



Numerical Error Analysis of EMC3-EIRENE Simulations in HSX

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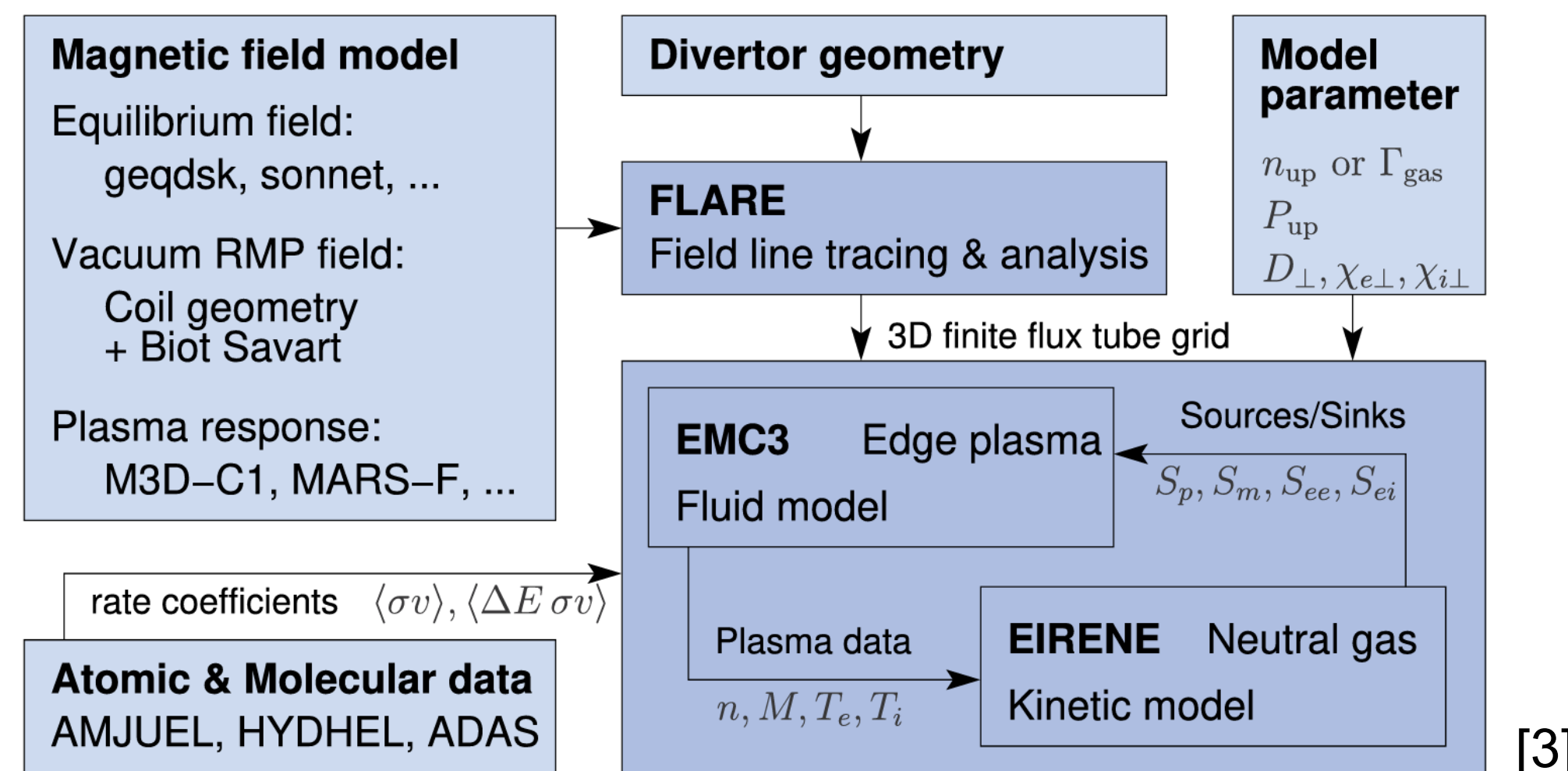


Motivation

- EMC3-EIRENE modeling guides divertor and edge designs in stellarators but numerical error and uncertainty estimates are lacking [1, 2]
- Goal: quantify and reduce EMC3-EIRENE numerical errors in HSX to better assess its use and capabilities

EMC3-EIRENE

- 3D Coupled Monte Carlo–Monte Carlo plasma edge code
- EMC3 solves Braginskii fluid equations
- EIRENE solves Boltzmann-type equation for neutral source terms



