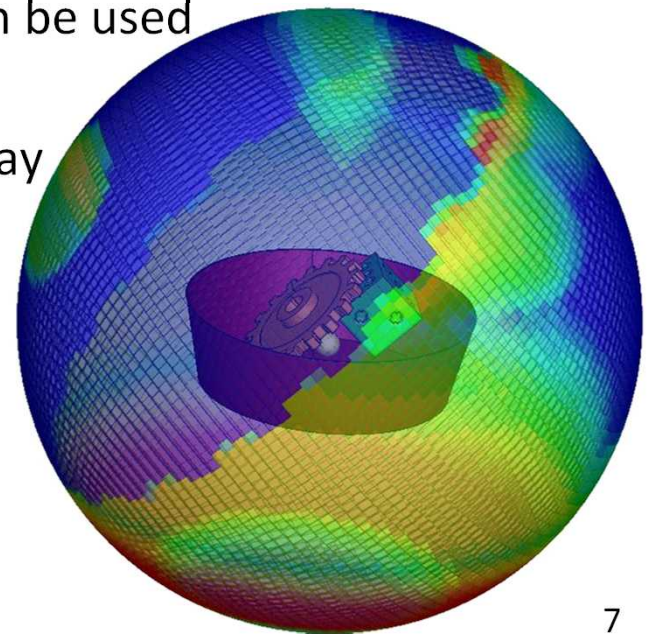
Traditional (Forward) Transport

- Many of typical capabilities of a Monte Carlo transport code
- Magnetic and Electric Fields
 - Magnetic fields in materials and voids
 - Electric fields only in voids
- Continuous-energy or multigroup cross sections
 - XGEN code for continuous energy
 - CEPXS code for multigroup
- Energy and charge deposition, photon and electron flux, electron emission, pulse-height



Multigroup and Adjoint Capability

- The 1D and 3D codes have a multigroup capability that also allows adjoint mode calculations
 - Uses cross sections generated by the included CEPXS code
- Adjoint advantages:
 - Assessing dose from multiple source spectra in a single calculation.
 - Generating dose response functions that can be used long after the initial calculation
 - A direction-sphere output capability to display a dose-direction map
- There is also an associated ray-tracing capability
 - Allows fast scoping of complex geometries



ITS 6.4 is Available Through RSICC

- ITS version 6.4 is now available through RSICC
- US Government-Use-Only license.
 - You must be a US government entity or have a government contract.
- Includes source code.
- Combinatorial geometry is all Fortran (dynamic arrays).
- CAD and Facet-based geometry is C++
 - CAD requires separate ACIS® license for libraries (<http://www.spatial.com>)
 - Facet-based geometry source is included but requires CUBIT to generate the facet files (www.cubit.sandia.gov)
 - There may be other ways to generate facets and convert to the required format.

Future Enhancements and Ongoing Research

- Below 1 keV transport for electrons and photons
 - Currently only photon absorption is active below 1 keV
- Enhanced low-energy cross sections beyond independent atom approximation
- Tally on a mesh (not transport on a mesh)
- Generalized Boltzmann Fokker-Planck moment-preserving scattering kernels alternative to condensed history for electrons
- Radiation transport in stochastic media
- Explore other parallel paradigms like threading and using GPUs to make use of next generation massively parallel architectures
- Replace ACIS library CAD capability with open source CAD library

Time Binning Basics

- Only in development version, not in RSICC released version
- Time-binned sources
 - Each time bin can have a different spectrum
 - Delta-function sources can be easily approximated
 - Biasing in time is not currently planned
- Time-binned tallies
 - Independent of source time binning
 - Currently only charge and energy deposition in released version
 - Other tallies may be enabled in development versions
- Each particle's time is tracked from birth to death
 - Secondary particles are born with the time of their creation
 - Particle banks store time of creation for those not immediately followed

