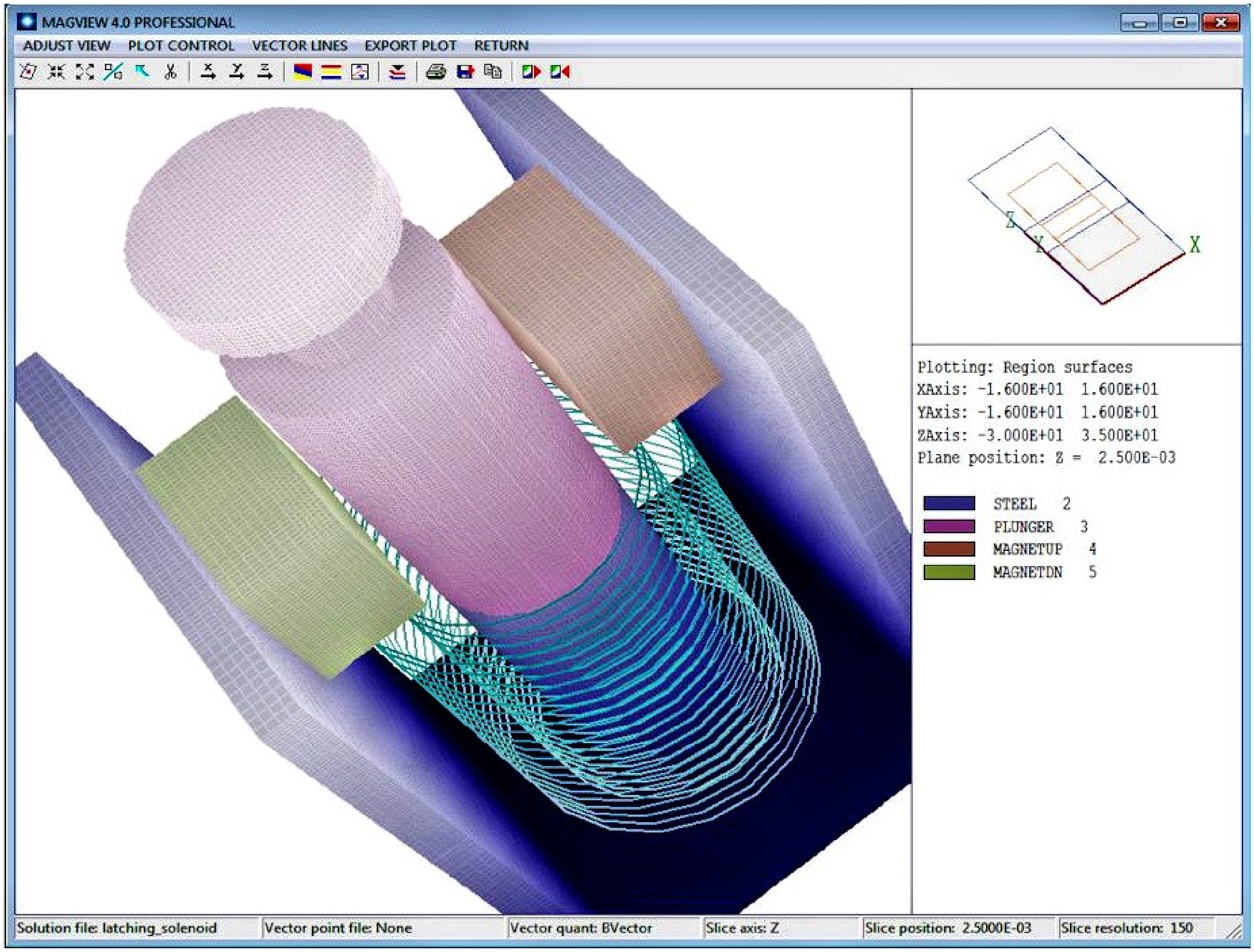

Xenos

Integrated simulation code suite for electron-beam and X-ray devices