- Numerical errors described as: $\epsilon_{num} = \epsilon_t + \epsilon_b + \epsilon_s + \epsilon_d$ (Described in each section of poster)

- 3 separate modules of code \Rightarrow 3 origins of error

$$\epsilon_{total\ num} = \epsilon_{ene} + \epsilon_{str} + \epsilon_{EIR} \quad [4]$$

- Error is estimated by finding L1-norm error for volumetric data along field lines

$$\epsilon_{L1} = \frac{\sum_{n=1}^N |f_n - f_{n,ref}|}{\sum_{n=1}^N |f_{n,ref}|}$$

$f_{n,ref}$ - Most numerically accurate solution

Time Integration Error (ϵ_t)

- The time integration error is the result of EMC3 following MC particles through random walks Δr described as

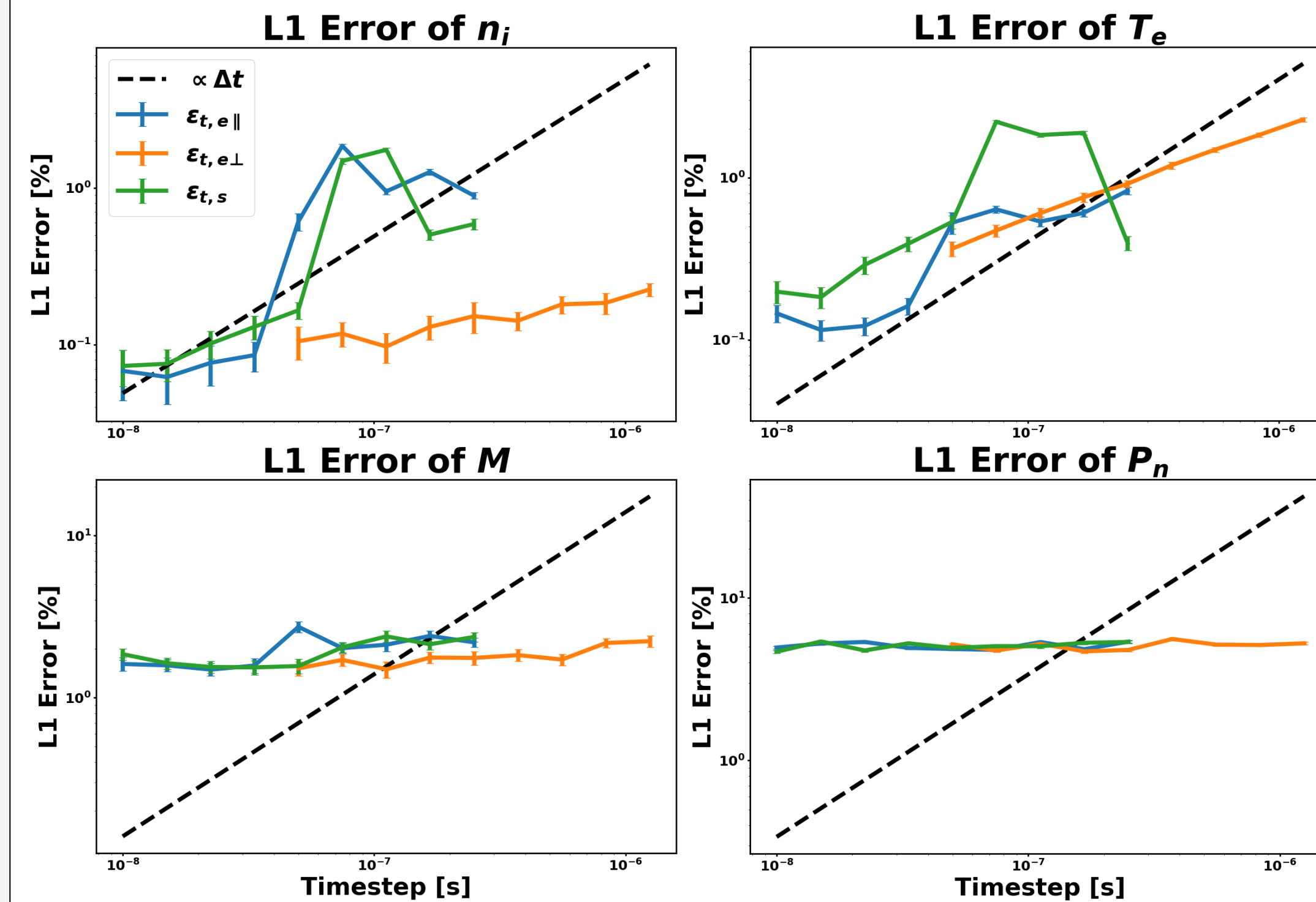
$$\Delta r = \sqrt{2\beta_{\parallel}\Delta t\xi_{\parallel}} + \alpha_{\parallel}\Delta t + \sqrt{2\beta_{\perp}\Delta t\xi_{\perp}} + \alpha_{\perp}\Delta t \quad [5]$$

