XENOS: X-RAY MONTE CARLO CODE SUITE

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Abstract

Xenos is an integrated 3D code suite for the design of X-ray sources and electron beam devices. The component programs run under 64-bit versions of Windows. **Xenos** has unique features compared to other Monte Carlo systems: 1) representation of geometry and deposited dose on a finite-element mesh, 2) inclusion of full 3D electric and magnetic fields in simulations, 3) an integrated user environment for input preparation and output analysis and 4) extended parallel-computing support for high-accuracy solutions. **Xenos** utilizes the full capabilities of multi-core computers and allows parallel computations on multiple independent computers.

CODE SUITE ORGANIZATION

Xenos [1] is a integrated suite of codes to simulate electron beam and X-ray devices for a range of medical, industrial and research applications. The suite employs **Penelope-2006** [2] for material interaction physics and Field Precision technology for geometry definition, calculations of electric/magnetic fields, electron beam transport and thermal solutions. Component programs run under 64-bit versions of Windows with support for multi-core machines. The codes handle both 2D and 3D geometries, but this talk concentrates on the more advanced 3D programs.
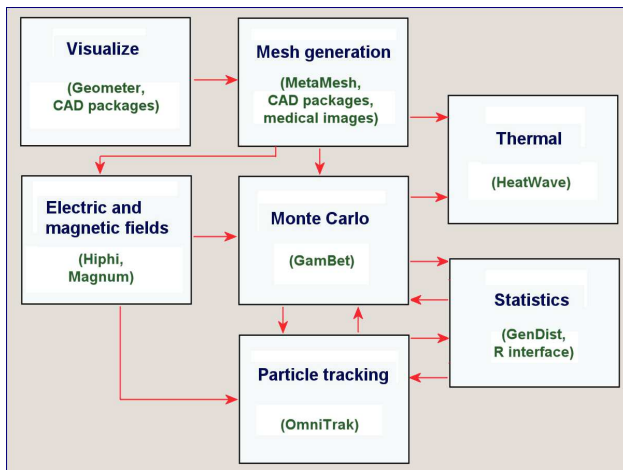

Figure 1: Organization of the **Xenos** suite, 3D components

Figure 1 shows relationships between 3D component programs of the **Xenos** suite. Each may act as a standalone solver or as a step in a coupled solution. The arrows represent file transfers of three types:

- Physical quantities organized on a mesh (*e.g.*, deposited energy distribution from a Monte Carlo calculation ported to a thermal solution).

- Model particle lists (*e.g.*, electron beam solution input to a Monte Carlo calculation.).

- Control parameters for the physical solutions

Separation of functions into individual programs offers three advantages: 1) the component programs may be used for stand-alone solutions, 2) users can access and modify intermediate results and 3) batch files or scripts may be used to modify the content of control files in optimization loops.

FINITE-ELEMENT MESH FEATURES

All physical solutions in **Xenos** are performed on finite-element meshes generated by a common mesh generator, **MetaMesh**. The meshes define geometric objects by dividing space into regions composed of elements. The physical properties of regions may vary with the solution type. For example, they represent electrodes, dielectrics and space charge in electrostatic solutions. In Monte Carlo calculations, regions represent different material types, voids or volumes to calculate deposited energy.

Xenos uses meshes that are both *conformal* and *structured*, a type unique to the suite (Fig. 2). The term *conformal* implies that elements are individually shaped to provide accurate representations of non-planar surfaces. The term *structured* means that elements in the mesh have a logical relationship that allows location of neighboring elements by simple index operations. In this case, the foundation mesh is cubic whereas the actual elements are generalized hexahedrons that conform to complex surfaces. A structured mesh has a key advantage over an unstructured mesh in this application. In both the Monte Carlo and charged-particle beam solutions, element searches occupy the bulk of the computational effort.
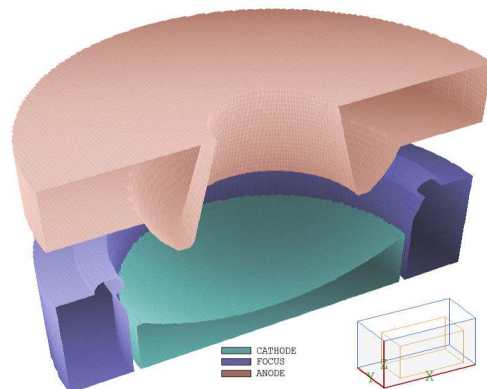

Figure 2: Structured, conformal mesh from STL data.

