Optimizing the performance of fusion reactors at exascale

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PPPL PRINCETON PLASMA PHYSICS LABORATORY

PSFC MIT Plasma Science & Fusion Center

Fusion 101: star power!

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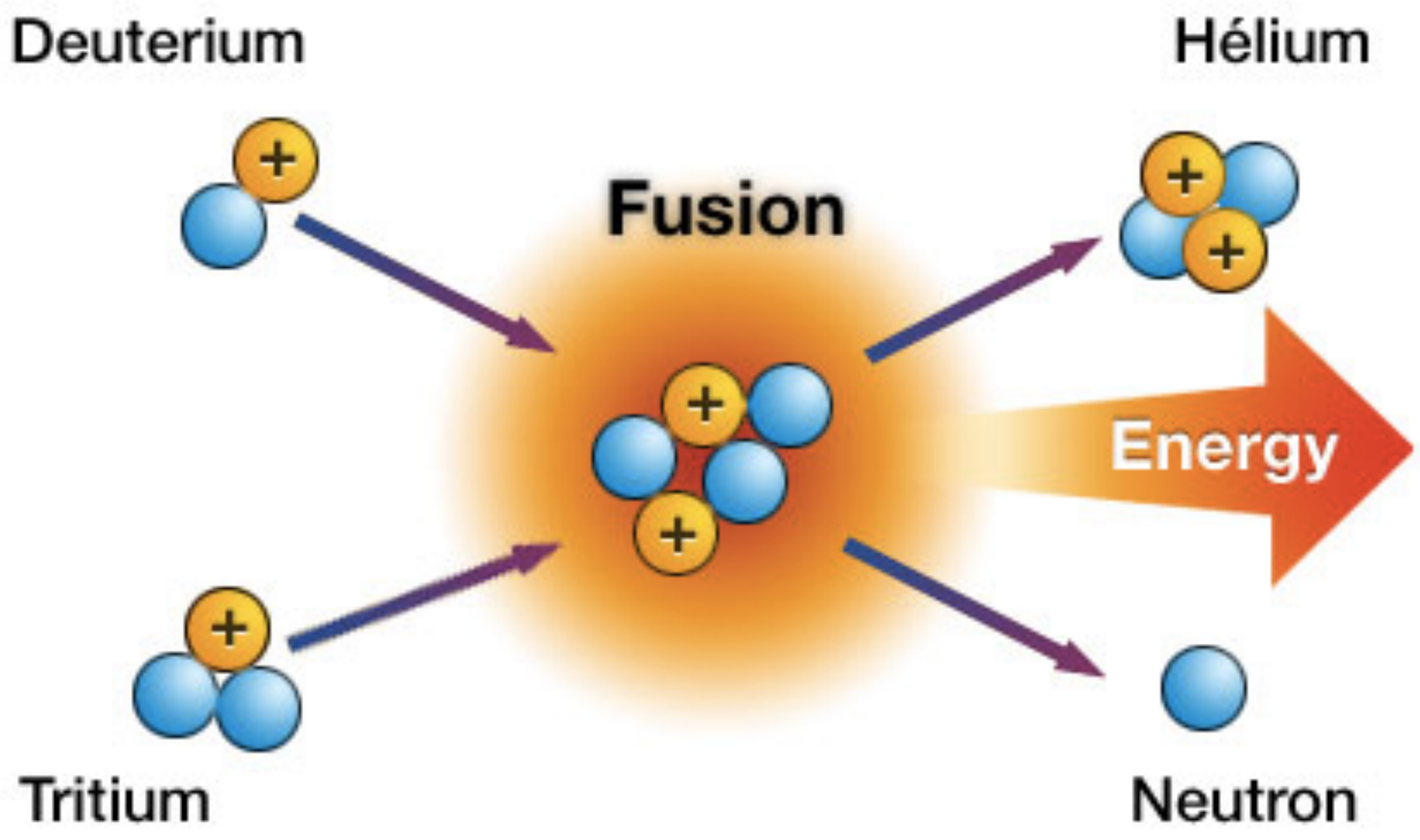
- **Fusion** is the energy that powers the stars



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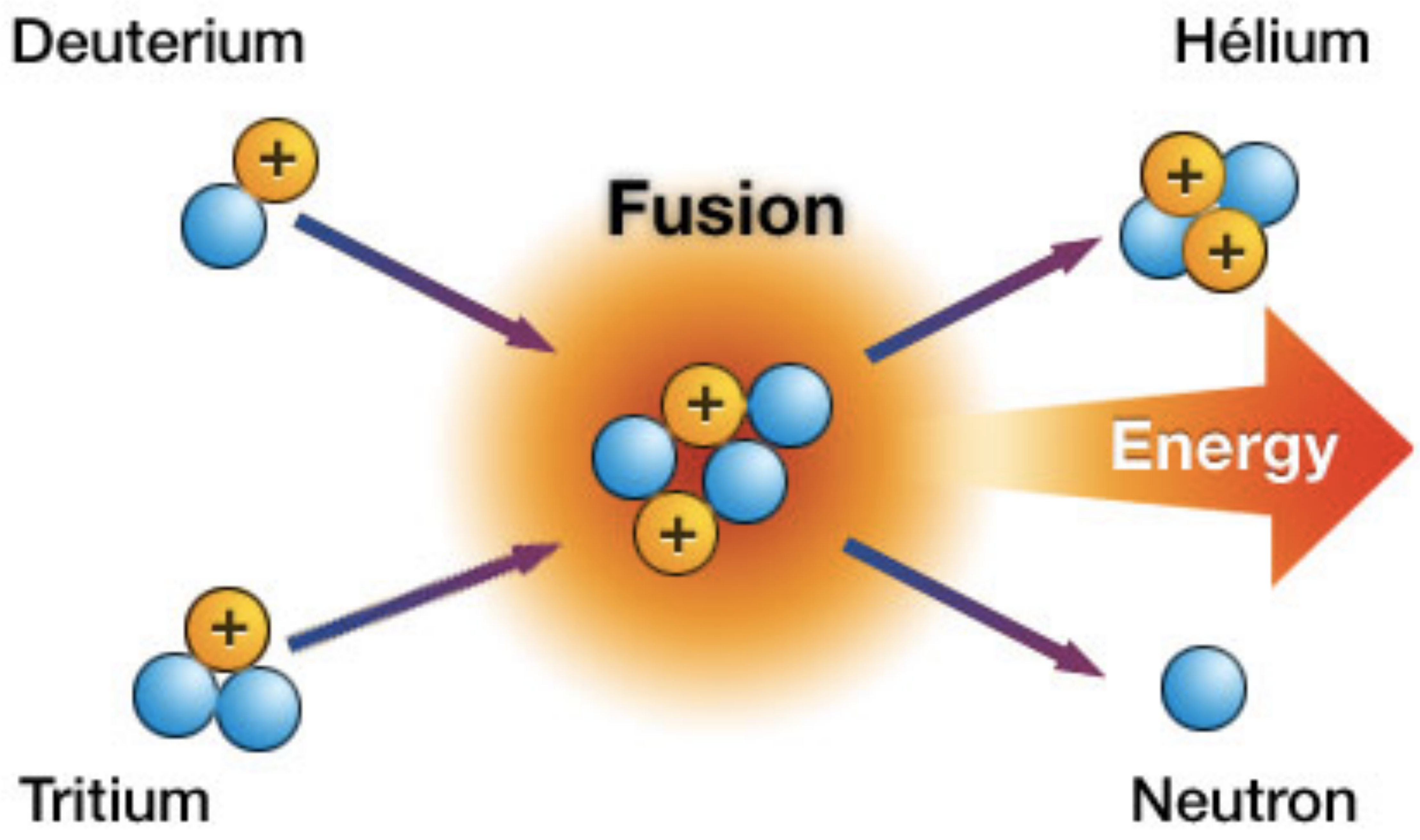

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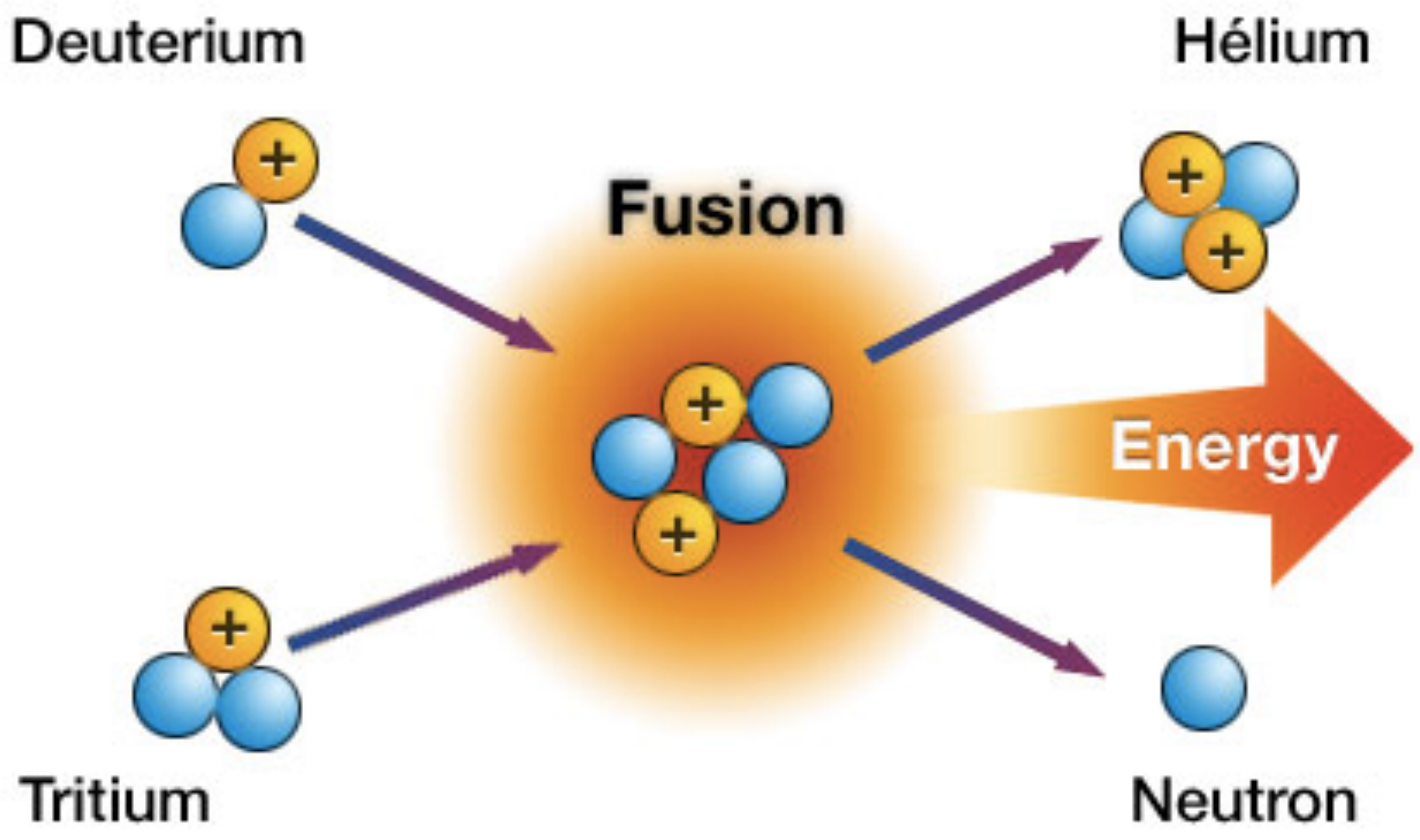

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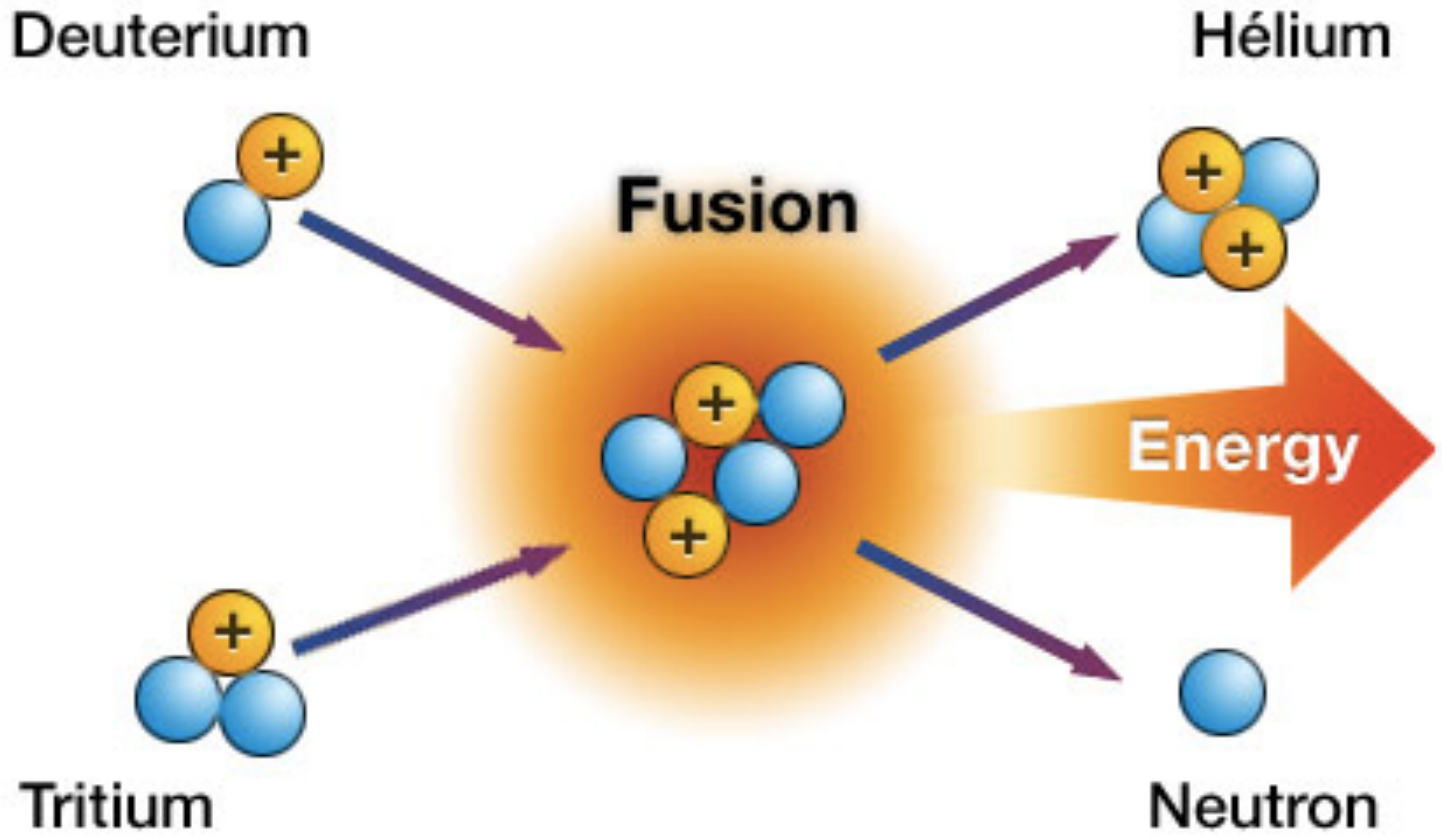