- Δt is inputted timestep, β_{\parallel} and β_{\perp} are diffusion coefficients, α_{\parallel} and α_{\perp} are convection coefficients, ξ_{\parallel} and ξ_{\perp} are 1D and 2D random unit vectors
- Time integration error expected to scale linear to selected timestep

$$\epsilon_t \propto \Delta t$$

\parallel & \perp Δt in energy module of EMC3
 Δt in streaming module of EMC3

- Three inputted timesteps: $\Delta t_{e\parallel}$, $\Delta t_{e\perp}$, Δt_s



Reference solution is an order of magnitude finer than smallest shown timesteps

- n_i and T_e scale roughly linear to timestep
- Mach number M independent of timestep (currently investigating)
- Neutral pressure P_n independent of timestep (neutral quantities have little dependence on plasma modules)

Discretization Error (ϵ_d)

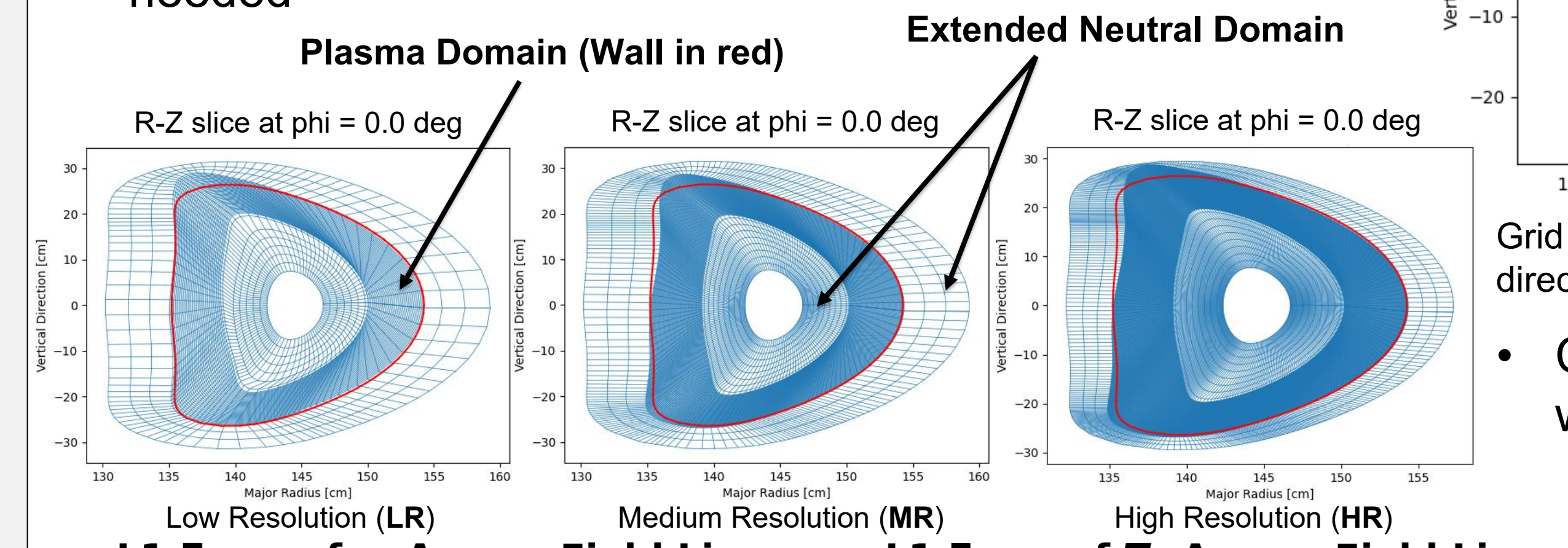
- The discretization error is the result of solving continuous equations at finite points in space

