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(U) A Rigorous Verification Strategy for a Continuum Plasma Code

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CCR Center for Computing Research

U.S. DEPARTMENT OF ENERGY

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Continuum plasma modeling

- Target application: Source Region Electromagnetic Pulse (SREMP)
  - At high altitudes (low density), PIC plasma modeling is ideal
  - At low to moderate altitude, atmospheric density is higher and continuum plasma modeling is more efficient
- Taking moments of the Boltzmann equation yields a general collisional multi-fluid plasma model with equations for each species α:

$$\frac{\partial \rho_\alpha}{\partial t} + \nabla \cdot (\rho_\alpha \mathbf{u}_\alpha) = \sum \Gamma^{\mathrm{src}}$$

$$\frac{\partial (\rho_\alpha \mathbf{u}_\alpha)}{\partial t} + \nabla \cdot (\rho_\alpha \mathbf{u}_\alpha \otimes \mathbf{u}_\alpha + p_\alpha I + \Pi_\alpha) = q_\alpha n_\alpha (\mathbf{E} + \mathbf{u}_\alpha \times \mathbf{B}) + \sum \mathbf{R}^{\mathrm{src}}$$

$$\frac{\partial \varepsilon_\alpha}{\partial t} + \nabla \cdot ((\varepsilon_\alpha + p_\alpha)\mathbf{u}_\alpha + \Pi_\alpha \cdot \mathbf{u}_\alpha + \mathbf{h}_\alpha) = q_\alpha n_\alpha \mathbf{u}_\alpha \cdot \mathbf{E} + \sum Q^{\mathrm{src}}$$

where Γ^{src}, $\mathbf{R}^{\mathrm{src}}$, and Q^{src} are source terms.
This system couples with Maxwell's equations for electromagnetics.

Verification roadmap

- Use linear plasma wave solutions for verification to build confidence in the code across a wide parameter space
  - Explore the linear regime of the relevant equations
  - Build a basis for confidence in nonlinear problems

Plasma Type	Equations	Status
Cold single-fluid	Electron continuity & momentum; Maxwell	Complete
Warm single-fluid	Electron continuity, momentum & energy; Maxwell	Complete
Cold collisional	Electron continuity & momentum w/source term; Maxwell	Planned
Warm two-fluid	Coupled electron & ion continuity, momentum & energy; Maxwell	Started

Simplified continuum plasma model

- The general collisional multi-fluid model is highly complex and challenging to analyze with source terms
- Start verification with a simplified ideal electron plasma:

$$\frac{\partial \rho_e}{\partial t} + \nabla \cdot (\rho_e \mathbf{u}_e) = 0$$

$$\frac{\partial (\rho_e \mathbf{u}_e)}{\partial t} + \nabla \cdot (\rho_e \mathbf{u}_e \otimes \mathbf{u}_e + p_e I) = \frac{q_e \rho_e}{m_e} (\mathbf{E} + \mathbf{u}_e \times \mathbf{B})$$

$$\frac{\partial \varepsilon_e}{\partial t} + \nabla \cdot (\varepsilon_e \mathbf{u}_e + p_e \mathbf{u}_e) = \frac{q_e \rho_e}{m_e} \mathbf{E} \cdot \mathbf{u}_e$$

$$\nabla \times \mathbf{B} = \mu_0 \frac{q_e}{m_e} \rho_e \mathbf{u}_e + \frac{1}{c^2} \frac{\partial \mathbf{E}}{\partial t} \qquad \nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$$

$$\nabla \cdot \mathbf{B} = 0 \qquad \nabla \cdot \mathbf{E} = \frac{q_e}{\epsilon_0} (\rho_e / m_e - n_0)$$

  - This is a set of nonlinear dispersive hyperbolic equations in 11 unknowns (3D), and looks like the Euler equations with a coupling to Maxwell's equations through the Lorentz force term.

Linear single-fluid waves

- Perturbation analysis: simplify and linearize the system
  - Cold plasma case with zero temperature (no energy equation)
  - Warm plasma case with finite temperature and ideal gas law
  - Quasi-neutral by implied static ion species
- Static equilibrium state:

$$\rho_e^0,\ \mathbf{B}_0,\ [p_e^0]$$

- Small perturbation δ from reference state:
  - Nonlinear terms are dropped [$O(\delta^2)$]
  - Fluid velocity small compared to phase velocity
- Solve as pseudo-1D periodic problem with wave vector **k** defined in the x-direction
- Yields a set of solutions described by an oscillation frequency and a wavenumber

$$\begin{aligned}
\rho_e &= \rho_e^0 + \bar{\rho}_e e^{i(k_x x - \omega t)} \\
u_x^e &= \bar{u}_x^e e^{i(k_x x - \omega t)} \\
u_y^e &= \bar{u}_y^e e^{i(k_x x - \omega t)} \\
u_z^e &= \bar{u}_z^e e^{i(k_x x - \omega t)} \\
p_e &= p_e^0 + \bar{p}_e e^{i(k_x x - \omega t)} \\
E_x &= \bar{E}_x e^{i(k_x x - \omega t)} \\
E_y &= \bar{E}_y e^{i(k_x x - \omega t)} \\
E_z &= \bar{E}_z e^{i(k_x x - \omega t)} \\
B_x &= B_x^0 \\
B_y &= B_y^0 + \bar{B}_y e^{i(k_x x - \omega t)} \\
B_z &= B_z^0 + \bar{B}_z e^{i(k_x x - \omega t)}
\end{aligned}$$

Solving for dispersion relations

- Functions that relate oscillation frequencies to wavenumber
  - Derived by substituting the perturbed solution form into the plasma system and solving the momentum equations to yield a matrix determinant problem
  - Roots of the determinant equation define the wave solutions
- Three groups of solutions exist:
  - Longitudinal waves: Electrostatic pressure/density waves
  - Transverse waves: Electromagnetic waves
  - Hybrid waves: Electromagnetic waves coupled to electrostatic waves
- Depend on fundamental plasma frequencies and length scales:
  - Plasma frequency: $\omega_{pe} = \sqrt{\frac{q_e^2 n_0}{\epsilon_0 m_e}}$
  - Cyclotron frequency: $\omega_{ce} = \frac{q_e B_0}{m_e}$ (a function of background B field)
  - Debye length: $\lambda_{De} = \sqrt{\frac{\epsilon_0 k_B T}{n_0 q_e^2}}$ and skin depth: $d_e = c/\omega_{pe}$

Example: zero B_0 field

- Simplifies the determinant to yield the dispersion relations:

$$\underbrace{\left(\frac{\omega^2}{\omega_{pe}^2} - \gamma\lambda_{De}k_x^2 - 1\right)}_{\text{LEP}}\underbrace{\left(\frac{\omega^2}{\omega_{pe}^2} - d_e k_x^2 - 1\right)^2}_{\text{TEM}} = 0$$

- Frequencies that satisfy the LEP or TEM terms are valid linear waves
- Select a wavenumber and solve for frequency to derive solutions:
  - Choose a sinusoidal perturbation and turn the crank…

$$\rho_e = m_e n_0 \left(1 + \delta \sin\left(k_x x - \omega t\right)\right)$$

  - Electric field can then be derived assuming a neutralizing background ion field

$$E_x = \delta \frac{n_0 q_e}{k_x \epsilon_0} \cos(k_x x - \omega t)$$

  - The remaining fields are similarly derived

Longitudinal electron plasma wave

- Cold LEP wave is an oscillation at the plasma frequency
- Electrostatic coupling between electrons and static background ions
- Magnetization along direction of propagation has no effect on electrostatic interaction (i.e., same wave when $\mathbf{B}_0 = 0$ and $\mathbf{B}_0 \parallel \mathbf{k}$)

Dispersion Relation

$$\frac{\omega^2}{\omega_{pe}^2} = 1 + \gamma k_x^2 \lambda_{De}^2$$

Analytical Solution

$$\rho_e = m_e n_0 (1 + \delta \sin(k_x x - \omega t)$$

$$u_x^e = \delta \frac{\omega}{k_x} \sin(k_x x - \omega t)$$

$$u_y^e = 0$$

$$u_z^e = 0$$

$$p_e = p_0 \left(1 + \gamma \delta \sin(k_x x - \omega t)\right)$$

$$E_x = \delta \frac{q_e n_0}{\epsilon_0 k_x} \cos(k_x x - \omega t)$$

$$E_y = 0$$

$$E_z = 0$$

$$B_x = B_0$$

$$B_y = 0$$

$$B_z = 0$$

Transverse electromagnetic waves

- TEM waves are oscillations normal to the wave vector
- Independent of temperature
- A coupled electromagnetic wave driving an electron current in the transverse direction
- The magnetized version with background field pointing along the current drive is the linearly polarized ordinary wave (O-wave), with the same dispersion relation

Dispersion Relation

$$\frac{\omega^2}{\omega_{pe}^2} = 1 + d_e^2 k_x^2$$

Analytical Solution

$$\rho_e = m_e n_0$$
$$u_x^e = 0$$
$$u_y^e = -\delta \frac{q_e}{m_e \omega} \cos(k_x x - \omega t)$$
$$u_z^e = 0$$
$$p_e = p_0$$
$$E_x = 0$$
$$E_y = \delta \sin(k_x x - \omega t)$$
$$E_z = 0$$
$$B_x = 0$$
$$B_y = B_0$$
$$B_z = \delta \frac{k_x}{\omega} \sin(k_x x - \omega t)$$

TEM circularly polarized waves

- Circularly polarized TEM when background B-field is parallel to the wave

LCP Dispersion Relation

$$\frac{\omega^2}{\omega_{pe}^2} = \frac{1}{1 + \omega_{ce}/\omega} + d_e^2 k_x^2$$

RCP Dispersion Relation

$$\frac{\omega^2}{\omega_{pe}^2} = \frac{1}{1 - \omega_{ce}/\omega} + d_e^2 k_x^2$$

Note: RCP has upper & lower branches

Analytical Solution

$$\rho_e = m_e n_0$$

$$u_x^e = 0$$

$$u_y^e = -\delta \frac{q_e}{m_e \omega} \left(\frac{\omega^2}{\omega_{pe}^2} - d_e^2 k_x^2 \right) \cos(k_x x - \omega t)$$

$$u_z^e = \delta \frac{q_e}{m_e \omega_{ce}} \left(\frac{\omega^2}{\omega_{pe}^2} - d_e^2 k_x^2 - 1 \right) \sin(k_x x - \omega t)$$

$$p_e = p_0$$

$$E_x = 0$$

$$E_y = \delta \sin(k_x x - \omega t)$$

$$E_z = \delta \frac{\omega}{\omega_{ce}} \frac{\left(\frac{\omega^2}{\omega_{pe}^2} - d_e^2 k_x^2 - 1 \right)}{\left(\frac{\omega^2}{\omega_{pe}^2} - d_e^2 k_x^2 \right)} \cos(k_x x - \omega t)$$

$$B_x = B_0$$

$$B_y = -\delta \frac{k_x}{\omega_{ce}} \frac{\left(\frac{\omega^2}{\omega_{pe}^2} - d_e^2 k_x^2 - 1 \right)}{\left(\frac{\omega^2}{\omega_{pe}^2} - d_e^2 k_x^2 \right)} \cos(k_x x - \omega t)$$

$$B_z = \delta \frac{k_x}{\omega} \sin(k_x x - \omega t)$$

TEM extraordinary (X) wave

- Extraordinary TEM wave when background B-field is normal to the wave

Dispersion Relation

$$\left(\frac{\omega^2}{\omega_{pe}^2} - \gamma\lambda_{De}^2 k_x^2 - 1\right)\left(\frac{\omega^2}{\omega_{pe}^2} - d_e^2 k_x^2 - 1\right) = \frac{(\omega_{ce}^y)^2}{\omega^2}\frac{\omega^2}{\omega_{pe}^2}\left(\frac{\omega^2}{\omega_{pe}^2} - d_e^2 k_x^2\right)$$

Note: X has upper & lower branches

Analytical Solution

$$\rho_e = m_e n_0 \left(1 + \delta \sin(k_x x - \omega t)\right)$$

$$u_x^e = \delta \frac{\omega}{k_x} \sin(k_x x - \omega t)$$

$$u_y^e = 0$$

$$u_z^e = -\delta \frac{\omega}{k_x} \frac{\omega_{pe}^2}{\omega \omega_{ce}} A_0 \cos(k_x x - \omega t)$$

$$p_e = p_0 \left(1 + \gamma\delta \sin(k_x x - \omega t)\right)$$

$$A_0 = \left(\frac{\omega^2}{\omega_{pe}^2} - \gamma\lambda_{De}^2 k_x^2 - 1\right)$$

$$A_1 = \left(\frac{\omega^2}{\omega_{pe}^2} - d_e^2 k_x^2\right)$$

$$E_x = \delta \frac{q_e n_0}{\epsilon_0 k_x} \cos(k_x x - \omega t)$$

$$E_y = 0$$

$$E_z = \delta \frac{\omega}{k_x} B_0 \frac{\omega_{pe}^2}{\omega_{ce}^2} \frac{A_0}{A_1} \sin(k_x x - \omega t)$$

$$B_x = 0$$

$$B_y = B_0 \left(1 - \delta \frac{\omega}{k_x} \frac{\omega_{pe}^2}{\omega_{ce}^2} \frac{A_0}{A_1} \sin(k_x x - \omega t)\right)$$

$$B_z = 0$$

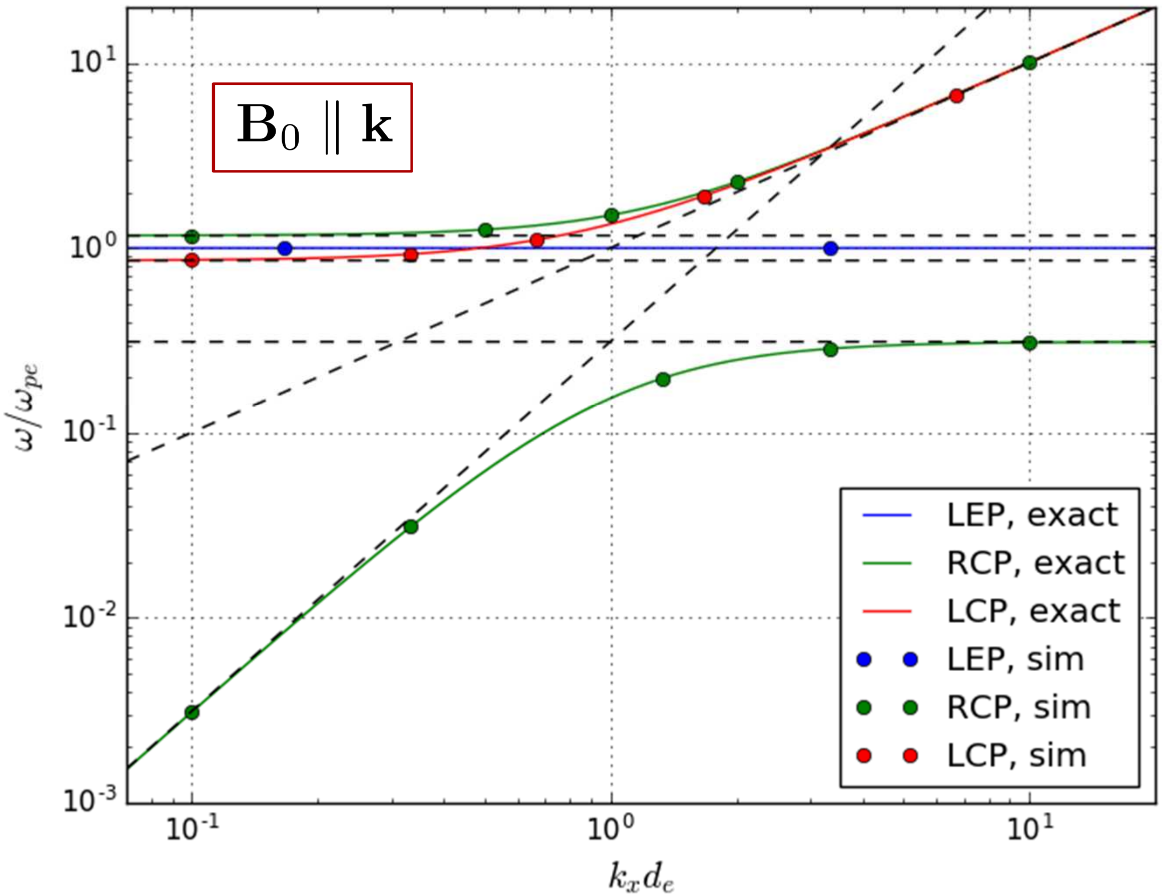
Note that background magnetic field is perpendicular to the current drive here

Numerical solution

- EMPIRE/Drekar:
  - Compatible second-order FEM discretization of the plasma system
  - Coupled monolithic implicit or explicit time integration (see J. Shadid's talk)
  - Sophisticated physics-based block preconditioners (see E. Phillips' poster)
- Verification tests:
  - Examine long-time solution behavior: matching the dispersion relation and checking convergence to expected wave frequency
  - Convergence to the analytic wave solution with mesh refinement
- Implementation observations:
  - Variable scaling is helpful when handling huge variations in magnitudes (can span $O(10^{-15})$ to $O(10^{5})$ in the same simulation)
  - Setting appropriate linear and nonlinear solver tolerances is essential for achieving solution stability and convergence

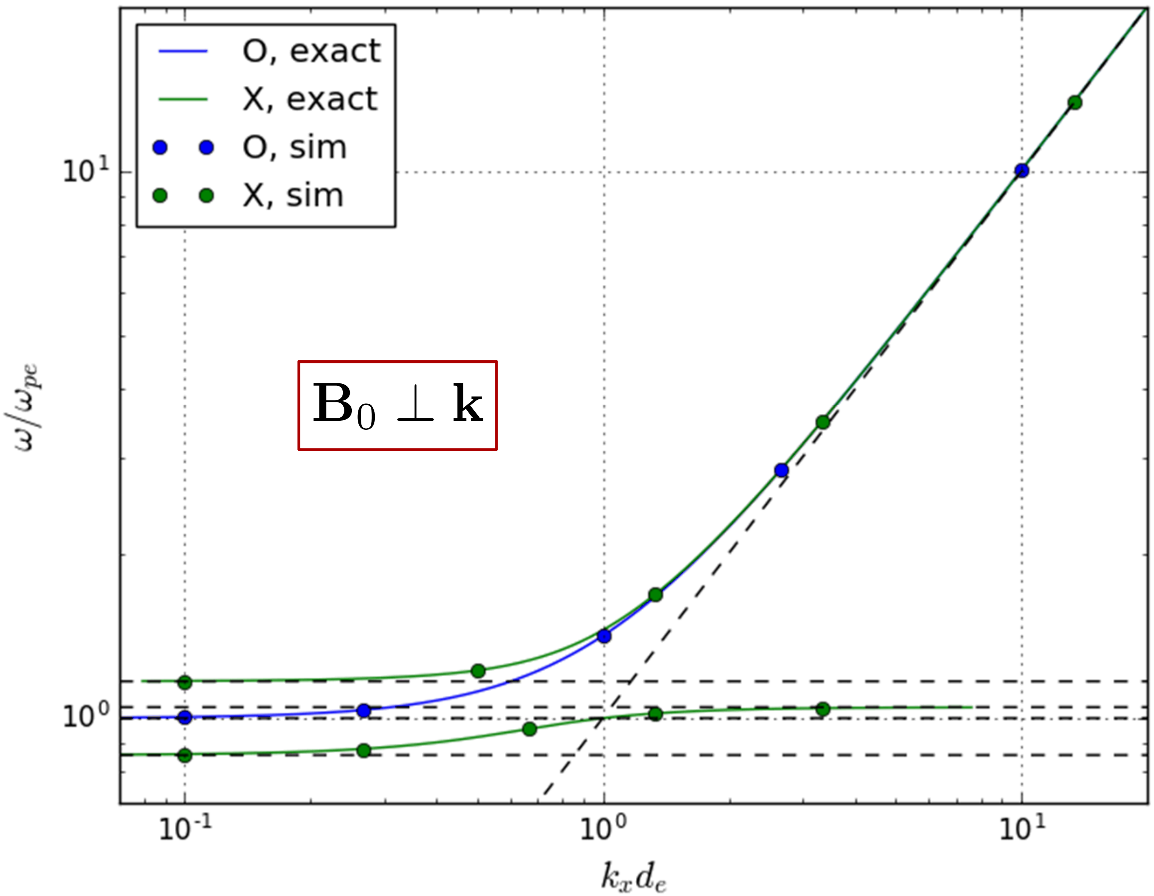
Cold plasma dispersion relations

- Dispersion relations for waves aligned with the magnetic field



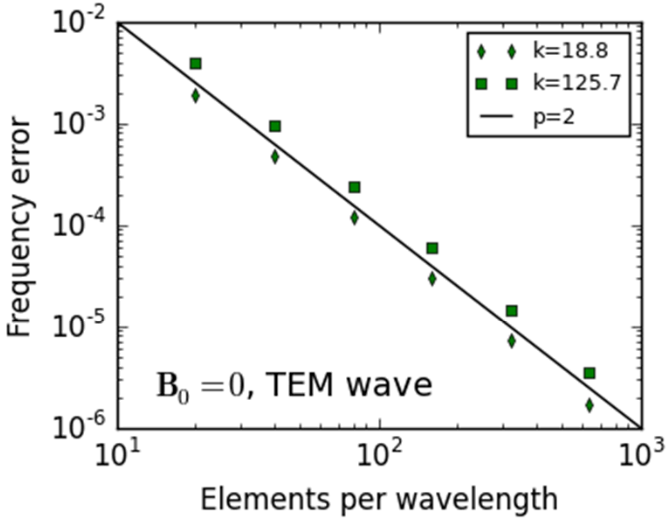
Cold plasma dispersion relations

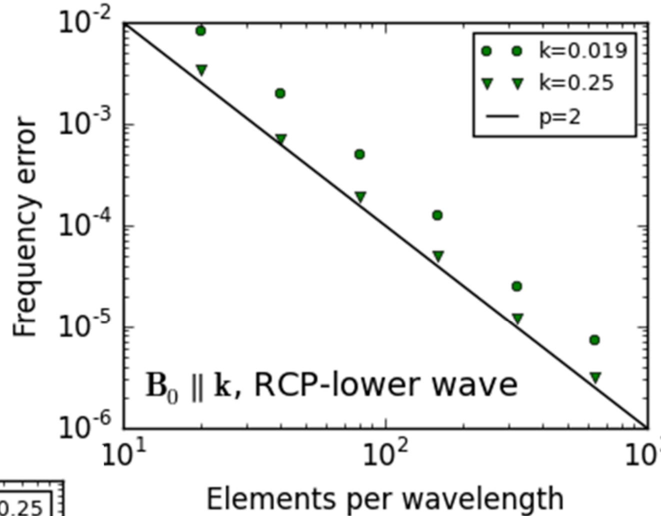
- Dispersion relations for waves normal to the magnetic field

