Development of MH4D for Simulation of Emerging Concept Fusion Experiments

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Main Ideas

- PSI-Center: further developing a tetrahedral mesh MHD simulation code to model Emerging Concept (EC) experiments (MH4D: Lionello & Schnack, 2004)
  - represent the complex 3-dimensional geometry of many EC experiments
  - using existing programs for gridding, parallel implementation, and visualization
- Current status
  - vacuum fields in code
  - input/output in General Mesh Viewer (GMV) format (Ortega, 2000)
  - preliminary simulations of HIT-SI and ZAP experiments with near experimental parameters

Code: Resitive MHD Model

$$\frac{\partial \mathbf{A}}{\partial t} = -\mathbf{E} \qquad \mathbf{B} = \boldsymbol{\nabla} \times \mathbf{A} \qquad \mathbf{J} = \boldsymbol{\nabla} \times \mathbf{B}$$

$$\mathbf{E} = -\mathbf{v} \times \mathbf{B} + \eta \mathbf{J}$$

$$\frac{\partial \rho}{\partial t} = -\boldsymbol{\nabla} \cdot \rho \mathbf{v}$$

$$\rho \left(\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} \right) = -\boldsymbol{\nabla} p + \mathbf{J} \times \mathbf{B} + \nu \nabla^2 \mathbf{v}$$

$$\frac{\partial p}{\partial t} + \mathbf{v} \cdot \boldsymbol{\nabla} p = -\gamma p \boldsymbol{\nabla} \cdot \mathbf{v} + \boldsymbol{\nabla} \cdot \mathbf{q} + Q$$

Alfvén velocity: $V_A = B/\sqrt{\rho}$
Alfvén transit time: $\tau_A = (2\pi r_{axis})/V_A$
Resistive diffusion time : $\tau_R = 1/(\eta\lambda^2)$

Lundquist number: $S = \tau_R/\tau_A$

Include Vacuum Fields

Assume external fields:

$$\dot{\mathbf{A}} = -\mathbf{E}_{int}$$

$$\text{and} \qquad \mathbf{B}_{total} = \mathbf{B} + \mathbf{B}_{ext}$$

$$\Rightarrow \dot{\mathbf{A}} = \mathbf{v} \times (\mathbf{B} + \mathbf{B}_{ext}) - \eta \mathbf{J} + \mathbf{E}_{ext}$$

$$\Rightarrow \rho \left(\frac{D\mathbf{v}}{Dt} \right) = -\nabla p + \mathbf{J} \times (\mathbf{B} + \mathbf{B}_{ext}) + \nu \nabla^2 \mathbf{v}$$

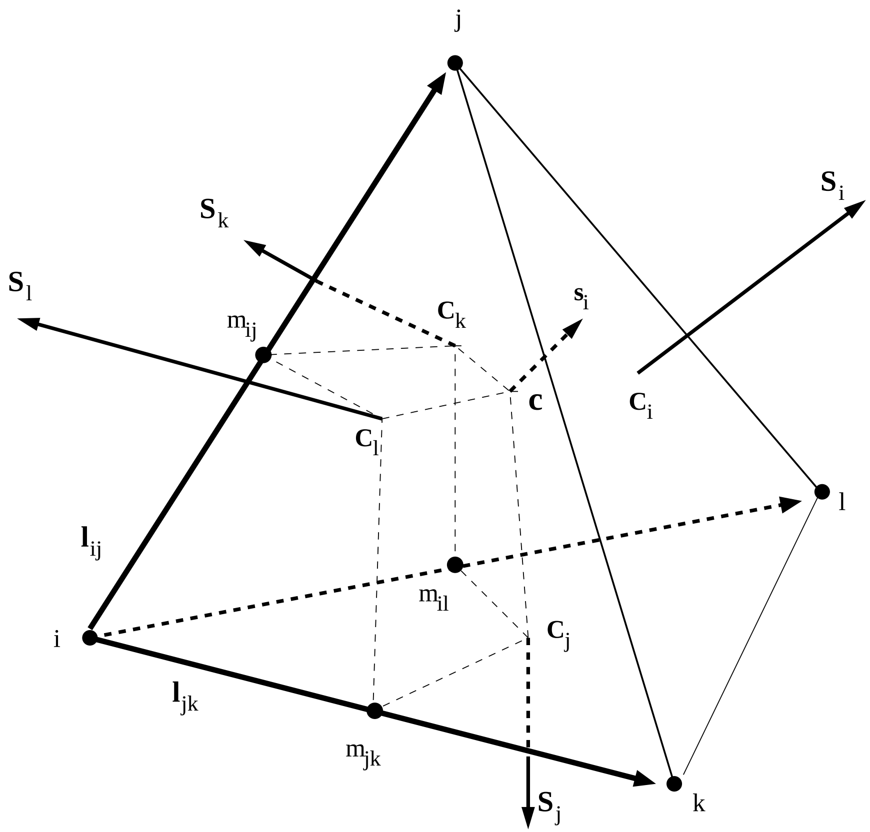
where

$$\mathbf{E}_{ext} = \text{Volt}_{coeff} \left(\mathbf{v}_{f1} \sin(\omega t) + \mathbf{v}_{f2} \cos(\omega t) \right)$$

$$\mathbf{B}_{ext} = \text{Flux}_{coeff} \left(\mathbf{v}_{f1} \sin(\omega t) + \mathbf{v}_{f2} \cos(\omega t) \right)$$

If $\mathbf{B}_{ext}$ is time dependent then its induced electric field must be included in $\mathbf{E}_{ext}$.