- Dominant error term**

$$\epsilon_d \propto h^{p_d}$$

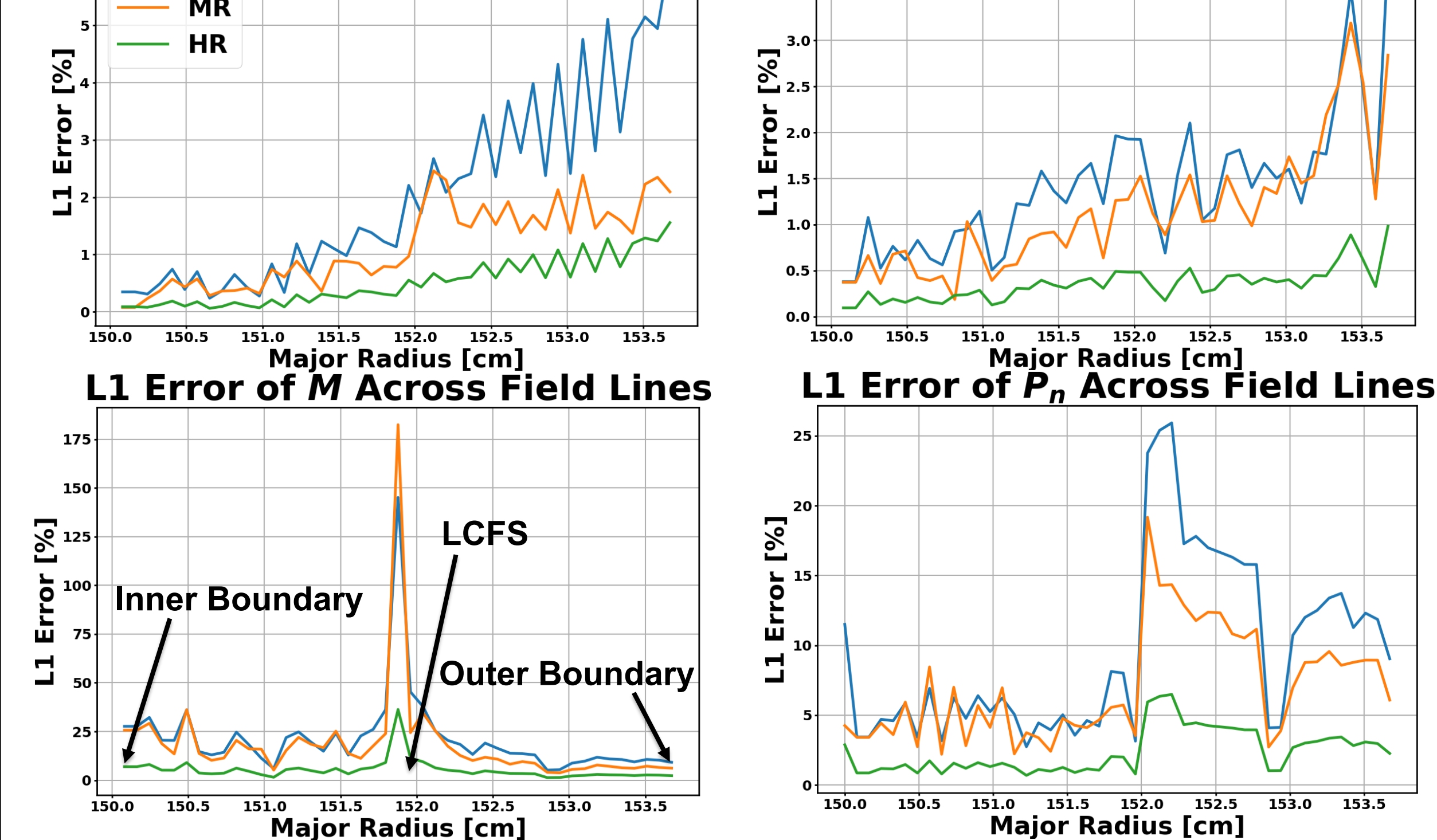
- h is some measure of grid spacing, p_d is the order of convergence ($p_d \approx 2$ expected for MC codes)