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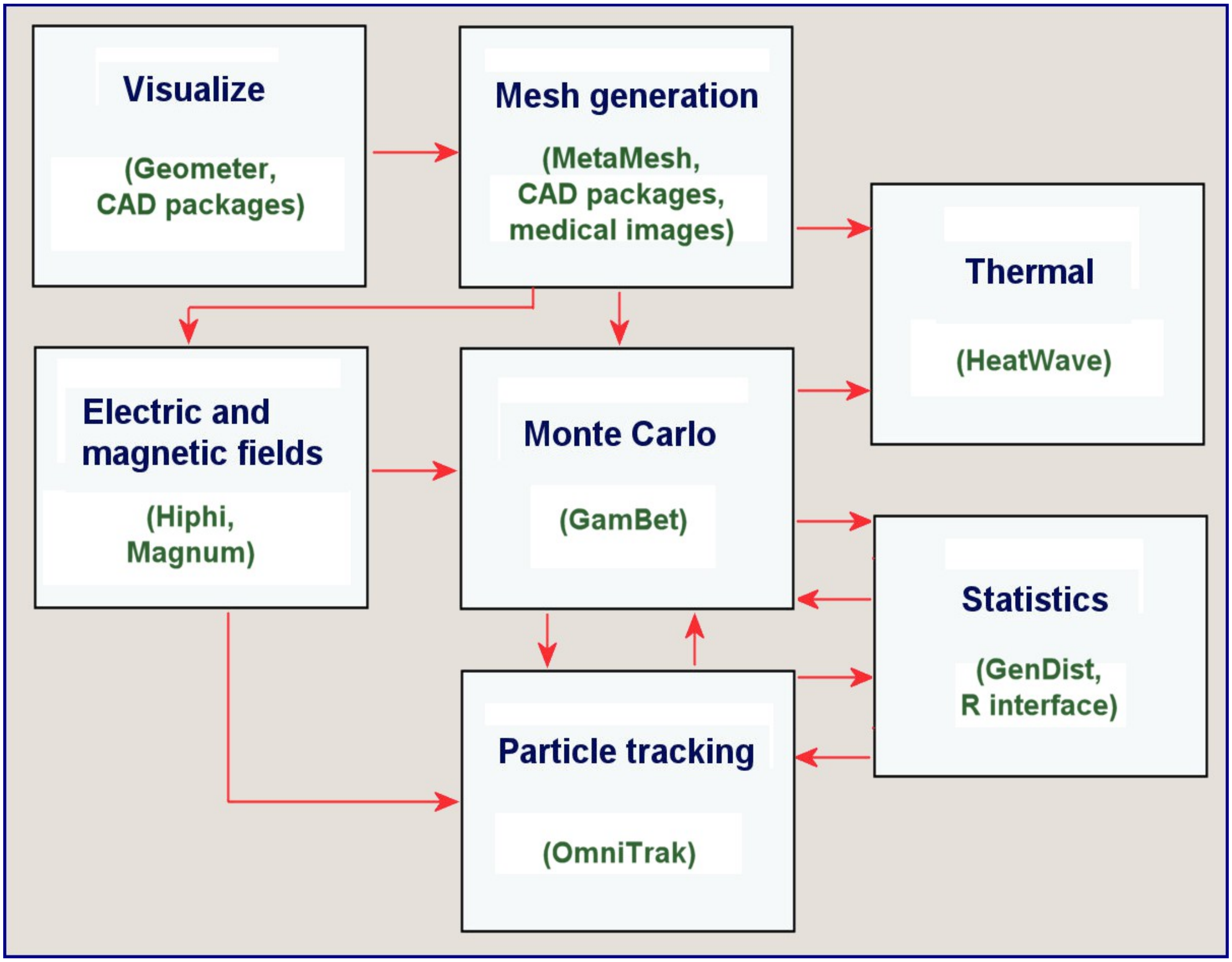
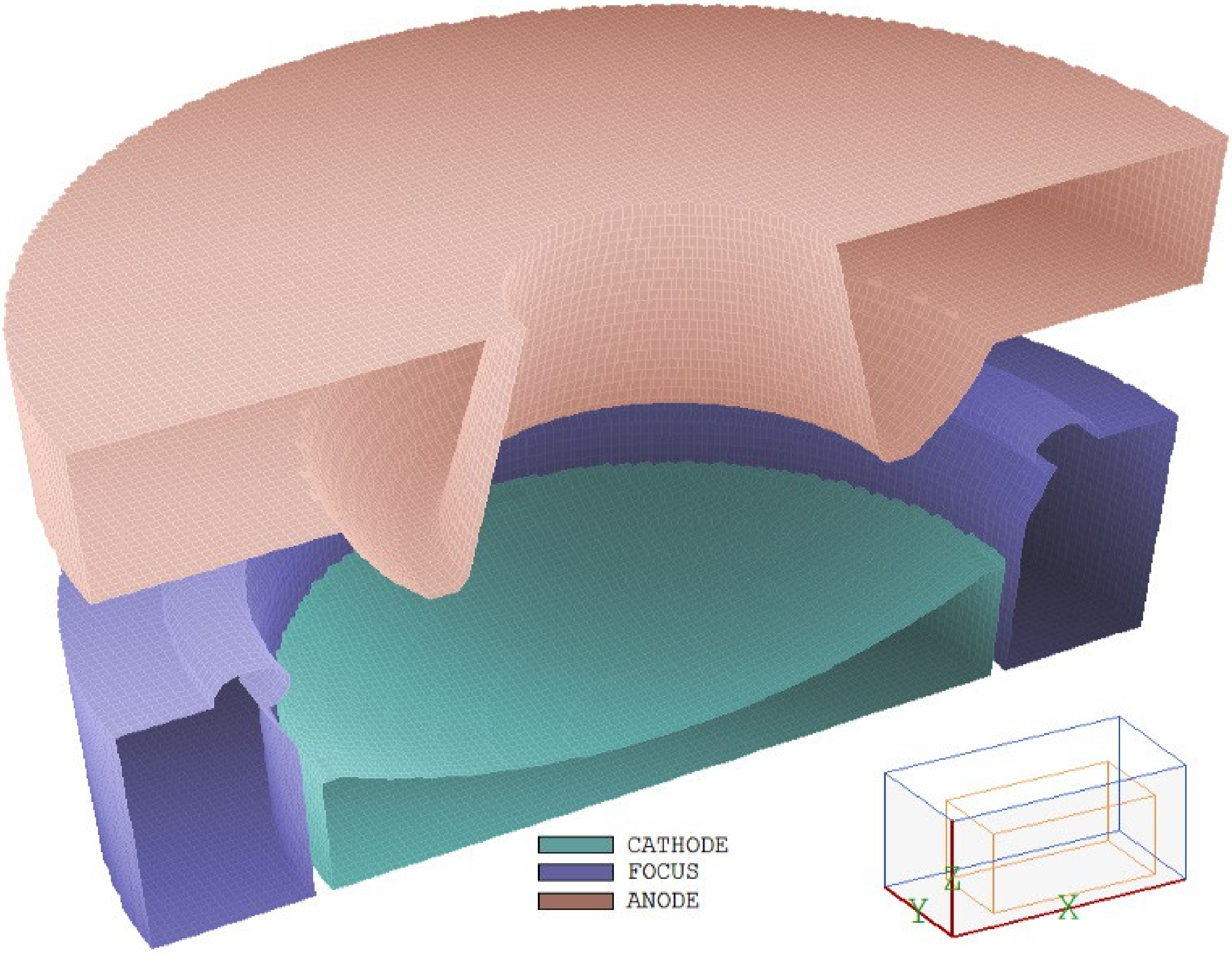