Tetrahedral Grid



- Sides are labeled by index of their opposite vertex
- **c**: centroid of tetrahedron
- m_{ij}: midpoint of edge $\mathbf{l}_{ij}$
- C_i: centroid of side i
- $\mathbf{S}_i$: vector area of side i
- $\mathbf{s}_i$: vector area of dual median surface
- V_c: volume of tetraderon c

$$\mathbf{s}_i = \frac{1}{3}\mathbf{S}_i \qquad V_c = \frac{1}{6}\mathbf{l}_{ij} \cdot (\mathbf{l}_{ik} \times \mathbf{l}_{il}) = -\frac{1}{3}\mathbf{l}_{ij} \cdot \mathbf{S}_j$$

Finite Volume Formalism

Integral relations to define differential operators

Gradient:

$$\int_V \nabla f dV = \int_S \hat{\mathbf{n}} f dS$$

Divergence:

$$\int_V \boldsymbol{\nabla} \cdot \mathbf{F} dV = \int_S \hat{\mathbf{n}} \cdot \mathbf{F} dS$$

Curl in 2D

$$\int_s \mathbf{n} \cdot \boldsymbol{\nabla} \times \mathbf{F} dS = \oint_C \mathbf{F} \cdot d\mathbf{l}$$

Curl in 3D

$$\int_V \nabla \times \mathbf{F} dV = \int_S \hat{\mathbf{n}} \times \mathbf{F} dS$$

Magnetic Field

Vector potential $\mathbf{A}$ defined on vertices

- $\mathbf{A}$ varies linearly within tetrahedron

$$\int_V \mathbf{B} dV = \int_V \boldsymbol{\nabla} \times \mathbf{A} dV = \int_S d\mathbf{S} \times \mathbf{A}$$

$$\Rightarrow B_\tau V_\tau = \sum_{s=1}^{4} \mathbf{S}_s \times \bar{\mathbf{A}}_s$$

In terms of vertices:

$$\mathbf{B}_\tau = -\frac{1}{3V_\tau} \sum_{\nu(\tau)} \mathbf{S}_\nu \times \mathbf{A}_\nu$$

$\mathbf{B}_\tau$: constant within tetrahedron τ
$\bar{\mathbf{A}}_s$: average of $\mathbf{A}$ over the 3 vertices of side S
V_τ: volume of tetrahedron τ
$\nu(\tau)$: indices of the 4 vertices of tetrahedron τ
$\mathbf{S}_\nu$: outward directed side opposite vertex ν

Divergence of B

Using Gauss' theorem to dual median volume element surrounding vertex ν

$$(\nabla \cdot \mathbf{B})_\nu \, v_\nu = \frac{1}{3} \sum_\tau \mathbf{B}_\tau \cdot \mathbf{S}_{\nu(\tau)}$$

$$= \frac{1}{3} \sum_\tau \frac{1}{V_\tau} \sum_{\gamma(\tau)} \bar{\mathbf{A}}_\gamma \cdot (\mathbf{S}_\nu \times \mathbf{S}_\gamma)$$

$v_\nu = \sum_{\tau(\nu)} \frac{1}{3} V_\tau$: volume of dual median volume element
$\tau(\nu)$: indices of the tetrahedra sharing vertex ν
$\nu(\tau)$: index of the side of tetrahedron τ opposite vertex ν
$\gamma(\tau)$: indices of the 4 sides of tetrahedron τ

- Contributions from common sides of adjoining tetrahedra cancel

$$(\nabla \cdot \mathbf{B})_\nu = 0$$

Another Derivation of B

A varies linearly within tetrahedron

$$\mathbf{A}(\mathbf{x}) = \sum_\nu \mathbf{A}_\nu \left(1 - \frac{1}{3V_\tau}\mathbf{S}_\nu \cdot (\mathbf{x} - \mathbf{x}_\nu)\right)$$

Take curl of **A**

$$B_\alpha = \varepsilon_{\alpha\beta\gamma}\frac{\partial A_\gamma}{\partial x_\beta}$$

$$\Rightarrow \mathbf{B}_\tau = -\frac{1}{3V_\tau}\sum_{\nu(\tau)} \mathbf{S}_\nu \times \mathbf{A}_\nu$$

Same as finite volume represenation.

Current Density

Apply Stoke's to dual median volume element

$$\int_V \mathbf{J} dV = \int_V \boldsymbol{\nabla} \times \mathbf{B} dV = \int_S \hat{\mathbf{n}} \times \mathbf{B} dS$$

Use B in terms of $\mathbf{A}$

$$\mathbf{J}_\nu \upsilon_\nu = \frac{1}{3} \sum_{\tau(\nu)} \mathbf{S}_{\nu(\tau)} \times \mathbf{B}_\tau$$

$$\mathbf{J}_\nu \upsilon_\nu = \sum_{\tau(\nu)} \sum_{\nu'(\tau)} \mathfrak{M}^\tau(\nu, \nu') \cdot \mathbf{A}_{\nu'}$$

$$\mathfrak{M}^\tau(\nu, \nu') = \frac{1}{9V_\tau} \left[\left(\mathbf{S}_{\nu(\tau)} \cdot \mathbf{S}_{\nu'(\tau)} \right) \mathbf{I} - \mathbf{S}_{\nu'(\tau)} \mathbf{S}^T_{\nu(\tau)} \right]$$

$\mathfrak{M}^\tau$ is symmetric, self adjoint and the discrete "curl-curl" operator

Variational Principle (VP)

- begin with functional: $I(\mathbf{A}) = \frac{1}{2}\left[(\boldsymbol{\nabla} \times \mathbf{A})^2 - 2\mathbf{J} \cdot \mathbf{A}\right] dV$
- minimize I w.r.t variations $\delta\mathbf{A}$, let $\mathbf{A} \rightarrow \mathbf{A} + \epsilon\delta\mathbf{A}$

$$I\left(\mathbf{A} + \epsilon\delta\mathbf{A}\right) = \frac{1}{2}\int\left[(\boldsymbol{\nabla} \times \mathbf{A})^2 - 2\mathbf{J} \cdot \mathbf{A}\right] dV$$

$$+\epsilon \underbrace{\int(\boldsymbol{\nabla} \times \mathbf{A} \cdot \boldsymbol{\nabla} \times \delta\mathbf{A} - \mathbf{J} \cdot \delta\mathbf{A})dV}_{C}$$

$$+\frac{\epsilon^2}{2}\int(\boldsymbol{\nabla} \times \delta\mathbf{A})^2 dV$$

I has minimum at $\epsilon = 0$ only if $C = 0$. Vector identities and integration by parts imply

$$\int \delta\mathbf{A} \cdot \left(\boldsymbol{\nabla} \times \boldsymbol{\nabla} \times \mathbf{A} - \mathbf{J}\right) dV = -\int_S \delta\mathbf{A}_t \cdot (\mathbf{B} \times \hat{\mathbf{n}}) dS$$

$$\text{where} \quad \mathbf{A}_t = (\mathbf{I} - \hat{\mathbf{n}}\hat{\mathbf{n}}) \cdot \mathbf{A}$$