- To analyze, 3 grids of proportionally higher resolution are needed



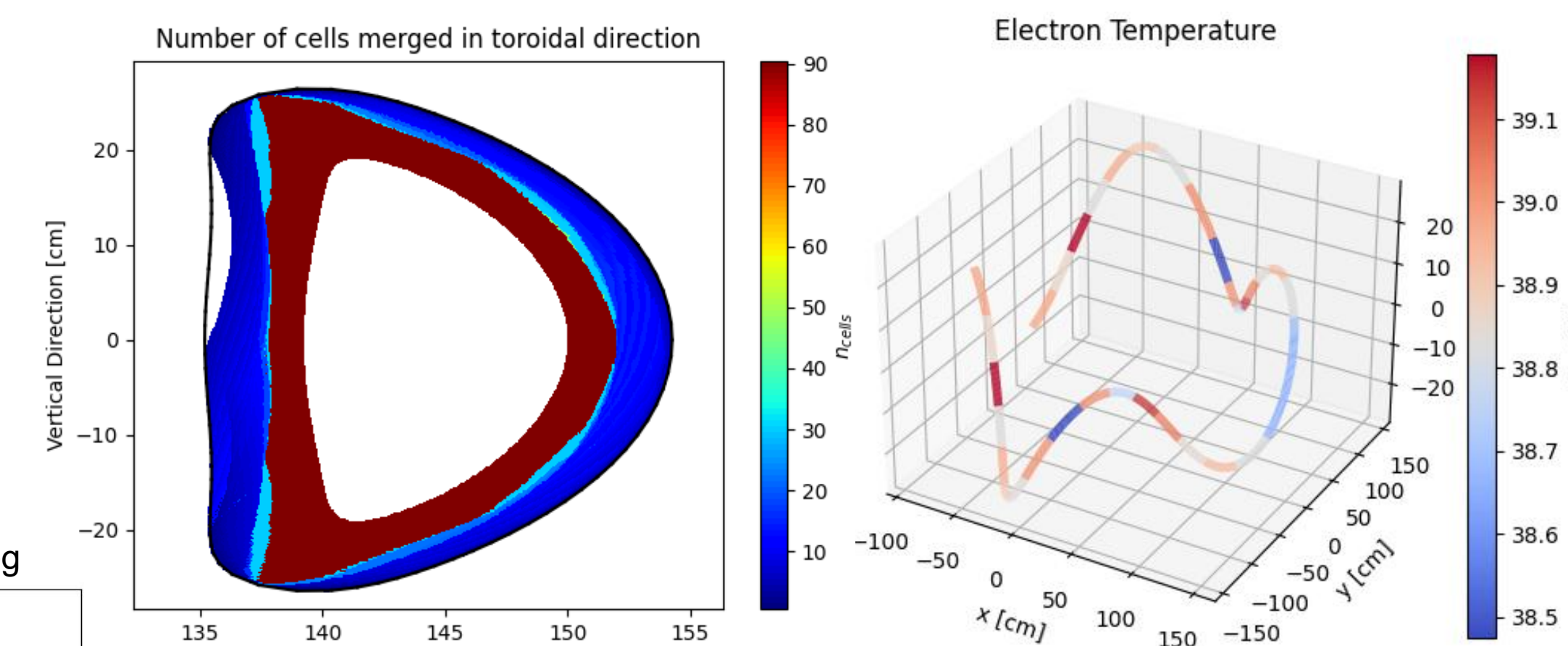
Plasma Domain (Wall in red) Extended Neutral Domain

Low Resolution (LR) Medium Resolution (MR) High Resolution (HR)



- Error taken with respect to continuum value estimated using Richardson Extrapolation: $f_{true} \approx \frac{4}{3}f_{HR} - \frac{1}{3}f_{MR}$ [6]

- Grid cells often merged in field aligned direction to reduce the computational requirements of simulations
- This drastically lowers grid fidelity inside LCFS



Grid Cells merged in field aligned direction in EMC3-EIRENE simulation T_e profile along field line in merged grid cells

- Cell merging introduces additional discretization error which is especially noticeable in neutral quantities