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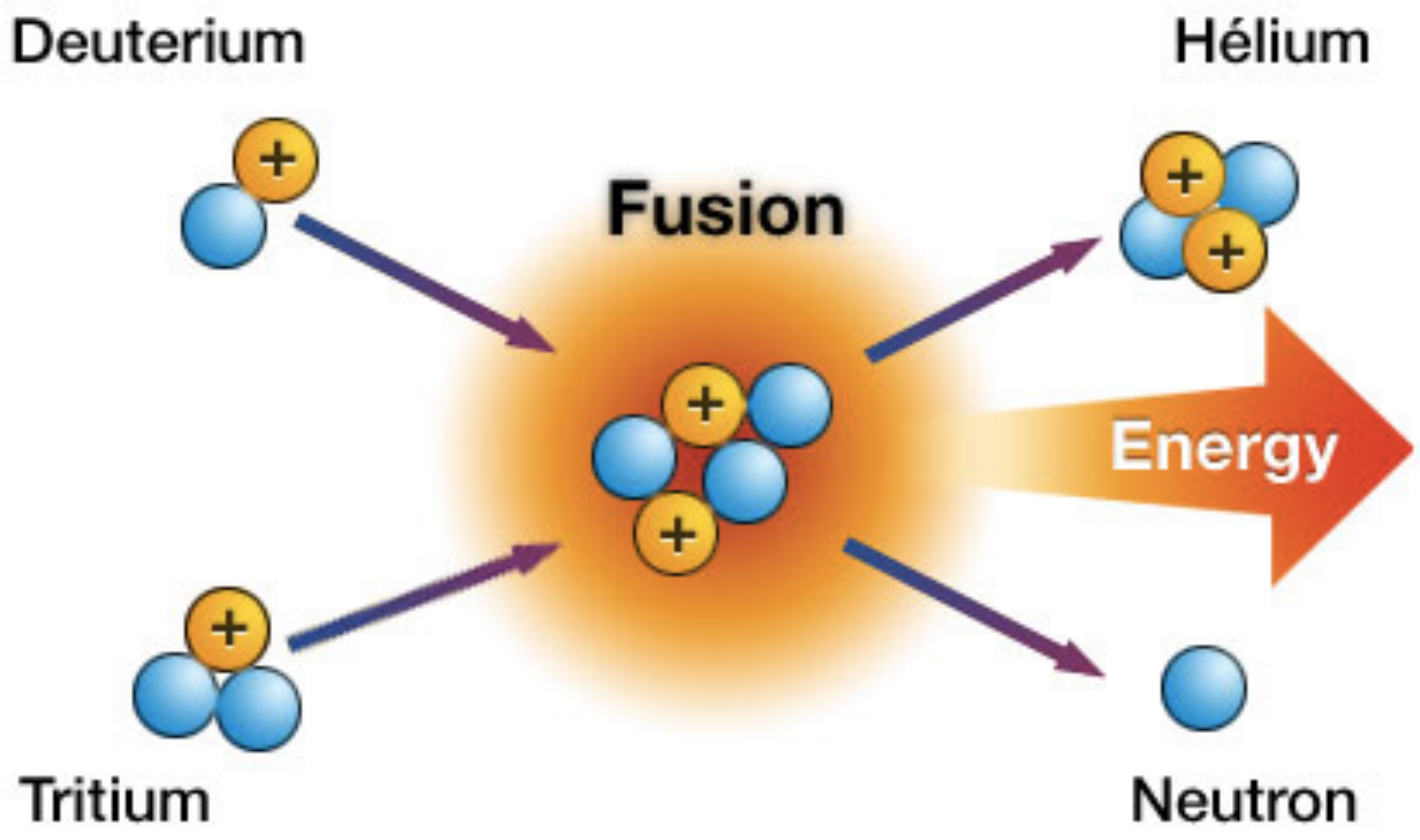

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- The development of **fusion** as a viable commercial energy source will be a game-changer for the **health of the planet** in the coming decades, because it is a clean and virtually limitless energy source
    - Minimal carbon footprint, no long-lived radioactive byproducts, safe (no meltdown scenario)

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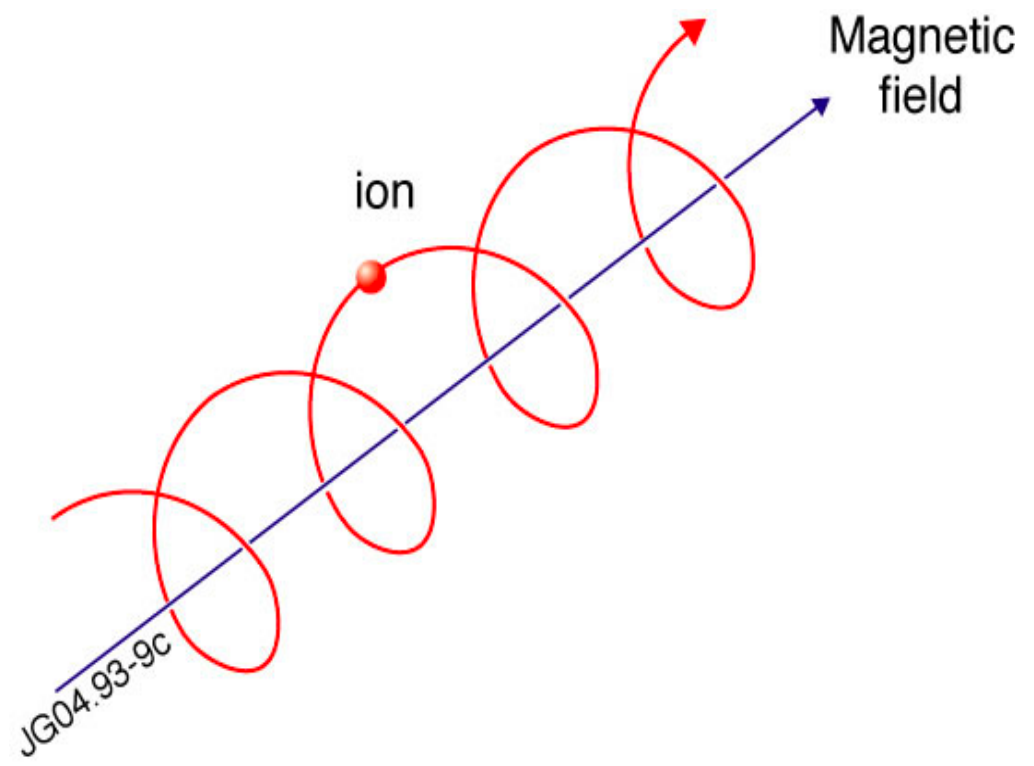

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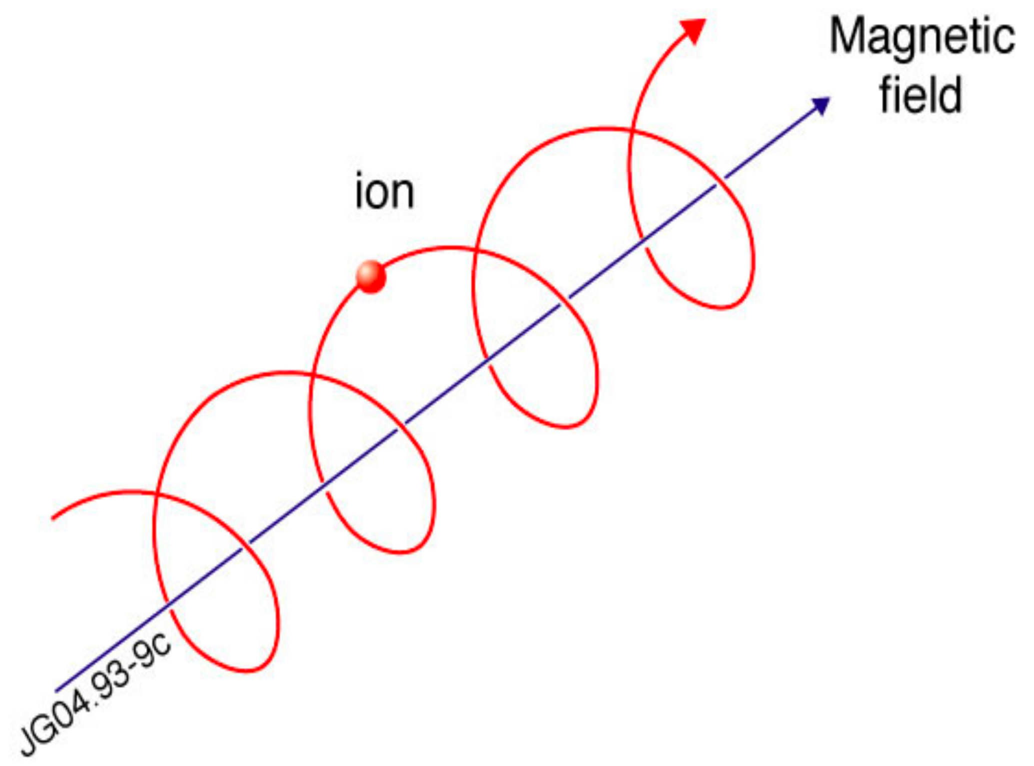

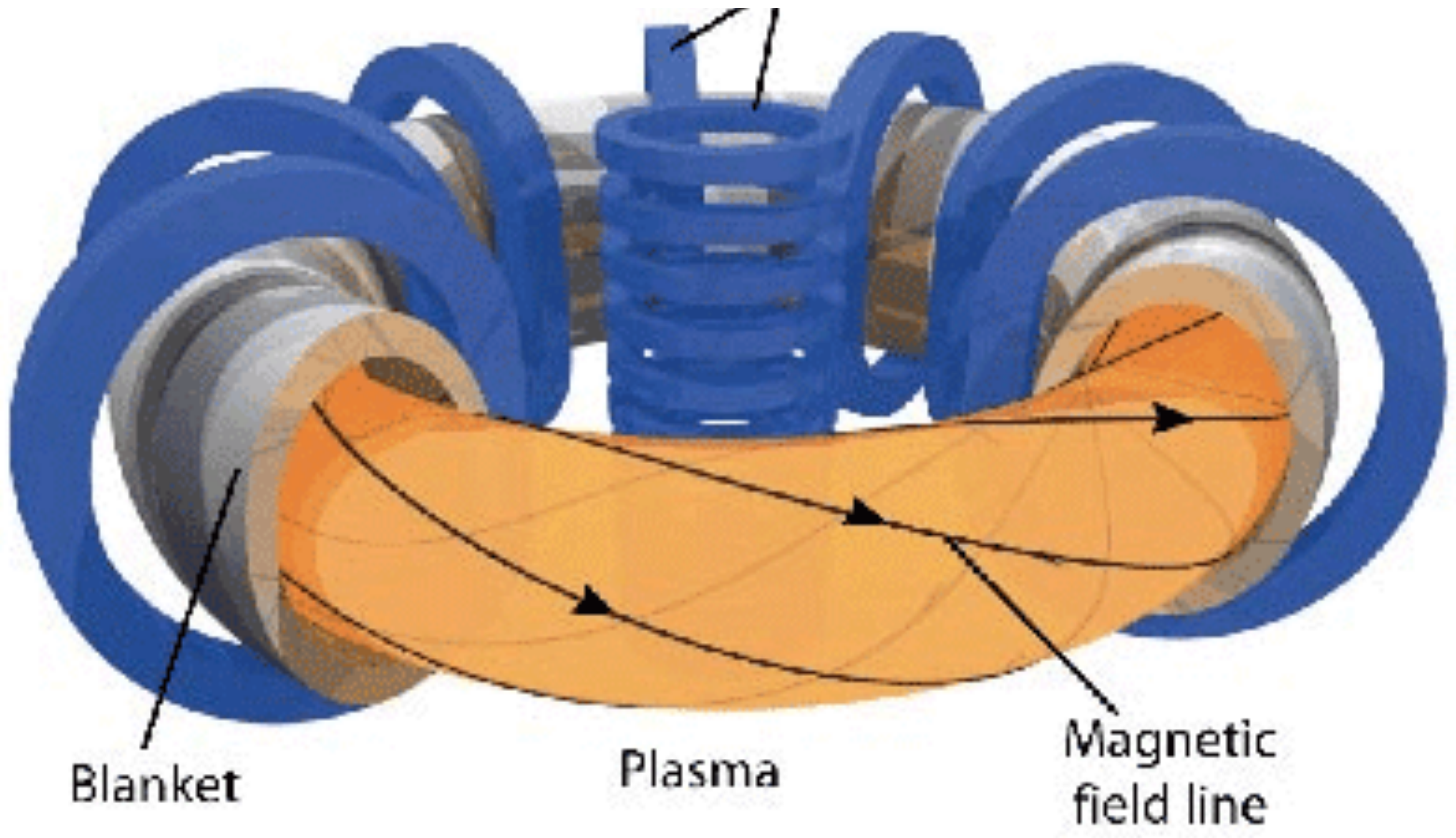

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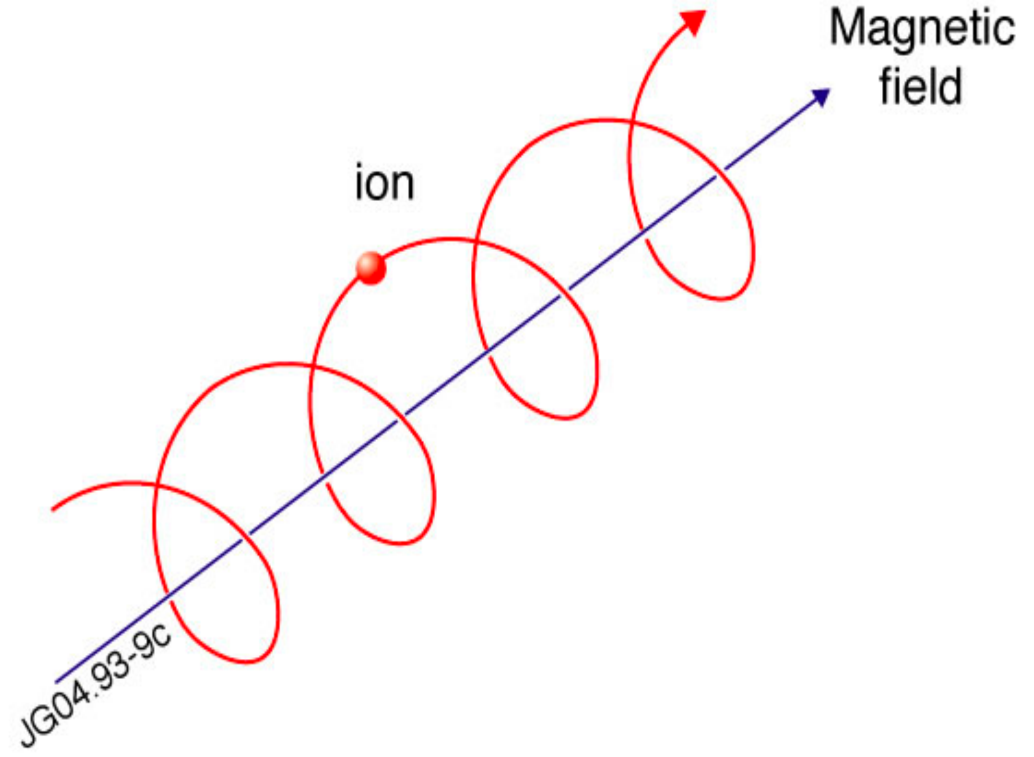