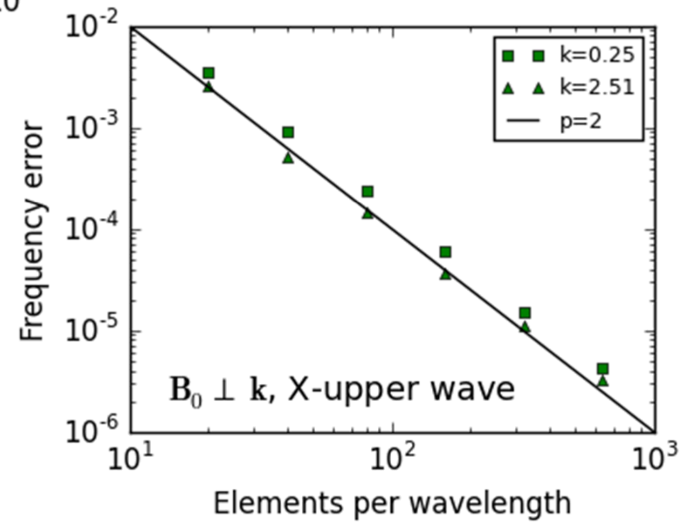


Cold plasma convergence

- Convergence to analytic frequency: verifies long-time behavior (over many cycles), but less sensitive to phase errors

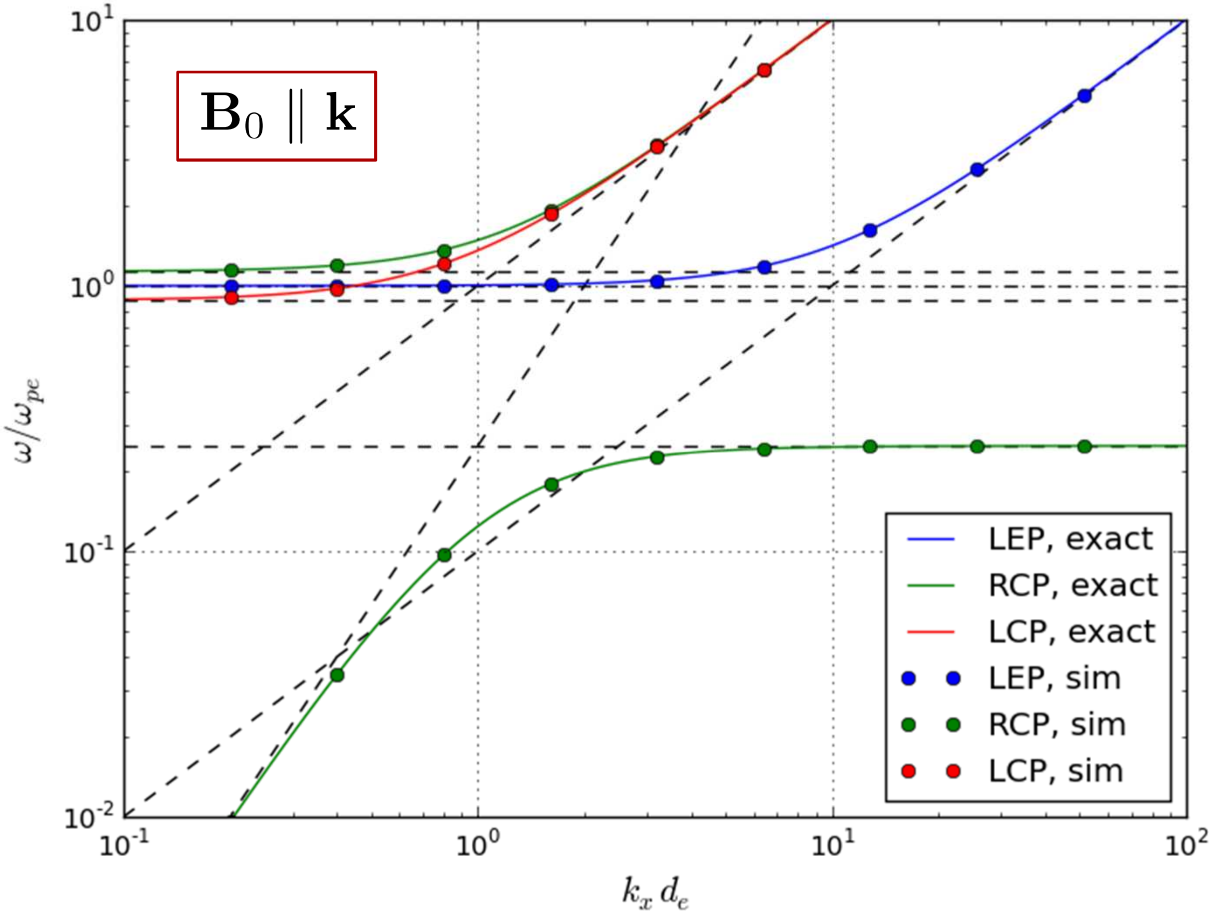






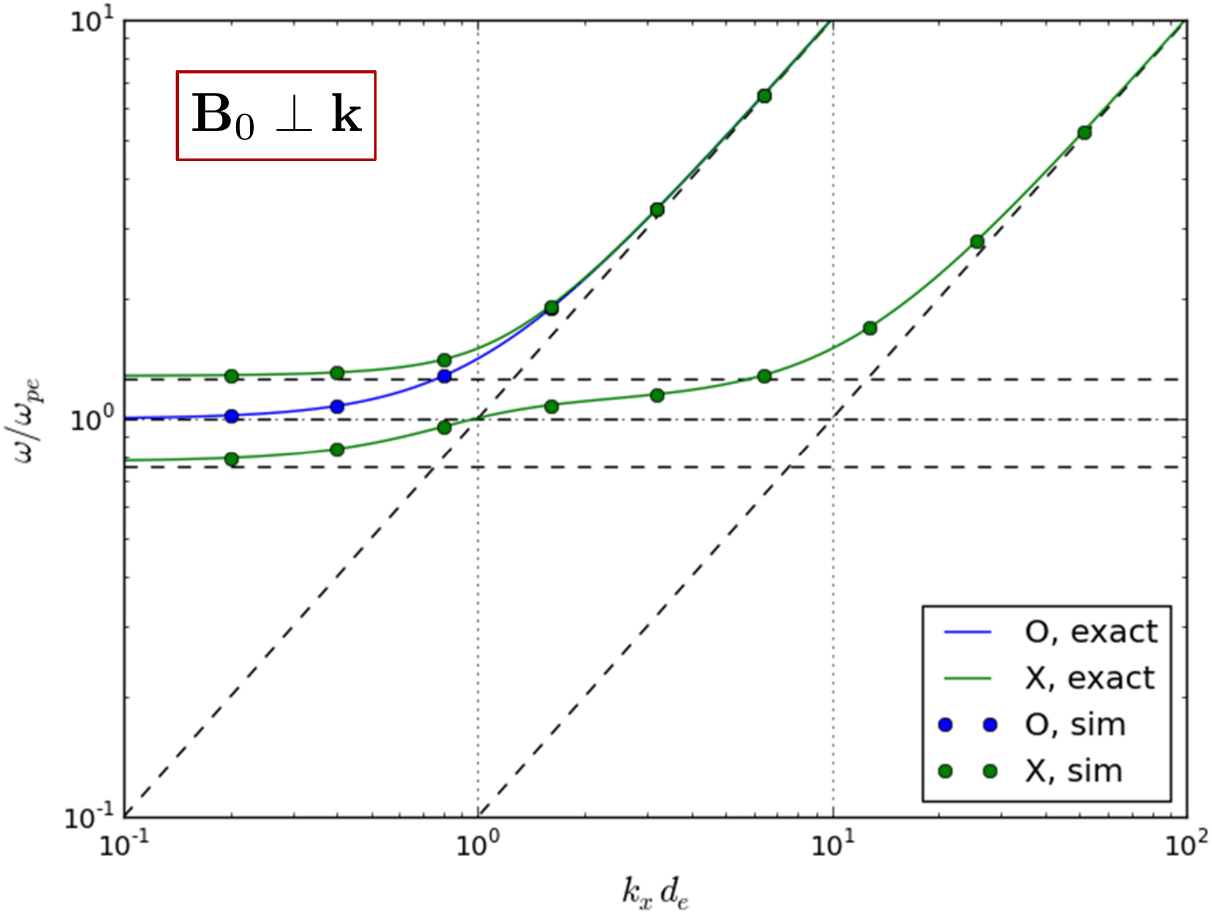
Warm plasma dispersion relations

- Dispersion relations for waves aligned with the magnetic field



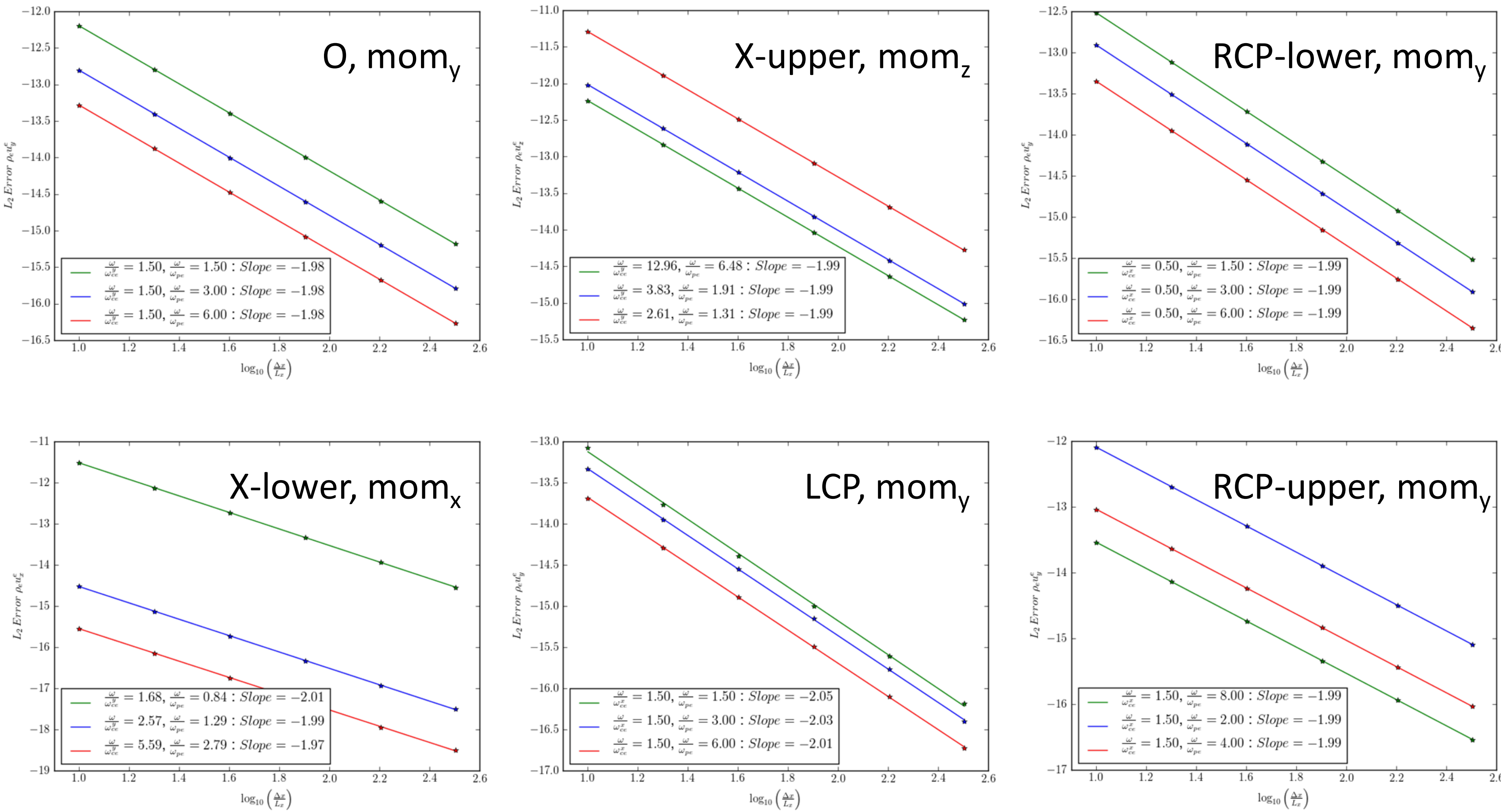
Warm plasma dispersion relations

- Dispersion relations for waves normal to the magnetic field



Warm plasma convergence

- Second-order L_2 convergence to the analytic sinusoidal solution



Cold collisional waves

- Add simple collision term for drag from a stationary neutral species:

$$\frac{\partial(\rho_e \mathbf{u}_e)}{\partial t} + \nabla \cdot (\rho_e \mathbf{u}_e \otimes \mathbf{u}_e) = \frac{q_e \rho_e}{m_e}(\mathbf{E} + \mathbf{u}_e \times \mathbf{B}) - \rho_e \mathbf{u}_e \nu_{en}$$

- Give waves dissipative character with increasing collision frequency due to appearance of an imaginary term in the dispersion relation:
  - LEP relation:

$$\omega = \sqrt{\omega_{pe}^2 - (\nu_{en}/2)^2} - i\nu_{en}/2$$

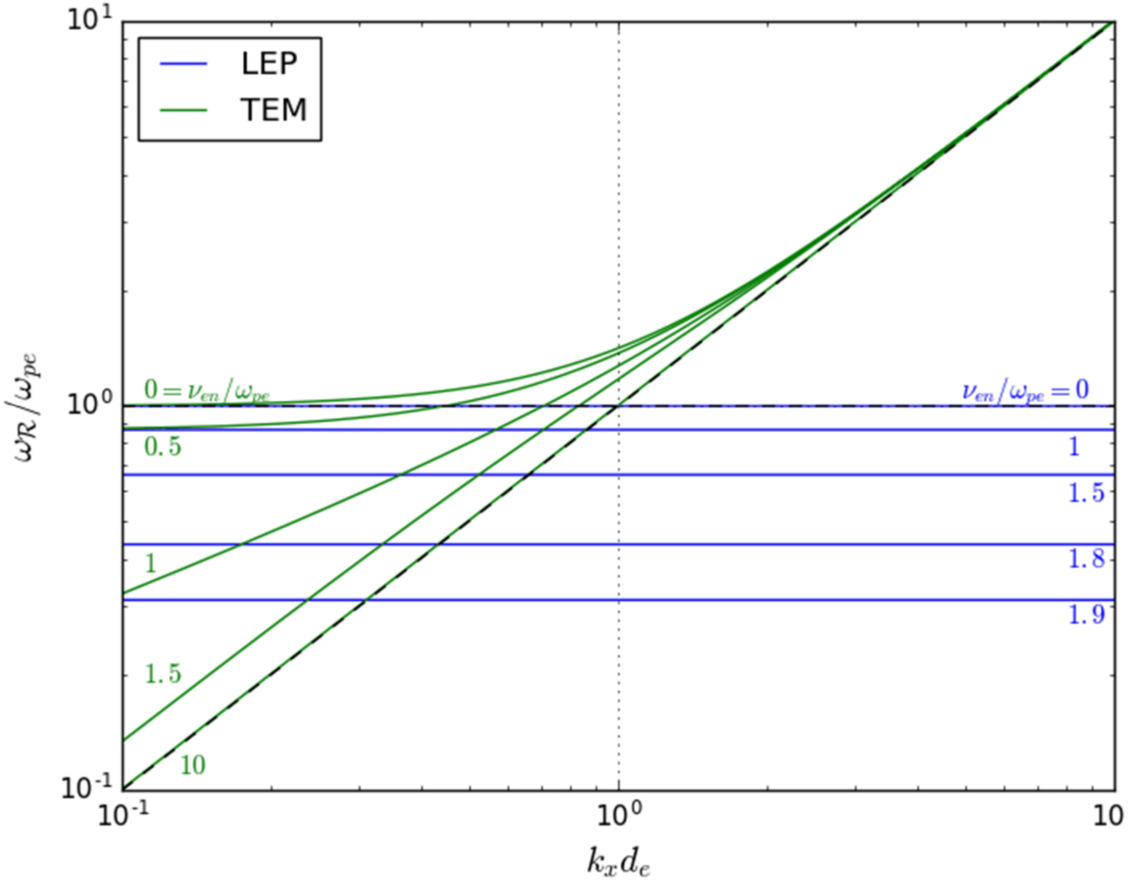
  - TEM relation:

$$c^2 k^2 = \omega^2 - \frac{\omega_{pe}^2}{1 + (\nu_{en}/\omega)^2} + i\frac{\omega_{pe}^2(\nu_{en}/\omega)}{1 + (\nu_{en}/\omega)^2}$$

  - Damping effect is controlled by the ratio of collision frequency to the plasma frequency