Organization

Xenos employs **Penelope-2006** for material interaction physics and Field Precision technology for geometry definition, calculations of electric/magnetic fields, electron beam transport and thermal solutions. The figure shows relationships between component 3D programs. 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).
- Particle lists (*e.g.*, electron beam solution as input to a Monte Carlo calculation.).
- Control parameters for the physical solutions.

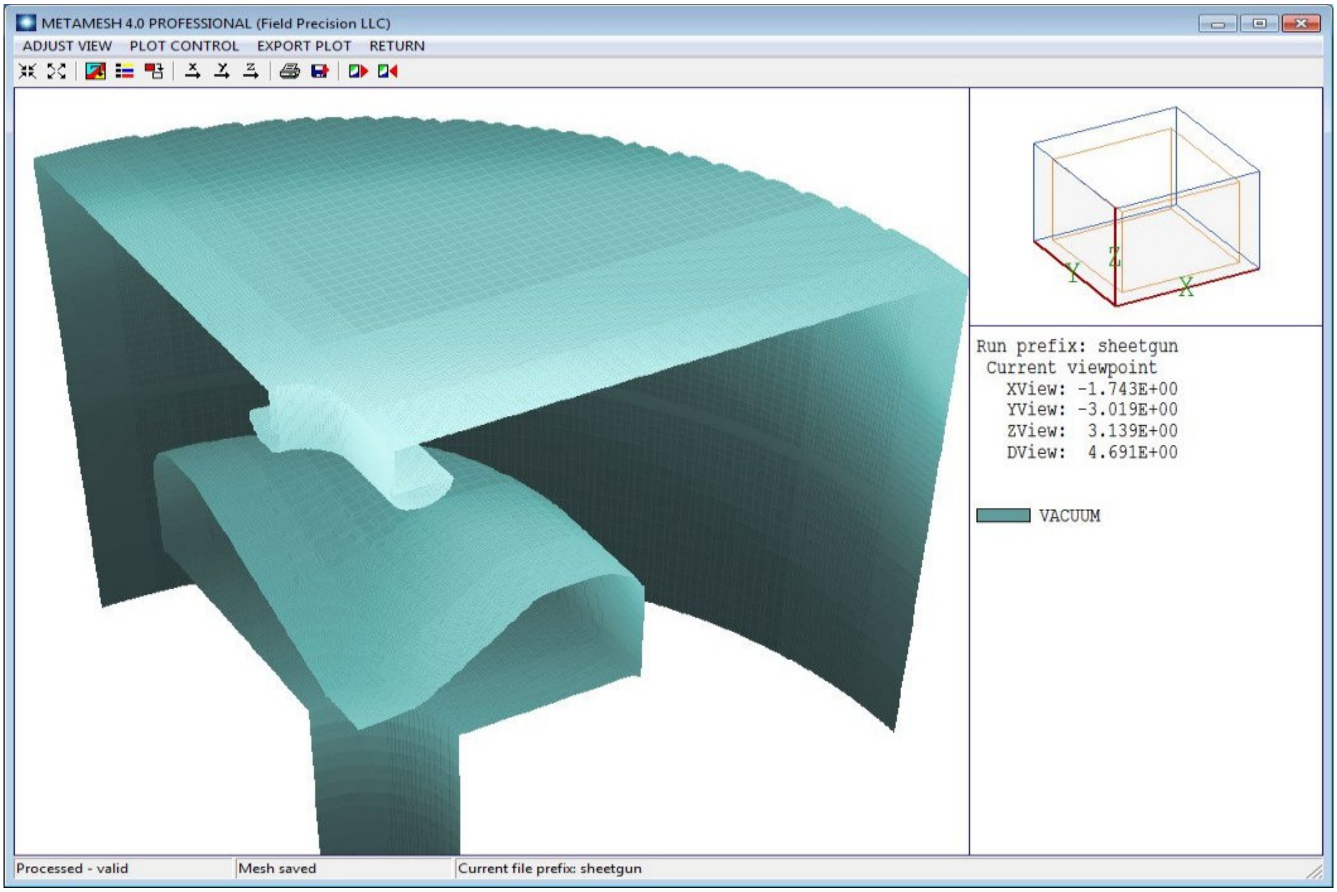


Finite-element mesh

Xenos uses meshes that are both *conformal* and *structured*, a type unique to the code suite.