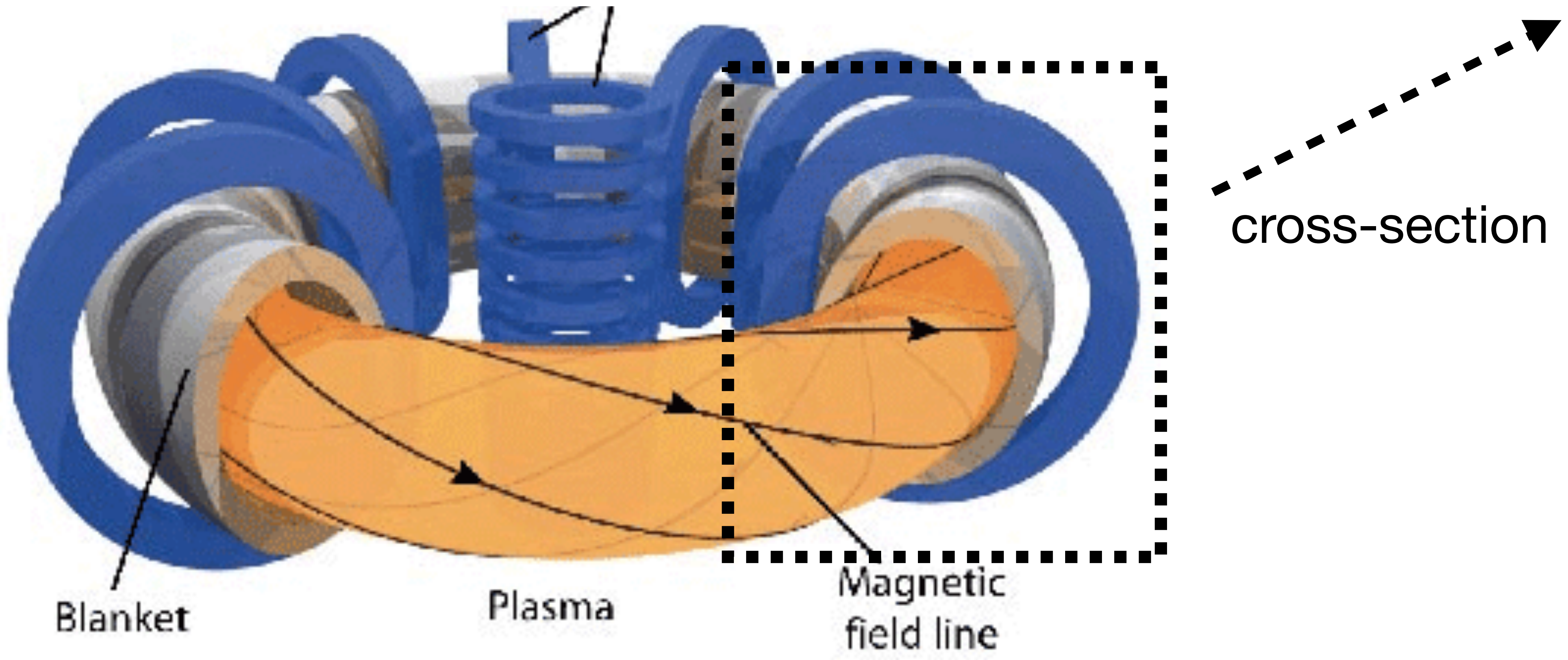

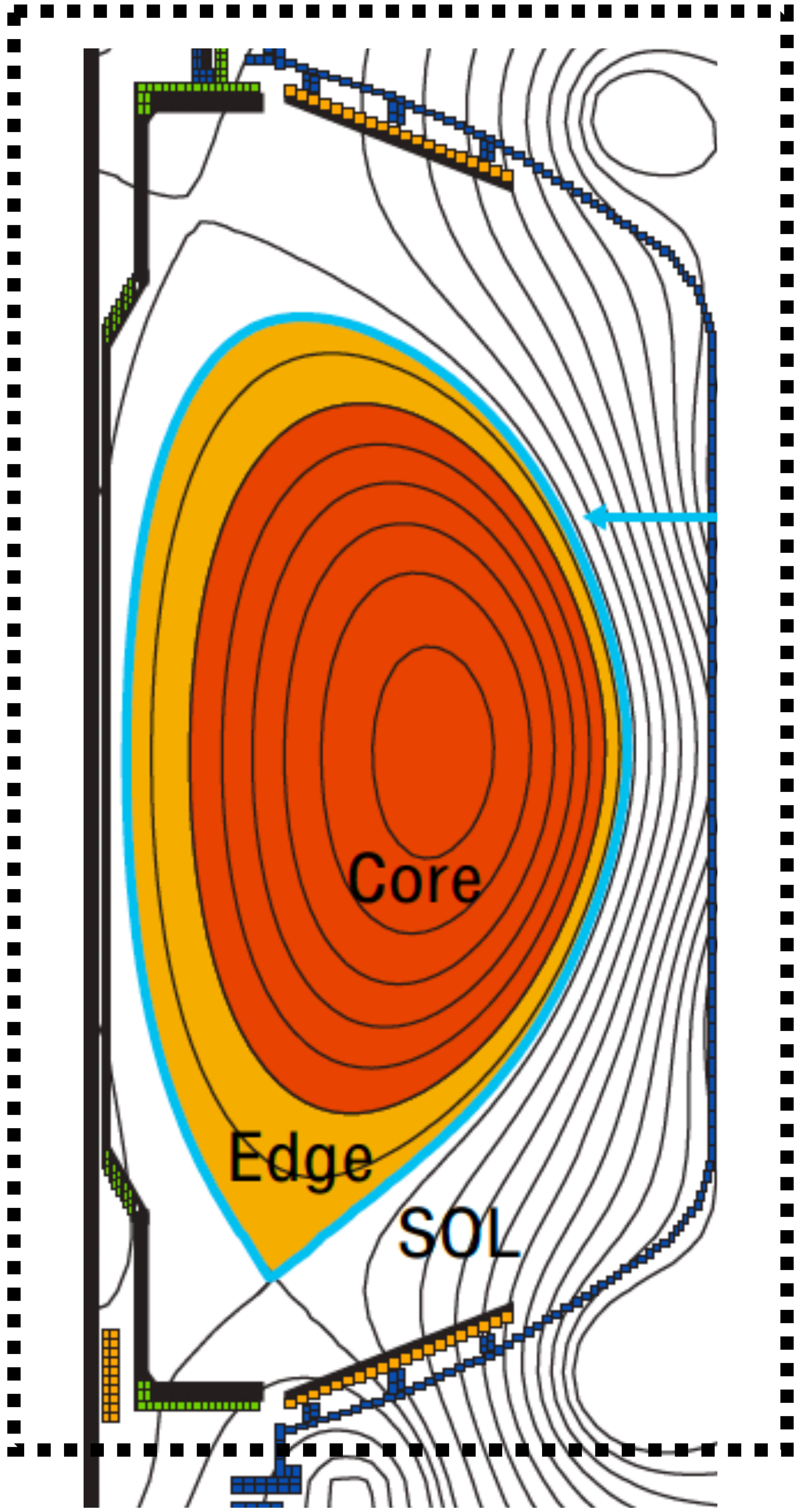

Figure adapted from Stoltzfus-Dueck (2009)

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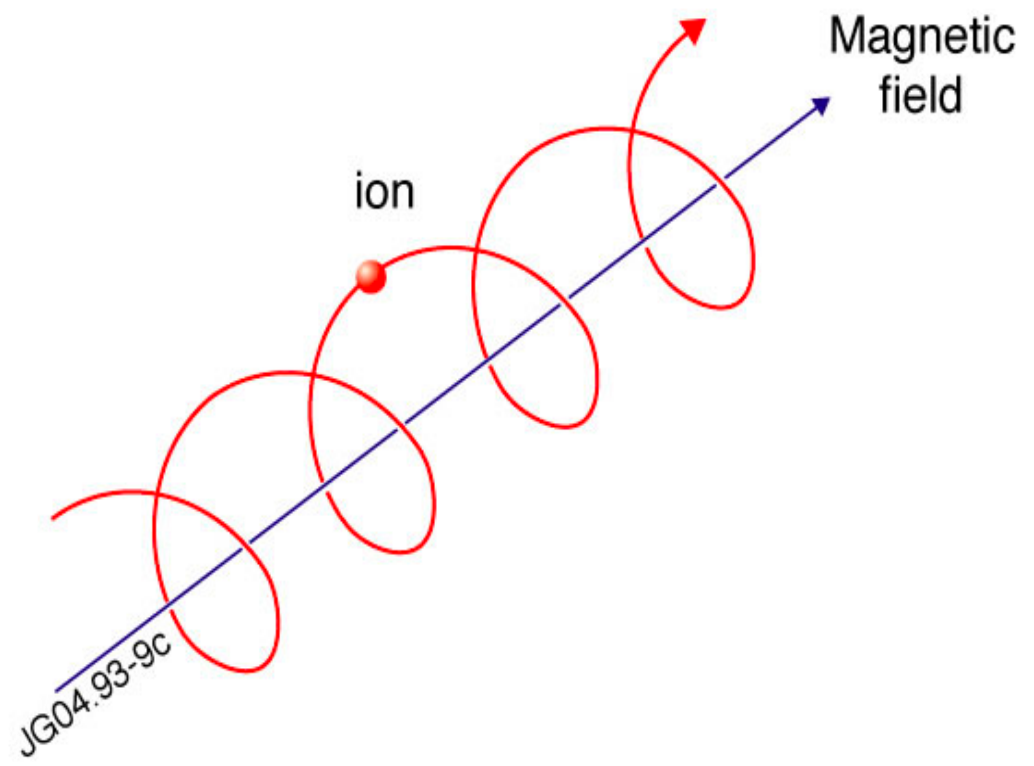
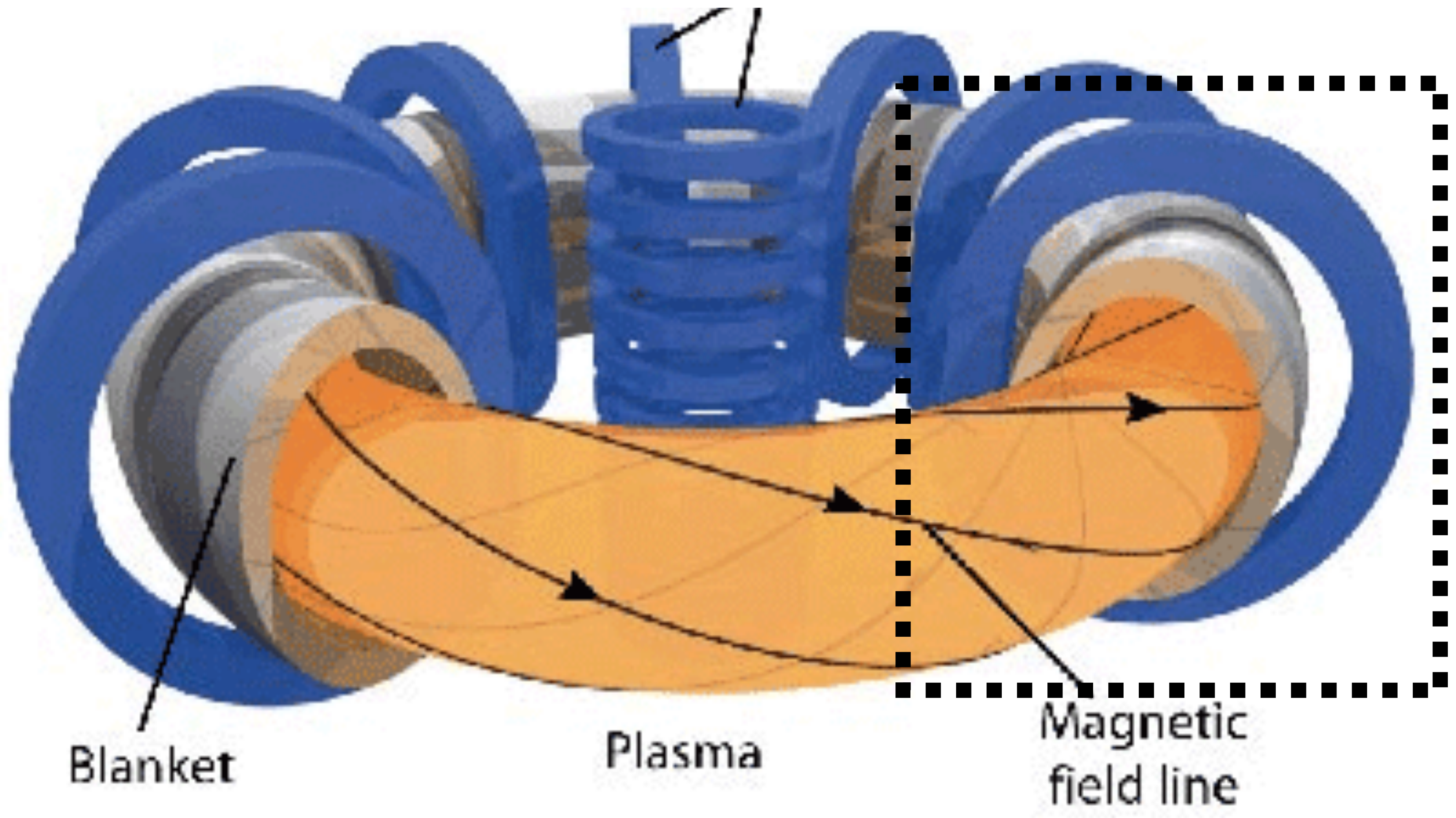
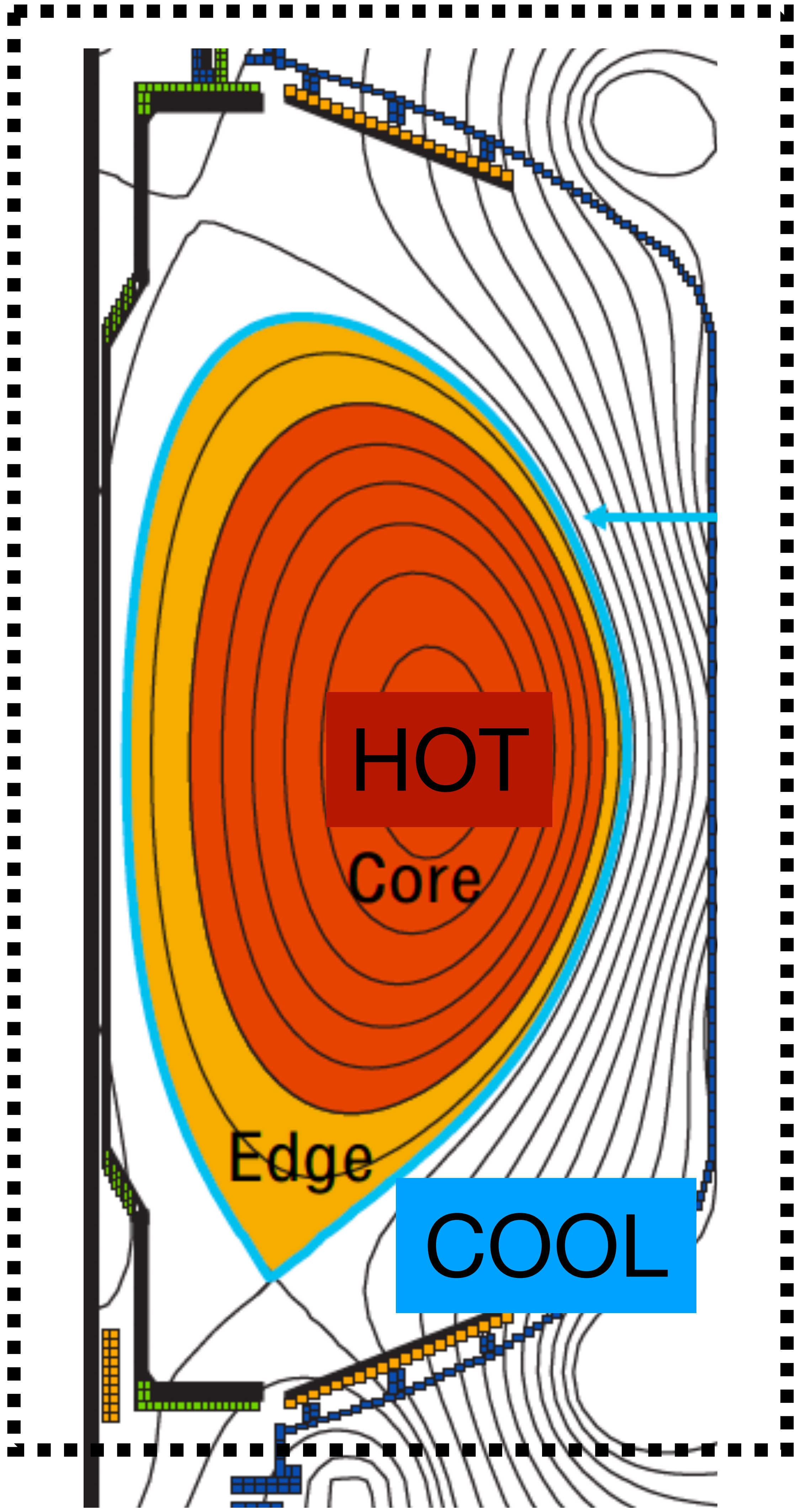
- The most advanced designs are donut-shaped: tokamaks & stellarators
    - In the “core”, the magnetic field lines are “closed”, wrapping around the concentric surfaces of the donut
    - Temperature gradients between hot core and cool walls are more than 1000x steeper than gradients handled by reentry tiles on spacecraft