- Let: $I(\mathbf{A}) = \frac{1}{2}\left[(\boldsymbol{\nabla} \times \mathbf{A})^2 - 2\mathbf{J} \cdot \mathbf{A}\right] dV$
- Minimum of $I(\mathbf{A})$ is solution to $\boldsymbol{\nabla} \times \boldsymbol{\nabla} \times \mathbf{A} = \mathbf{J}$ with $\mathbf{A}_t$ specified on boundary
- Minimize $I(\mathbf{A})$ on tetrahedral grid with N_ν vertices and N_τ tetrahedra.
  - Expand $\mathbf{A}(\mathbf{x})$ with basis $\alpha_\nu(\mathbf{x})$: $\mathbf{A}(\mathbf{x}) = \sum \mathbf{A}_\nu \alpha_\nu(\mathbf{x})$
  - Expand current density with delta functions: $\mathbf{J}(\mathbf{x}) = \sum_\nu v_\nu J_\nu \delta(\mathbf{x} - \mathbf{x}_\nu)$

VP gives discrete result

Discrete functional:

$$I = \frac{1}{2} \sum_{\nu} \sum_{\nu'} \mathbf{A}_\nu \cdot \mathfrak{M}(\nu, \nu') \cdot \mathbf{A}_{\nu'} - \sum_{\nu} \sum_{\nu'} v_\nu \mathbf{J}_\nu \cdot \mathbf{A}_{\nu'} \alpha_{\nu'}(\mathbf{x}_\nu)$$

$$\text{where} \quad \mathfrak{M} = \sum_{\tau} \mathfrak{M}^\tau$$

To minimize, $\frac{\partial I}{\partial \mathbf{A}_\mu} = 0, \ \forall \mu = 1, \ldots, N_\nu$

$$\Longleftrightarrow \sum_{\nu} \alpha_\mu(\mathbf{x}_\nu) v_\nu \mathbf{J}_\nu = \sum_{\tau} \sum_{\nu} \mathfrak{M}^\tau(\mu, \nu) \cdot \mathbf{A}_\nu, \ \forall \mu = 1, \ldots, N_\nu$$

Setting $\alpha_\mu(\mathbf{x}_\nu) = \delta_{\mu\nu}$ is the finite volume expression for solving **J** from **A**

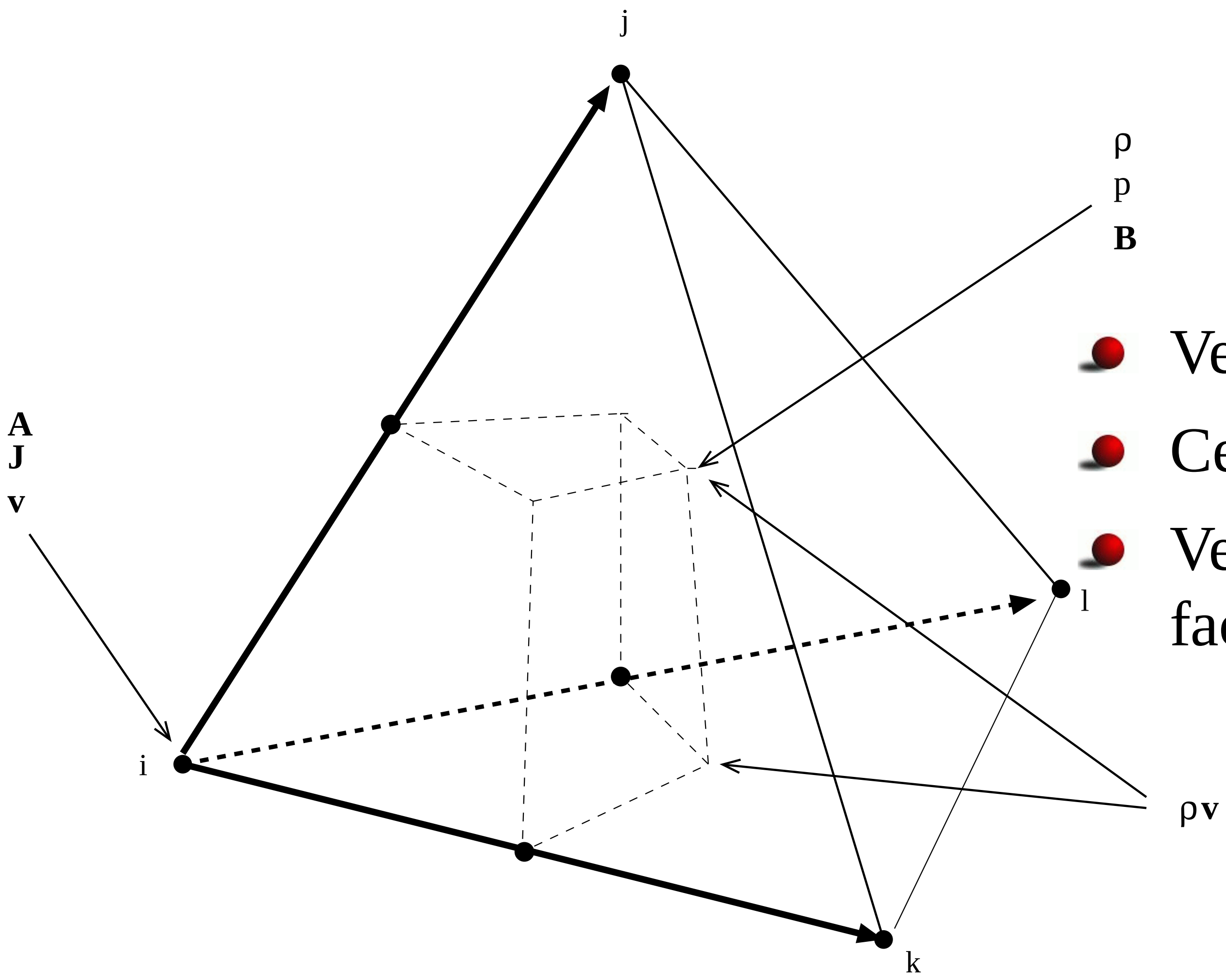
Boundary Condition

- Natural boundary condition,

$$\delta \mathbf{A}_t \cdot (\mathbf{B} \times \hat{\mathbf{n}}) = 0$$

- We must specify $\mathbf{A}_t = (\mathbf{I} - \hat{\mathbf{n}}\hat{\mathbf{n}}) \cdot \mathbf{A}$ on the boundary (Dirichlet)
- Item for further PSI-center development