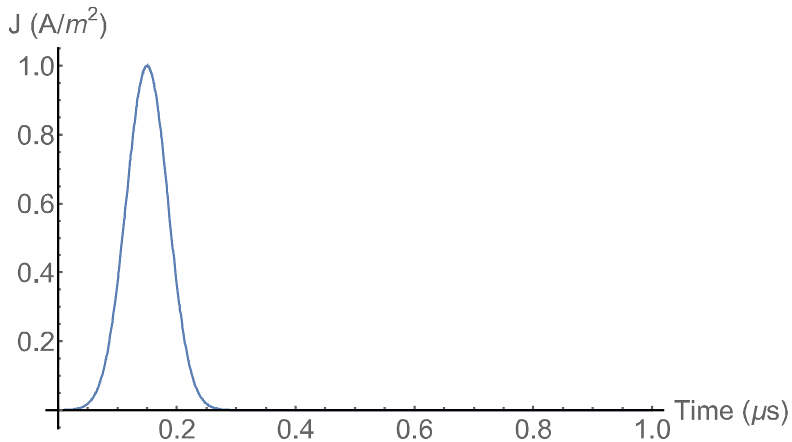
Collisional waves

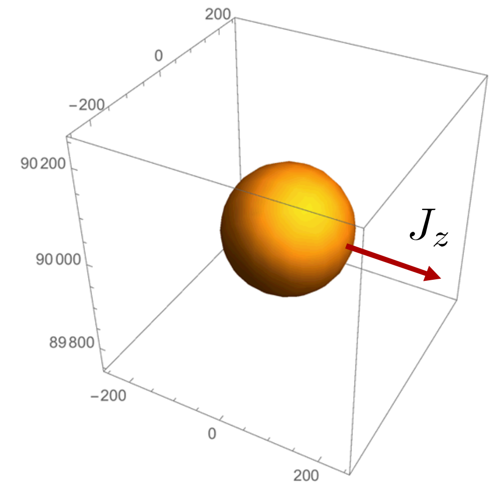
- Dispersion relation for a range of damping factors ν_{en}/ω_{pe}



Towards an SREMP simulation

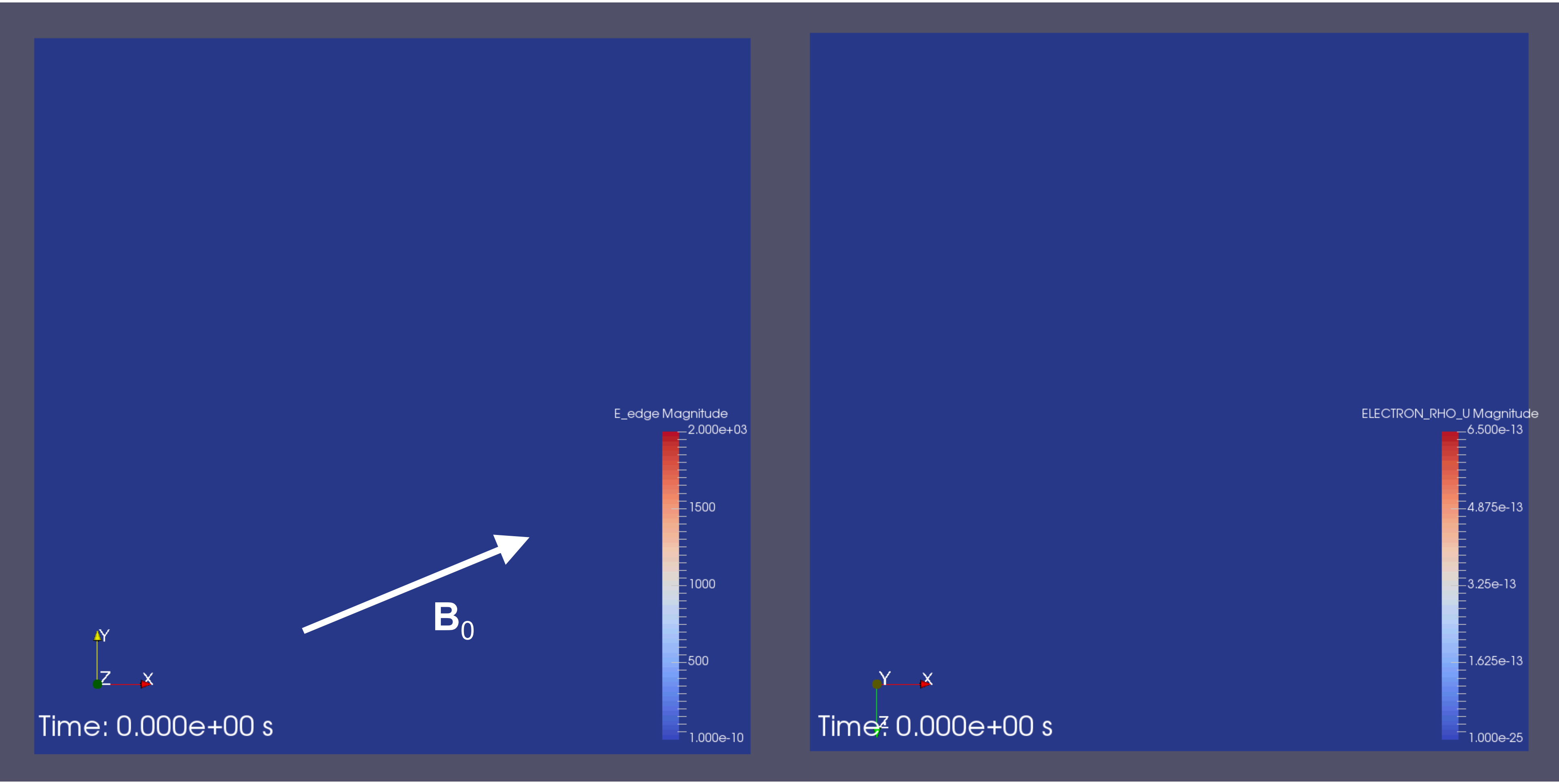
- A plasma wave system driven by an external current source
  - Gaussian profile in time and spherically distributed in space





  - Peak magnitude of 1 A/m^2
  - Source located at altitude of 90 km in a nominal atmosphere with quadratic variation in background electron density
  - Background magnetic field of 3×10^{-5} T at 22.5^o to the ground plane
  - 3D domain is a cube with 4 km sides, resolved to 50 m
  - Solved as a cold electron plasma (no energy equation)

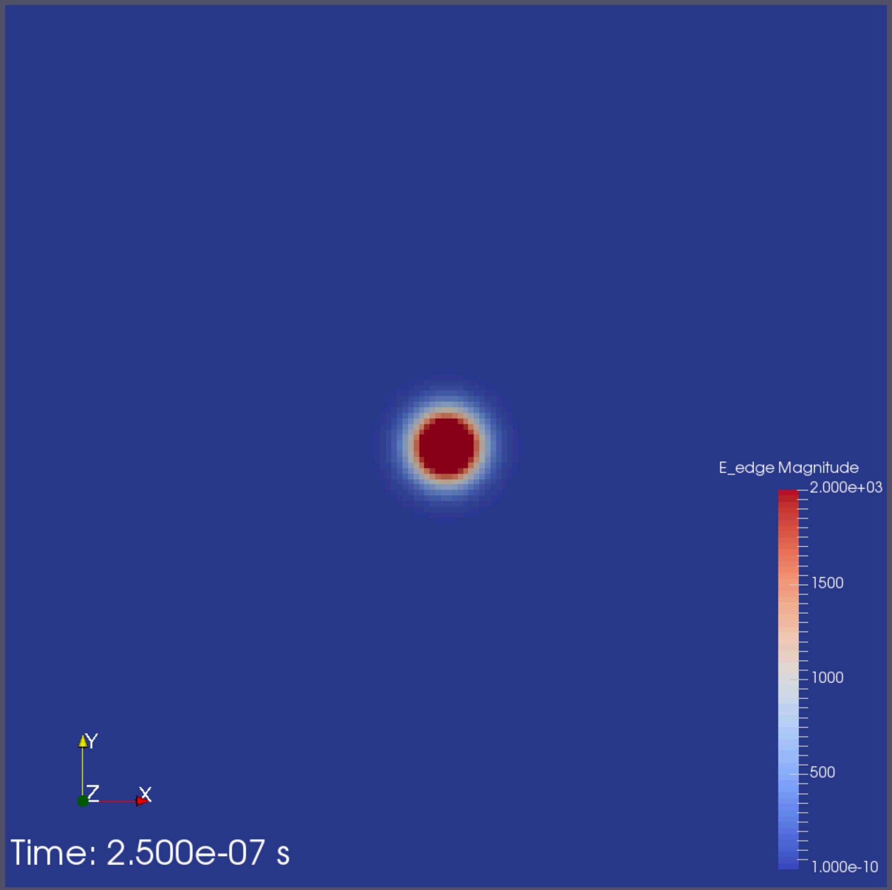
3D wave generator simulation

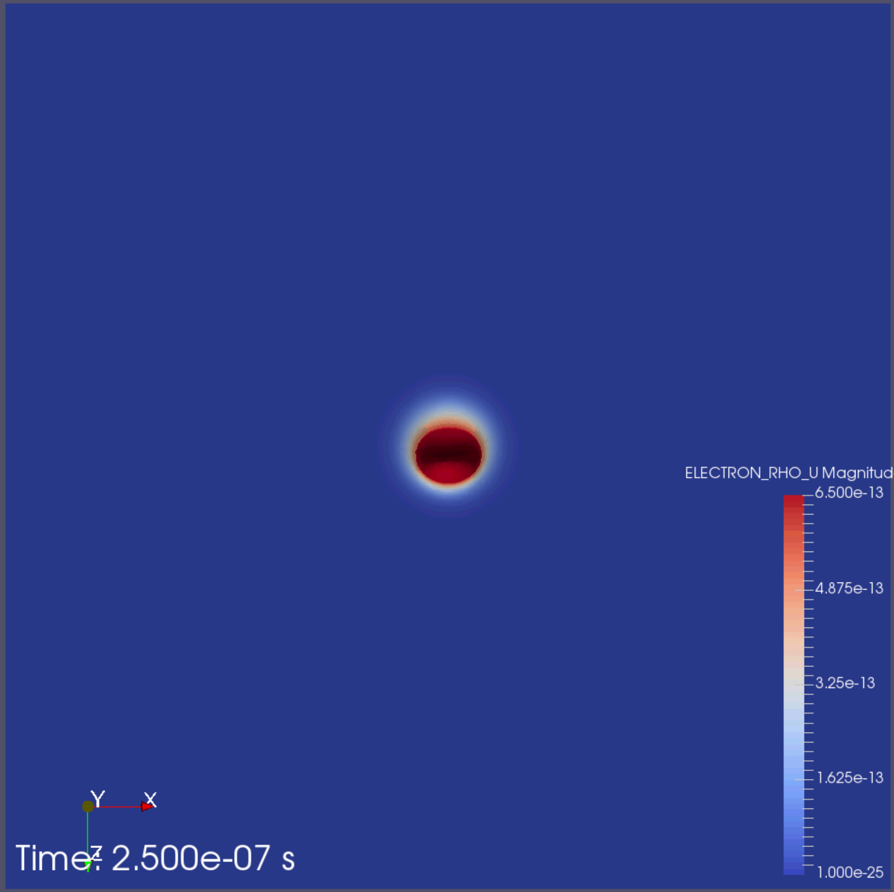


Electric field magnitude
Contours through altitude

Electron momentum magnitude
Projected onto $n_e = 3.5{\times}10^{10}$ contour
(approx. 90 km altitude plane)

3D wave generator simulation





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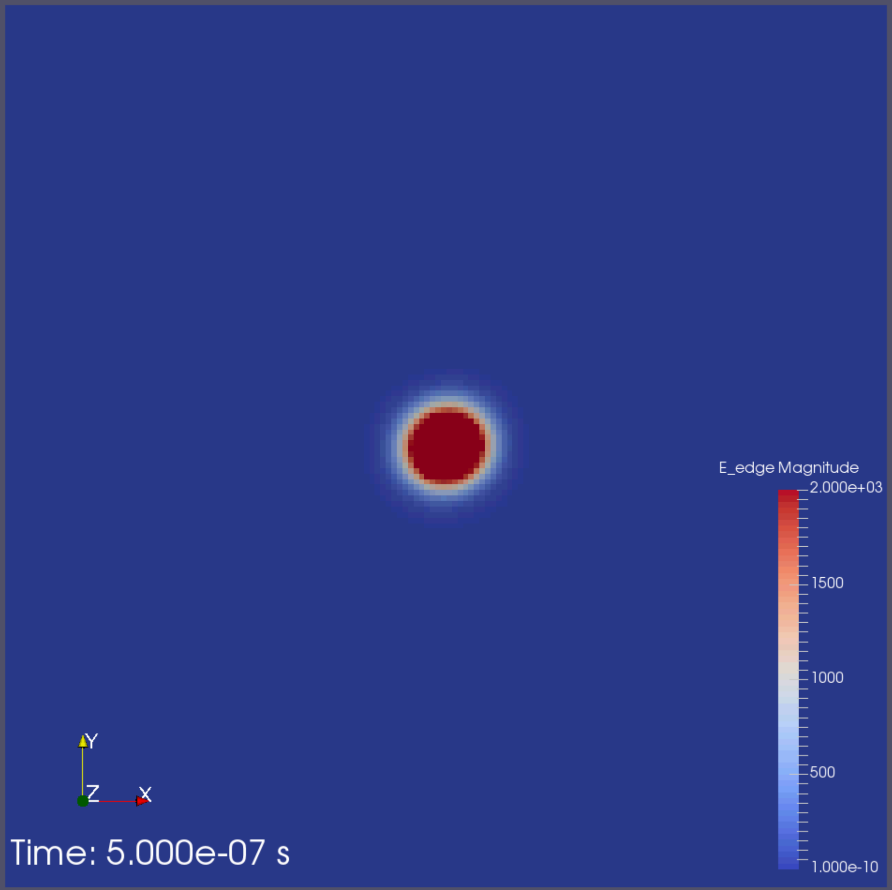

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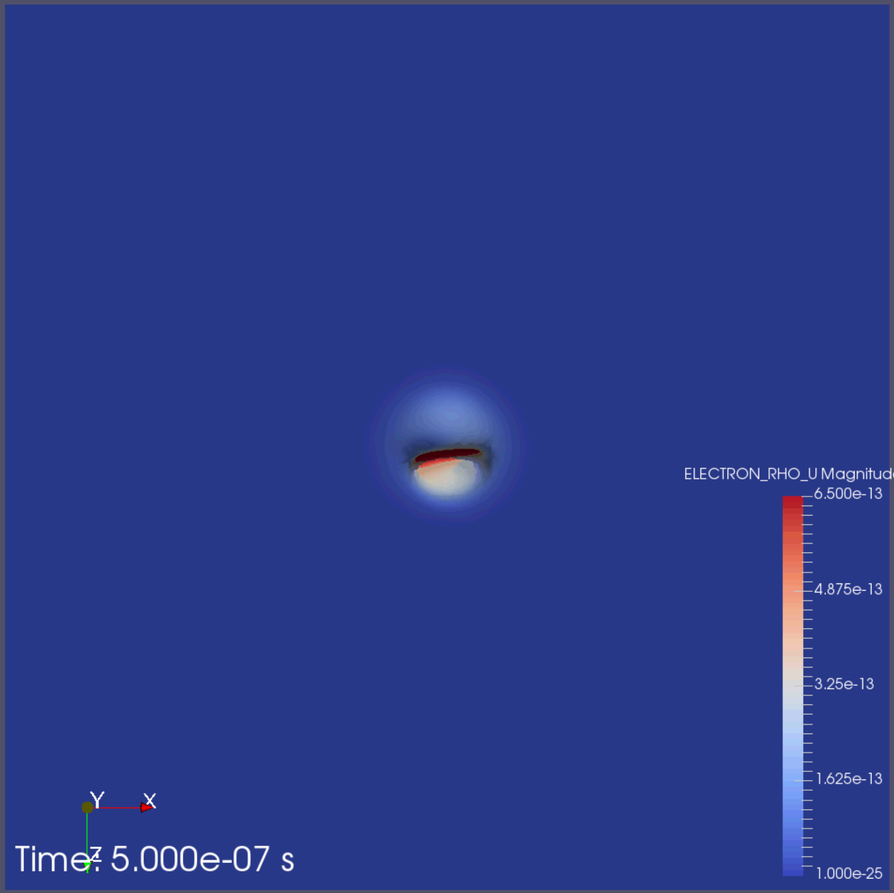

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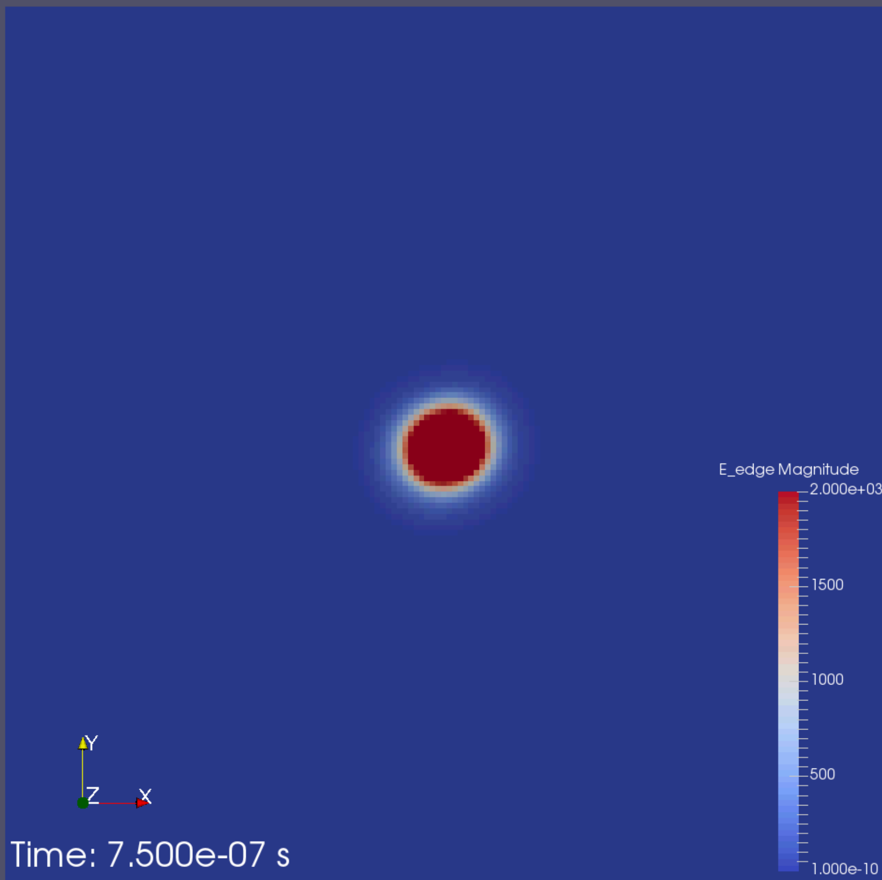

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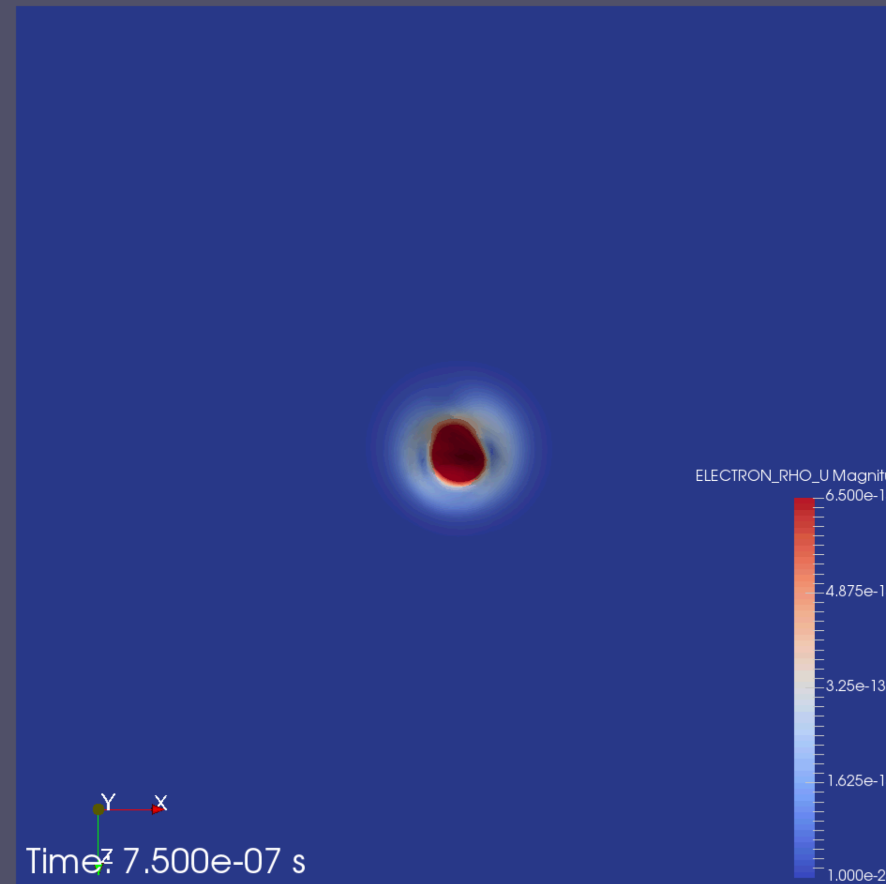