cross-section



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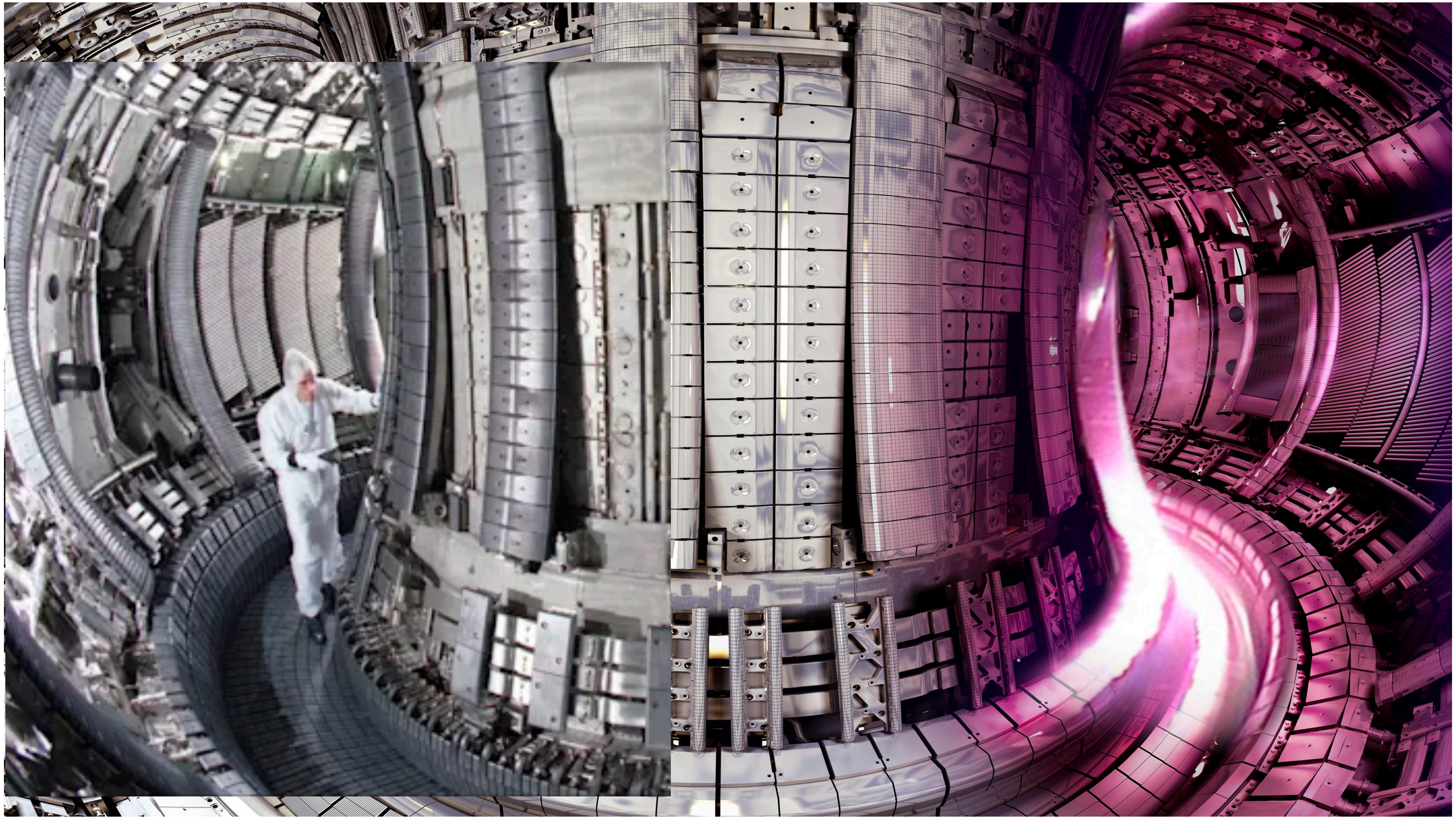
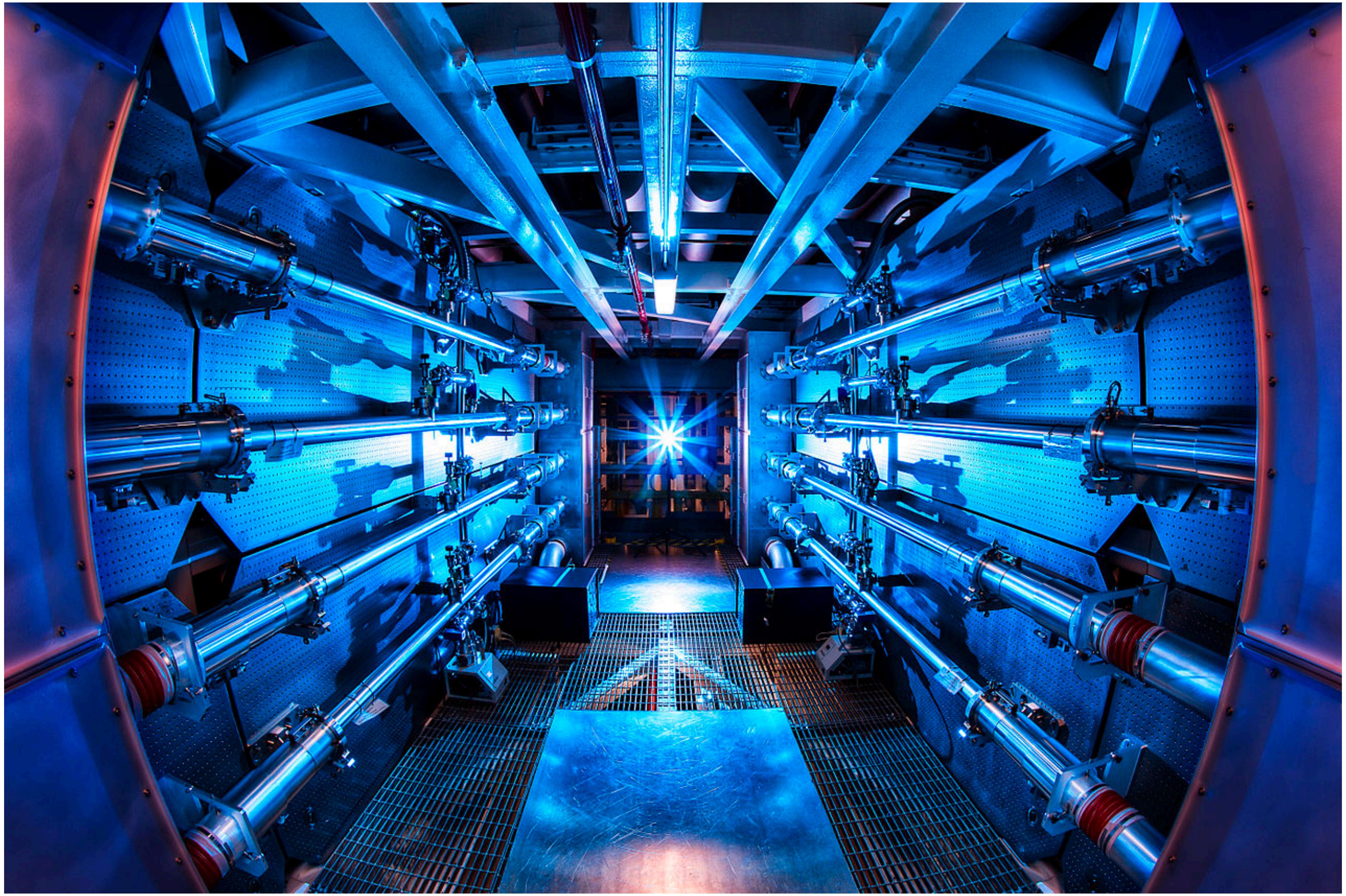
Exciting times in fusion: JET sets fusion power record

- The Joint European Torus (JET) tokamak recently set a record of 59 MJ of fusion power over 5 seconds (Q = 0.33)



Exciting times in fusion: NIF breaks even(?)

- National Ignition Facility (NIF) at LLNL uses inertial confinement fusion (shoots super-lasers at a tiny capsule to implode it)
- Produced 14 kJ of energy, more than the x-ray energy absorbed (break-even?), but still a small fraction of the 1.8 MJ laser energy



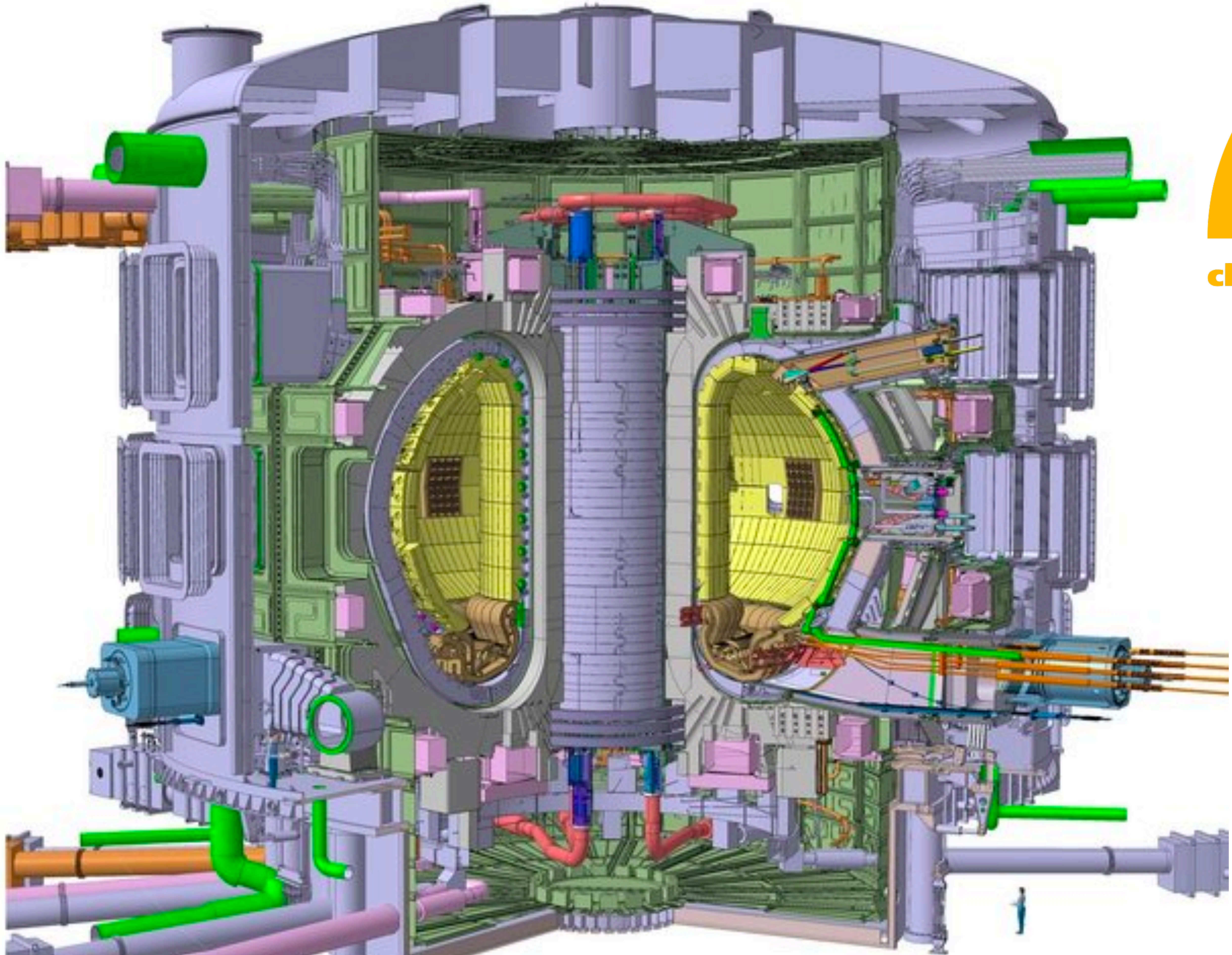
National Nuclear Security Administration

Exciting times in fusion: ITER on the way

- The ITER tokamak experiment will produce 500 MW of fusion power from 50 MW of heating power (Q = 10), with 400+ sec pulses
  - Under construction in France, projected to begin operation in 2025?, Q>1 in 2035. Massive international collaboration involving 35 nations. ~$25B