- 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 is a cubic mesh whereas the actual elements are generalized hexahedrons that conform to complex surfaces. A structured mesh has a key advantage over an unstructured mesh in X-ray applications. In both the Monte Carlo and electron-particle beam solutions, element searches occupy the bulk of the computational effort.



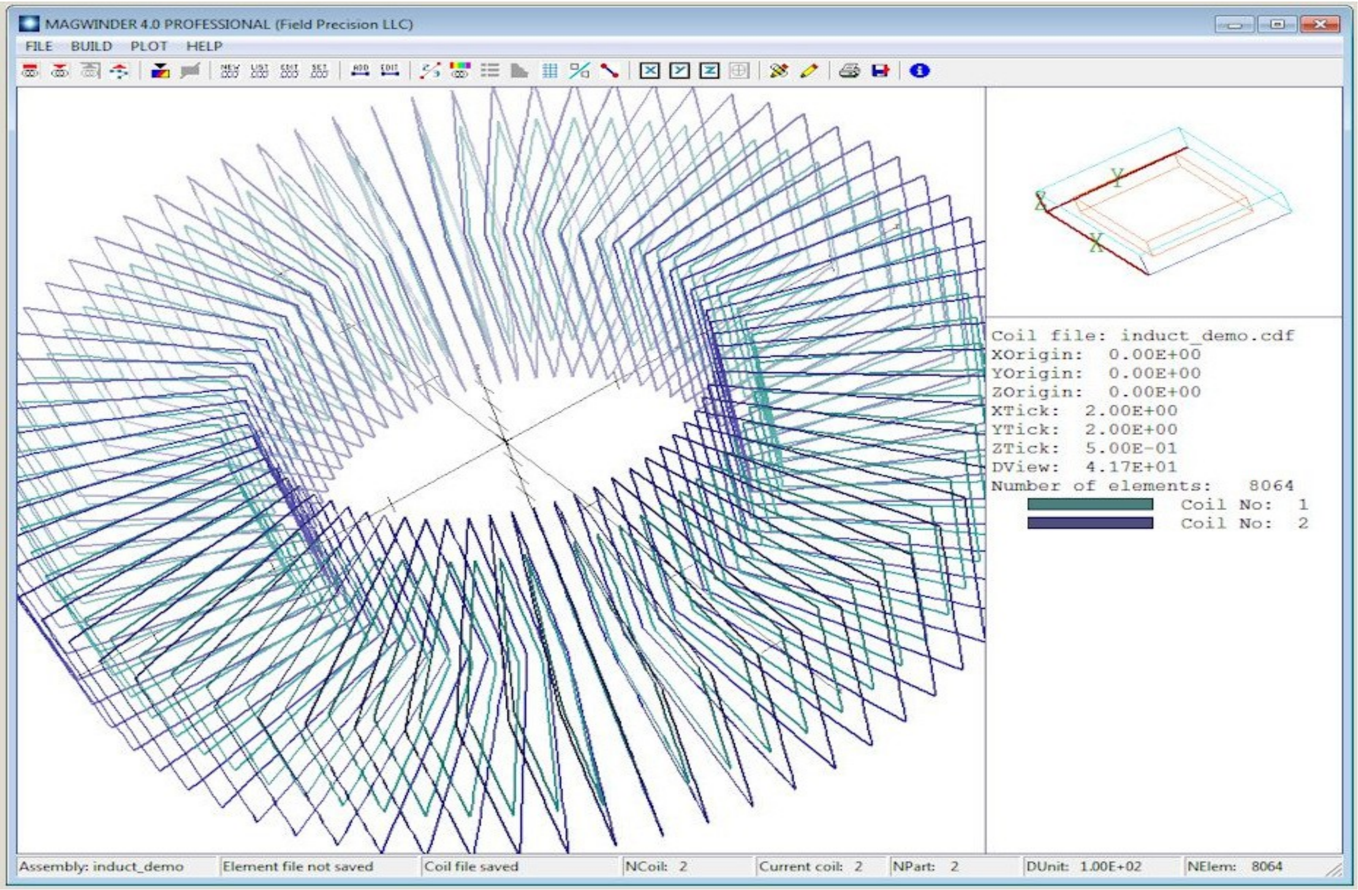
Geometry definition and mesh generation

Xenos has two components to build finite-element meshes:

- **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.