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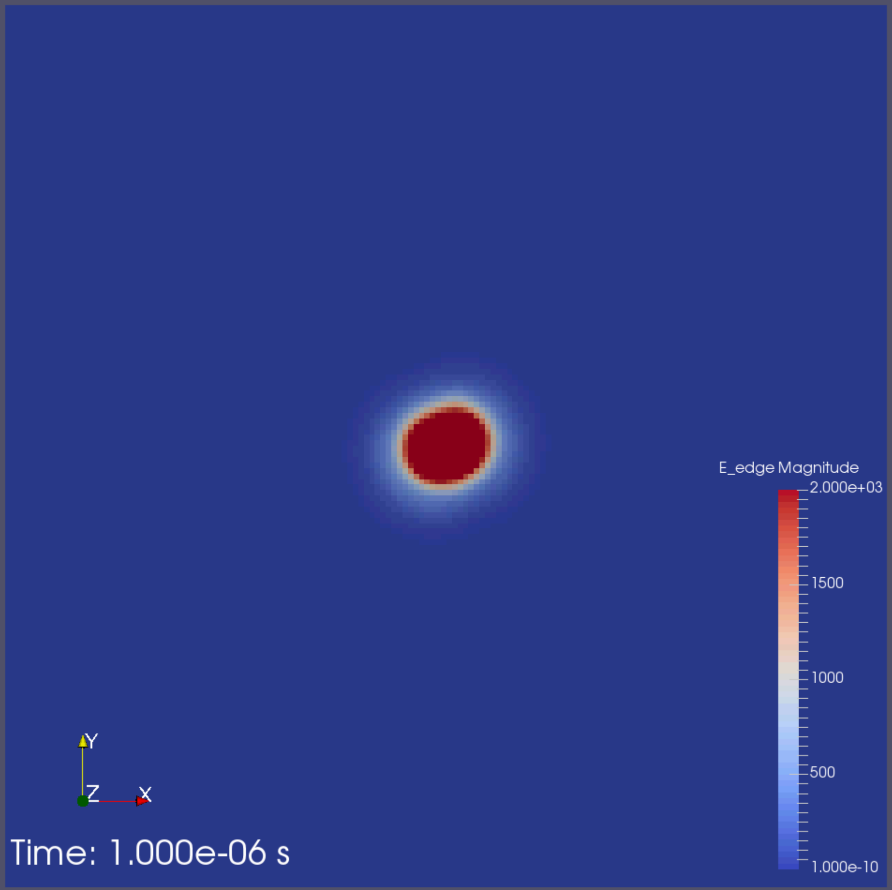

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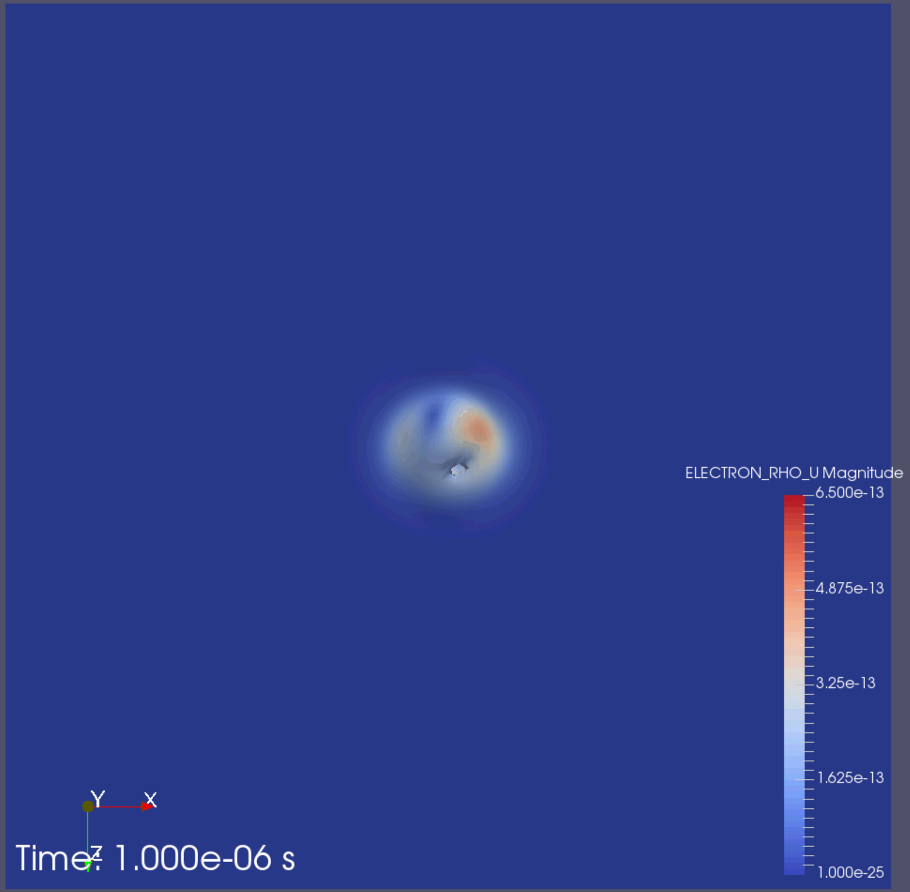

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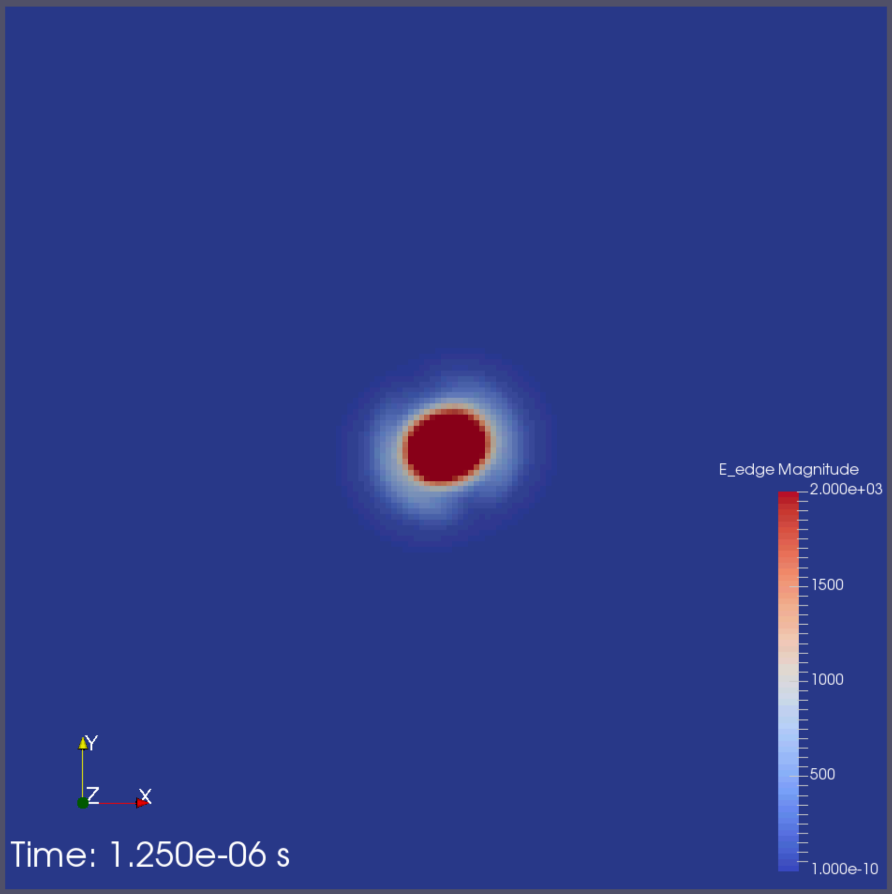

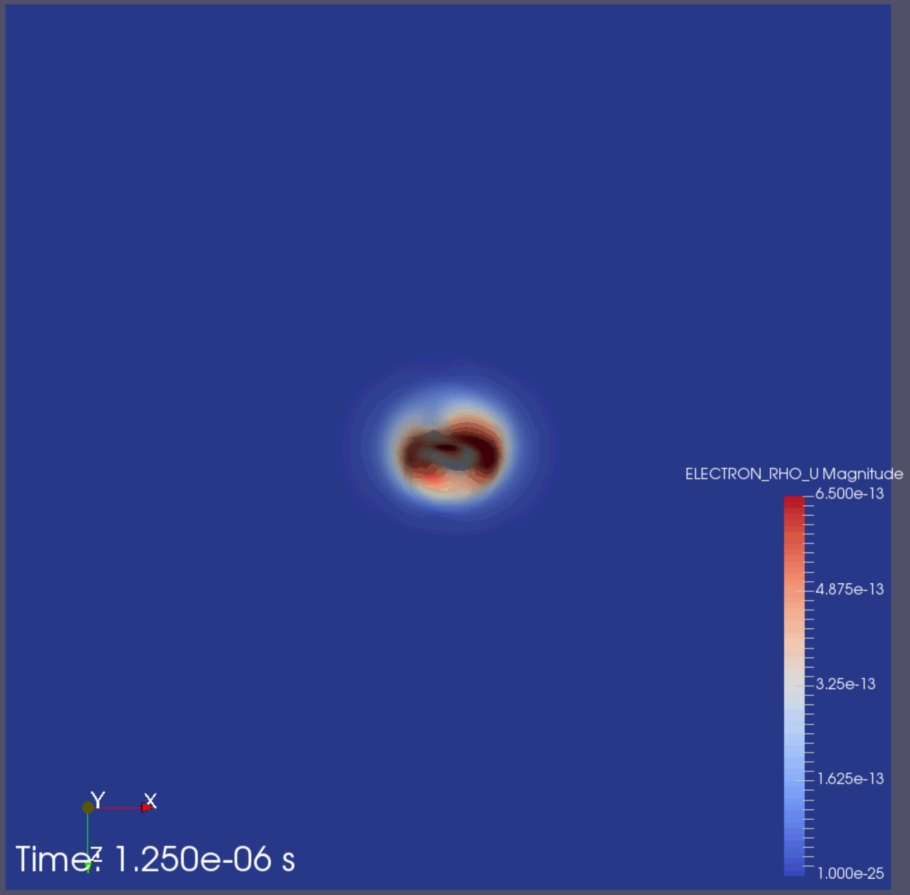

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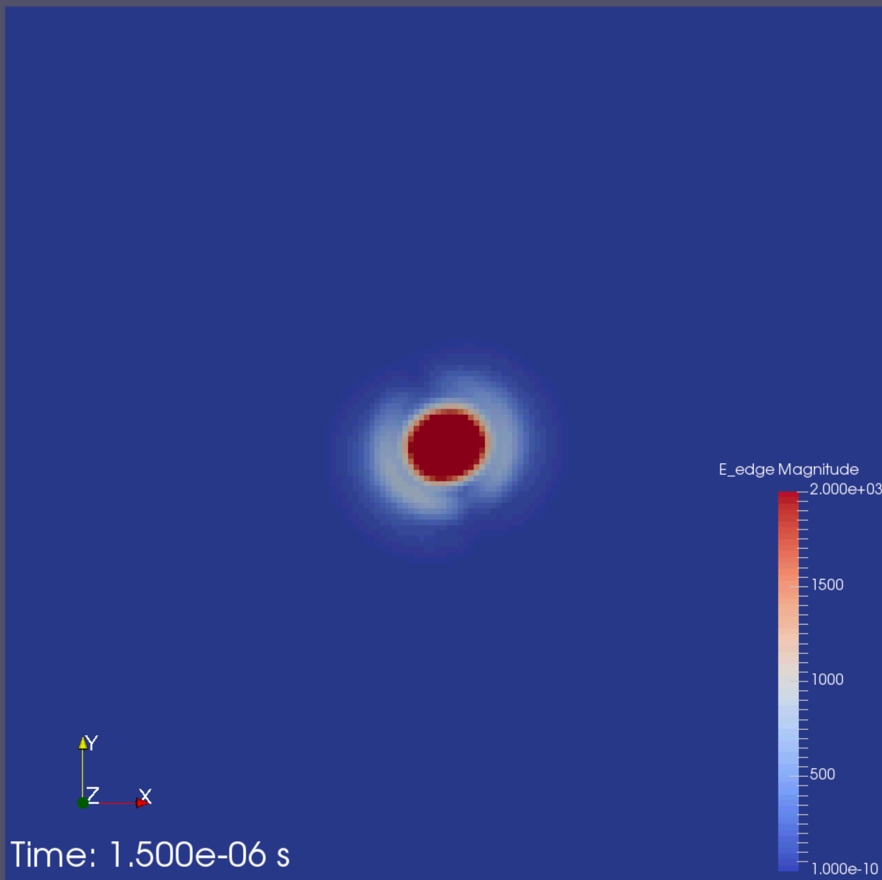

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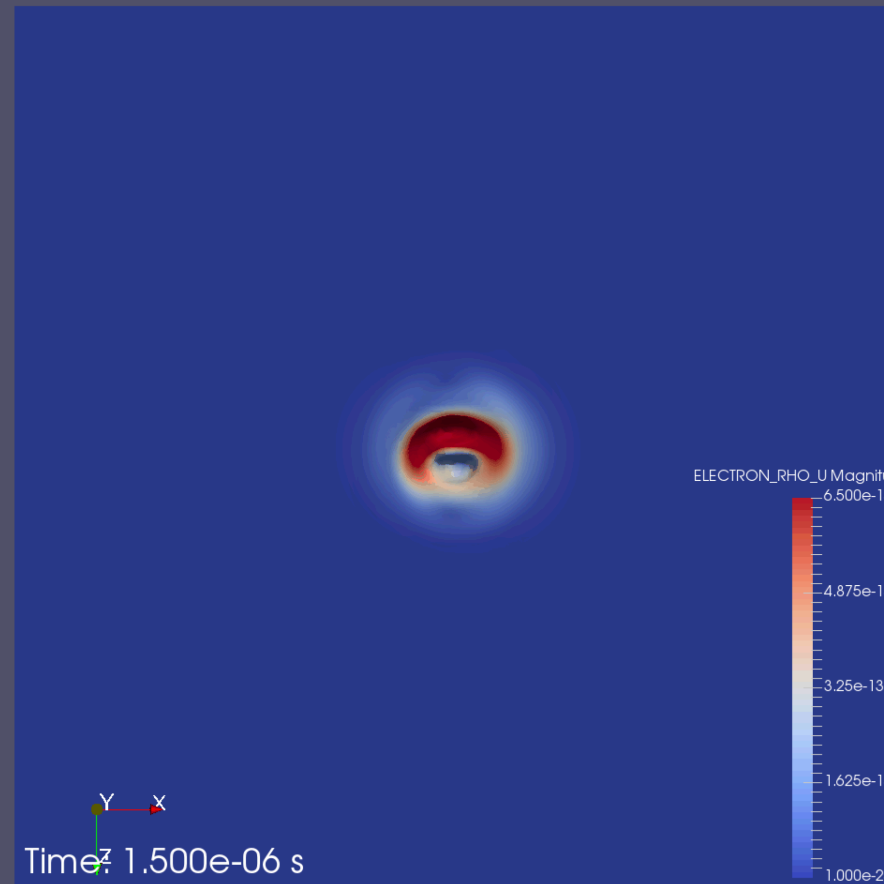

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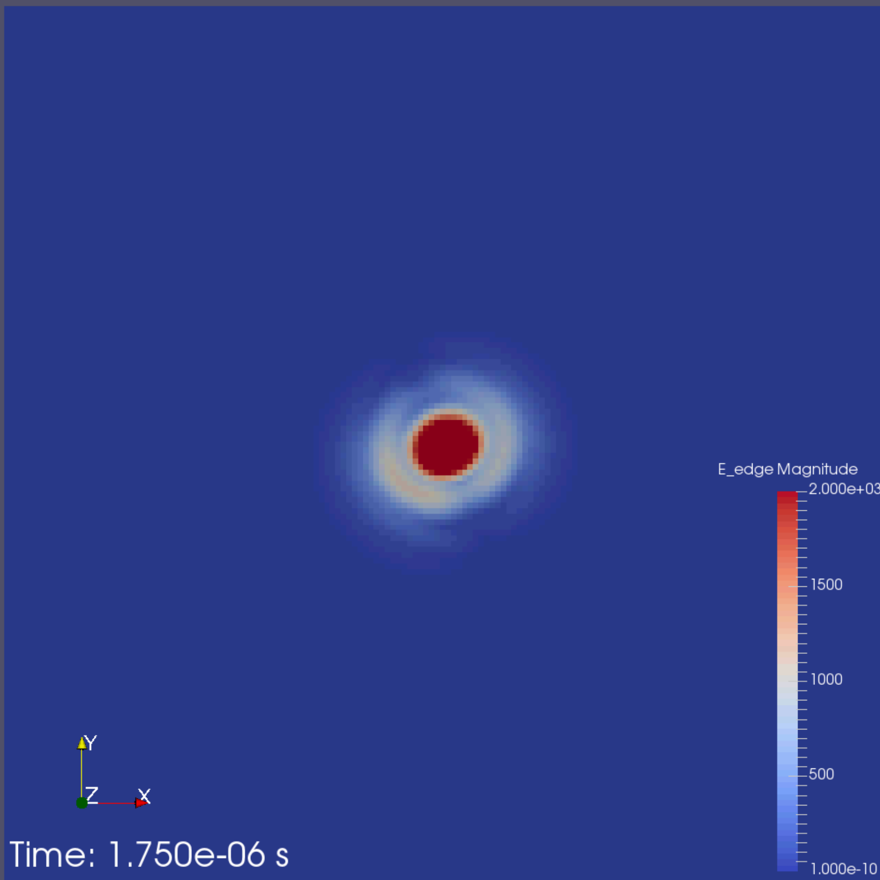

