Recent Advances in Beam Optics Analyzer

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Abstract: Recent advances in Beam Optics Analyzer include anisotropic materials implemented within the finite element framework, higher order interpolation for thermal and stress analyses, and smoother, more efficient shapelets method to construct current density on 3D surfaces

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Introduction

Beam Optics Analyzer (BOA) is a relativistic particle tracker with several finite element field solvers for electrostatics, heat transfer, magnetostatics and Helmholtz fields. It can track particles in either static or harmonic fields with space charge effects. It provides sophisticated emission models for field and thermionic emission. Thermal velocities, which exactly satisfy the Gaussian distribution by the Inverse Cumulative Distribution method, are included in the model. Its Mesher generates unstructured mesh with fine-grained control. Meshing adaptivity driven by smoothing field gradient can be enabled. Calabazas Creek Research (CCR) recently added stress analysis coupled thermal analysis to BOA making it a complete multiphysics platform. It uses the same CAD model for all analysis types, from magnetostatics, electrostatics, and beam simulation to heat transfer and stress analysis. Parts in the original CAD model can be enabled/disabled per analysis type, and changing material of one part in one analysis type is automatically carried over to other types.

A multiple beam IOT requires several modulating grids to generate RF currents, and each grid must be structurally sound under grid loading and irradiated by a high temperature emitter. These grids are commonly made of pyrolytic graphite, whose thermal conductivity and thermal expansion coefficient are highly directional. If we desire to change the grid material to molybdenum, which is much easier to fabricated, we need to be able to perform thermal and stress analyses of pyrolytic graphite grid and compare its structural characteristics to that of molybdenum. The IOT grid such as shown in Figure 1 is spherical and machined to many thin circular bars. To achieve the required accuracy with a manageable mesh size, field solvers with higher order of interpolation are also highly desirable. In this paper we will describe how BOA implements anisotropic thermal material properties with simulation results in linear and quadratic elements.

In addition, in X-ray target or e-beam lithography, accuracy representation of the beam power density is very critical. The power density, which is generated by particles depositing energies on terminal surfaces, is commonly obtained by interpolation of particle position to the mesh. The typical approach is to increase the number of particles and meshes to satisfy the required accuracy. A better and more efficient approach would be to obtain the desired accuracy for a particular spot size by adaptively increasing the order of interpolation without increasing the mesh size or number of particles.

Anisotropic Properties

To include material anisotropy in heat transfer, we start first with the finite element formulation of the heat conduction

$$\sum_{e=1}^{n_{el}} \int_{\Omega^e} \nabla W \cdot \mathbf{K} \nabla T \ d\Omega = \sum_{e=1}^{n_{el}} \int_{\Omega^e} Wf \ d\Omega + \int_{\Gamma_n^e} Wh \ d\Gamma \ (1)$$

where **T** is the unknown temperature, f the prescribed heat density, h the prescribed heat flux, W the weighting function, and **K** the thermal conductivity tensor in global coordinate system. For isotropic materials, the thermal conductivity is a scalar, but a positive definite tensor for anisotropic materials. Anisotropic thermal conductivitives are given in principal material axes, which are in general not aligned with the global axes, and vary from element to element. Therefore, a coordinate transform is required as follows

$$\mathbf{K} = \mathbf{Q}^{\mathrm{T}} \mathbf{k} \mathbf{Q} \tag{2}$$

where \mathbf{k} is thermal conductivity tensor in material coordinates, and \mathbf{Q} a proper orthogonal rotation matrix

$$\mathbf{Q}\mathbf{Q}^{\mathrm{T}} = \mathbf{Q}^{\mathrm{T}}\mathbf{Q} = \mathbf{I}, \quad \mathbf{Q}^{-1} = \mathbf{Q}^{\mathrm{T}}, \quad |\mathbf{Q}| = 1$$
 (3)

The principal thermal conductivity tensor \mathbf{k} is diagonal for orthotropic materials. The orthogonal matrix provides the global to material coordinate transformation

It varies from element to element, and can be constructed from local material axes $\{l, m, n\}$ as follows

 $\mathbf{x}' = \mathbf{O}\mathbf{x}$

$$\mathbf{Q} = \begin{bmatrix} \mathbf{l}^{\mathrm{T}} \\ \mathbf{m}^{\mathrm{T}} \\ \mathbf{n}^{\mathrm{T}} \end{bmatrix}$$
(5)

BOA requires users to enter the surface(s) of each anisotropic part for it to construct the material axes $\{l, m, n\}$ for each finite element. The most efficient implementation is to compute and store these material axes of all elements in every anisotropic part each time a new mesh is created.

We will present the heat transfer and stress analyses for an IOT grid with pyrolytic graphite and molybdenum.

Shapelets Method

In astronomy, the *shapelets* method has been used for the analysis of images and for weak gravitational lensing to measure the distribution of mass in the universe. For both applications, the shapelets method is found to be very efficient, highly accurate, linear, mathematically well-defined and optimally sensitive. Like shape functions in the finite element method, shapelets are complete and orthogonal polynomials with convenient recursion relations for construction of higher order functions, suitable for adaptation. Instead of Lagrange polynomials for the scalar finite element method, the shapelets are constructed from a circular Gaussian and Hermite polynomials. To apply shapelets method, we seek to construct from the discrete power density field produced by particle simulations the continuous current density profile on an arbitrary 3D surface. We seek to reconstruct the current density profile with a minimum of a-priori assumptions about the result. One way to accomplish this goal is to expand the discrete data in the form of a set of smooth orthogonal functions. Due to the Gaussian profile property of thermal electron beams, the natural choice for a basis set of functions are shapelets, which are the normalized product of Hermite polynomials and a Gaussian.

We will present the result of a smoothed, high ordered interpolated power density profile on an X-ray target.

Sample Problem

Figure 1 shows the model of an IOT grid with its boundary conditions. The grid bottom is heated by electron bombardment with 2.5W and irradiated by a 1050°C emitter. Its bottom edge is kept at 75°C, and top surface radiates to a 150°C heat sink. In stress analysis, the grid bottom edge is allowed to slide radially outward. The grid material is orthotropic pyrolytic graphite.



Figure 1. IOT grid thermal and stress model. Bottom edge is a slider

Figure 2 shows the grid temperature profile of linear elements with the maximum temperature of 659°C at the center. With this temperature profile, BOA calculates thermal stresses also with linear elements. For completeness, gravity is

also included as a body force in the model. The largest displacement moving toward the emitter is 0.18mm at the grid center.



Figure 2. Temperature profile of a pyrolytic graphite grid heated up by the intercepted electrons and irradiation by emitter



Figure 3. Grid displacement in the direction toward the emitter. Maximum at the center

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