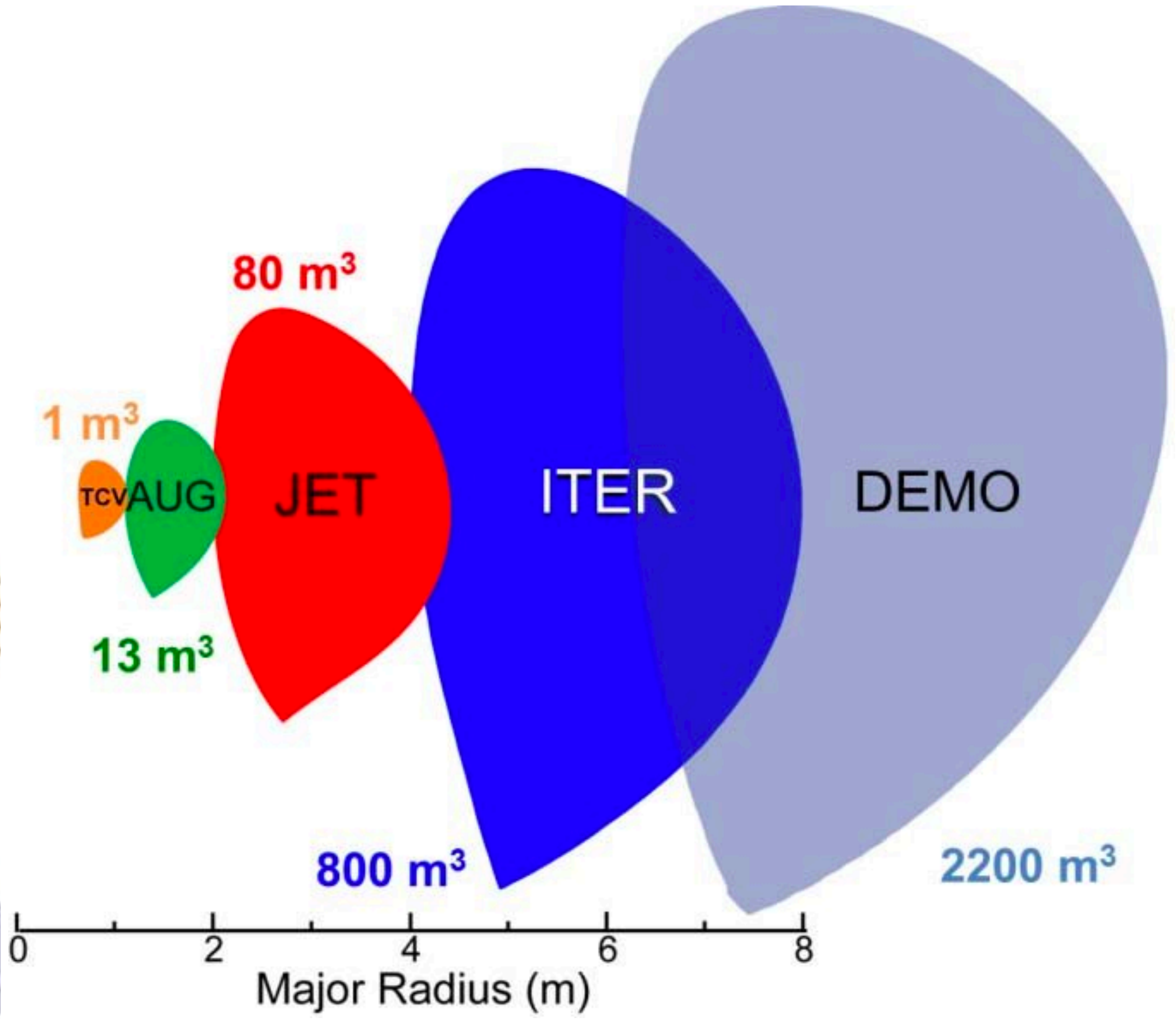
ITER = “The Way” in Latin

JET



ITER
(10x bigger by plasma volume than JET)

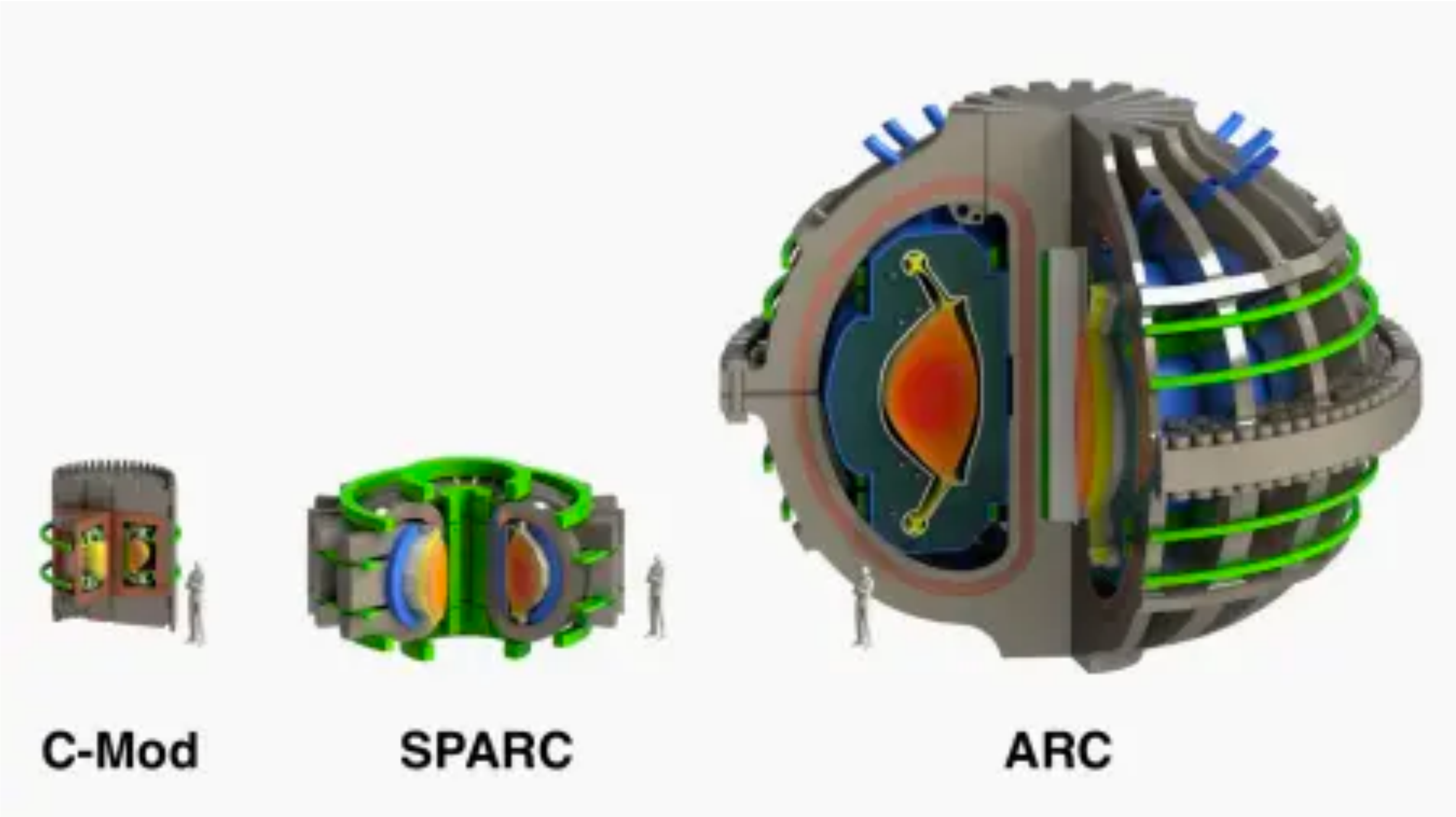
china eu india japan korea russia usa



Exciting times in fusion: SPARC/CFS go private

- MIT spin-off Commonwealth Fusion Systems (CFS) has begun building the SPARC tokamak
  - Stronger magnetic fields enabled by new high temperature superconducting magnets will give similar performance as ITER in a smaller device. Target is $Q>2$, could achieve $Q\sim10$.
    - Breakthrough: successful demonstration of 20T toroidal field magnet in late 2021.
  - Projected to begin operation in 2025, with $Q>1$ soon after.

Commonwealth Fusion Systems



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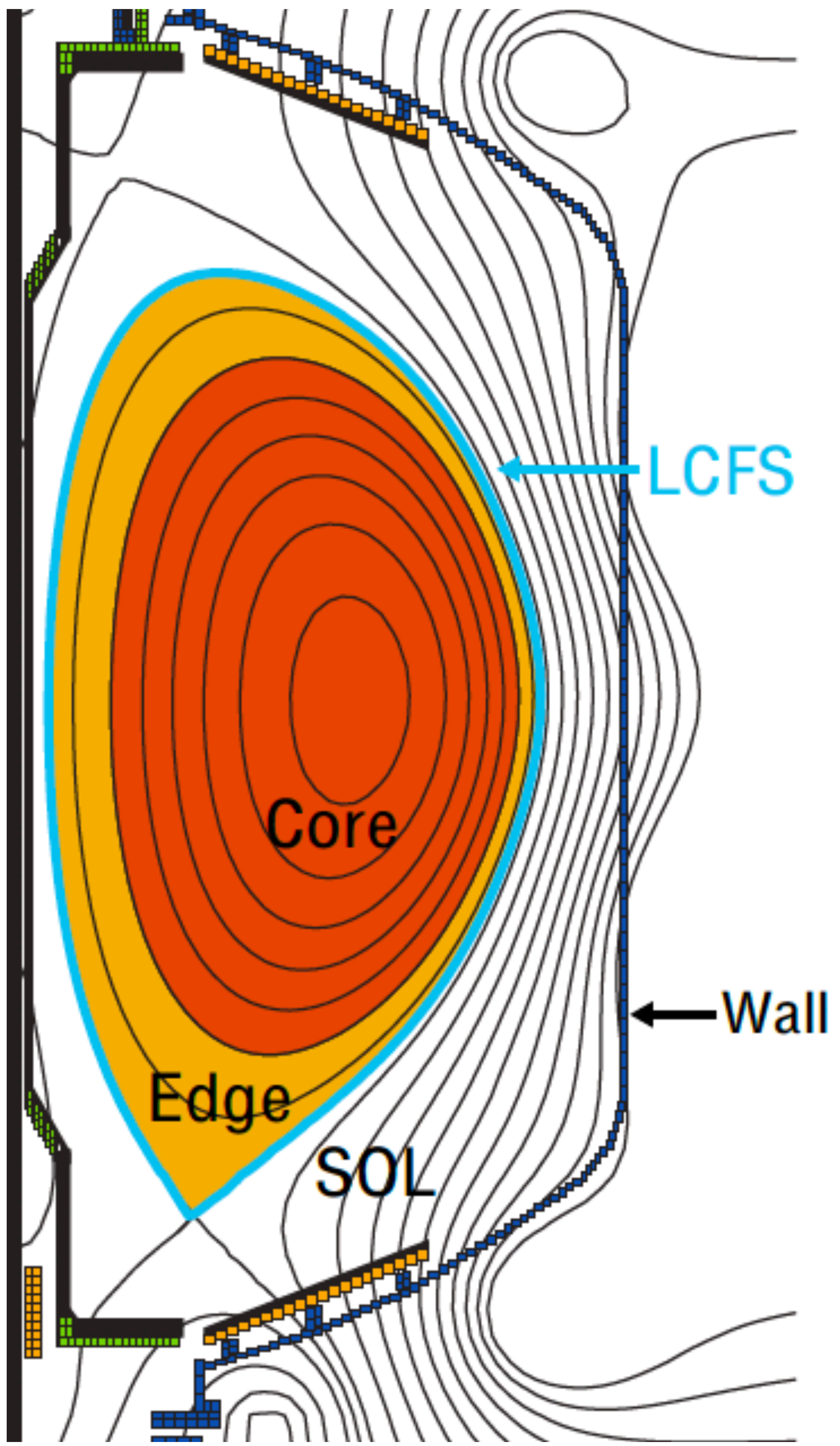

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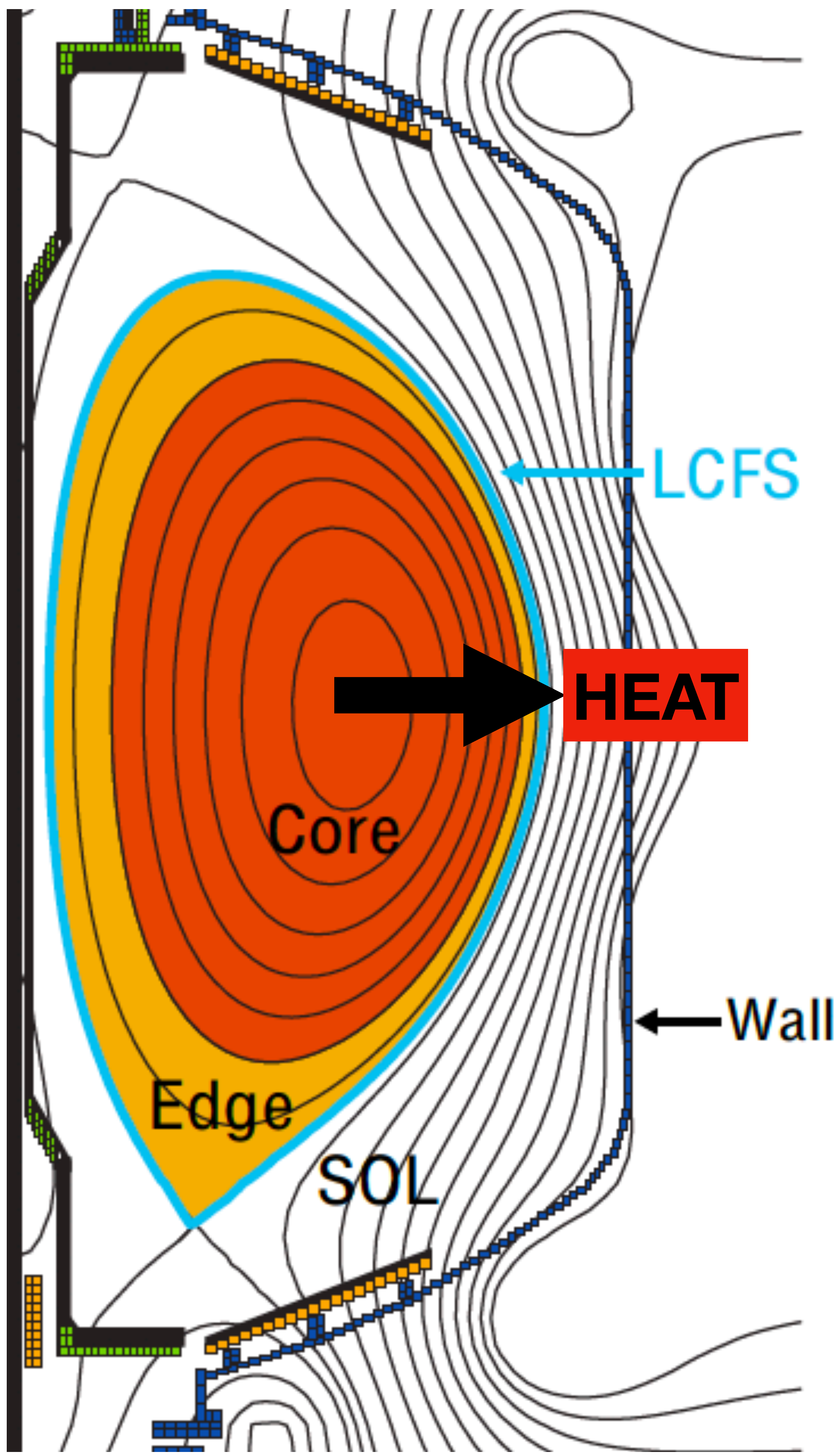
    - Nature doesn’t like temperature gradients that steep!