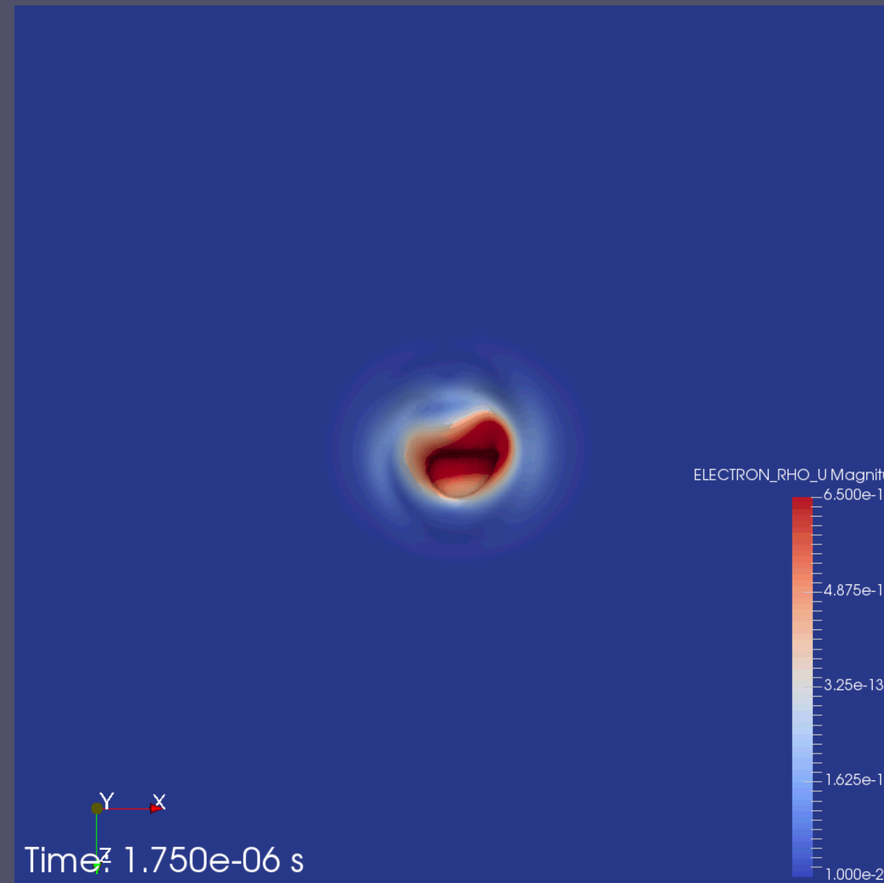

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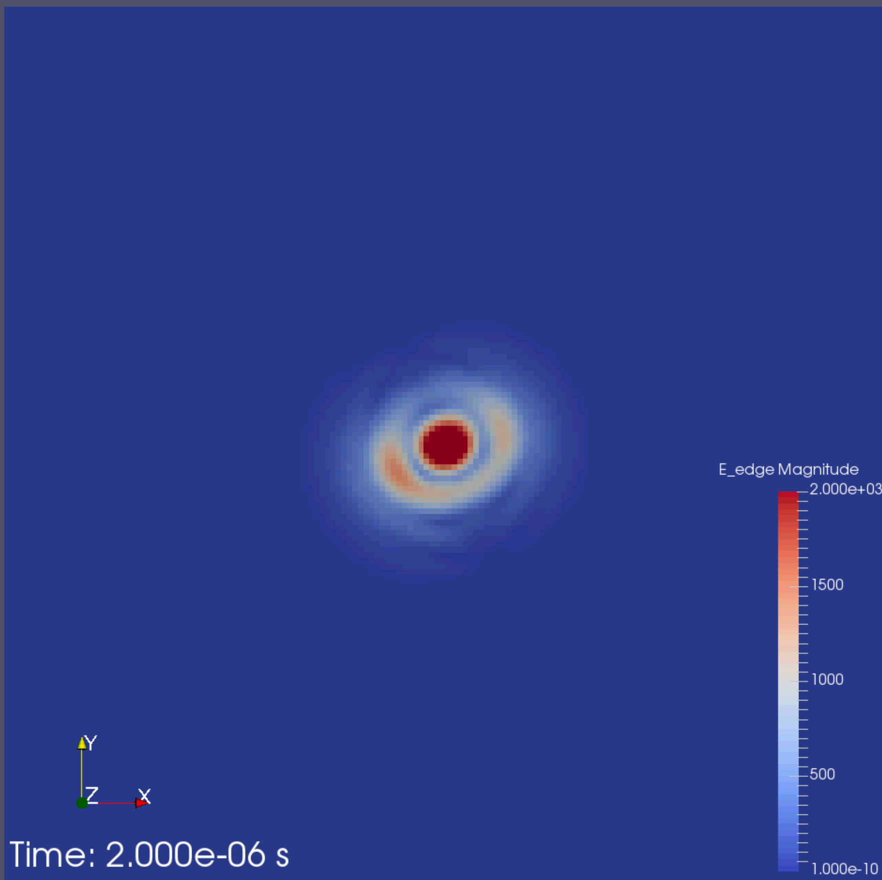

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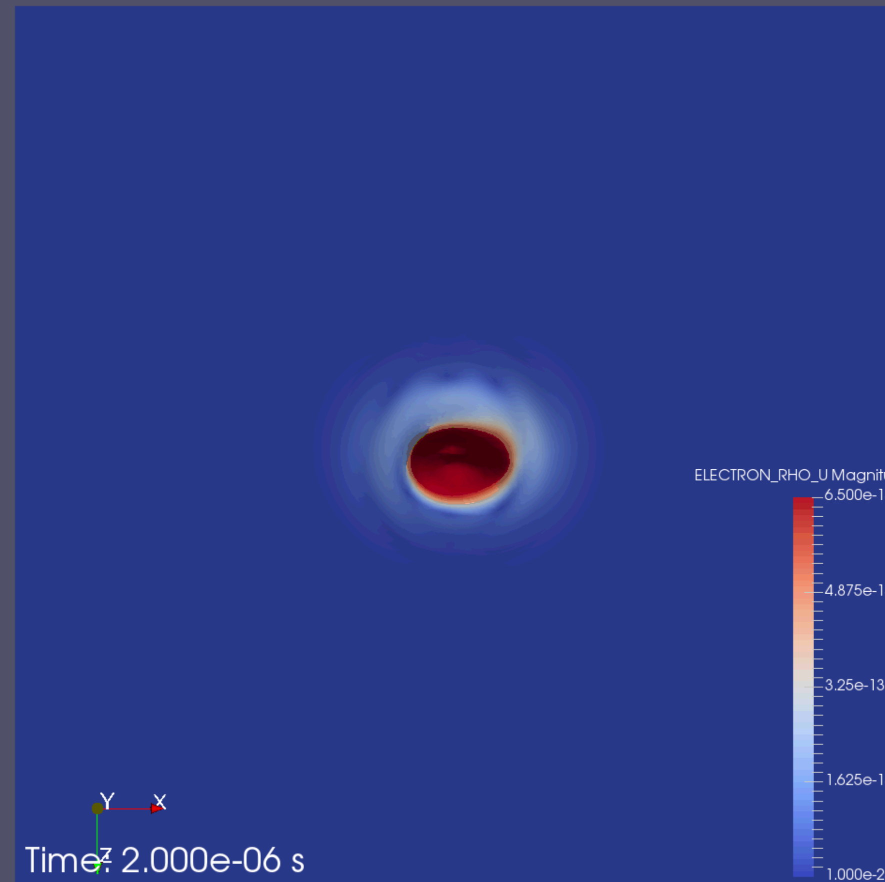

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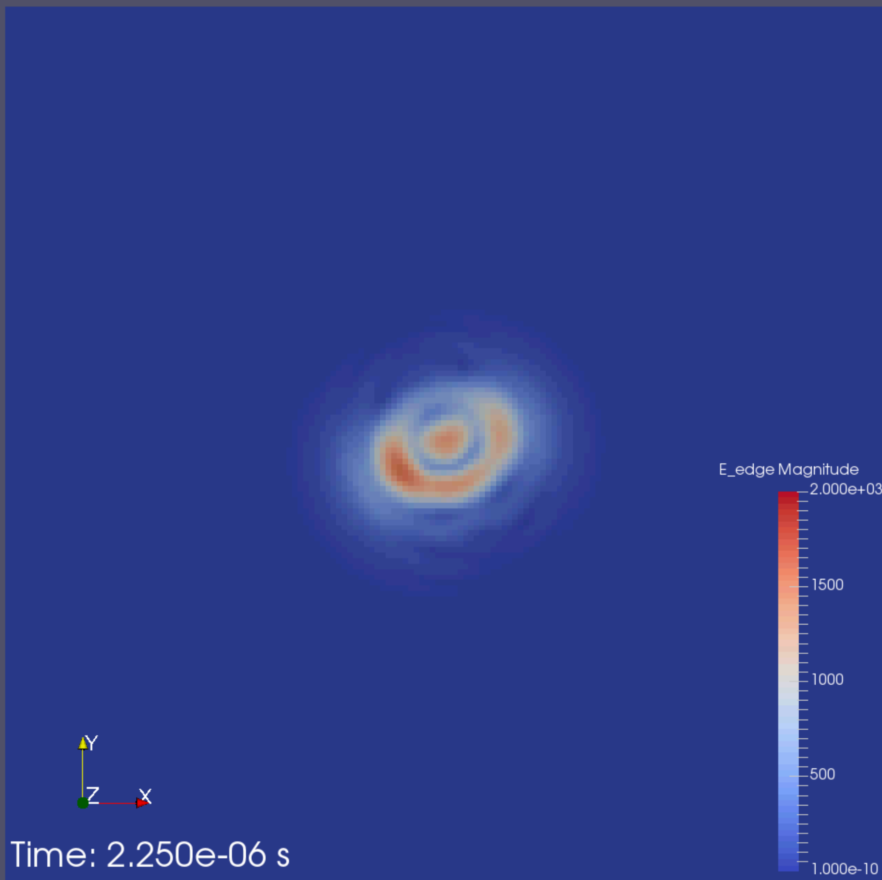
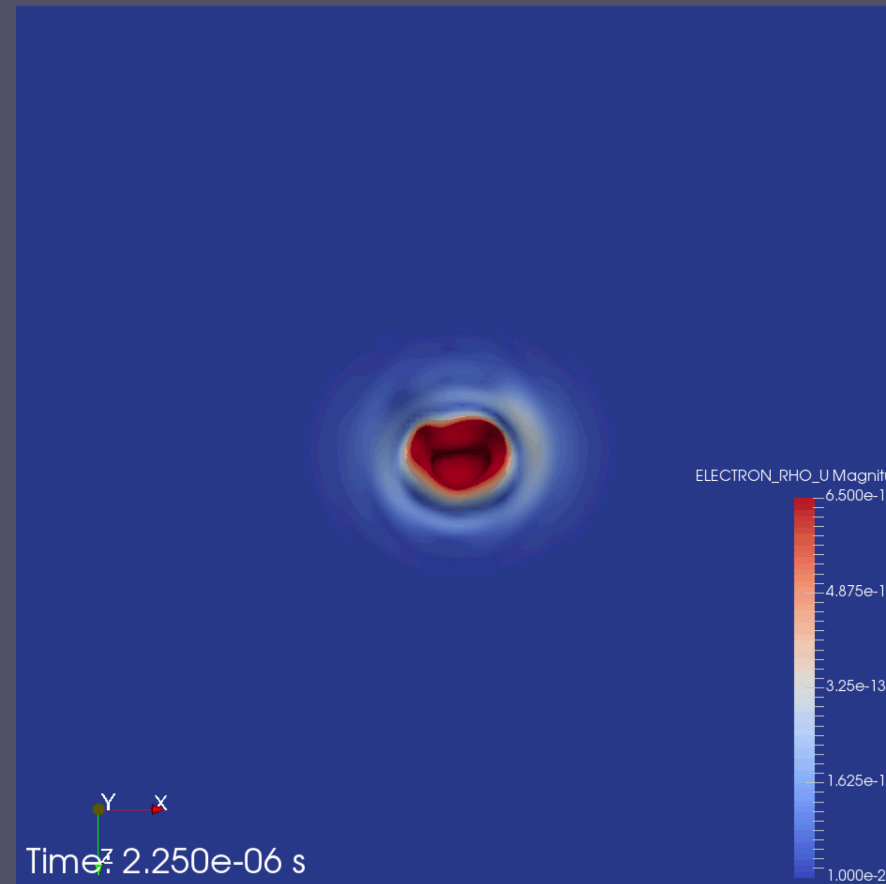
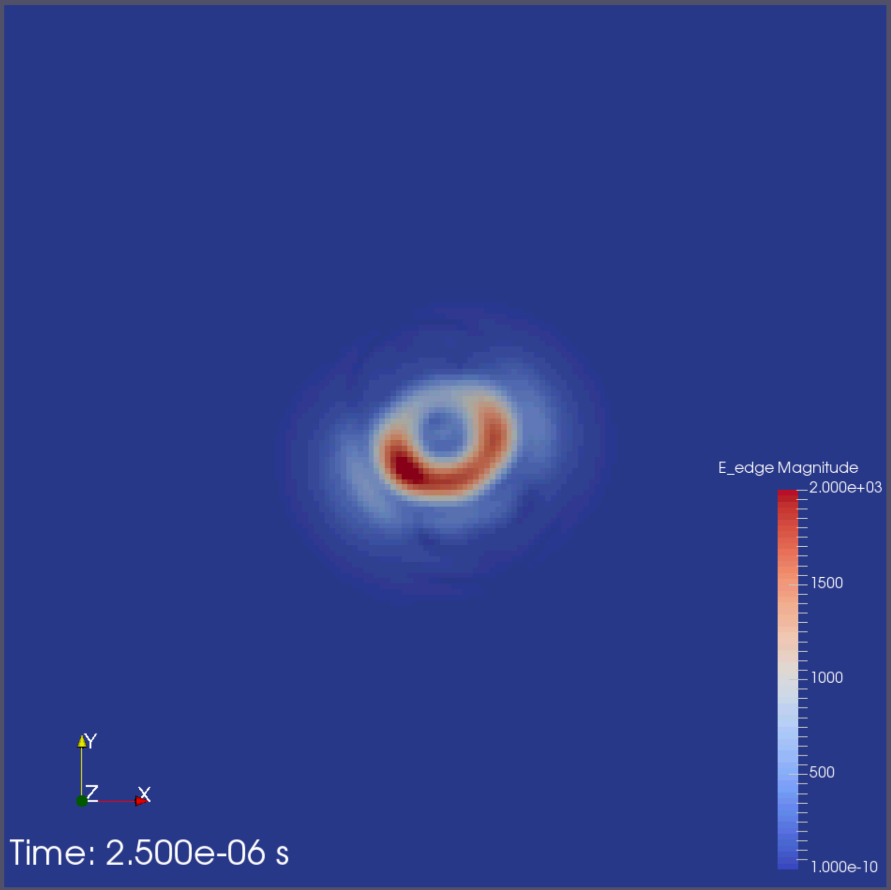


Electric field magnitude
Contours through altitude



Electron momentum magnitude
Projected onto $n_e = 3.5{\times}10^{10}$ contour
(approx. 90 km altitude plane)

3D wave generator simulation



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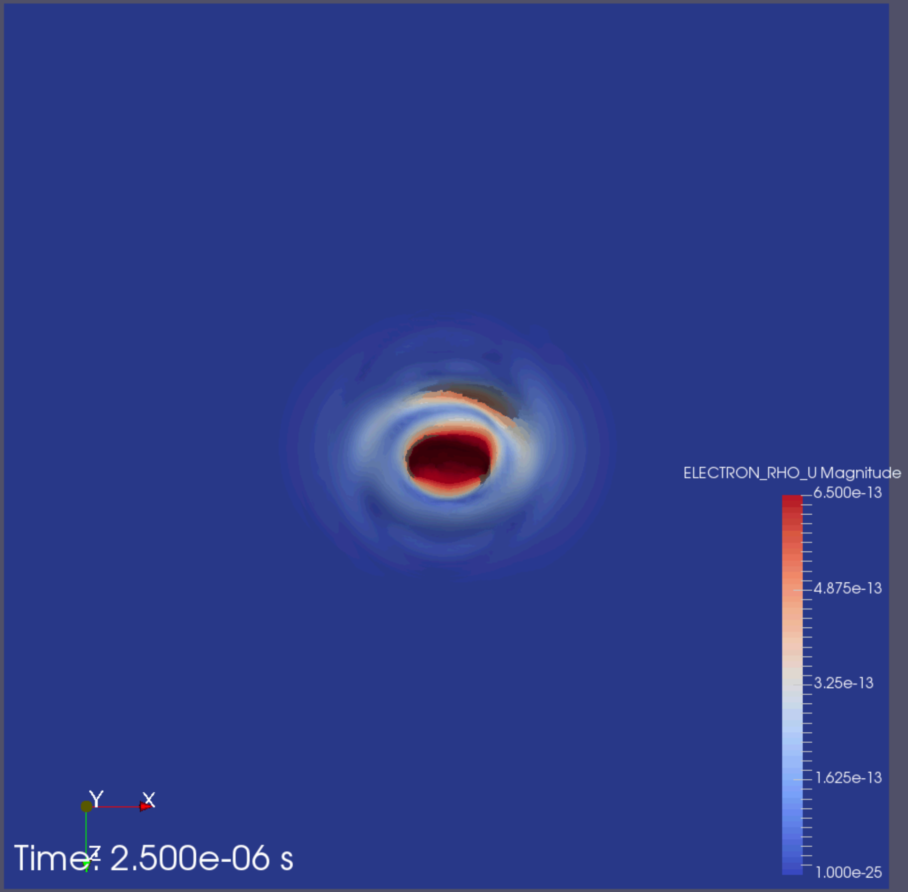

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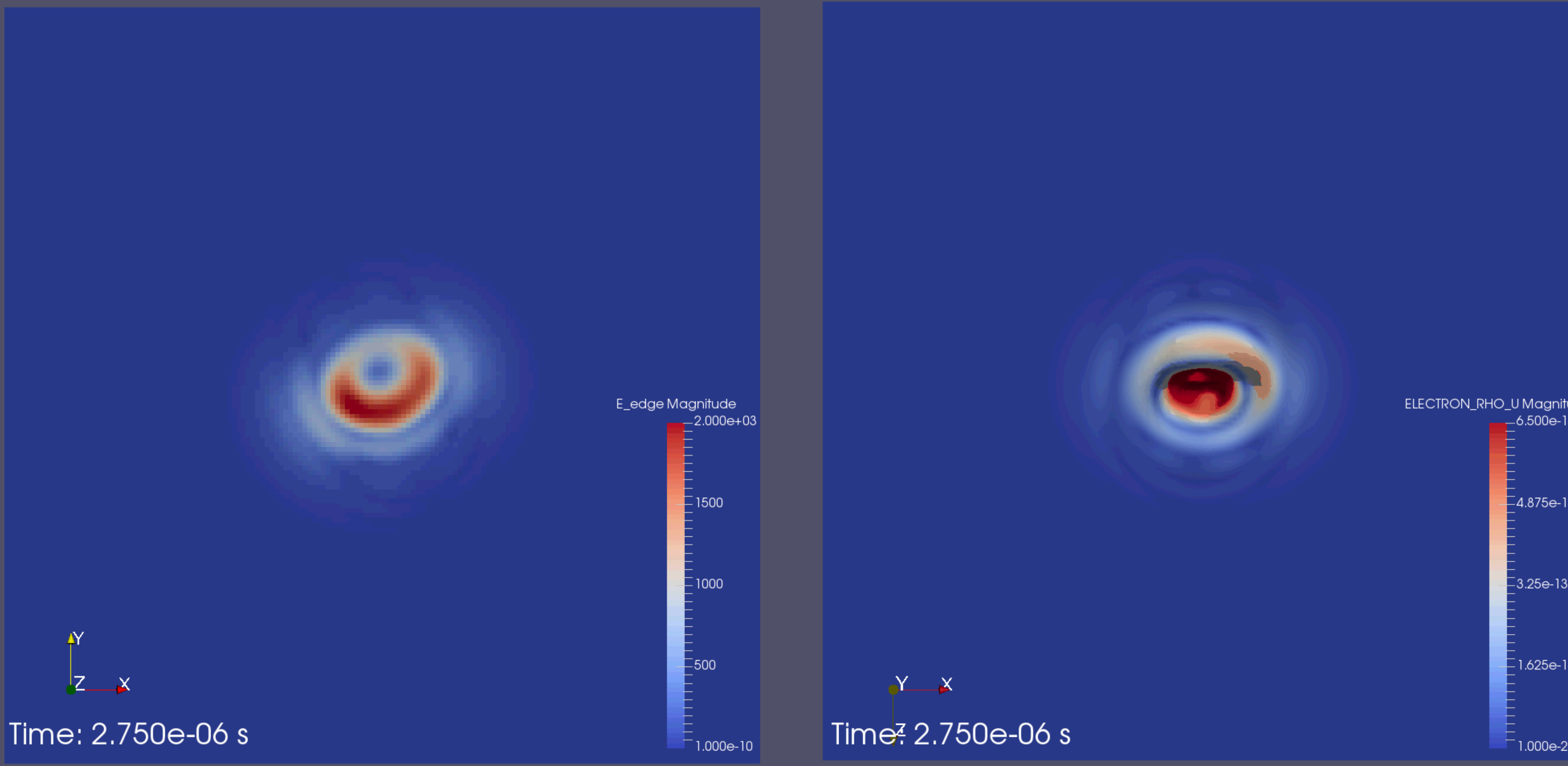