Particle Time Algorithms

- Photons are trivial: they all travel at the speed of light.
 - We ignore index of refraction on the speed of light in materials
 - We ignore relaxation times
- Electrons are not that simple
 - Speed varies with energy
 - Continuous slowing down approximation (CSDA)

Time t to travel distance s $t = \frac{s}{v} = \frac{s}{\beta c}$ $\beta = v/c$ v is electron speed
 c is speed of light

Electron slows over s : $t = \int_0^s \frac{ds'}{\beta(s)c}$

Change to energy variable: $t = \int_{E'}^{E_0} \frac{dE}{\beta c (dE/ds)}$

Electron Travel Time continued

Making the assumption that we can treat stopping power as a constant allows us to pull it out of the integral:

$$\Delta t = \frac{s}{\Delta E} \int_{E'}^{E_0} \frac{dE}{\beta c}$$

The assumption also allows us to derive an analytic expression. After some algebra and substituting $E_1 = E_0 - \Delta E$, the equation for Δt is finally implemented as

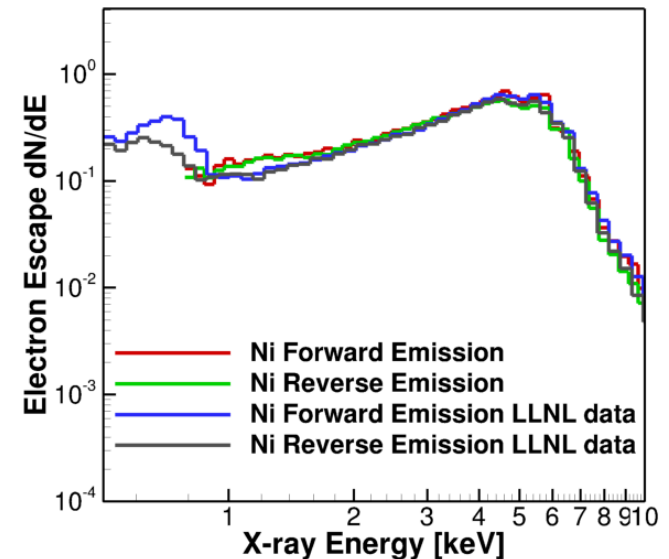
$$\Delta t = \frac{s}{c} \frac{(1 + \gamma_0 \gamma_1 (1 + \beta_0 \beta_1))}{(\gamma_0 \gamma_1 (\beta_0 + \beta_1))}$$

Where γ is the total electron energy, including rest mass, divided by the rest mass. This form of the equation works even when energy loss is zero.

Instead of just using total stopping power we sample energy loss, ΔE over the distance s , which includes energy straggling and energy loss due to bremsstrahlung photons .

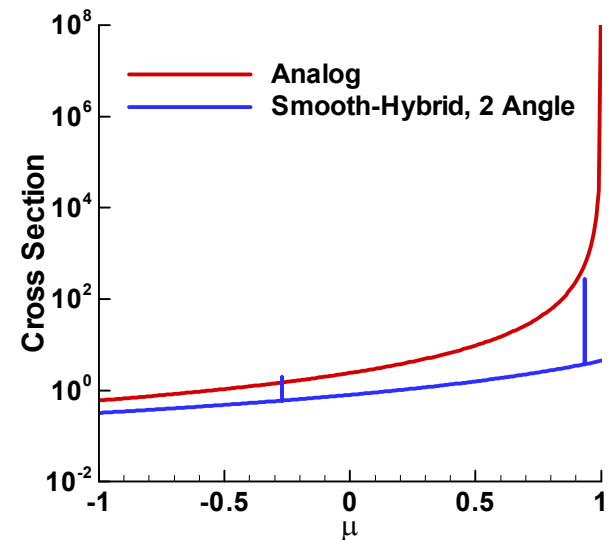
Low-Energy Transport

- Currently below-1-keV transport for photons implemented.
 - Absorption only
- Working on implementing full transport capability for both photons and electrons.
- Using Livermore data
- Research into methods to account for solid state effects
 - Hope to improve low energy cross section accuracy
 - On going effort