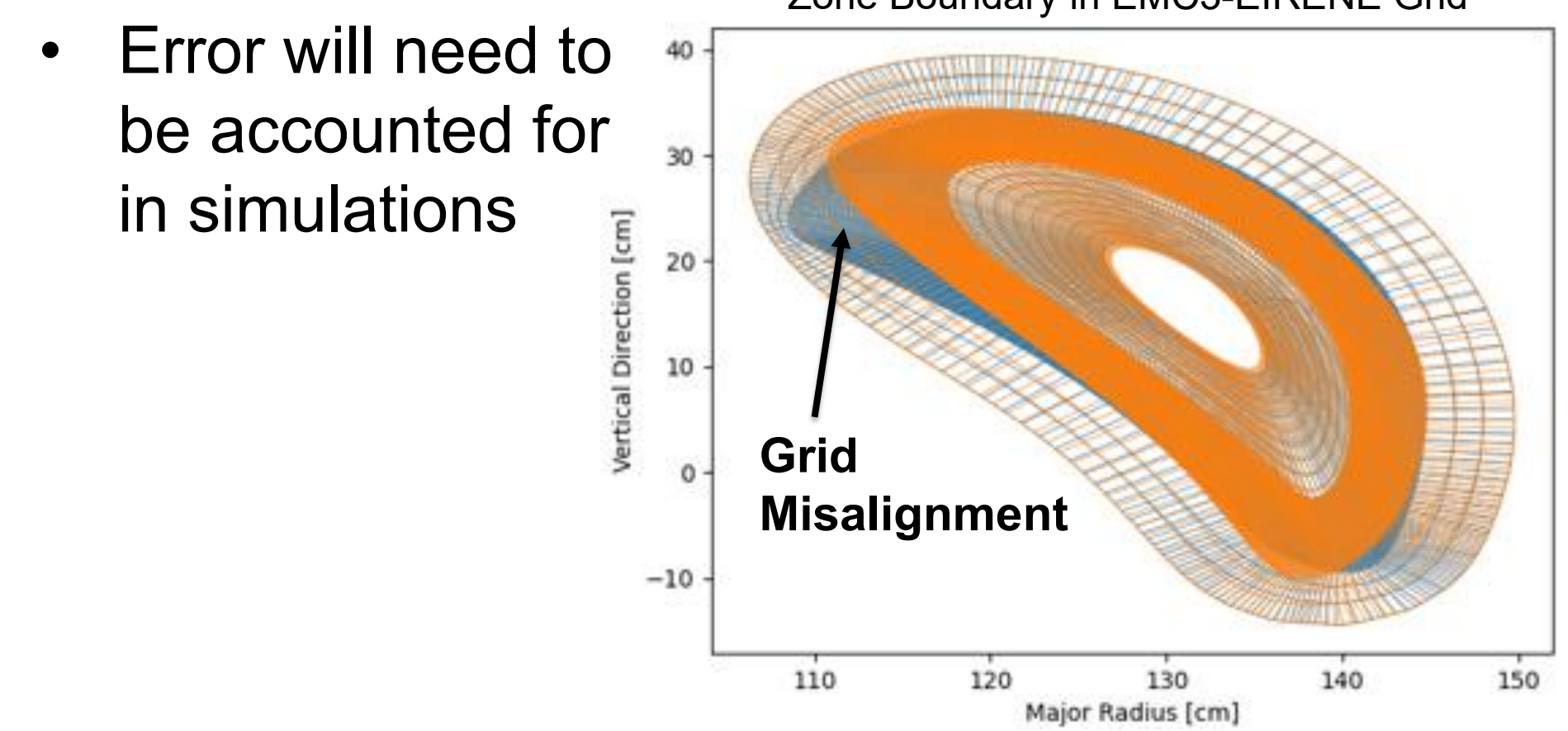
Plasma Data Error

n_i	4%
T_e	7%
M	54%

Neutral Data Error

n_H	32%
T_H	23%
P_n	33%

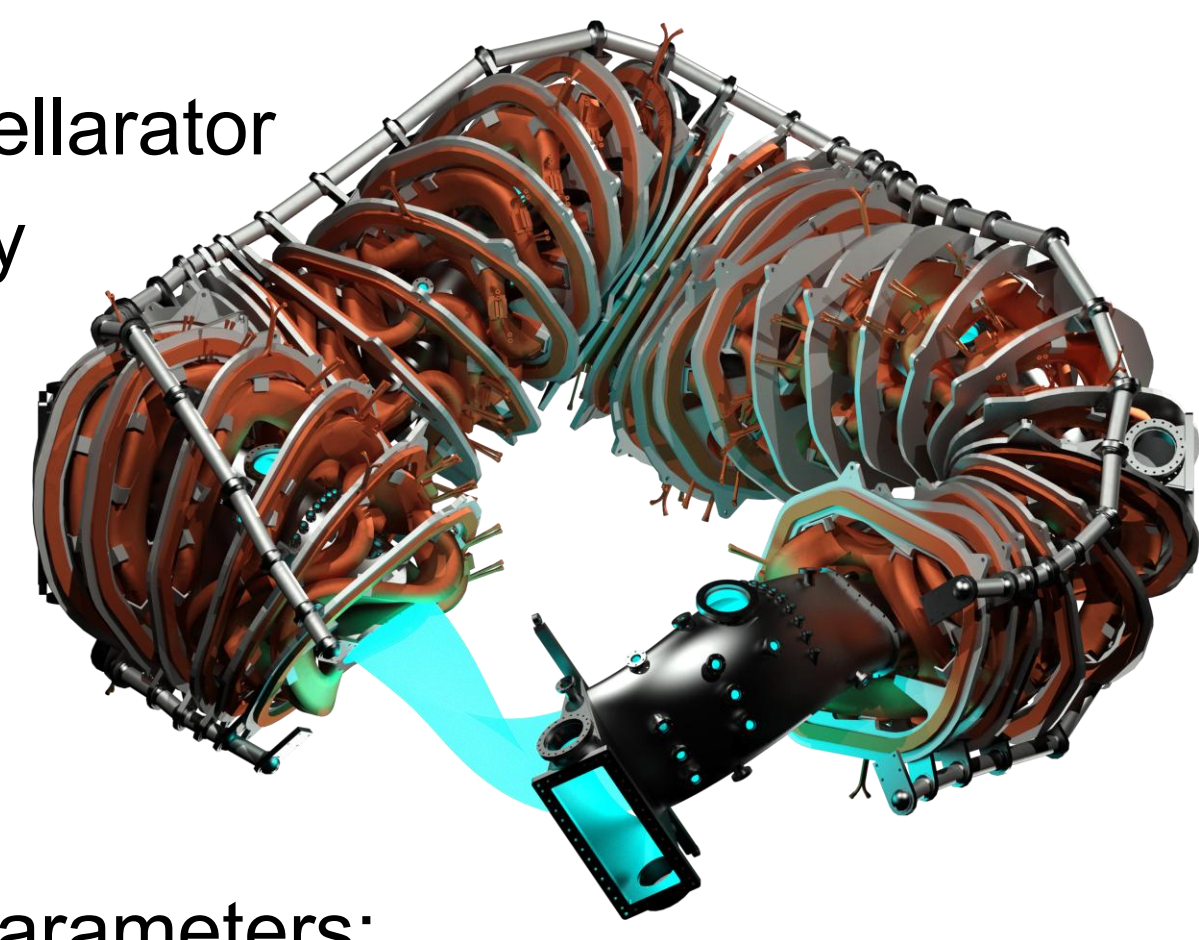
- Computational Mesh split into several toroidal zones. Zone boundaries can be misaligned and cause loss terms in simulations [7,8]



- Error will need to be accounted for in simulations
- The Discretization error is the most complex error as well as the most dominant error in EMC3-EIRENE