MetaMesh can import geometric data from a variety of sources to create a single mesh:

- Parametric solid-geometry models.
- Import of complex objects from 3D CAD programs via STL files.
- Mathematically-generated 3D surfaces.
- Solid bodies defined by generalized image files.
- Representations from unstructured, tetrahedron meshes.
- Planar surfaces from photographs.
- MRI data from Analyze 7.5 files
- Human phantom information (Zubal and GSF).

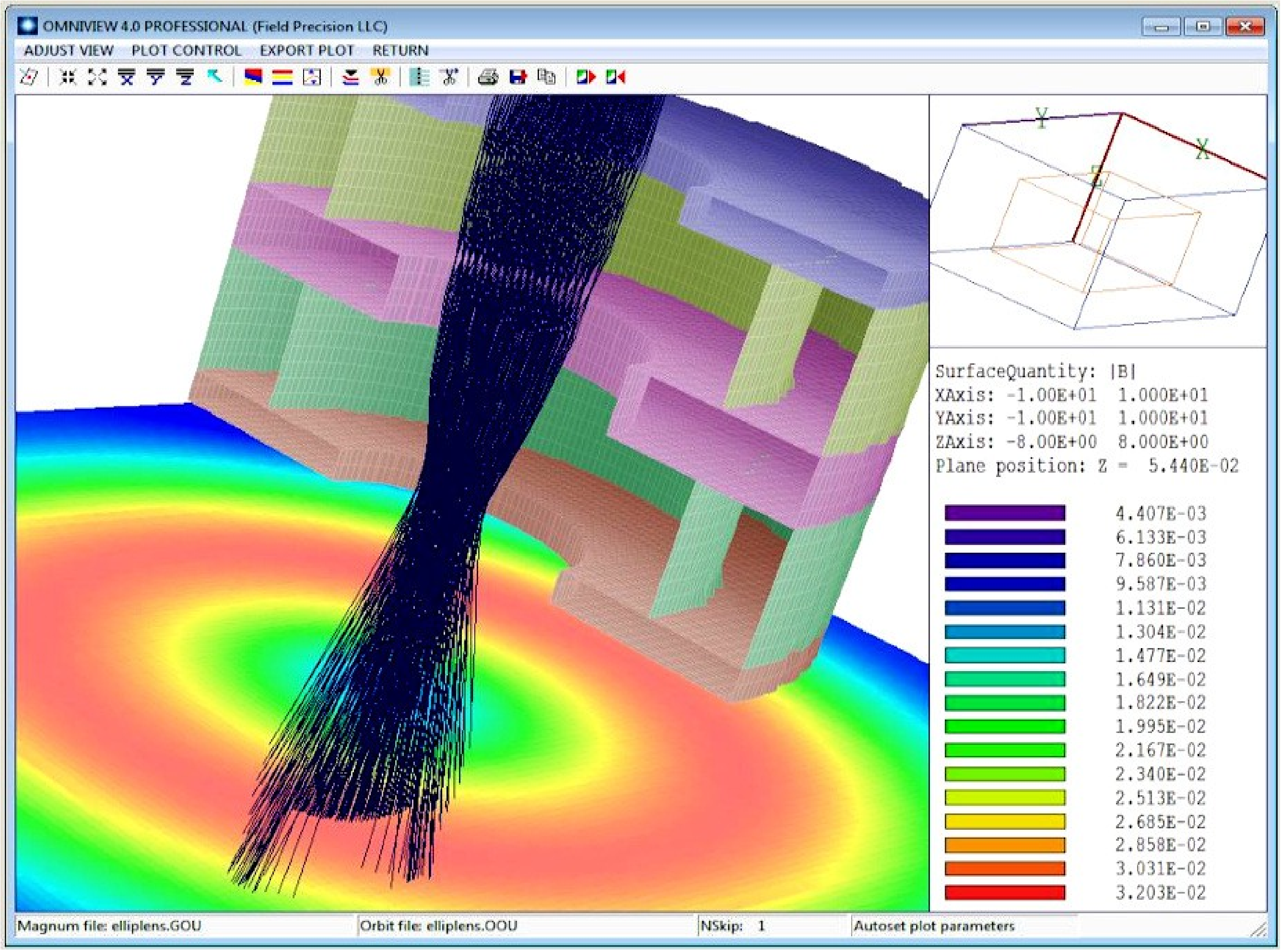


Electric and magnetic field calculations

HiPhi performs 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:

- Applied field definitions for electron or positron dynamics in the Monte Carlo radiation code **GamBet**
- Applied fields for the electron gun code **OmniTrak**.