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GEOMETRY DEFINITION AND MESH GENERATION

In **Xenos**, as in all finite-element codes, mesh generation represents a significant fraction of user effort. **Xenos** has two components to facilitate the task:

- **Geometer**: an interactive graphical environment for the definition and placement of regions in three-dimensional space.

- **MetaMesh**: an automatic generator that uses information from **Geometer** and other sources to create structured, conformal meshes.

An interesting feature of **MetaMesh** is the variety of information sources that may be combined to create a single mesh: 1) parametric solid-geometry models (as in conventional Monte Carlo packages), 2) import of complex objects from 3D CAD programs like **SolidWorks** via STL files (Fig. 2), 3) mathematically-generated 3D surfaces, 4) solid bodies defined by generalized image files, 5) representations from unstructured, tetrahedron meshes, 6) planar surfaces from photographs, 7) MRI data from Analyze 7.5 files and 8) human phantom information (Zubal and GSF). The last two methods were included for applications of **GamBet** to biological and medical research.

ELECTRIC AND MAGNETIC FIELDS

HiPhi is the **Xenos** component for 3D electrostatic solutions while **Magnum** handles magnetostatic solutions. Both programs include a dedicated interactive post-processor. Their output files serve two functions in the **Xenos** data chain: 1) applied field definitions for electron or positron dynamics in the Monte Carlo code **GamBet** or 2) applied fields for the electron gun code **OmniTrak**.

HiPhi and **Magnum** perform conventional finite-element field solutions on an unconventional mesh. The structured mesh offers the advantages of short solution times and efficient memory usage. **HiPhi** has several advanced features, including the option to define continuous variations of potential, dielectric constant or conductivity within a region. Features of **Magnum** include a parametric modeler to specify complex drive coils and procedures to handle non-linear materials like magnet steel (Fig. 3). Both programs include methods to find accurate field variations near small features within a global solution space. The post-processors are customizable. Users may define special quantities for analysis and plotting matched to their applications.

ELECTRON BEAM DESIGN

OmniTrak is used for the design and simulation of charged-particle guns and transport systems. Its main function in **Xenos** is tracking electrons and positrons in vacuum. **OmniTrak** may provide input to **GamBet** (*e.g.*, incident beams from electron guns) or follow the output from
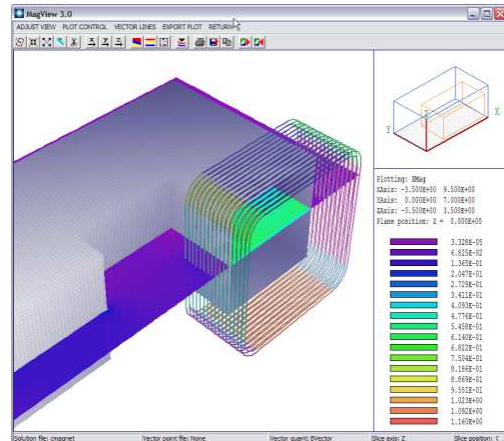
Figure 3: **Magnum** model of a permanent-magnet electron spectrometer.

GamBet (*e.g.*, positron sources). **OmniTrak** has two input source types: 1) electric and magnetic field distributions on independent conformal meshes, and 2) particle lists (e.g., incident beams) from **GenDist**, user programs or **GamBet** runs. **OmniTrak** can recalculate electric fields internally to account for self-consistent beam space-charge contributions. The code can also create particles to model space-charge limited emission, field emission and other processes. **OmniTrak** also determines magnetic fields of high-current relativistic electron beams.

Outputs from **OmniTrak** include particle distribution lists in user-defined planes, modified electric fields with space-charge, beam-generated magnetic fields, particle trajectory trace files and diagnostic files with statistical analyses. The program includes a post-processor to plot trajectories and fields. The particle lists may be ported to **GamBet**, with or without filtering by **GenDist**. As an example of a data chain [3], an initial **OmniTrak** run could represent a high-current electron beam incident on an exit foil. The distribution is input to **GamBet** to model scattering, backscattering and energy loss. **GenDist** removes positrons, photons and back-scattered electrons, leaving the electron distribution at the foil exit. These electrons are ported to **OmniTrak** for a transport solution. The absorbed power distribution in the foil is used as input to a **HeatWave** solution to determine heating. The entire run process can be performed in the background under batch file control.