Variables on Grid



- Vertices: $\mathbf{A}$, $\mathbf{J}$, $\mathbf{v}$
- Centroids: B, ρ, p
- Velocity averaged to faces or centroids

Partial Implicit Time Stepping

Large spectrum of eigenvalues associated with MHD operators
$\Rightarrow$ large range of time scales

$$\frac{\partial u}{\partial t} = \underbrace{\mathcal{M}\{u\}}_{\text{Full MHD Operator}} = \underbrace{\overbrace{\mathcal{F}\{u\}}^{\text{Fast time scales}}}_{\text{Alfvén waves, soundwaves}} + \underbrace{\overbrace{\mathcal{S}\{u\}}^{\text{Slow time scales}}}_{\text{interesting physics}}$$

To avoid time step restriction, treat "fast" part of operator implicitly

$$\frac{u^{n+1} - u^n}{\Delta t} = F u^{n+1} + S u^n$$

Quite difficult to achieve precise discrete representation

No need for operator S

F and M are known operators in MHD computations

$$\begin{aligned} \frac{u^{n+1}-u^n}{\Delta t} &= F u^{n+1} + \underbrace{(M-F)}_{S=M-F} u^n \\ &= M u^n + \Delta t F \left(\frac{u^{n+1}-u^n}{\Delta t} \right) \end{aligned}$$

Works for arbitrary operator F

Semi-Implicit Method

For an arbitrary operator G

$$\left(I - \underbrace{\Delta t G}_{\text{SI operator}}\right) u^{n+1} = \underbrace{(I + \Delta t M)\, u^n}_{\text{Explicit}} - \underbrace{\Delta t G}_{\text{SI operator}}\ u^n$$

Want to choose G for ease of inversion and inclusion of modes of interest

Semi-implicit MHD operator

- use of linearized, ideal MHD wave equation

$$\rho_0 \frac{\partial^2 \mathbf{v}}{\partial t^2} = \boldsymbol{\nabla} \times \boldsymbol{\nabla} \times (\mathbf{v} \times \mathbf{B}_0) \times \mathbf{B}_0$$

- large spectrum of normal modes
- anisotropic spatial operator
- modify equation of motion

$$\rho \frac{D\mathbf{v}}{Dt} = -\boldsymbol{\nabla} p + \mathbf{J} \times \mathbf{B} + \alpha \Delta t \mathbf{S} \left(\frac{\partial \mathbf{v}}{\partial t} \right)$$

where $\mathbf{S}(\mathbf{v}) = \boldsymbol{\nabla} \times \boldsymbol{\nabla} \times (\mathbf{v} \times \mathbf{B}) \times \mathbf{B}$

S is self-adjoint.

Discrete Semi-Implicit Operator

Use variational principle:

$$I(\mathbf{v}) = \frac{1}{2}\int \left[\left|\nabla\times(\mathbf{v}\times\mathbf{B})^2\right| + 2\mathbf{S}\cdot\mathbf{v}\right] dV$$

Let:

$$\mathbf{v}\times\mathbf{B} = \sum_j (\mathbf{v}_j\times\mathbf{B}_j)\alpha_j(\mathbf{x}),\quad \mathbf{v} = \sum_j \mathbf{v}_j\alpha_j(\mathbf{x}),\quad \mathbf{S} = \sum_j \mathbf{S}_j\delta(\mathbf{x}-\mathbf{x}_j)$$

Discrete variational principle:

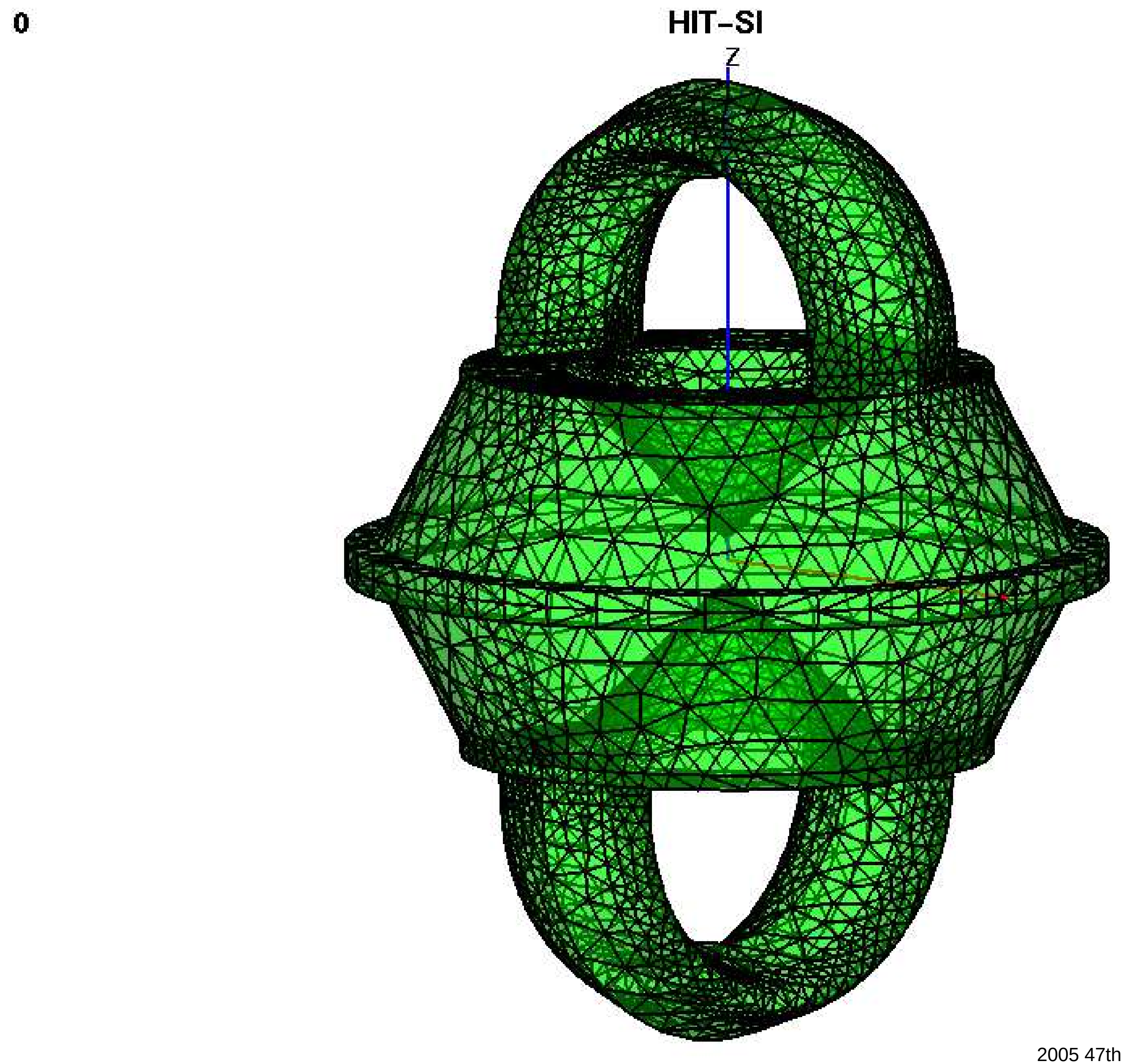
$$I(\mathbf{v}) = \frac{1}{2}\sum_k\sum_j \mathbf{v}_j\cdot\mathfrak{N}(j,k)\cdot\mathbf{v}_k + \mathbf{S}_k\cdot\mathbf{v}_k$$