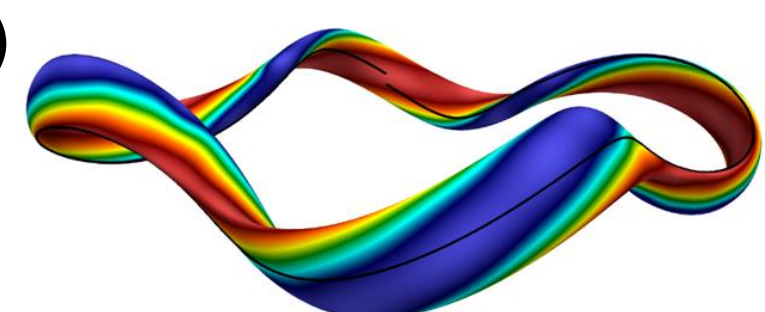
Helically Symmetric eXperiment

- HSX is an optimized stellarator
- Quasi-Helical symmetry
- 4-field symmetric
- Major radius: 1.2 m
- Minor radius: 12 cm
- Main Field: 1 T



- EMC3-EIRENE Input parameters:

- Magnetic geometry: quasi-helical symmetry
- Species: hydrogen (no impurities)
- Input power: 200 kW



Bias Error (ϵ_b) & Statistical Error (ϵ_s)