MONTE CARLO SIMULATIONS

Monte Carlo codes for X-ray science have two components: 1) an atomic physics engine (scattering, energy loss, photon generation,...) and 2) a geometry engine (material identification, dose distribution,...). In **GamBet**, the first function is performed by **Penelope-2006** [2]. The routines were developed at the University of Barcelona specifically for X-ray simulation (electrons, photons and positrons). **Penelope** handles generation of atomic cross sections, prediction of single-particle interactions with matter and cre-

ation of secondary particles. An outstanding feature is the ability to model low-energy interactions (≥ 100 eV) through a 150 MB database.

Field Precision technology handles run control and all matters related to the division of space. Tasks include the organization of input/output data for large distributions of particles, calculation of statistics, identification of material boundaries, generation of escape-particle records, variance reduction techniques, creation of records of spatial variations of dose and control of parallel operation.

GamBet has three modes of operation: 1) single particle (the standard approach of Monte Carlo codes), 2) continuous beam and 3) pulsed beam. For the second and third options, a current (or flux) is associated with the primary particles. The dose quantities in elements are respectively 1) eV/kg/primary, 2) J/kg/s and 3) J/kg. Unique features of **GamBet** compared with other Monte Carlo radiation codes include: 1) conformal meshes with accurate representations of material volumes with curved boundaries, 2) inclusion of 2D and 3D electric and magnetic fields on independent meshes, 3) interactive graphical post-processor to analyze dose distributions and selected particle histories, 4) bidirectional communication with the particle beam code **OmniTrak** and 5) connection to **HeatWave** for static and dynamic thermal simulations.

PARALLEL COMPUTING IN GAMBET

Although all **Xenos** solution programs support parallel operation on multi-core machines, parallel computing is particularly important in **GamBet** where a large number of showers may be necessary for statistical accuracy. The program utilizes two strategies for parallel operation.

- Multi-core calculations on single computer using the distributed memory method. With this choice, the reduction in computational time is almost linearly proportional to the number of cores. For a given run setup, **GamBet** starts an instance of the program with a unique random number seed in each core. When all runs are complete, the program combines escape particle, dose distribution and statistical data into single output files.

- Single or multi-core calculations on any number of individual computers. In this case, data organization is directed by the **GDE** (GamBet Distributed-computing Extension) utility. On the subsidiary computers, a special form of **GamBet** creates a binary file with a unique name that includes all information from the run. The files are ported to a central computer where a master program combines the information to produce standard **GamBet** output files with enhanced statistical accuracy. The process is flexible, allowing additional binary files to be added at a later time to improve ac-

curacy. The entire process may be automated to run in the background using batch files of Windows CMD commands or scripts.

THERMAL SOLUTIONS

The **HeatWave** program determines dynamic or static thermal flow in solid materials and biological media. It accepts profiles of deposited power from **GamBet** runs in the continuous-beam mode. **HeatWave** uses the **GamBet** geometric mesh with appropriate physical properties assigned to regions. A common application for X-ray source design is the determination of heating in targets and foils. In this case, user-defined temporal modulation functions may be applied to the power distribution to model pulsed or periodic beams. There is also an option to apply specified time-dependent spatial shifts of the thermal distribution to model rotating targets. Other special features of **HeatWave** include: 1) non-linear solutions with temperature-dependent material properties, 2) radiation boundaries (*e.g.*, modeling thermionic cathodes) and 3) perfusion contributions for biological calculations.

MONTE CARLO DATA ANALYSIS

As shown in Fig. 1, **Xenos** includes the statistical utility **GenDist**. The connecting arrows represent the transfer of particle lists – text files where each line documents particle parameters. There are two list formats: **OmniTrak** (PRT) and **GamBet** (SRC). The difference is that the **OmniTrak** file may include ions and macroparticles for other applications and the **GamBet** file may include photons.

GenDist performs these functions: 1) generation of large particle distributions based on parametric models in either the PRT or SRC format which may be ported to **GamBet** or **OmniTrak** to initiate electron beams or X-ray sources, 2) filtering of particle distributions to remove selected particles or shift the position and orientation of beams, 3) input of escape particle information from **GamBet** or distributions saved at specific locations from **OmniTrak** to perform statistical analyses and to generate plots and 4) conversion between PRT and SRC formats. The text format of the list files make it easy to perform advanced analyses with statistical packages like **R**.

REFERENCES

[1] **Xenos** technical information, `http://www.fieldp.com/xenos.html`

[2] F. Salvat, J.M. Fernandez-Varea and J. Sempau, PENELOPE-2006: A Code System for Monte Carlo Simulation of Electron and Photon Transport, (Proceedings of a Workshop/Training Course, July 4-7, 2006), NEA Number 6222.

[3] *X-ray Source Design with Xenos,* `http://www.fieldp.com/documents/xraysourcedesign.pdf`