    - Bigger reactors (e.g. ITER) or stronger magnetic fields (e.g. SPARC) can help



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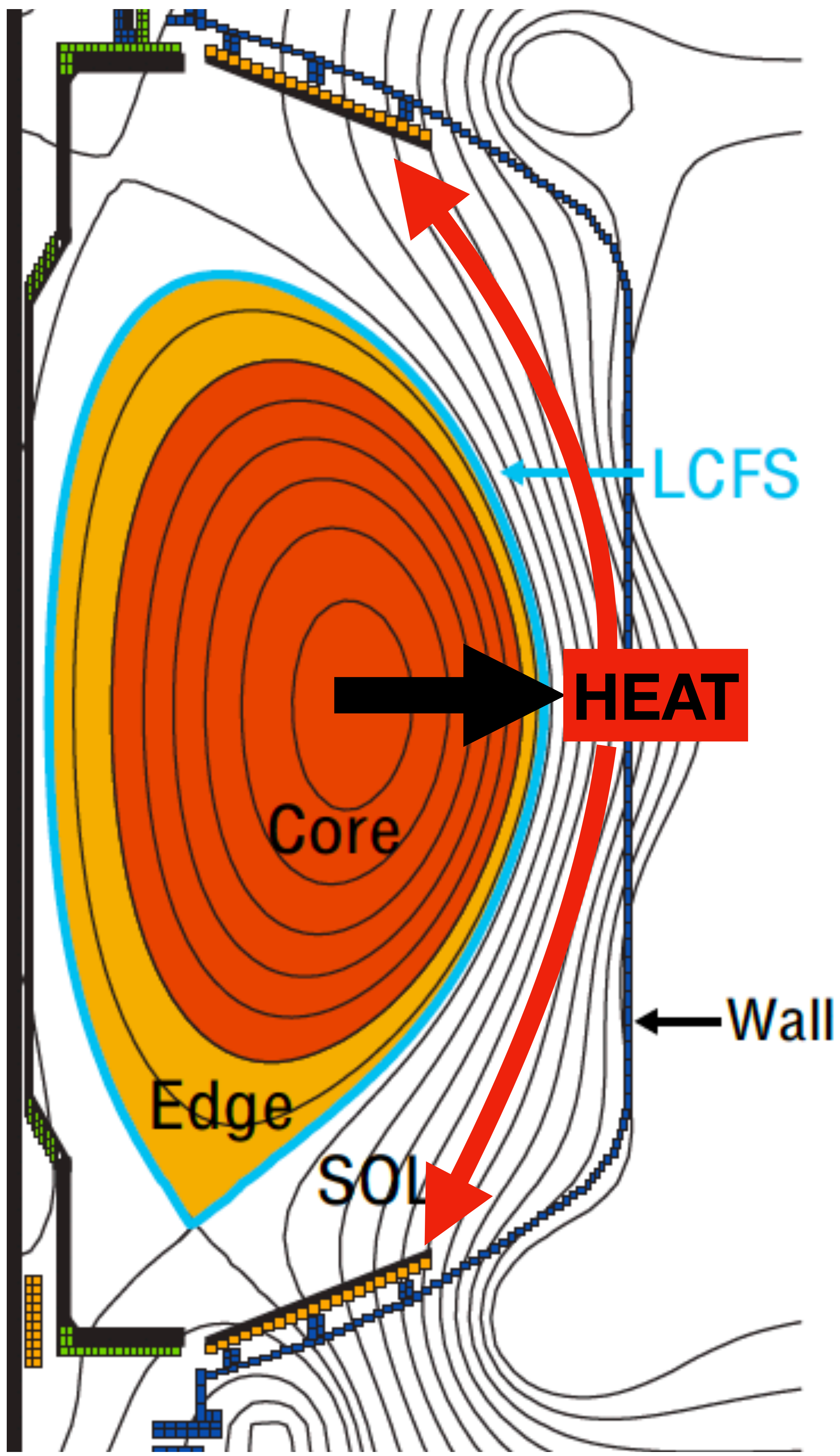

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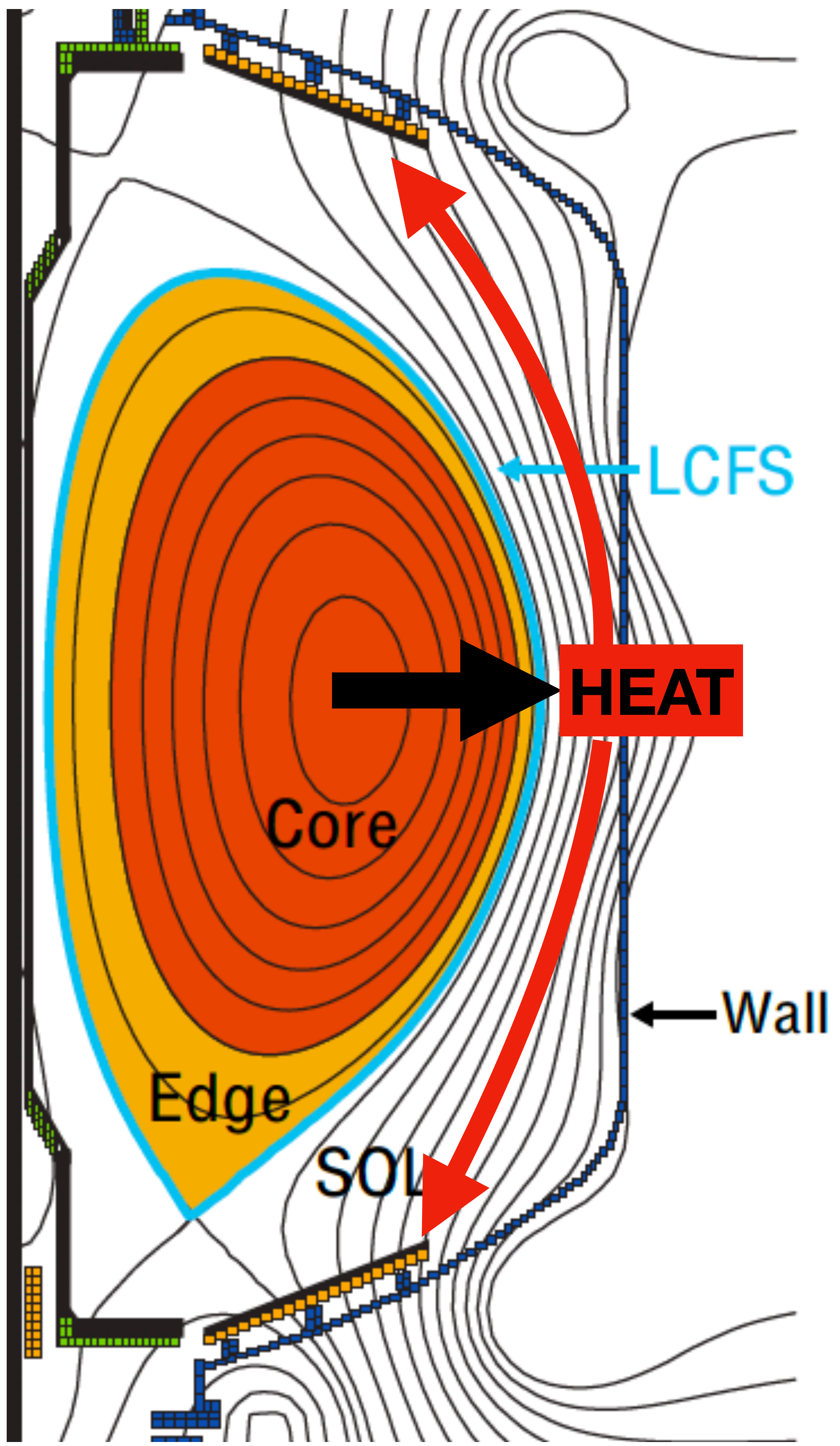
- Need a simultaneous **whole-device** solution to these coupled problems



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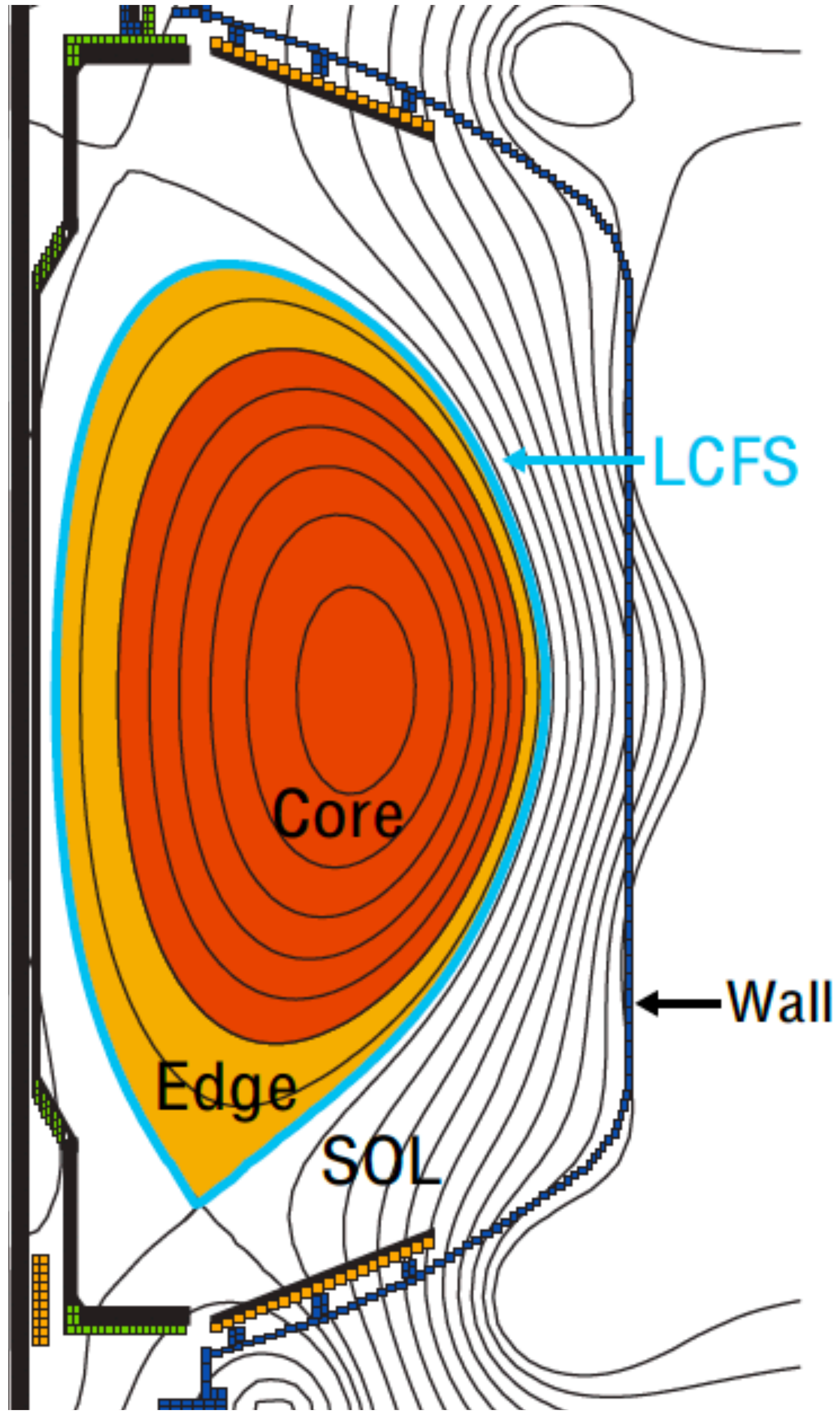
Whole-device modeling and optimization



Whole-device modeling and optimization

- **Whole-device turbulent transport modeling and optimization** are areas where **exascale high-performance computing** can make a large impact on the success of fusion by enabling the design of more efficient fusion reactors
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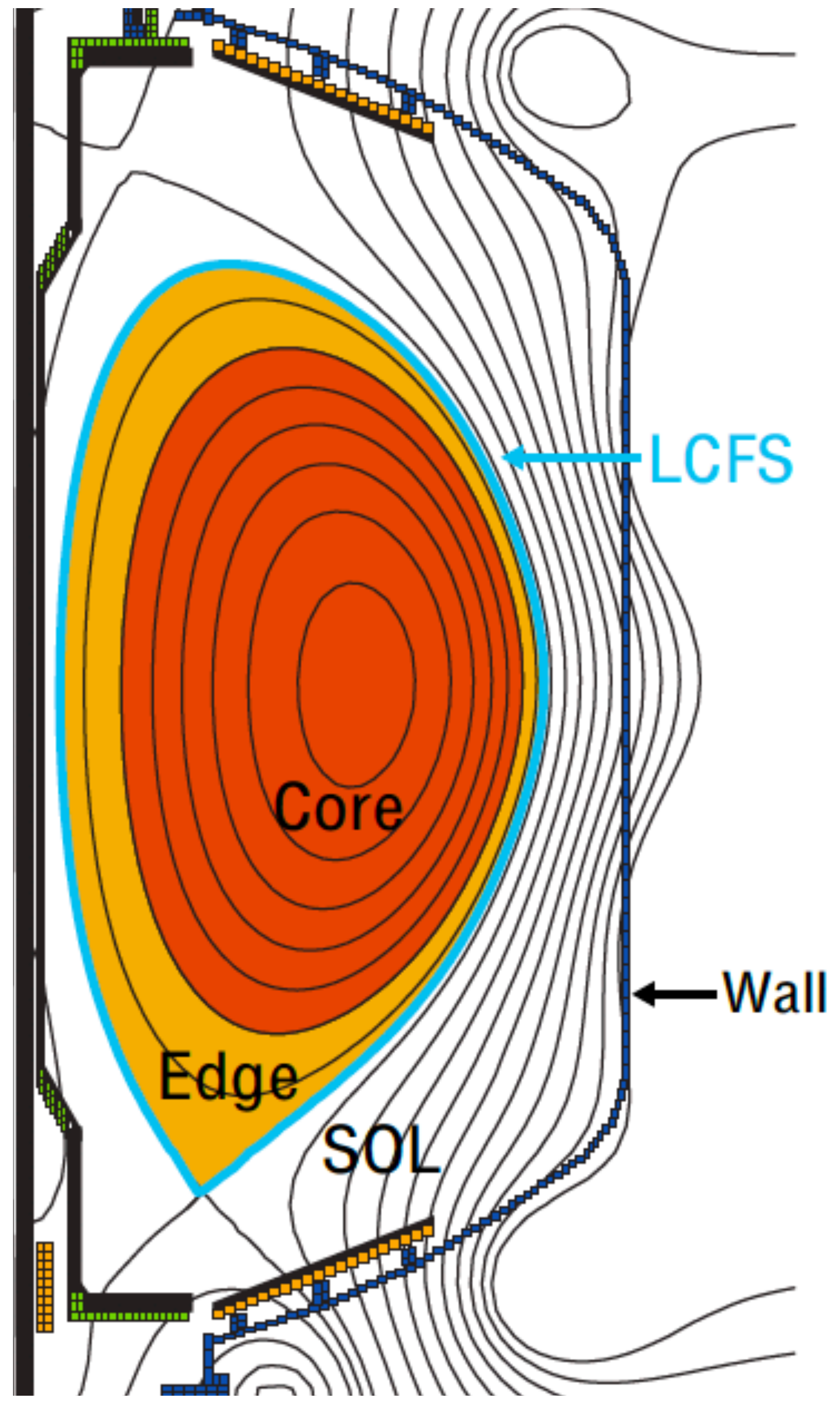