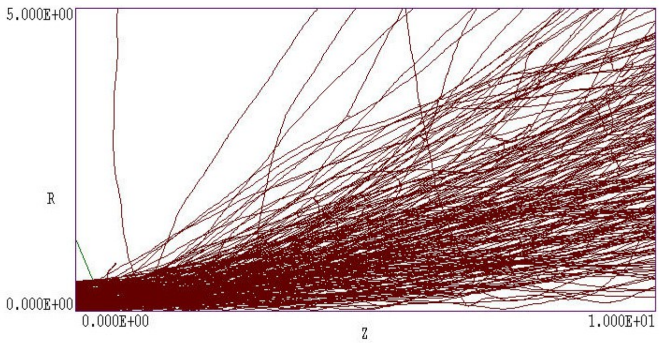
HiPhi and **Magnum** perform conventional finite-element field solutions on an unconventional mesh. The structured mesh offers the advantages of short solution times and efficient memory usage. **HiPhi** has several advanced features, including the option to define continuous variations of potential, dielectric constant or conductivity within a region. **Magnum** includes a parametric modeler **MagWinder** to generate complex drive coils.

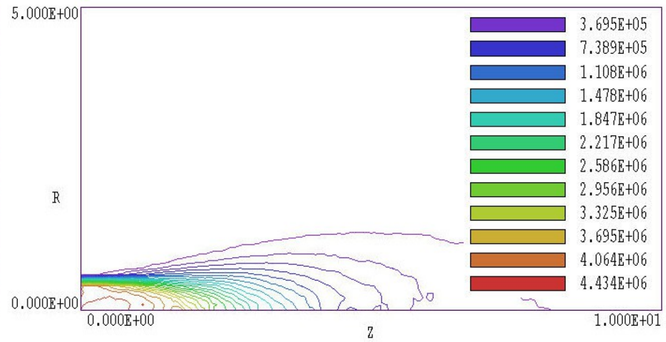


Electron beam modeling

OmniTrak handles the design of charged-particle guns and transport systems. Its function in **Xenos** is tracking electrons and positrons in vacuum. The code can recalculate electric fields internally to account for self-consistent beam space-charge contributions. It can also create particles to model space-charge limited emission, field emission and other processes. 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.

OmniTrak has two input source types: 1) electric and magnetic field distributions on independent meshes, and 2) particle lists (*e.g.*, incident beams) from **GenDist**, user programs or **GamBet** runs. **OmniTrak** provides input to **GamBet** via particle lists (*e.g.*, incident beams from electron guns), with or without filtering by **GenDist**.





Monte Carlo simulations

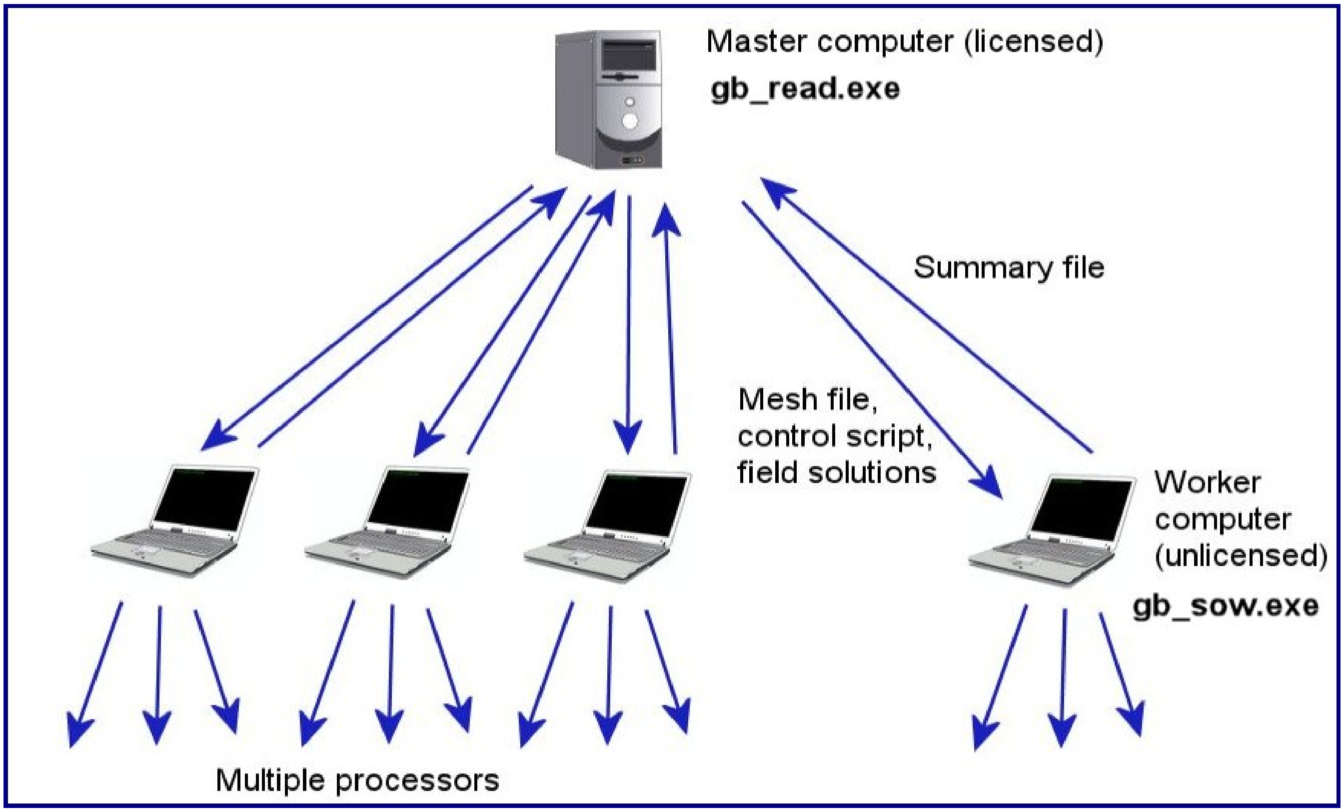
Monte Carlo codes for X-ray science have two components: 1) an atomic physics engine (scattering, energy loss, photon generation,...) and 2) a geometry engine (material identification, dose distribution,...).