where $\mathfrak{N}(j,k) = \mathbf{B}_j\times\mathfrak{M}(j,k)\times\mathbf{B}_k$ and is symmetric

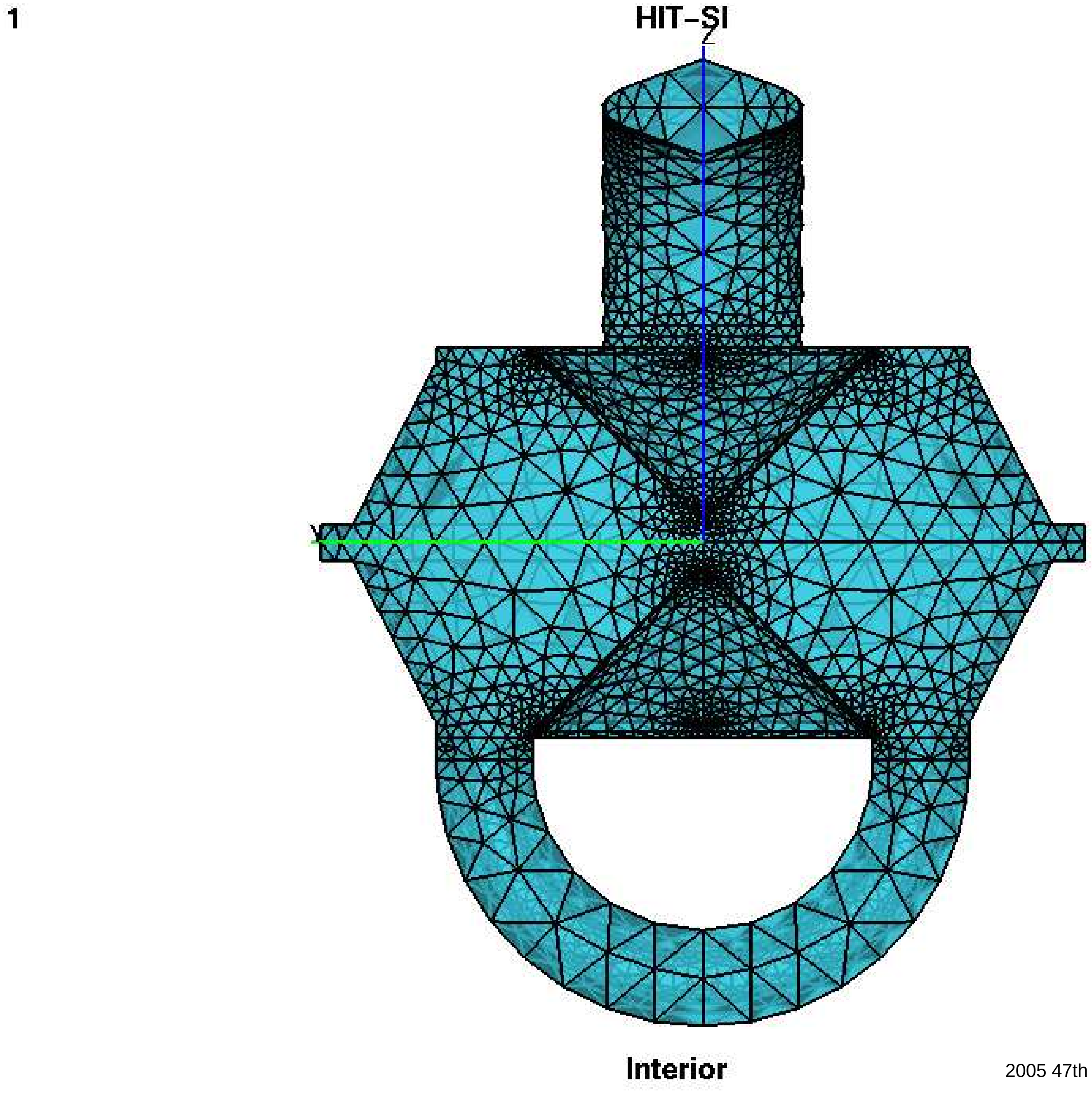
Minimization of $I \rightarrow$ discrete semi-implicit operator $\mathbf{S}_i$:

$$\frac{\partial I}{\partial \mathbf{v}_i} = 0 \iff \mathbf{S}_i = -\sum_j \mathfrak{N}(i,j)\cdot\mathbf{v}_j,\quad \forall\, i.$$