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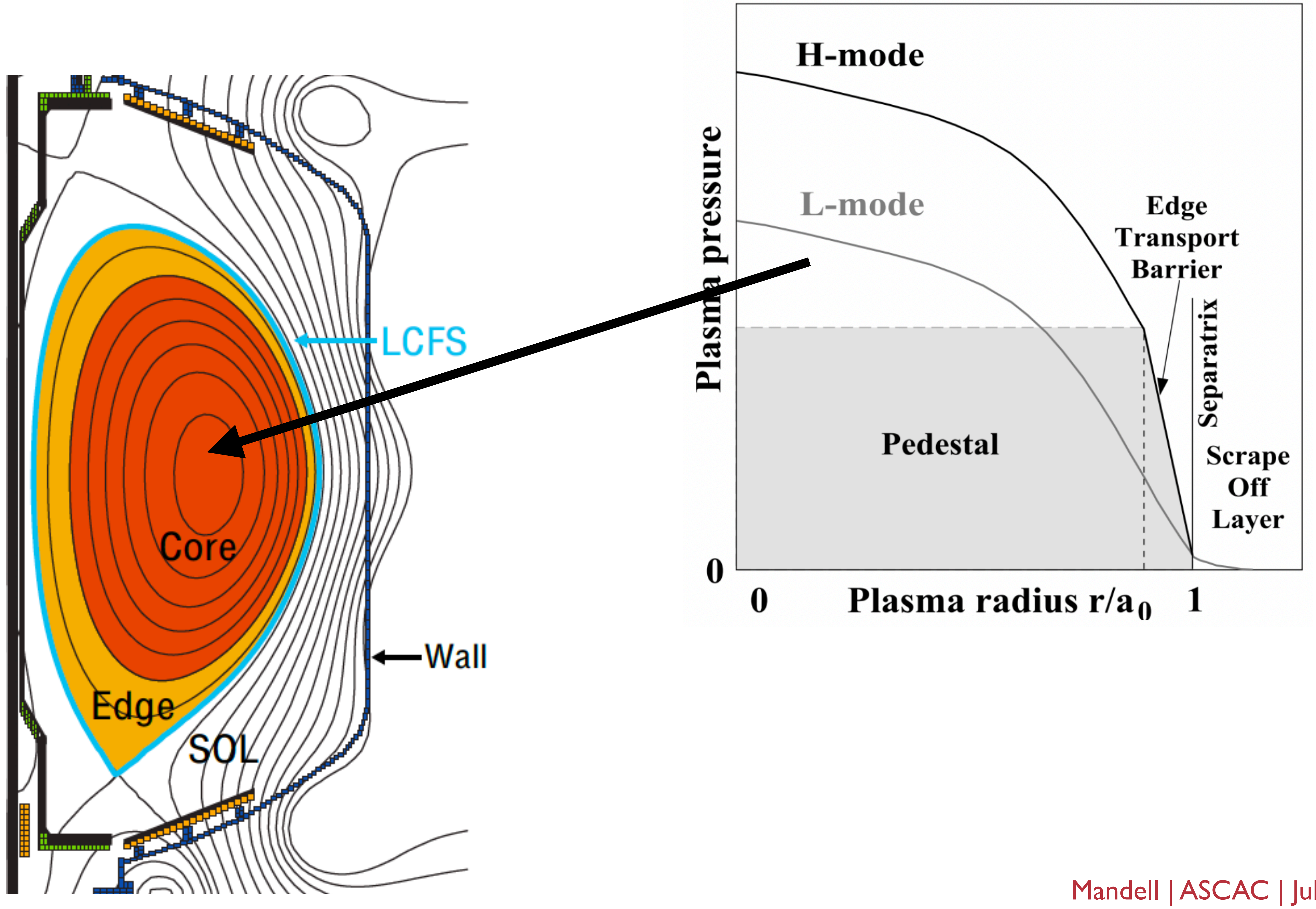

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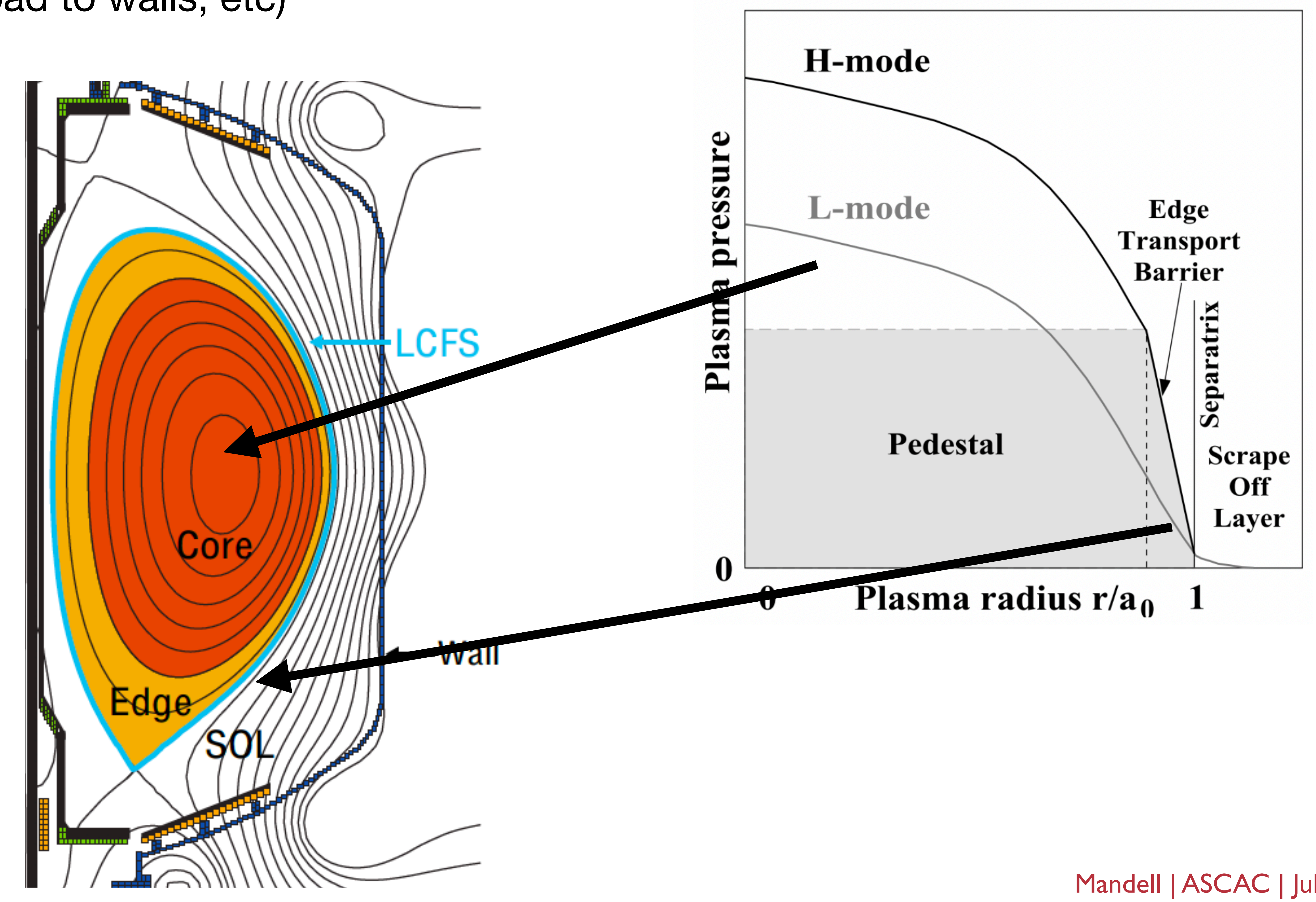

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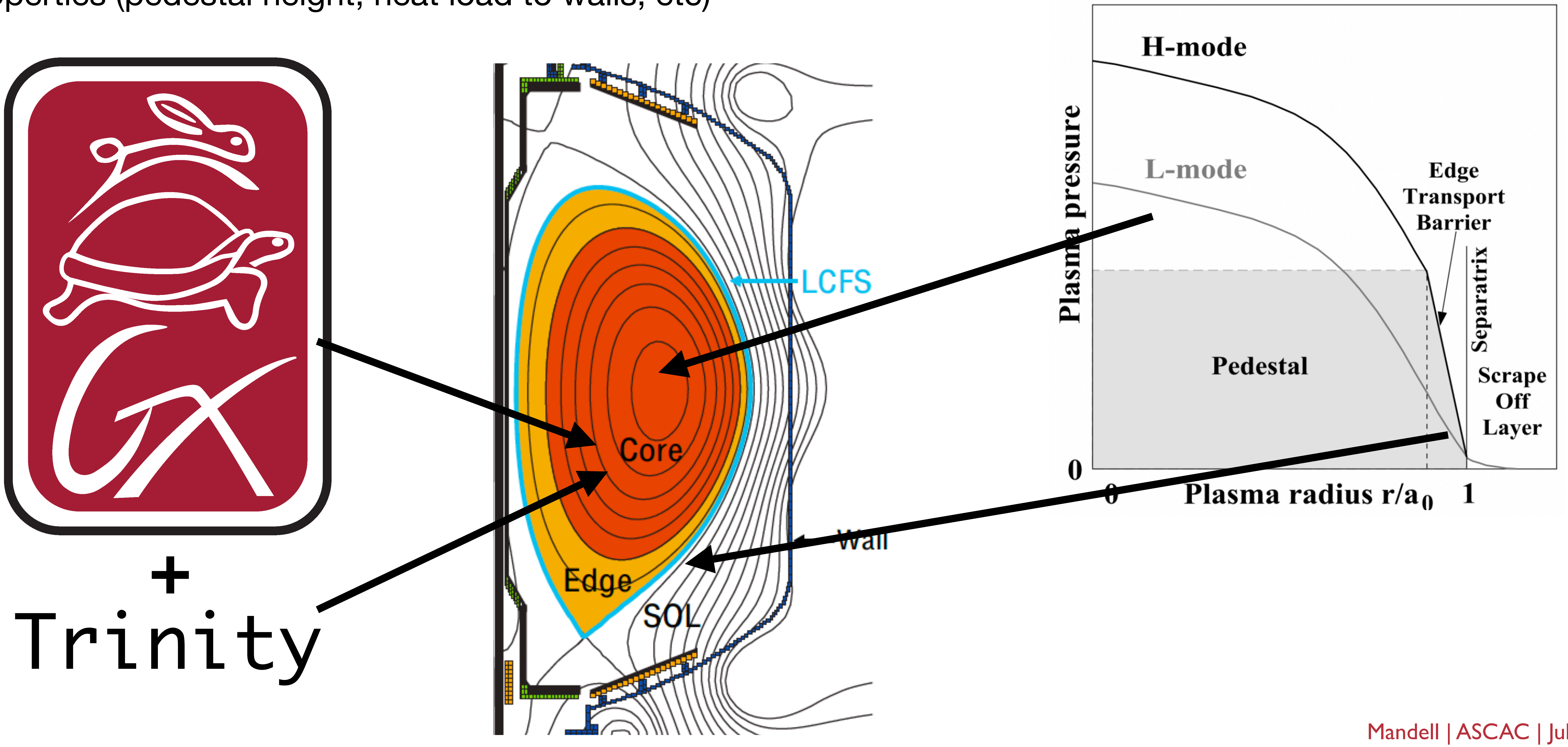

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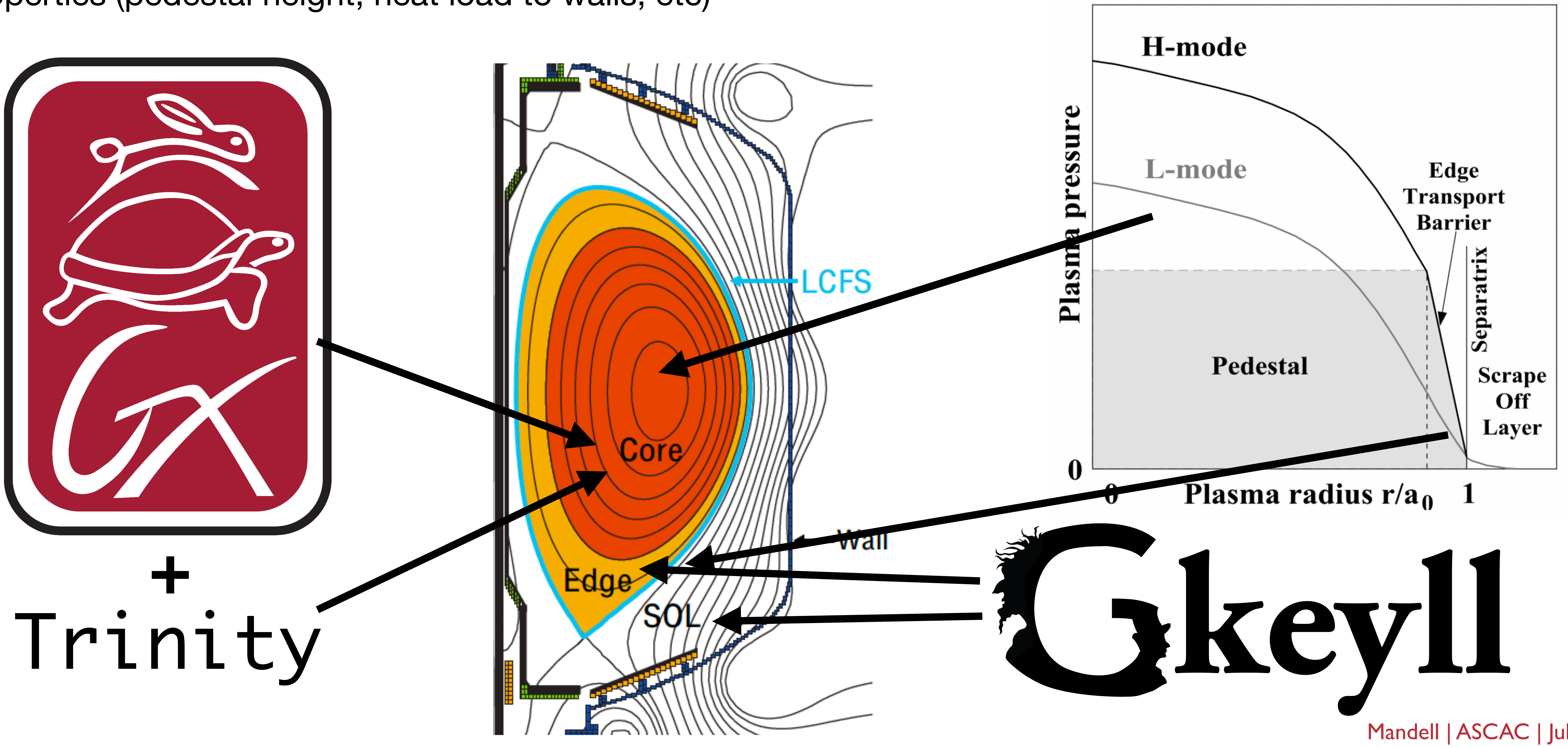