- In **GamBet**, the first function is performed by **Penelope-2006**, developed at the University of Barcelona. **Penelope** handles generation of atomic cross sections, prediction of single-particle interactions with matter and creation of secondary particles. A notable 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 in 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.

Some unique features of **GamBet**

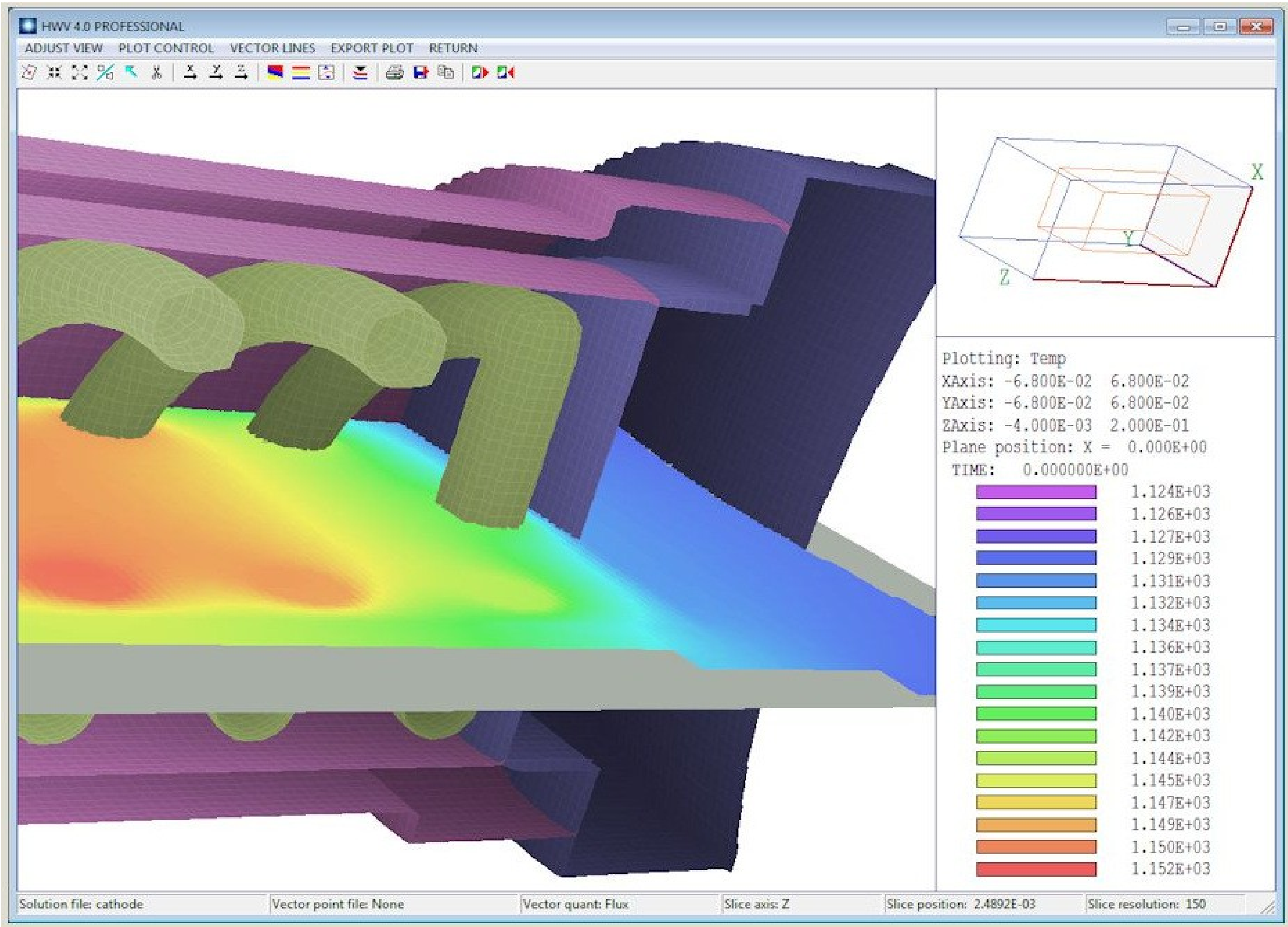
- Conformal meshes with accurate representations of curved boundaries,
- Inclusion of 2D and 3D electric and magnetic fields on independent meshes.
- Interactive graphical post-processor to analyze dose distributions and selected particle histories.
- Bidirectional communication with the particle beam code **OmniTrak**.
- Connection to **HeatWave** for static and dynamic thermal simulations.