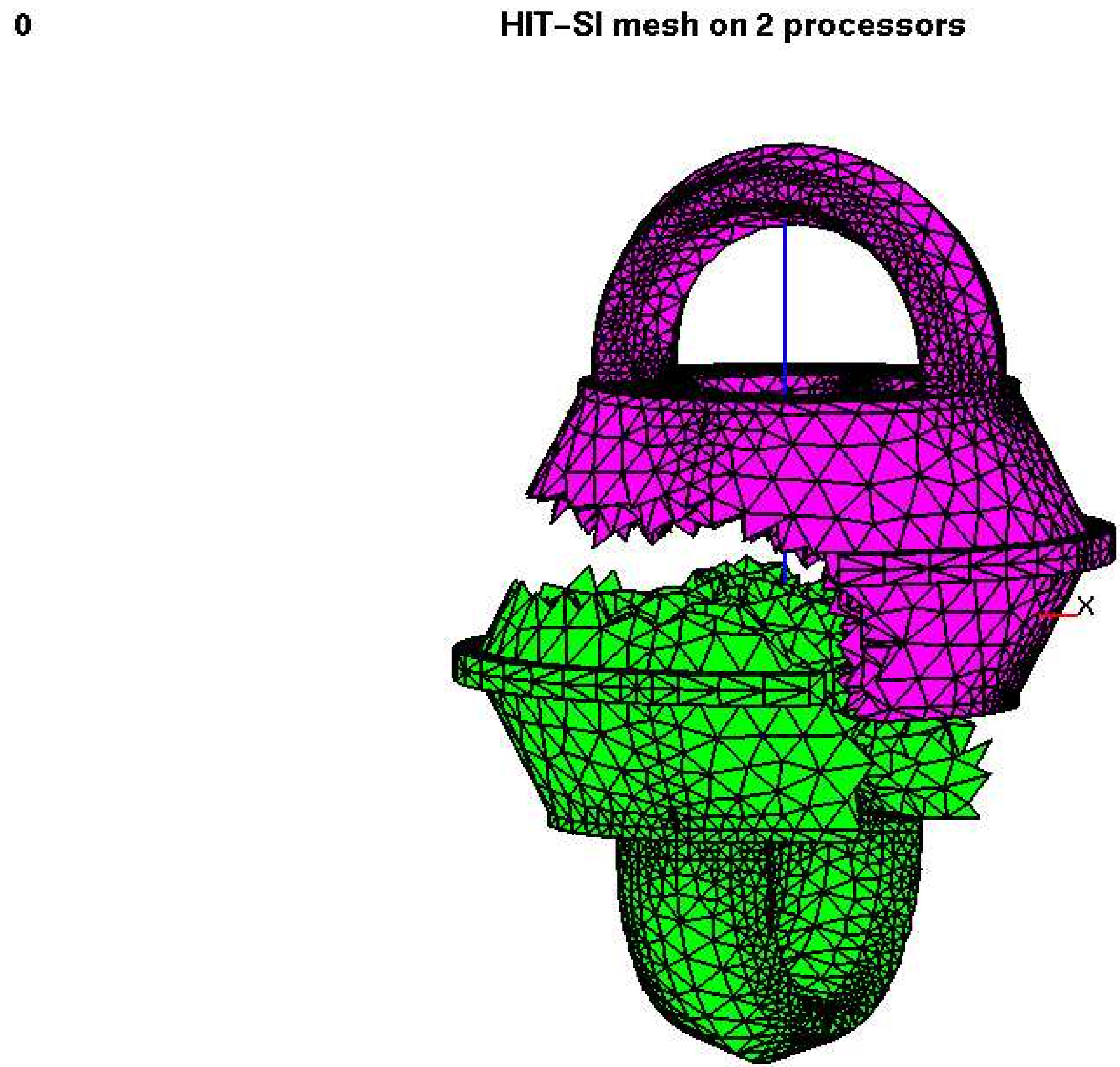
Tetrahedral Mesh for HIT-SI



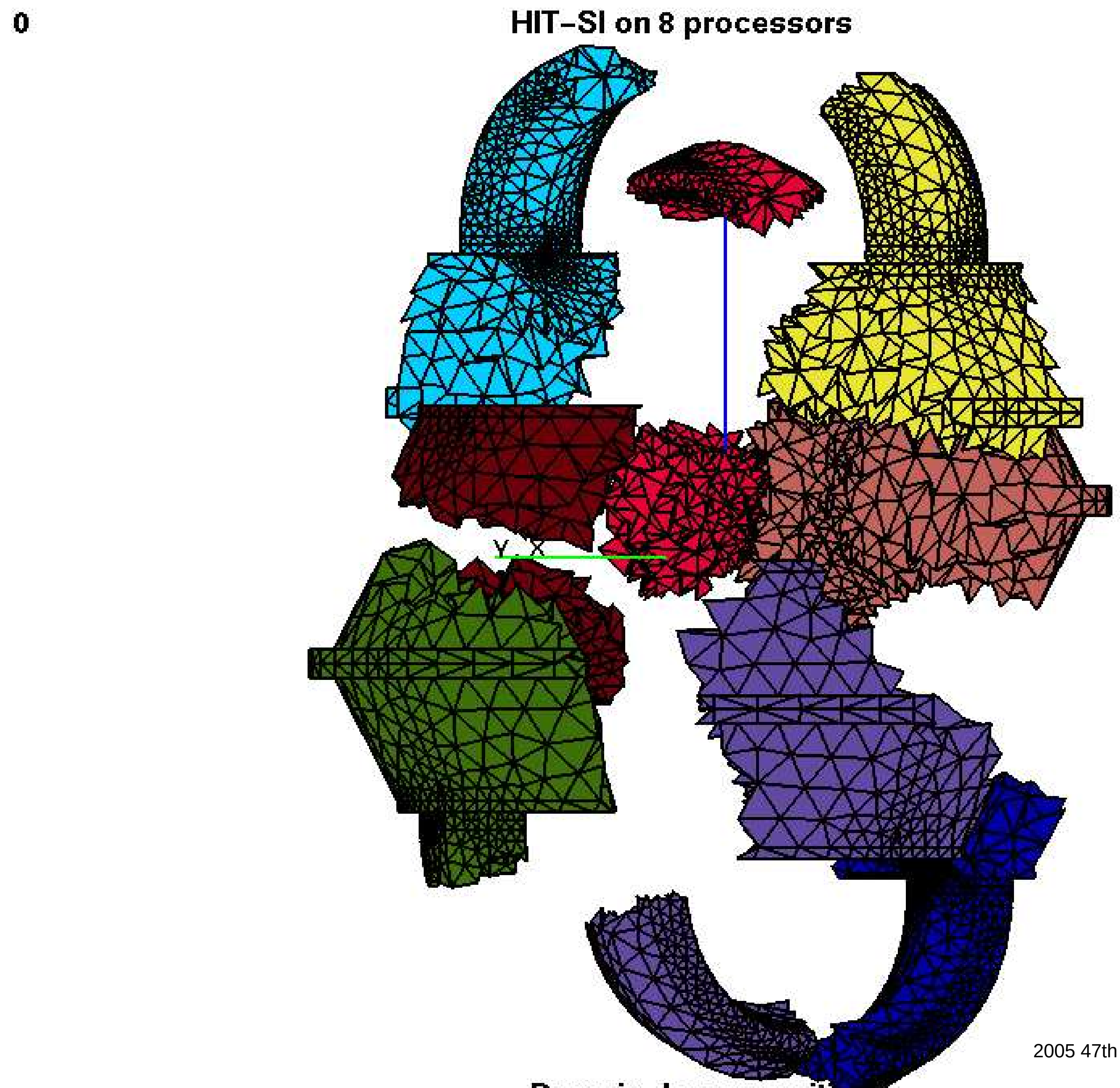
HIT-SI: y-z cut plane



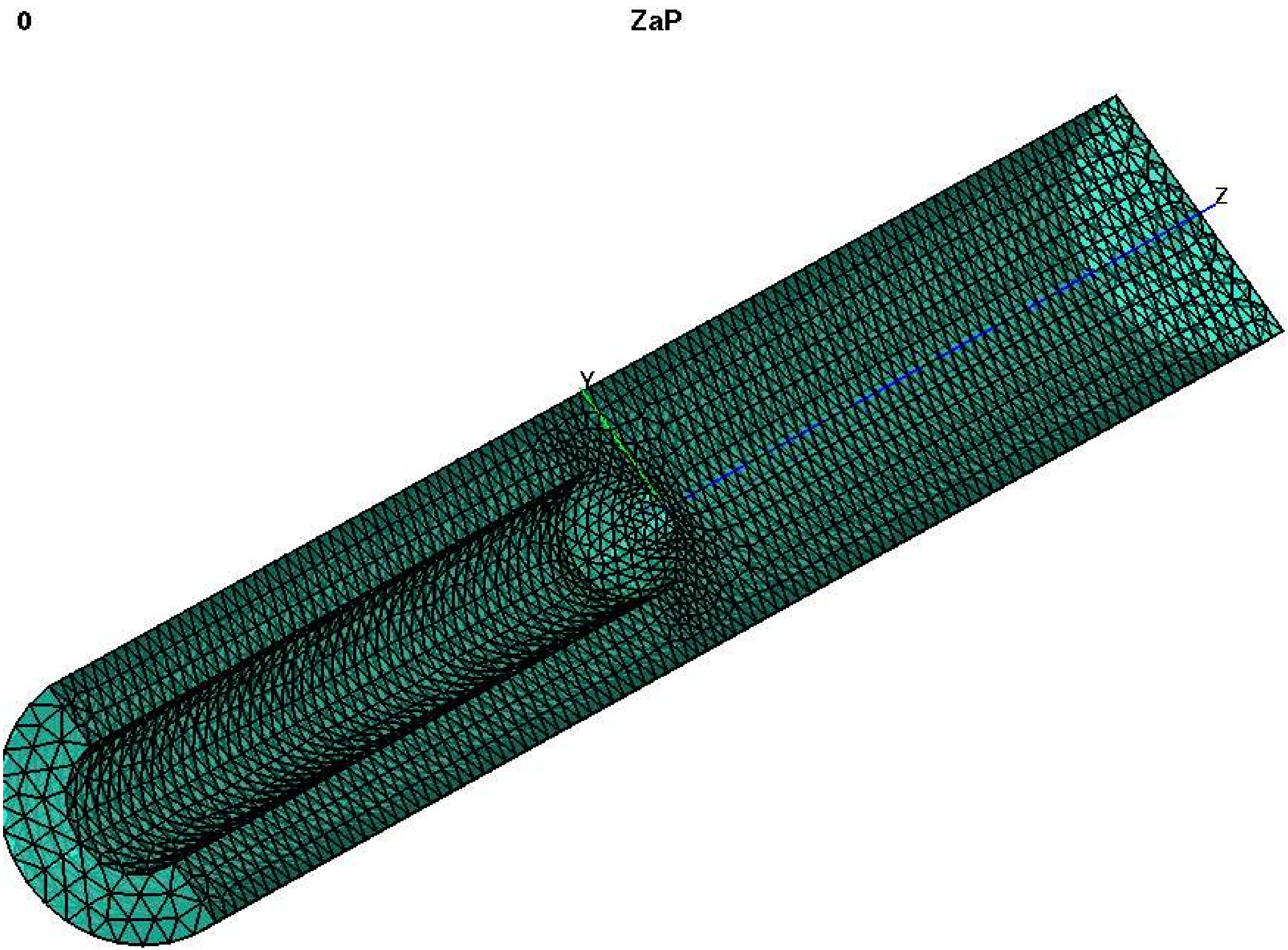
Domain decomposition



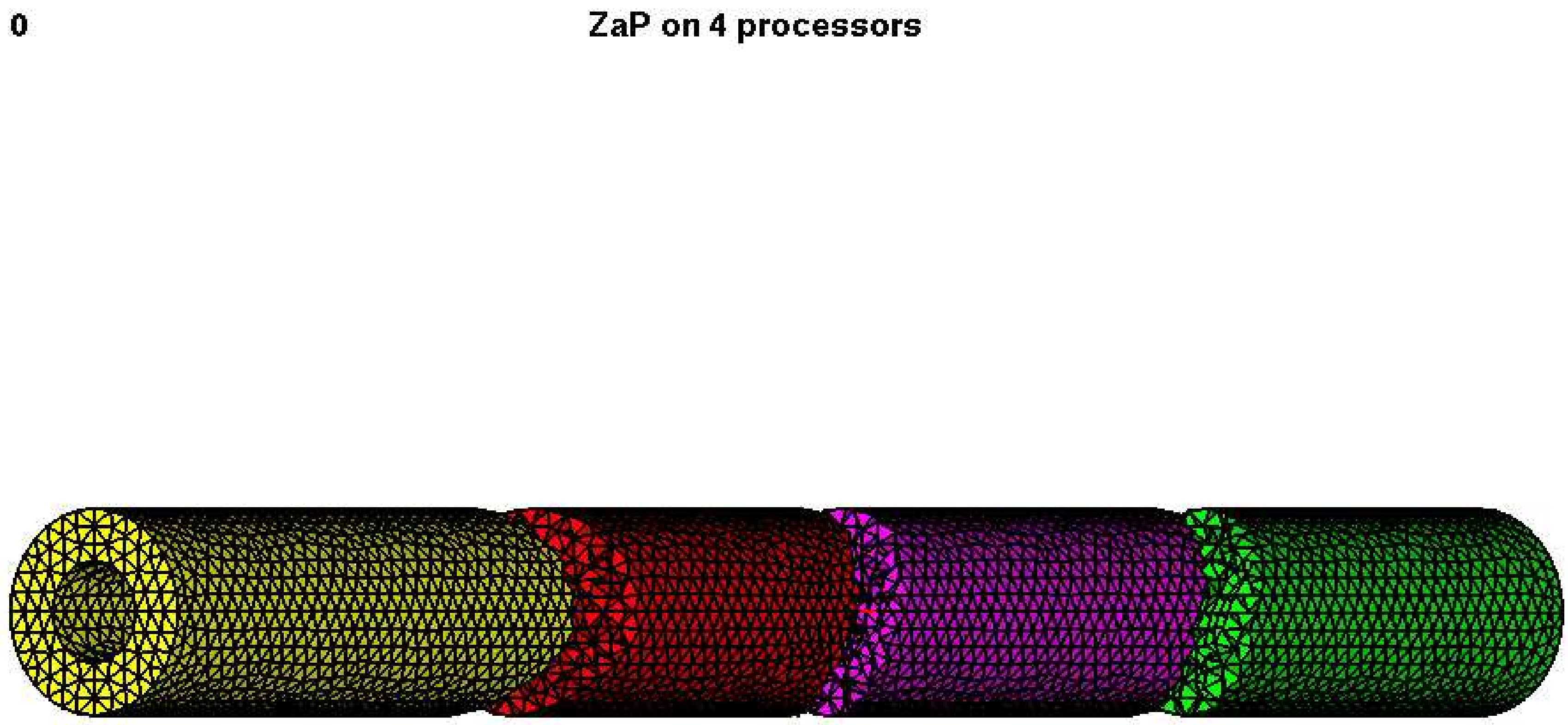
Domain decomposition



Tetrahedral mesh (1cm)



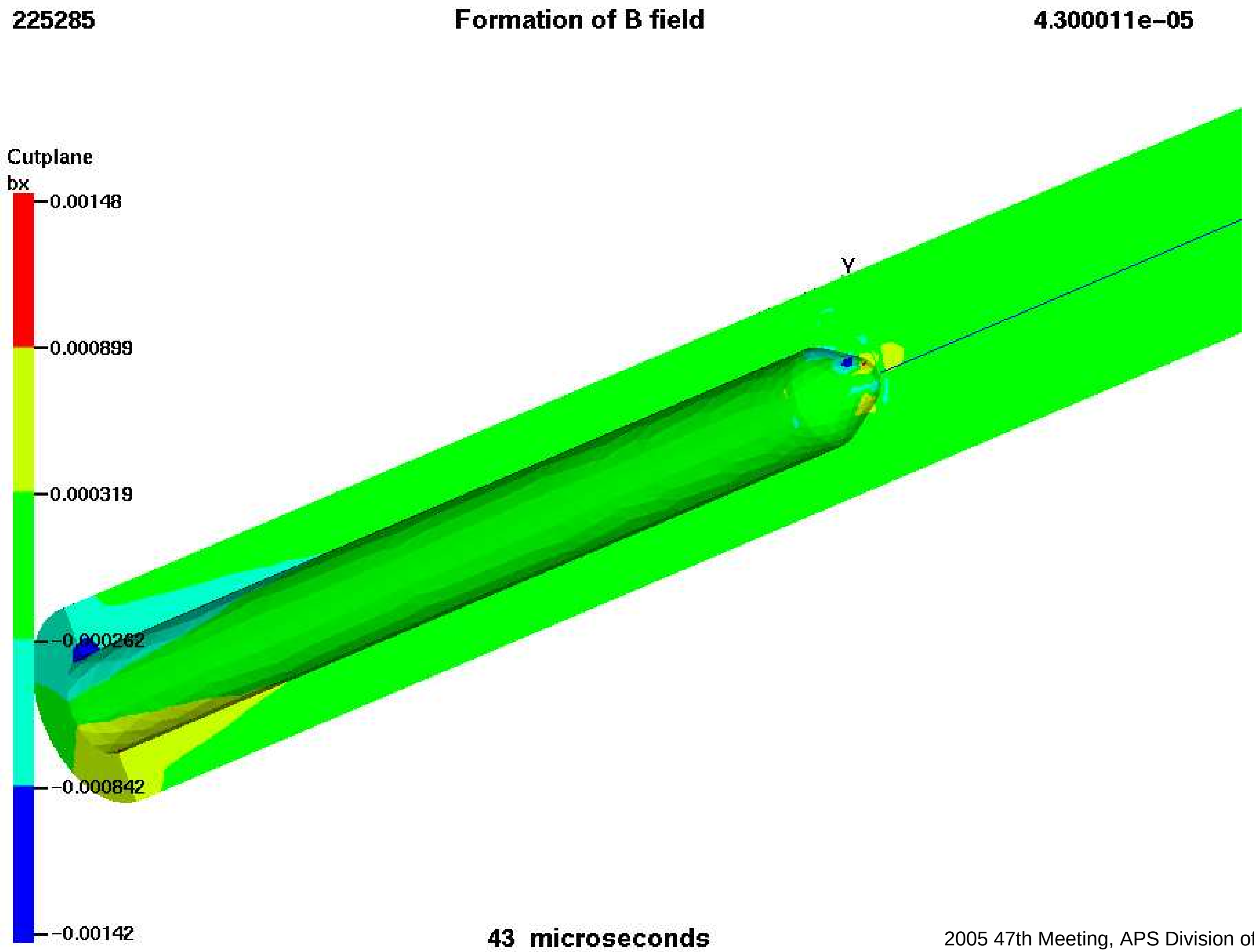
Domain decomposition



Simulation

$T = 10eV$, $n = 10^{-15}/cm^{-3}$

Applied $2kV$ from outer to inner electrode



MH4D computing

Tetrahedral mesh generation:

- T3D (Rypl, 2004)

Parallel implementations:

- MPI
- METIS (Karypis & Kumar, 1999) for domain decomposition
- PETSc (Baley et al., 2000) for preconditioned CG solver on unstructured grid

Visualization:

- General Mesh Viewer (GMV) (Ortega, 2000) for visualizing data on tetrahedral grid

Conclusion

The PSI-Center is refining the tetrahedral mesh MHD simulation code, MH4D, to model Innovative Confinement Concepts experiments.

Current refinement:

- GMV format
- vacuum fields

Current challenges:

- complicated boundary conditions
- neutral gas injection and ionization

Future challenges:

- regions of near zero density