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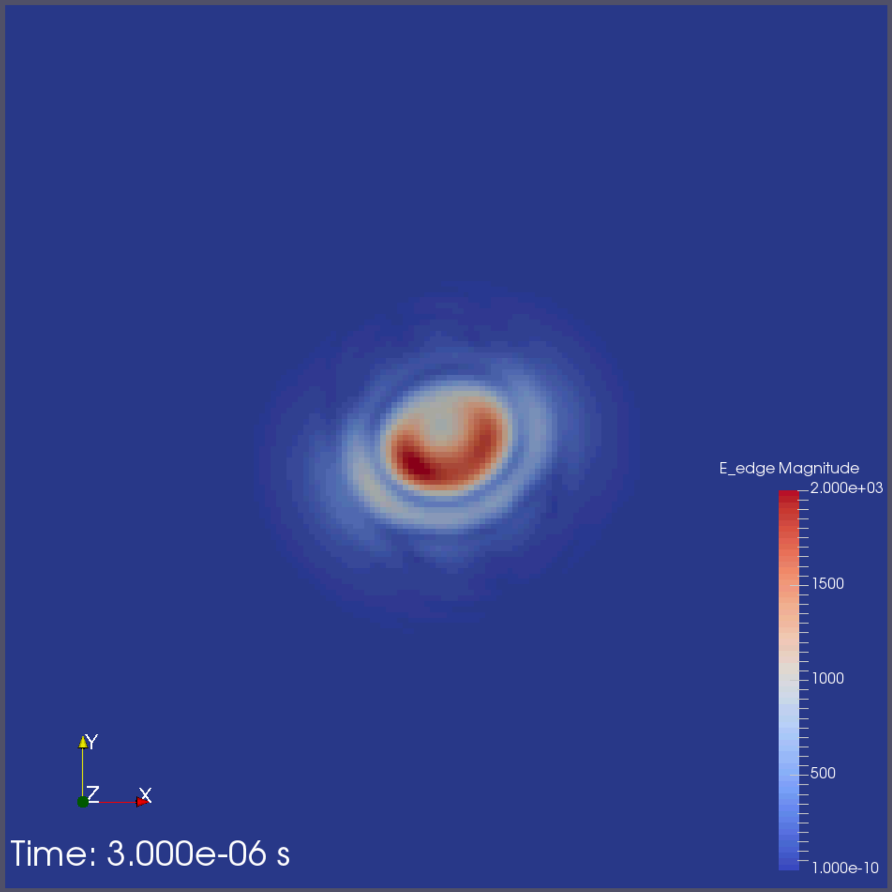

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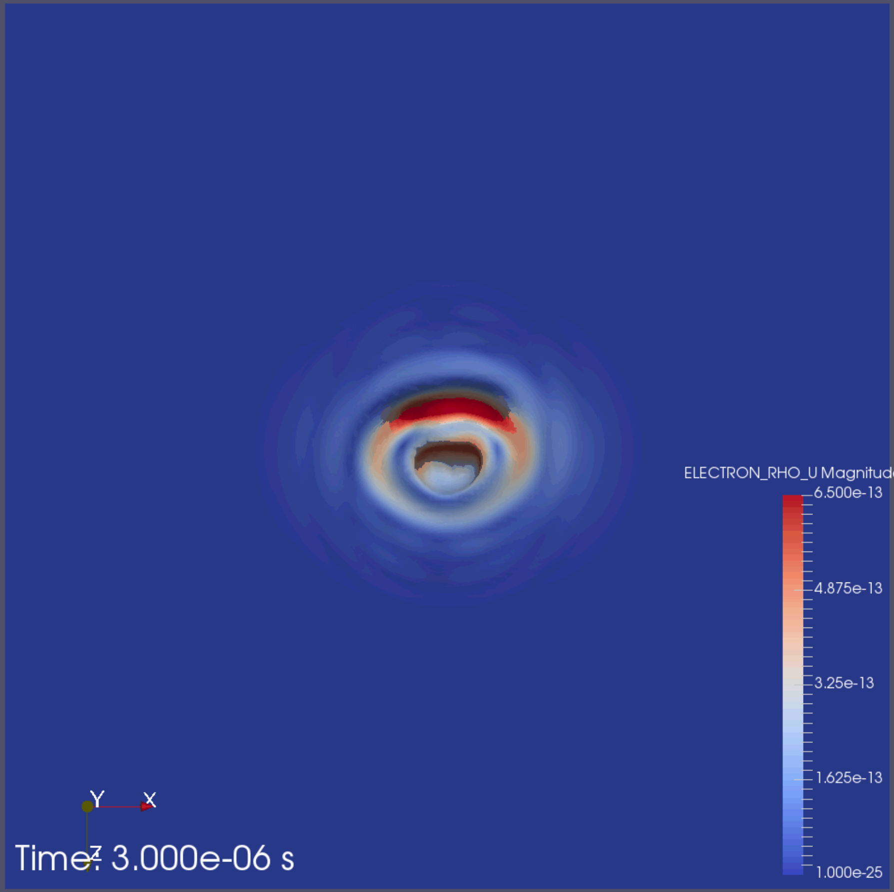

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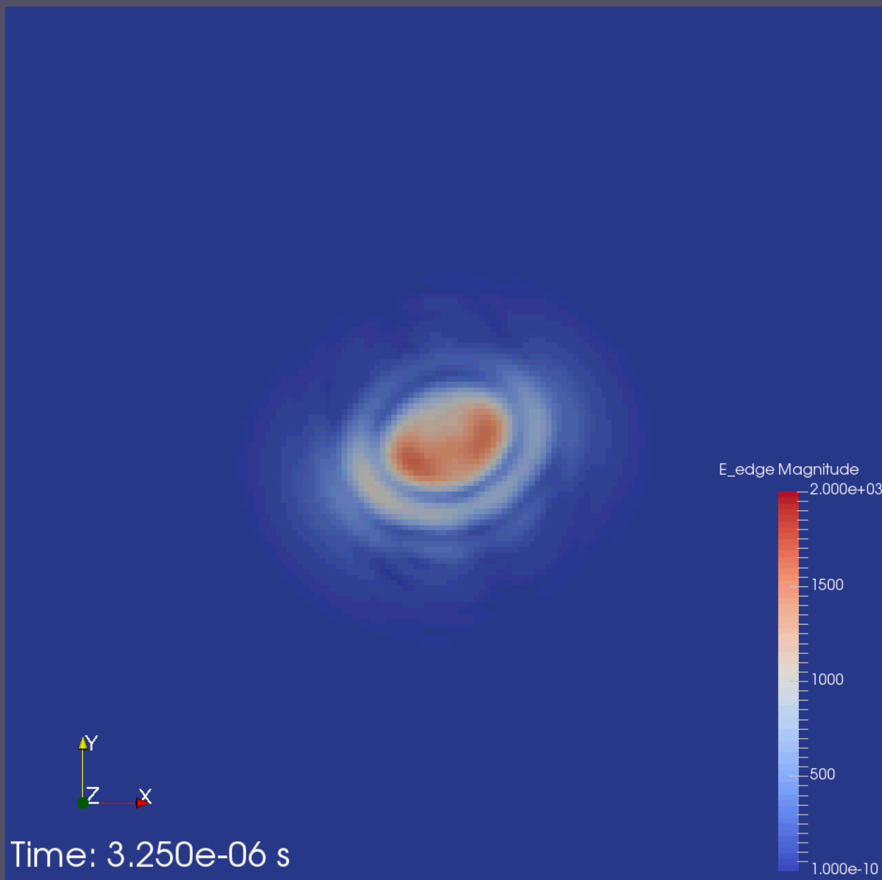

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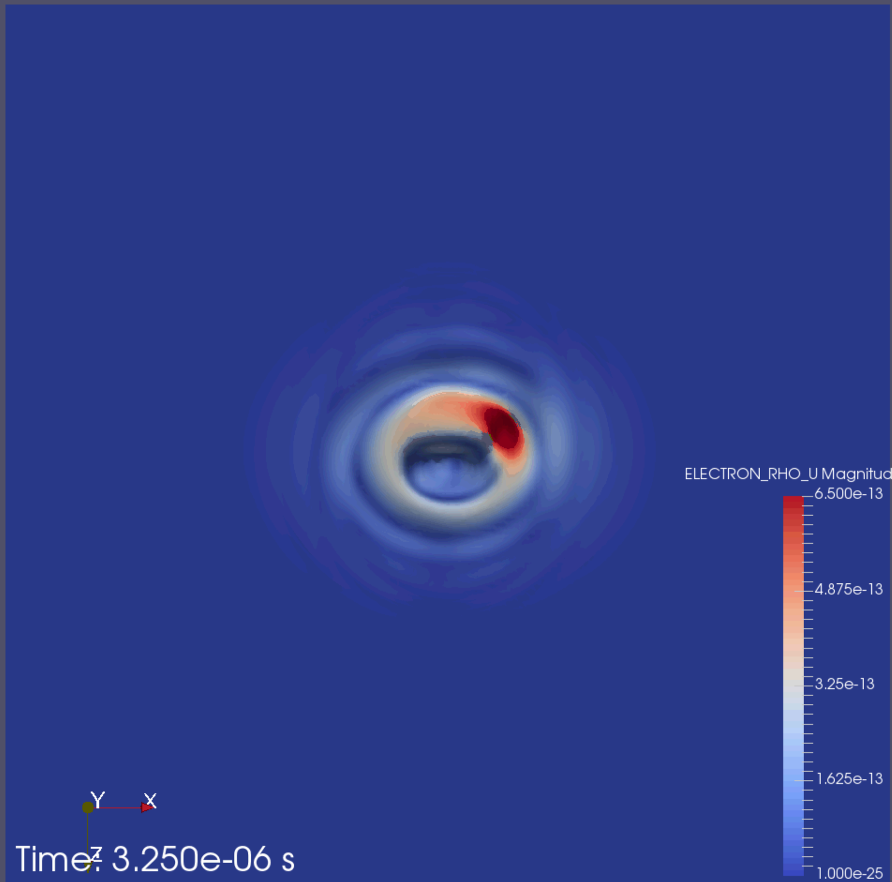

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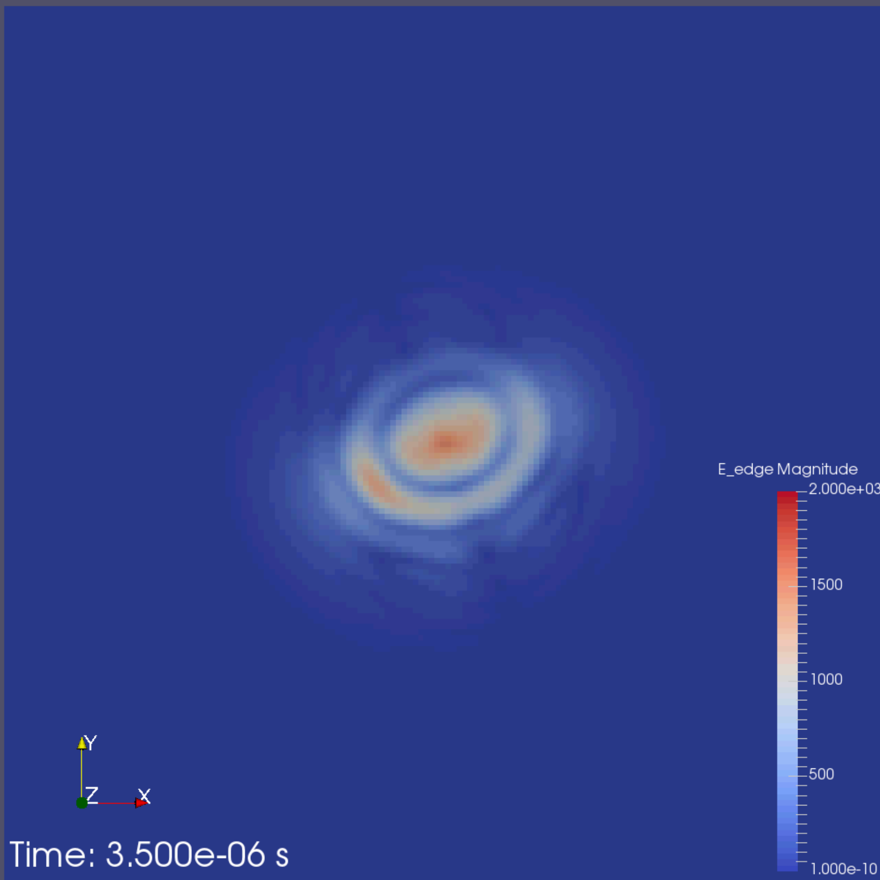

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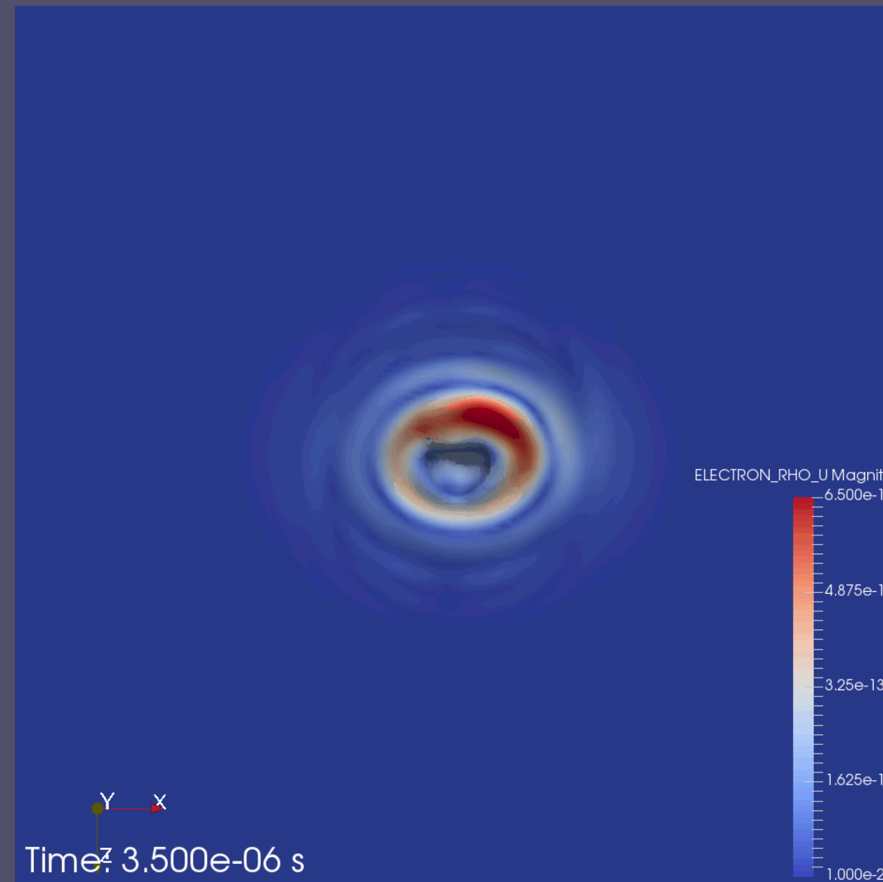

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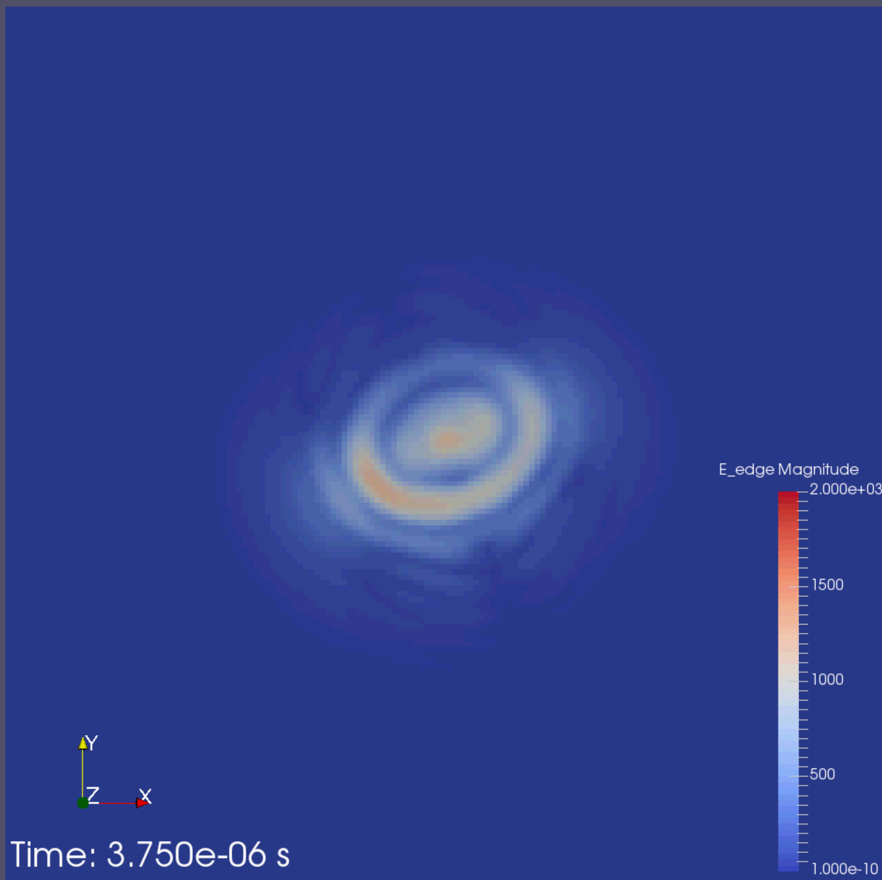
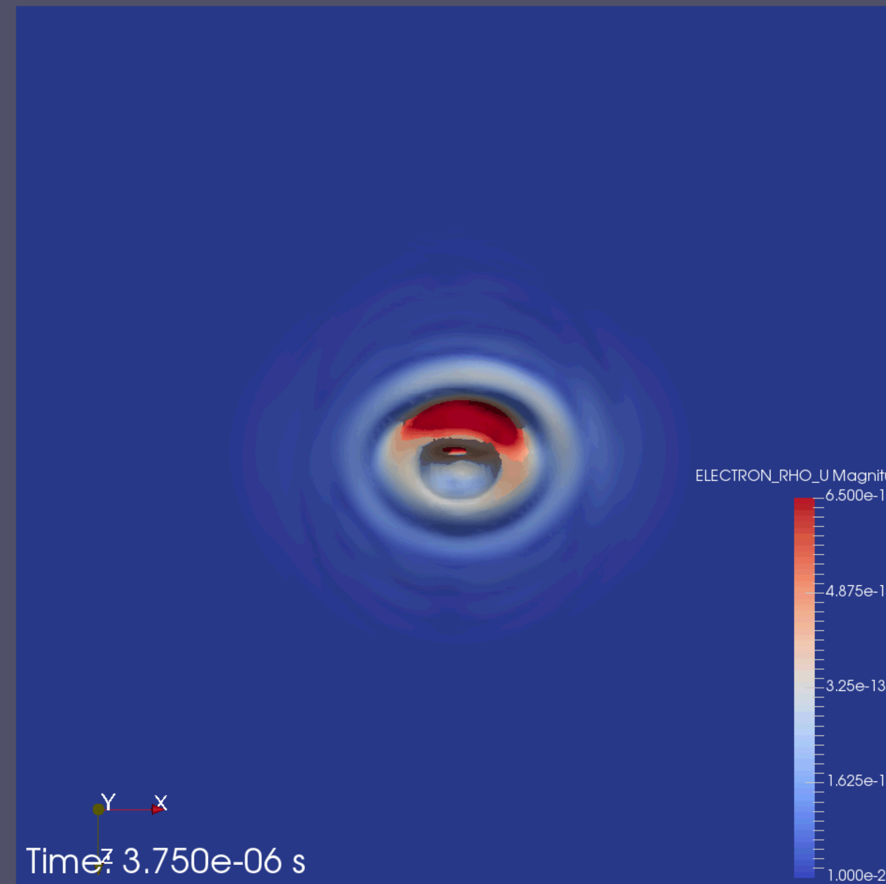
Sandia National Laboratories





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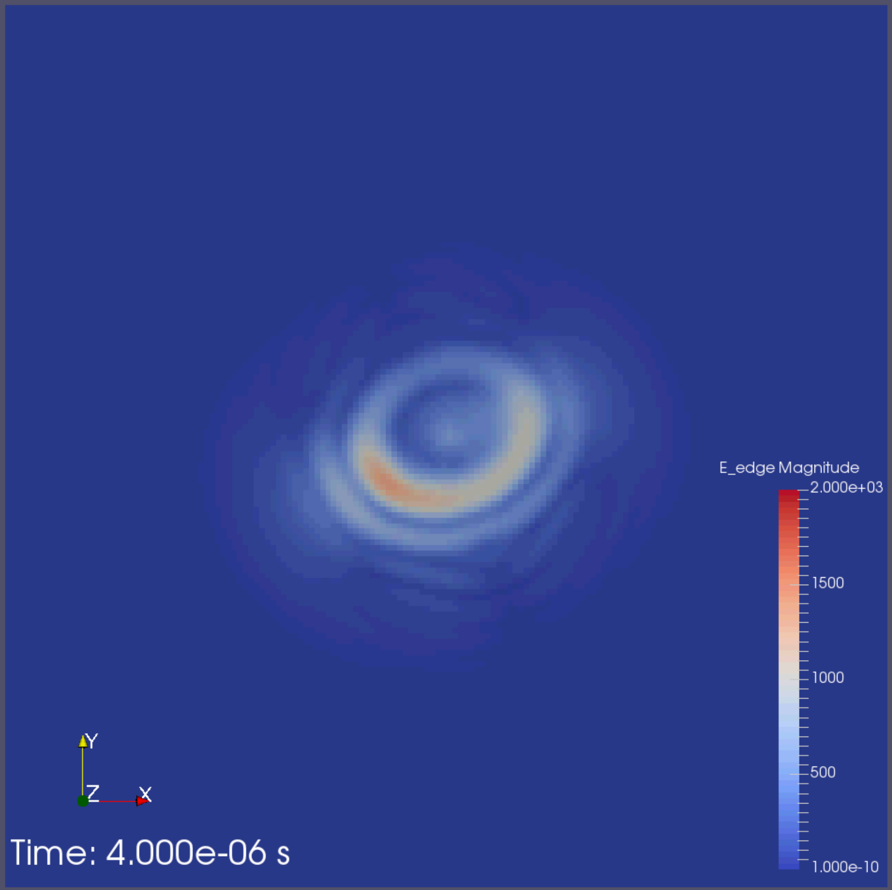