Alternate Electron Transport

- Generalized Boltzmann Fokker-Planck (GBFP)
 - Rigorously preserves cross section moments in the solution of a Boltzmann transport equation
 - Makes it look like a single-scattering method like photon transport
 - Shows promise in simplifying material boundary-crossing issues in electron transport
- Analog electron transport
 - Being implemented in conjunction with low-energy electron cross sections



Stochastic Media Transport

- Stochastic media problems arise when the mean chord lengths through materials are larger than the transport mean free path.
 - Think concrete, lungs, tree canopies, or foams
 - Material homogenization is a not truly adequate representation
- ITS team is investigating using the Levermore-Pomraning (LP) closure to the master equation for transport in stochastic media

$$\underbrace{\vec{\Omega} \cdot \nabla (p_i P_i)}_{\text{Streaming Term}} - \underbrace{\frac{\partial}{\partial \psi} [(\sigma_{ti} \psi)(p_i P_i)]}_{\text{Scatter and Absorption Removal Term}} + \underbrace{\frac{p_i \bar{P}_i}{\lambda_i} = \frac{p_j \bar{P}_j}{\lambda_j}}_{\text{Material Interface Terms}} - \underbrace{\frac{\partial}{\partial \psi} \int_0^\infty dE' \int_{4\pi} d\vec{\Omega}' \int_0^\infty d\psi' [\psi' \sigma_{si}(E' \rightarrow E, \vec{\Omega}' \cdot \vec{\Omega}) p_i P_{2i}(\psi, \psi')]}_{\text{Flux-Correlation-Based In-Scatter Term}}$$

Streaming Term

Scatter and Absorption Removal Term

Material Interface Terms

Flux-Correlation-Based In-Scatter Term
(Note: Flux correlations are lost if we “close” the infinite set of coupled correlation equations.)

Stochastic Media Transport

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 - Material homogenization is a not truly adequate representation
- ITS team is investigating using the Levermore-Pomraning (LP) closure to the master equation for transport in stochastic media
 - The material interface terms are closed with the LP approximation

$$\underbrace{\vec{\Omega} \cdot \nabla (p_i \Psi_i^{(1)})}_{\text{Streaming Term}} + \underbrace{\sigma_{ti} p_i \Psi_i^{(1)}}_{\text{Scatter and Absorption Removal Term}} + \underbrace{\frac{p_i \bar{\Psi}_i^{(1)}}{\lambda_i}}_{\text{Material Interface Terms}} = \underbrace{\frac{p_j \bar{\Psi}_j^{(1)}}{\lambda_j} + \int_0^\infty dE' \int_{4\pi} d\vec{\Omega}' \sigma_{si}(E' \rightarrow E, \vec{\Omega}' \cdot \vec{\Omega}) p_i \Psi_i^{(1)}(\vec{r}, \vec{\Omega}', E')}_{\text{In-Scatter Term}}$$

Tally-On-A-Mesh

- Not transport on a mesh
 - Avoid boundary-crossing issues
 - Avoid having to refactor code to optimize for mesh transport
- Use an unstructured FEM mesh as a tally structure
 - Like ITS subzoning mentioned earlier
 - Subzoning structures do not match mesh models used for mechanical analyses.
- Issues
 - Storage associated with mesh may destroy our domain replication parallel strategy.
 - Mesh boundaries do not exactly match curved boundaries of CG or CAD geometry representation.
- We are hopeful we can start the project in FY15

Summary

- Fully-coupled electron-photon Monte Carlo transport
- 1D, 2.5D, or 3D
- Continuous-energy or multigroup cross sections
- Forward and Adjoint Modes
- Multiple geometry representations
- Massively parallel
- ITS Version 6.4 currently available through RSICC
 - Government-Use-Only license
 - Separate ACIS® license required for CAD capability
 - User support is available through its-support@sandia.gov

Questions?