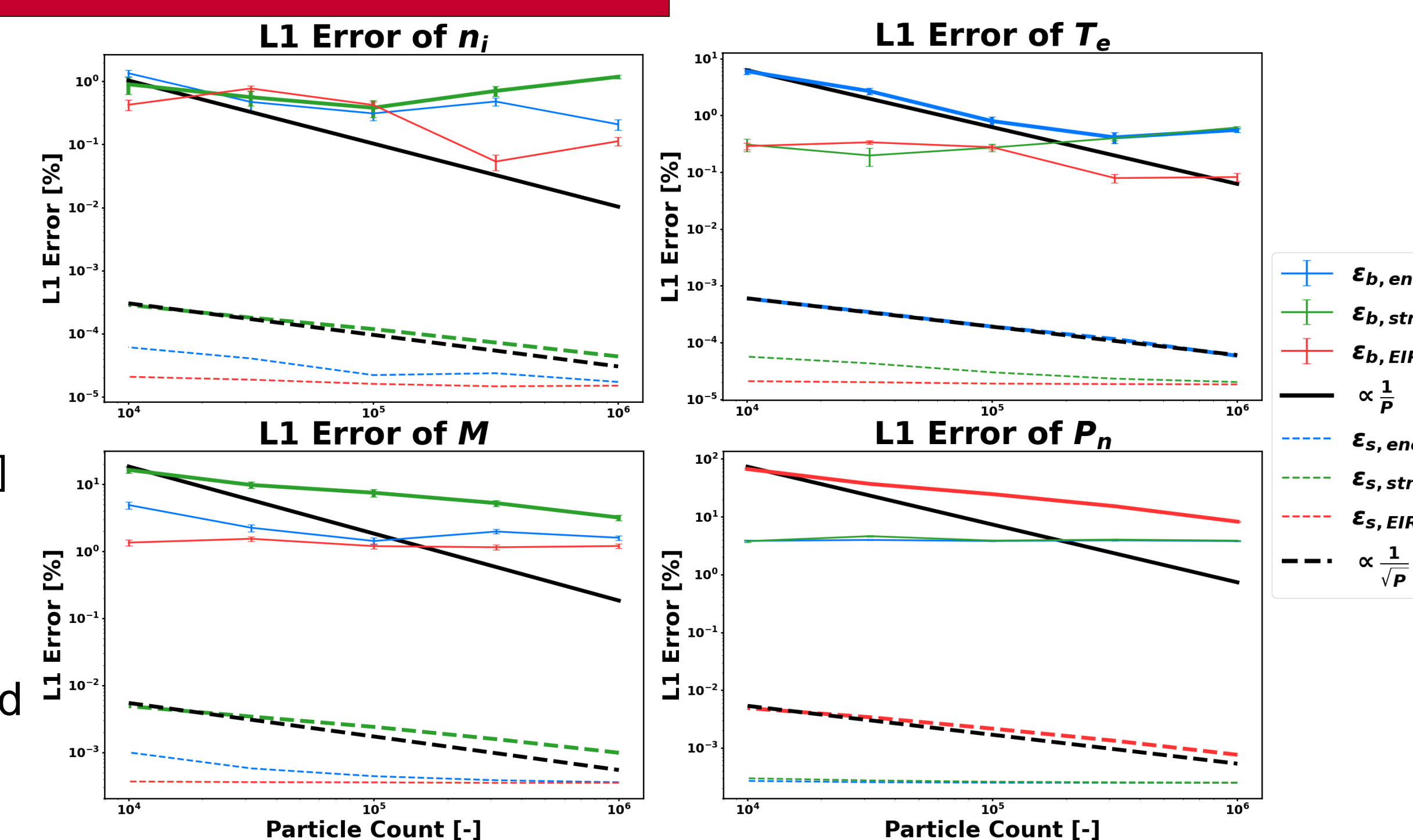
- The bias error is composed of the convergence and deterministic errors due to finite MC particles

$$\epsilon_b \propto \frac{1}{P}$$

- The statistical error is characterized by the standard deviation σ

$$\sigma_1 \propto \frac{1}{\sqrt{P}} \quad \epsilon_s \approx \sigma = \frac{\sigma_1}{\sqrt{I}} \propto \frac{\sqrt{T}}{\sqrt{PI}} \quad [4]$$

- P is particle count, σ_1 is sample standard deviation, I is iteration count solution is averaged over, T is correlation time (accounts for solution dependence iteration to iteration)



Summary & Future Work

- The time integration and statistical error generally follow predicted scaling. The bias error exhibits weaker correlation with theoretical reduction rates.
- The discretization error has been characterized, and local regimes of high error have been identified.
- These results are similar to what was found in [4] for DIII-D geometry.
- Plan to quantify error due to cell merging, zonal boundary misalignment, and EMC3-EIRENE's impurity module.
- Plan to analyze error in different HSX magnetic configurations, density regimes, and in the lofted wall scheme of HSX [9]

References

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