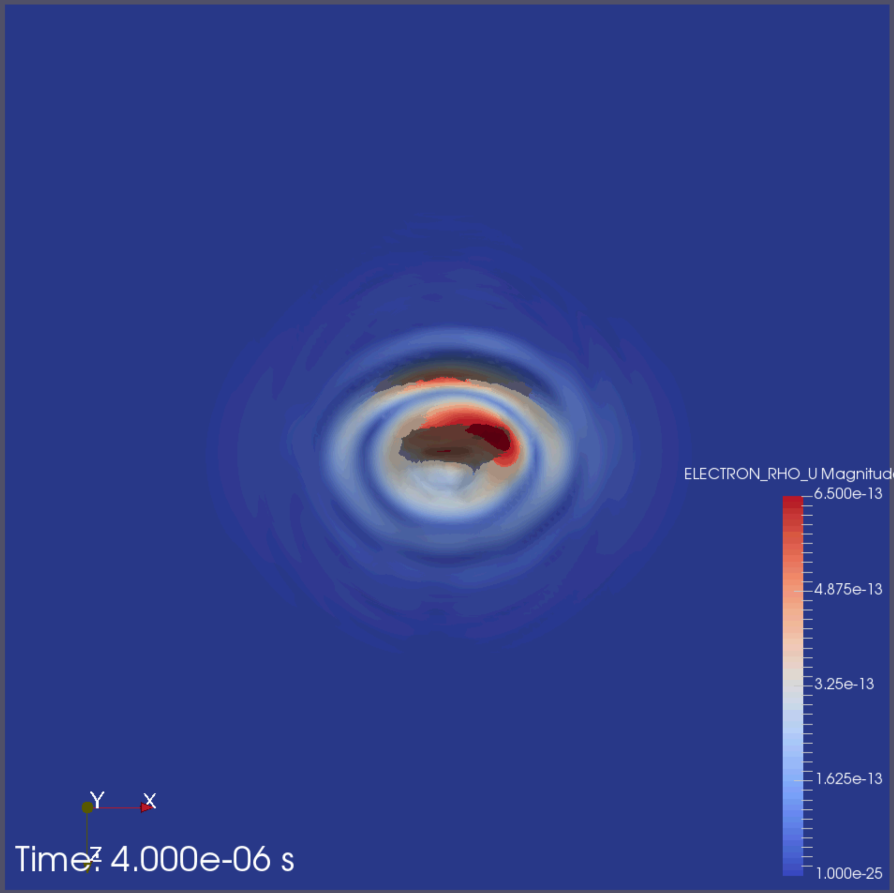

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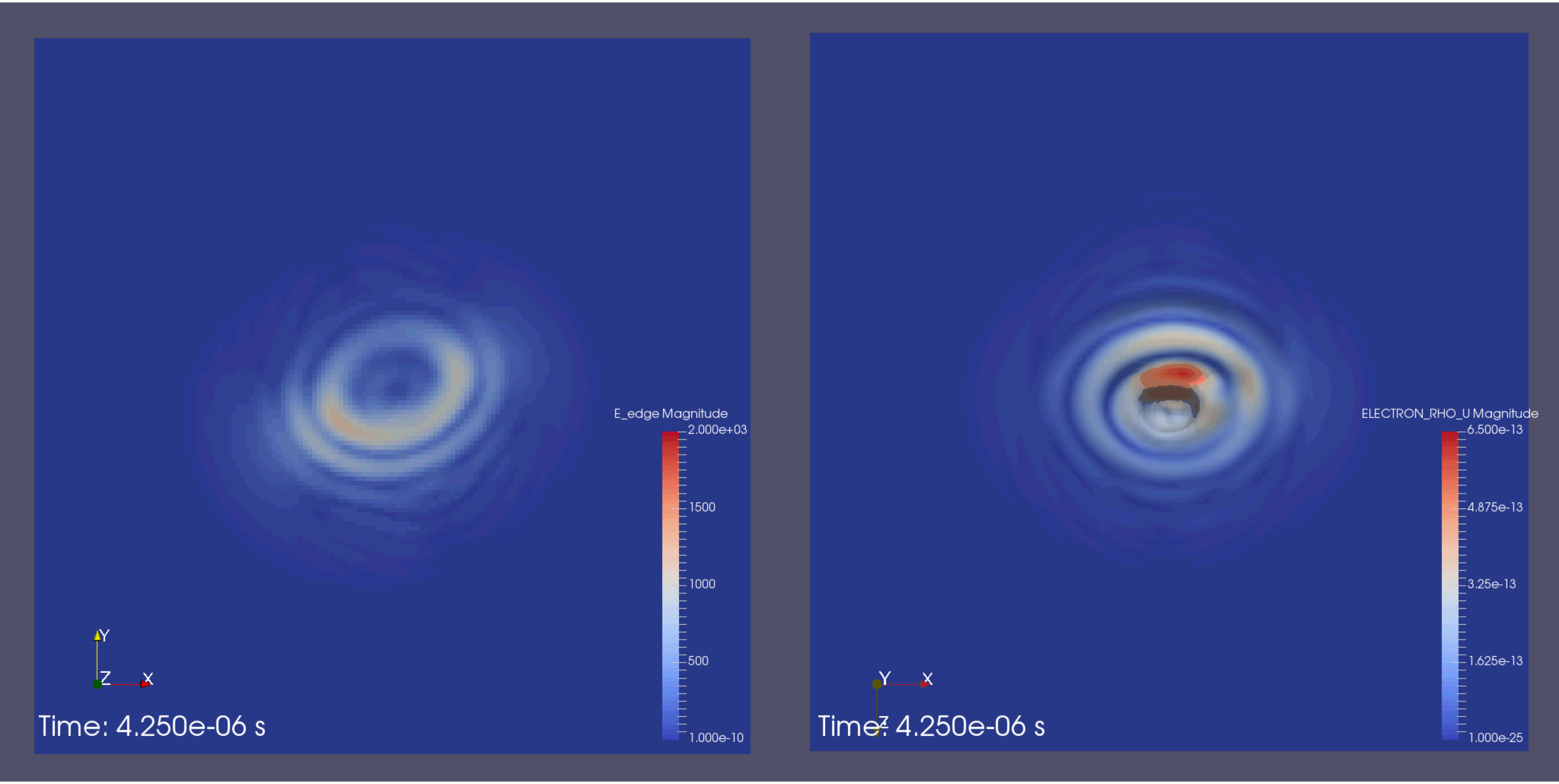

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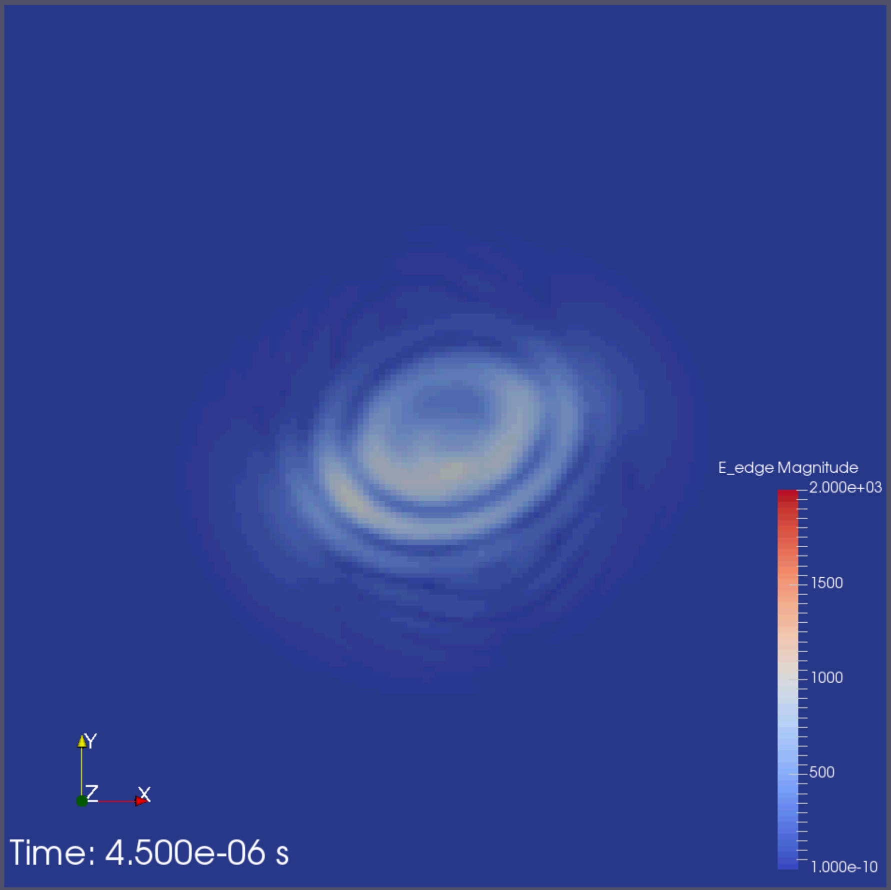

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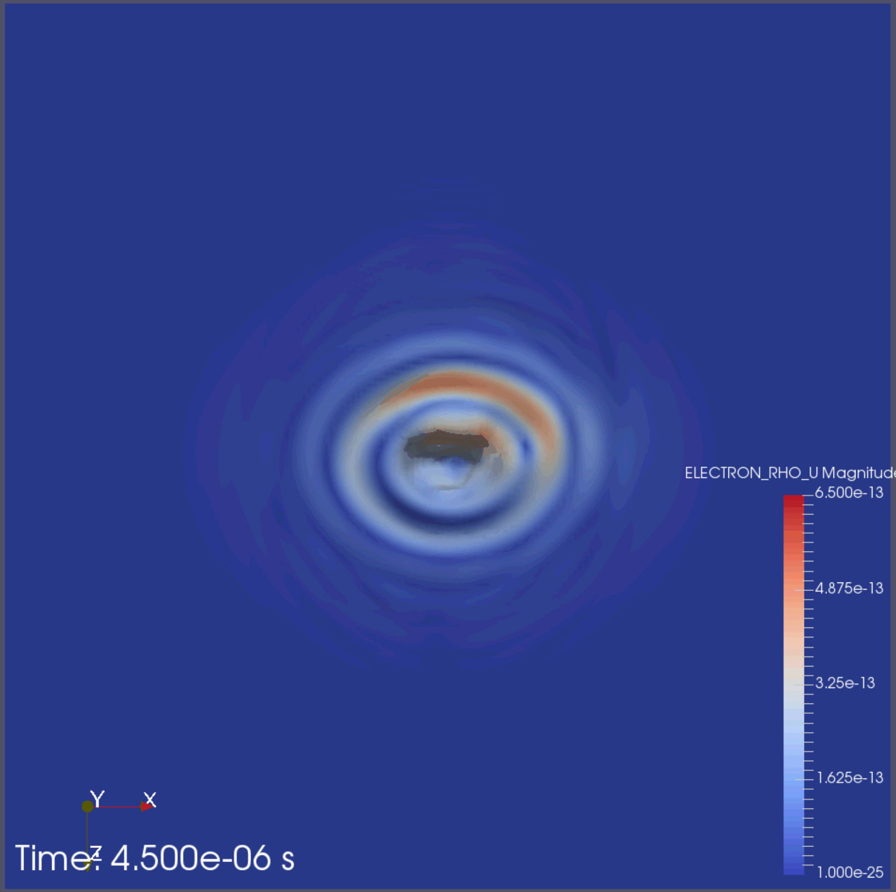

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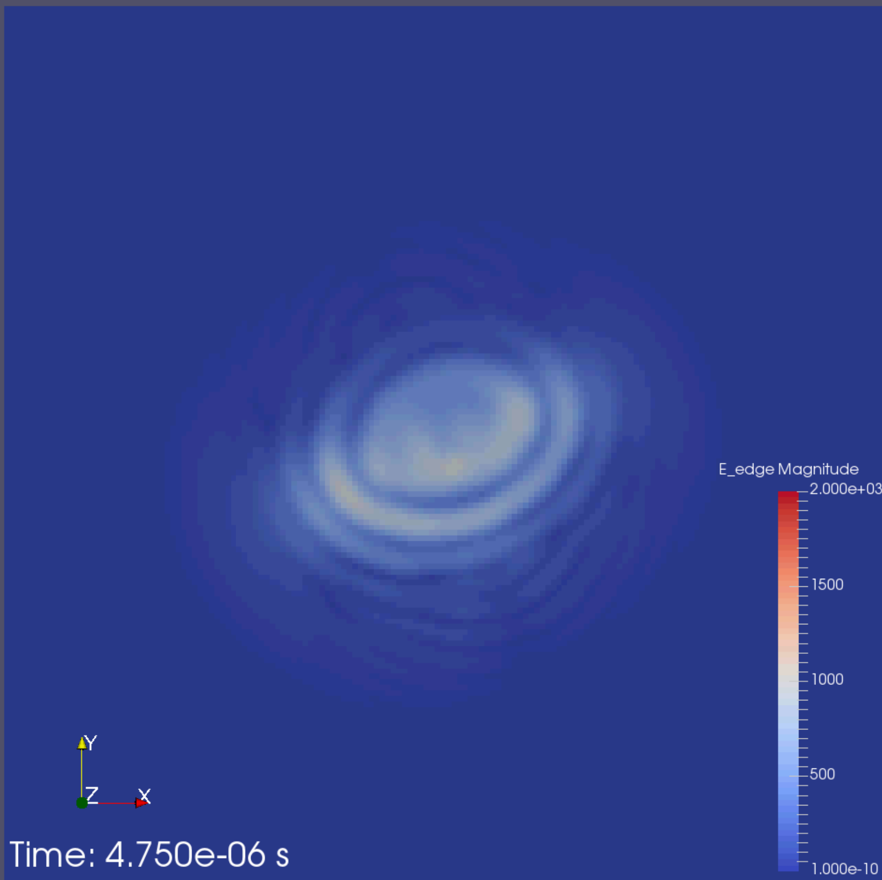

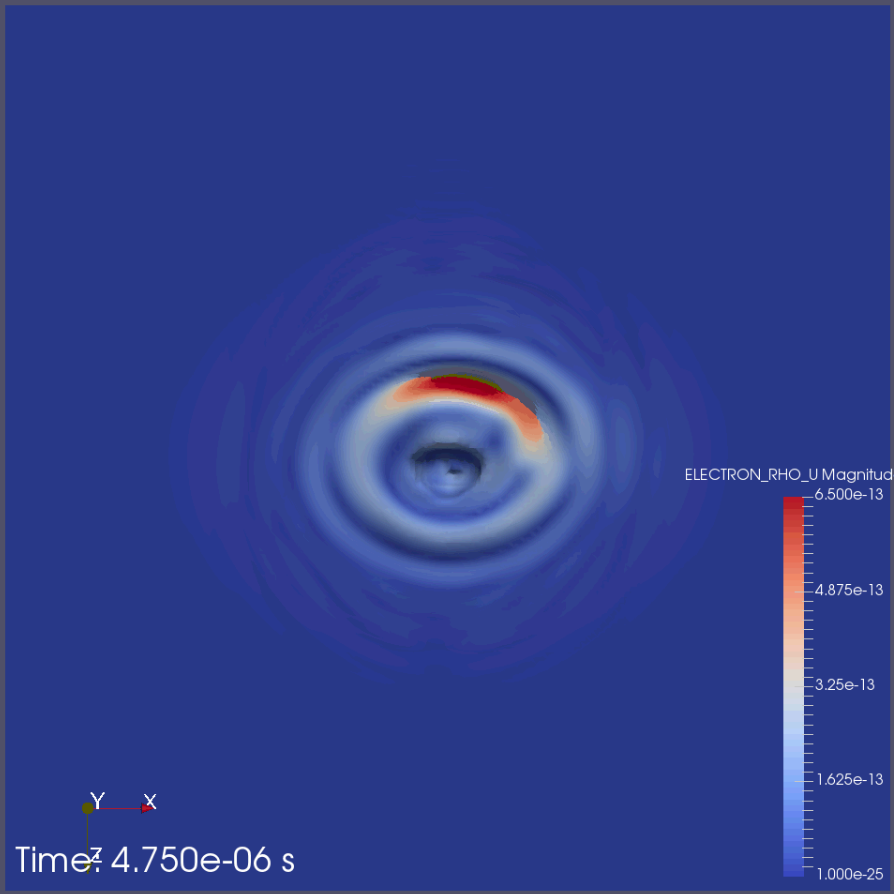

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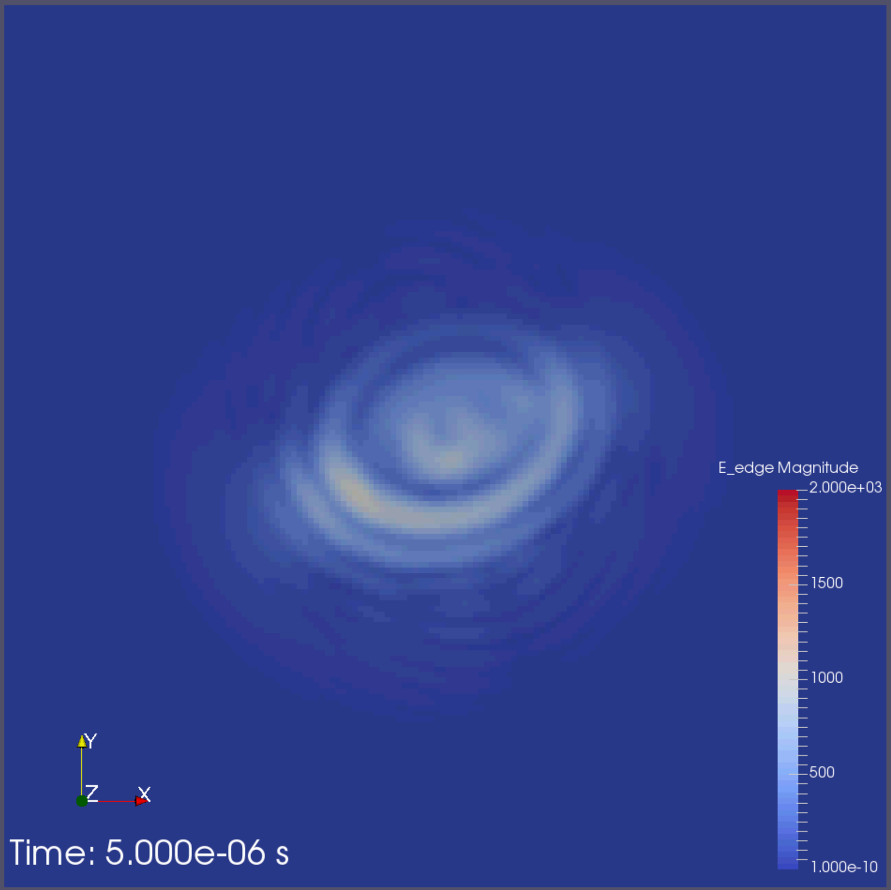