Parallel computing in GamBet

Parallel computing is particularly important in a Monte Carlo code where a large number of showers may be necessary for statistical accuracy. **GamBet** utilizes two strategies for parallel operation.

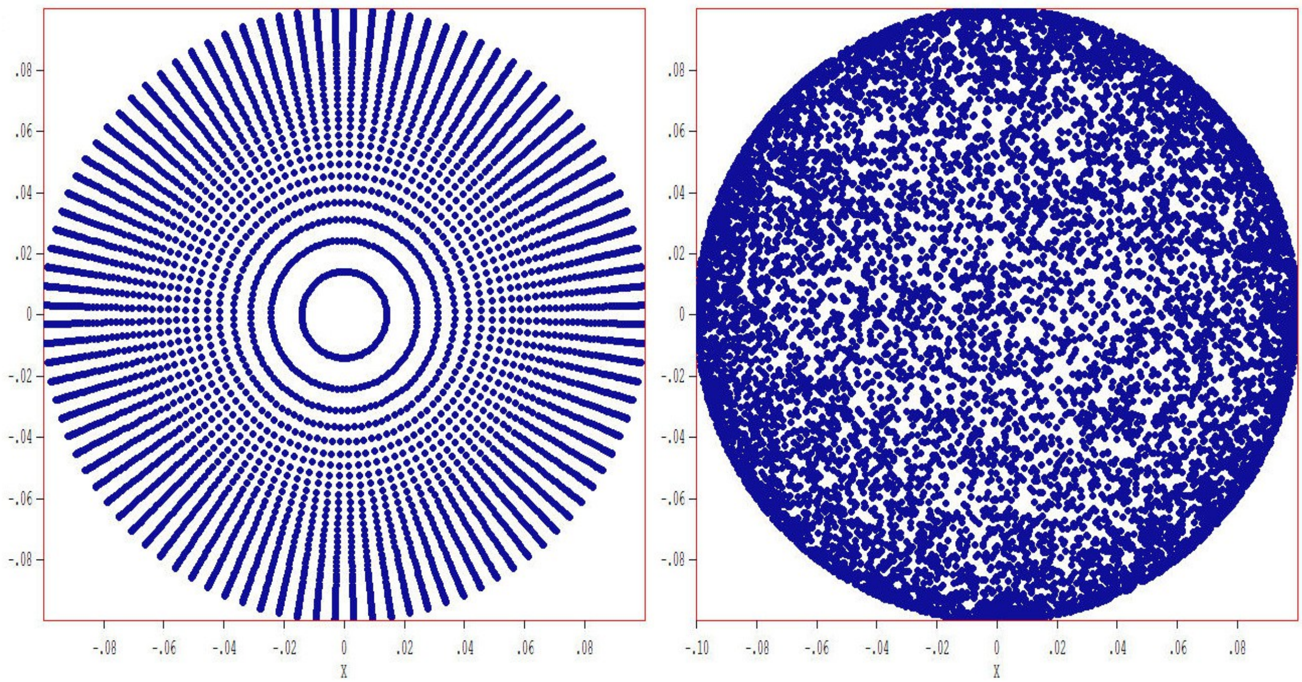
- Multi-core calculations on a single computer using the distributed memory method. With this choice, the reduction in computational time is almost linearly proportional to the number of cores. For a given run setup, **GamBet** starts an instance of the program with a unique random number seed in each 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 worker 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 accuracy.



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** calculations 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 beams. There is also an option to apply specified time-dependent spatial shifts to model rotating targets. Other special features of **HeatWave** include:

- Non-linear solutions with temperature-dependent material properties,
- Radiation boundaries (*e.g.*, modeling thermionic cathodes).
- Perfusion contributions for biological calculations.



Monte Carlo data analysis

Xenos includes the statistical utility **GenDist** which connects to **GamBet** and **OmniTrak** via model particle list files (text files where each line documents particle parameters). There are two list formats: PRT for **OmniTrak** and SRC for **GamBet**. The differences are that the **OmniTrak** file may include ions and macroparticles for other applications and the **GamBet** file may include photons. The text format of the list files make it easy to perform extended functions with statistical packages like **R**.

GenDist performs the following functions:

- Generation of large particle distributions based on parametric models in either the PRT or SRC format. These may be ported to **GamBet** or **OmniTrak** to initiate electron beams or X-ray sources
- Filtering of particle distributions to remove selected particles or shift the position and orientation of beams.
- Input of escape particle information from **GamBet** or distributions saved at specific locations from **OmniTrak** to perform statistical analysis and to generate plots.
- Conversion between PRT and SRC formats.