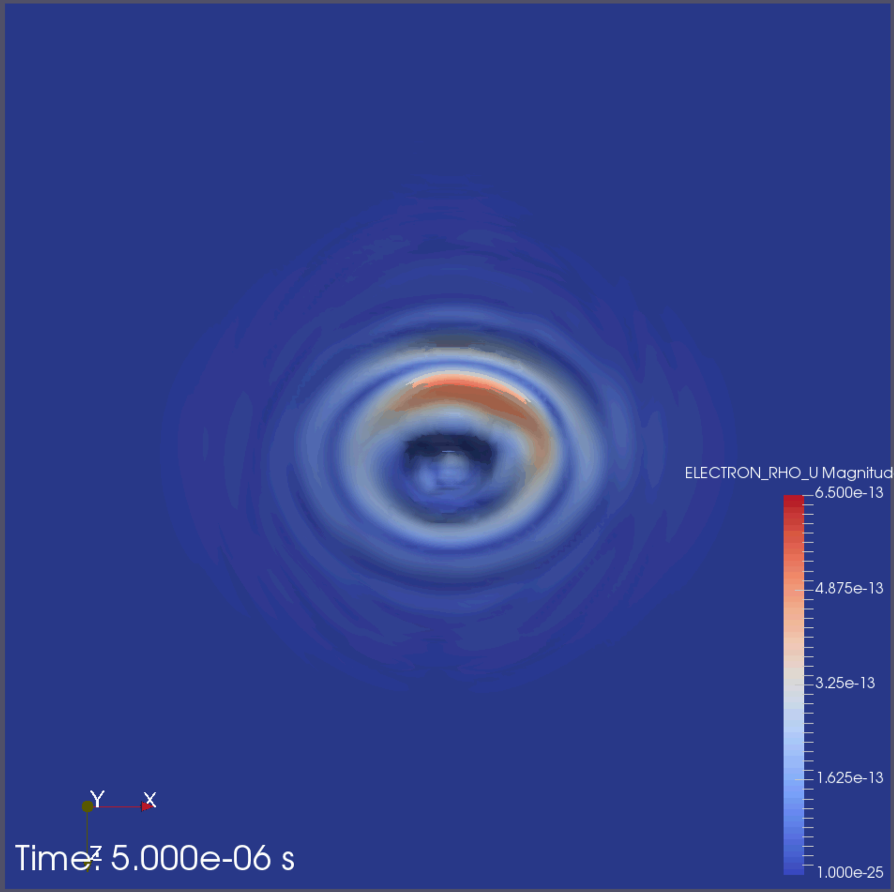

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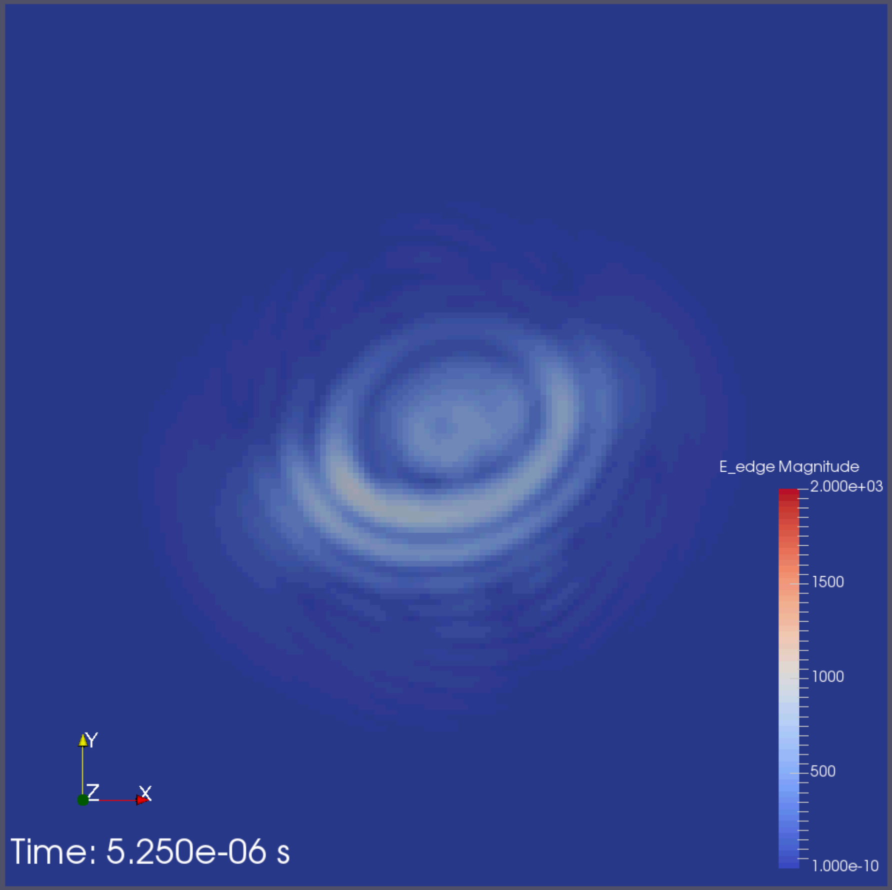

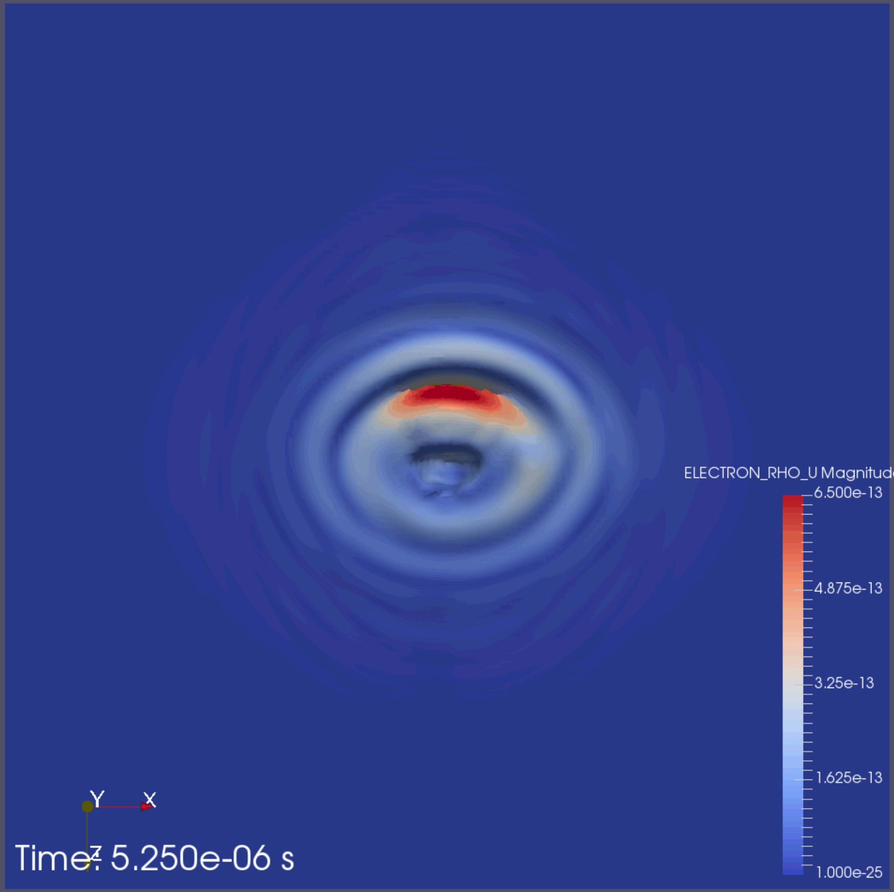

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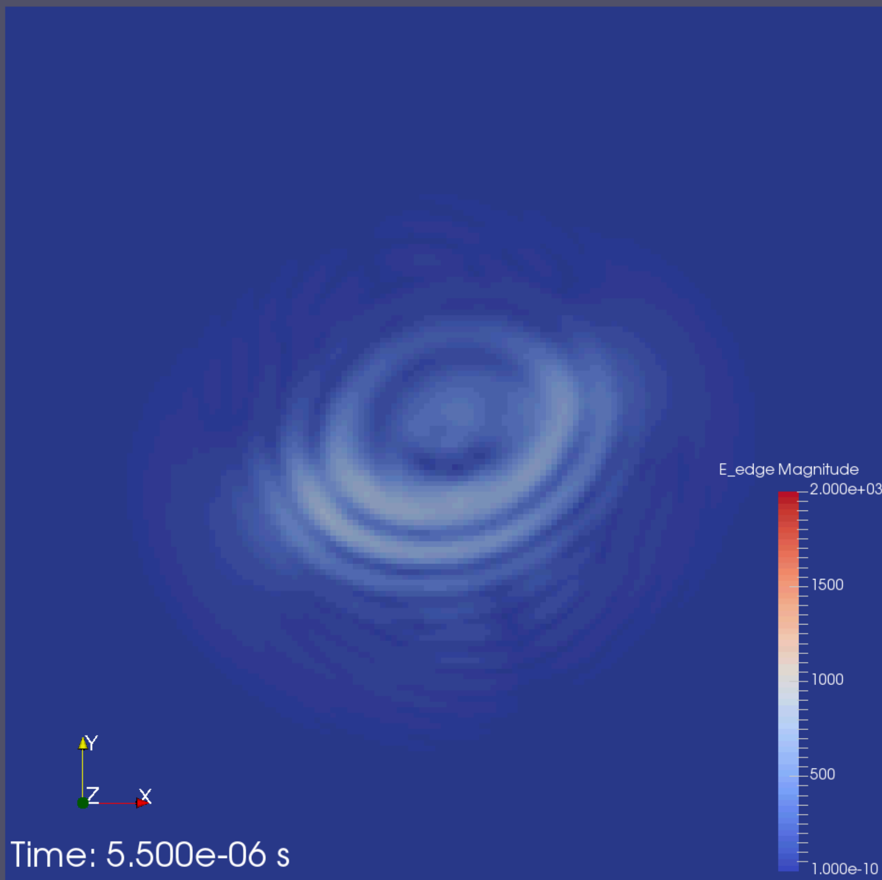

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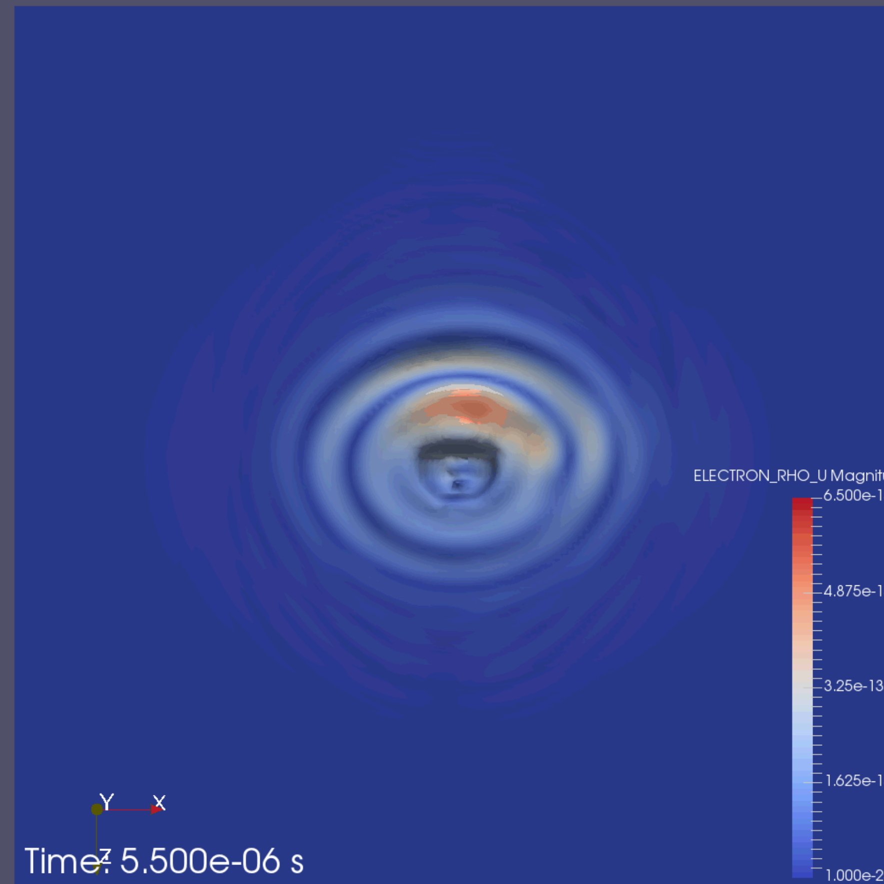

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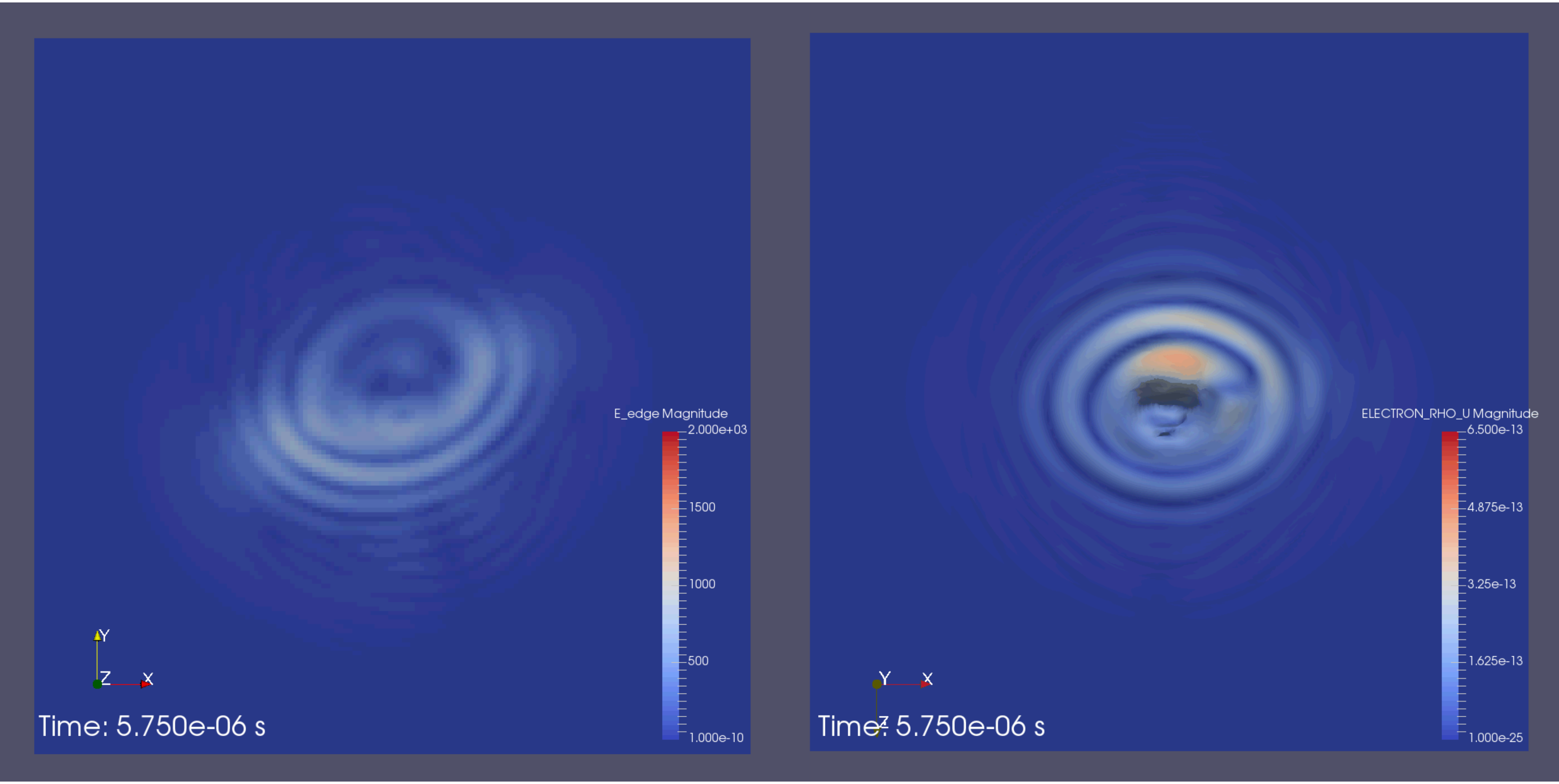

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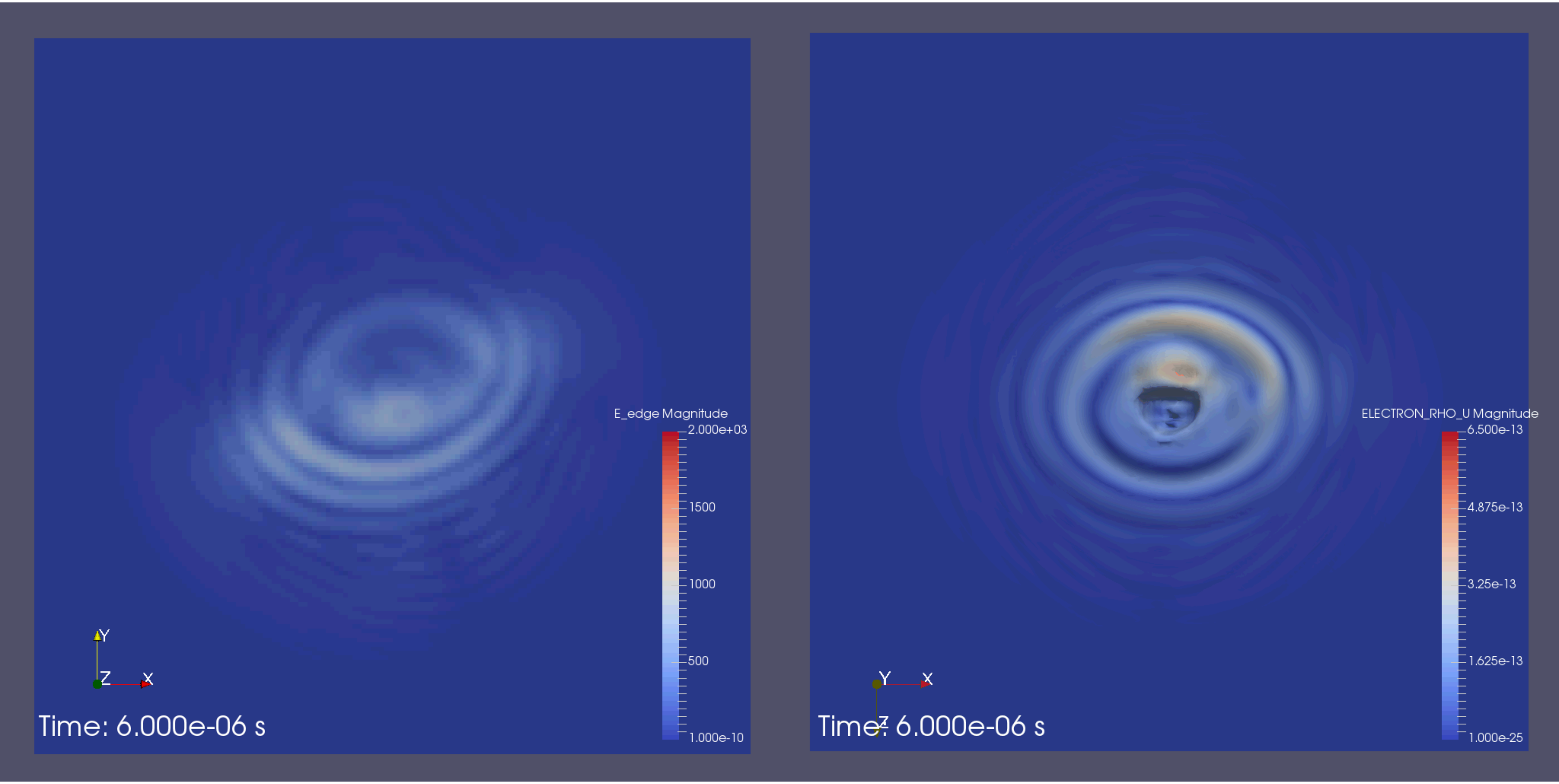

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Summary

- Developing a verification hierarchy based on linear plasma waves
  - Analyzes linear processes describing dispersive phenomena, a necessary step to gain confidence in strongly nonlinear plasma dynamics
  - Tests exercise a variety of couplings between terms in the equations
  - Lessons learned in problem setup, numerical solution controls
  - Demonstrated convergence in multiple contexts
  - Will be adding two-fluid versions
- Validation problems exercising nonlinearities remain to be explored:
  - Fast magnetic reconnection problem under development
- Progressing towards a “real” SREMP problem
  - Plasma wave generator demonstrates highly dispersive wave dynamics