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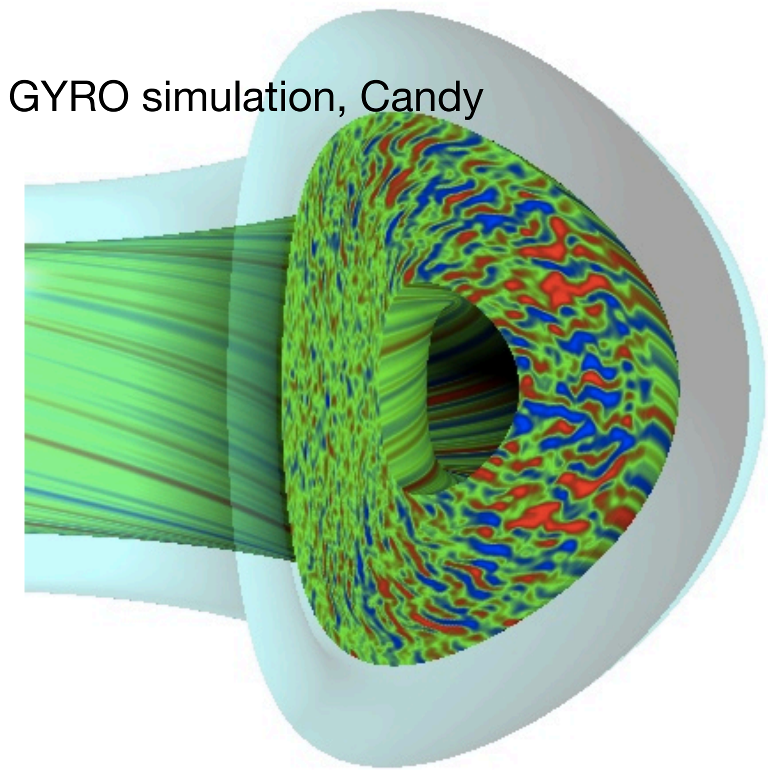
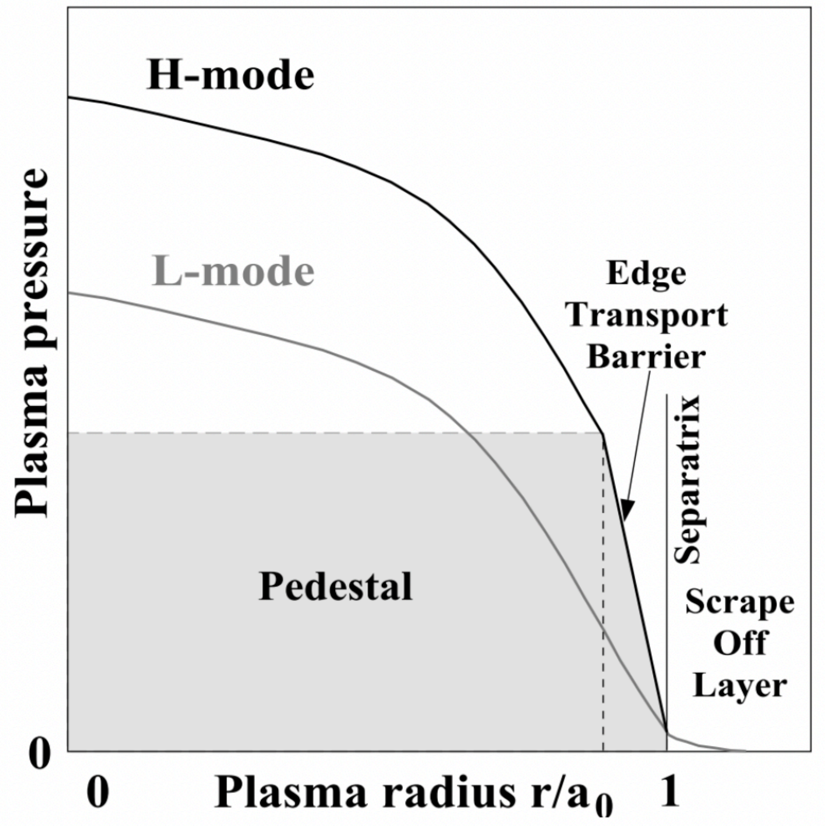


small-scale turbulence



slowly-varying background profiles

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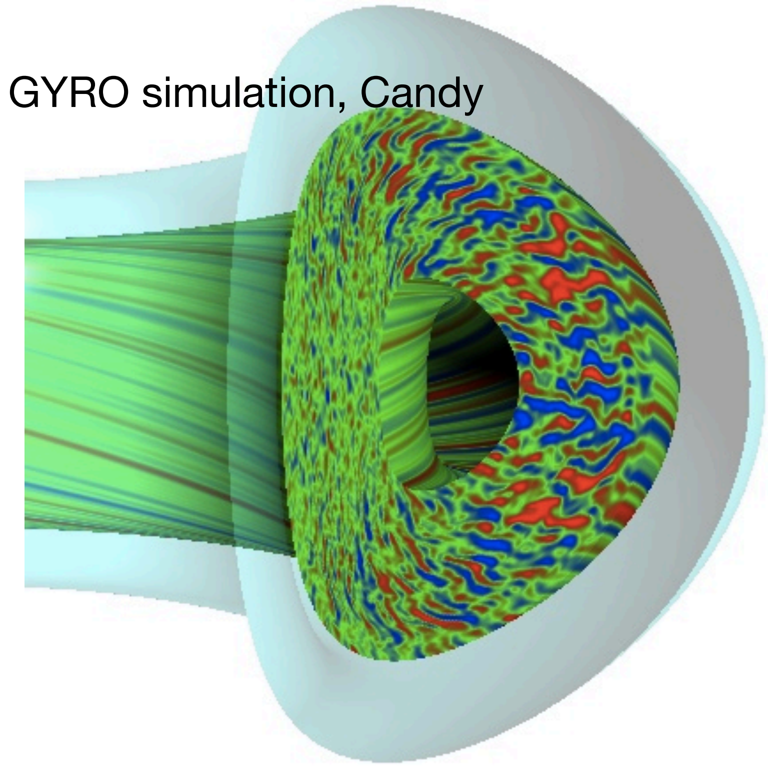
- A fusion reactor has an **enormous range of scales**. In the core, we have **turbulence at micro-scales** and background **profile evolution (transport) at macro-scales**, separated by several orders of magnitude

GYRO simulation, Candy



$$L_{\text{turb}} \sim \rho_i \sim 0.1 - 0.5 \text{ mm} \xleftrightarrow{\sim 10^3 - 10^4} L_{\text{transp}} \sim a \gtrsim 1 \text{ m}$$

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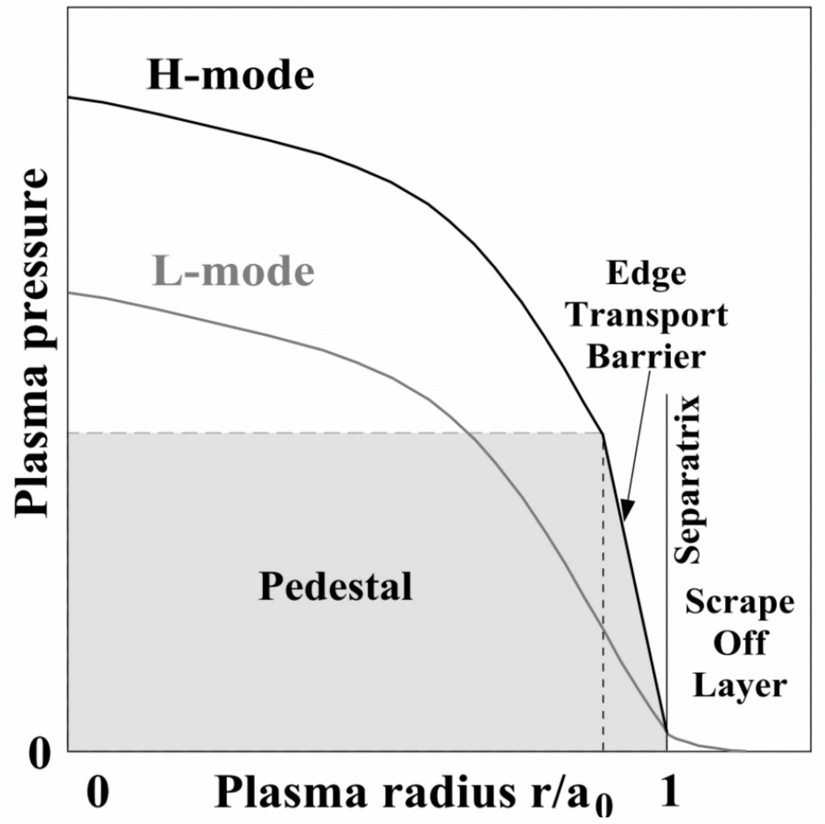

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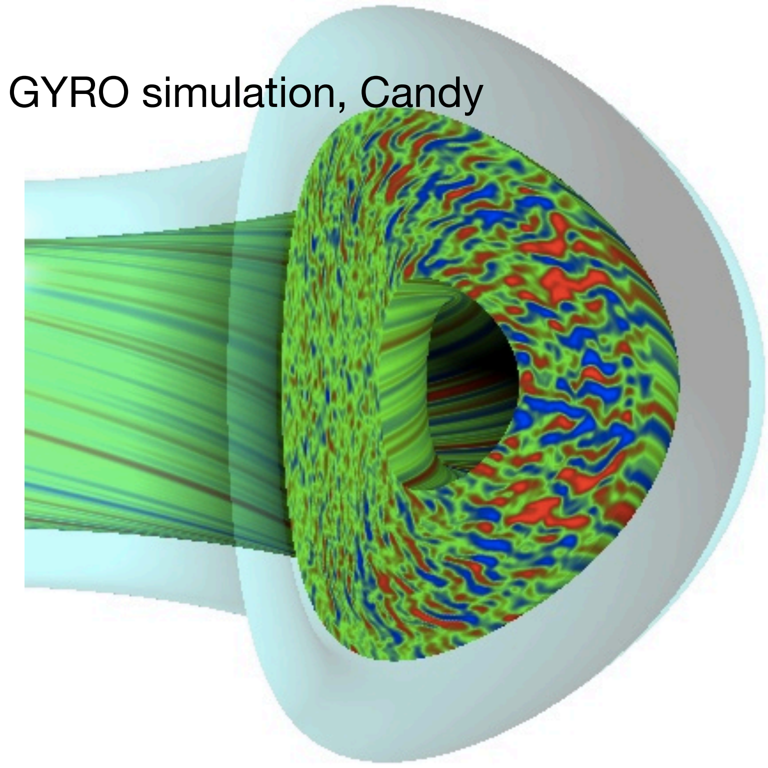

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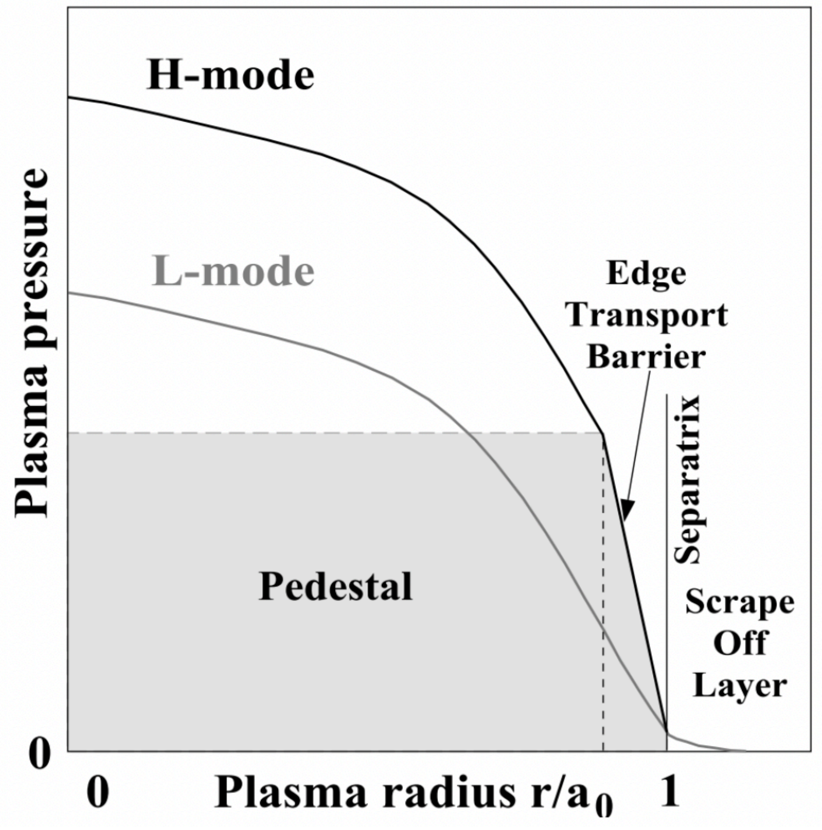

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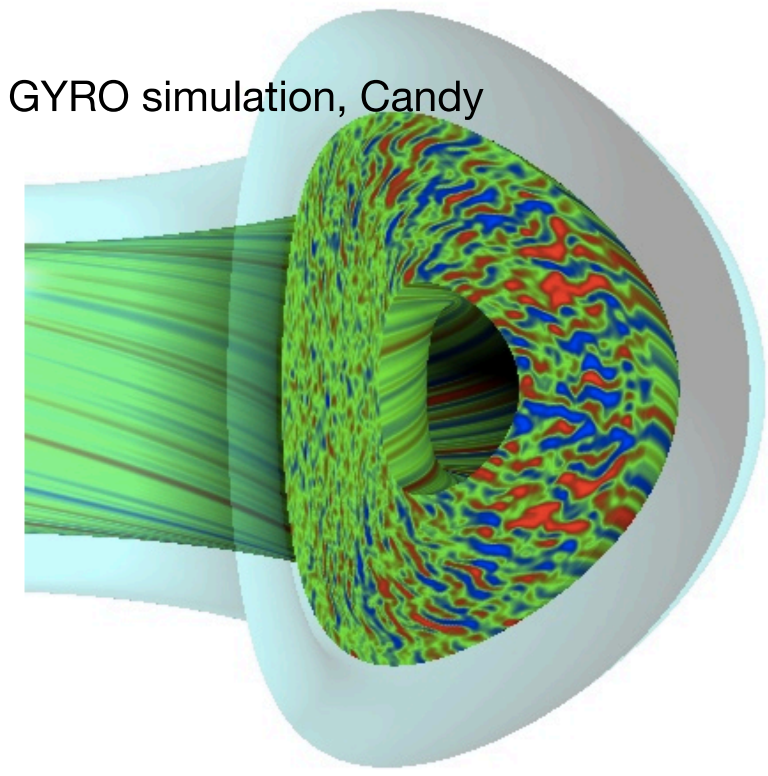
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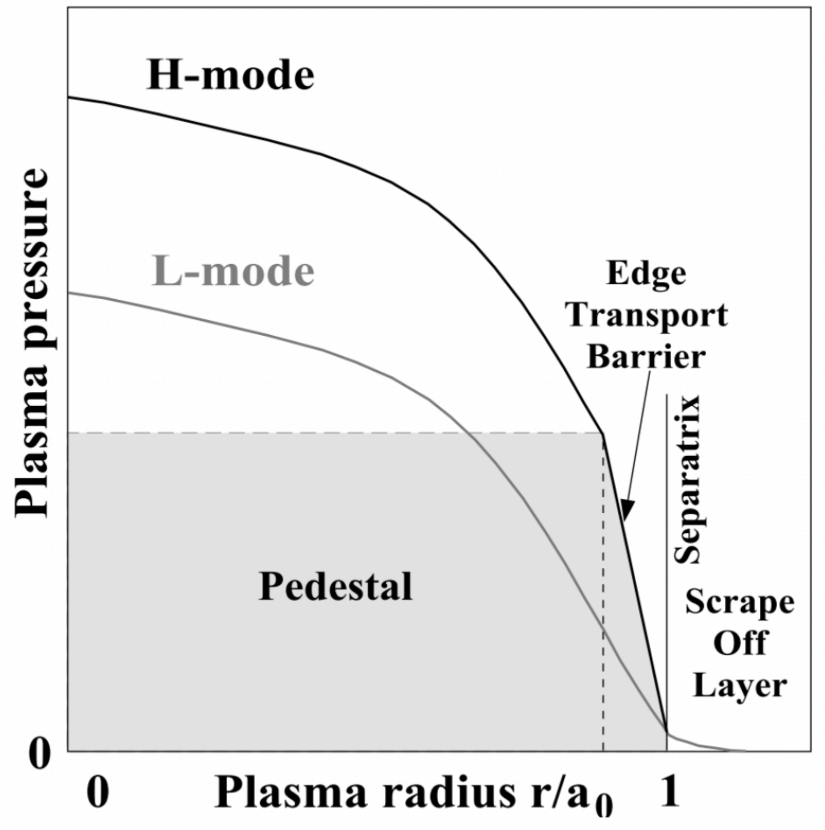

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- Modeling this range of scales with a brute-force 5D+time discretization would then require

$$N \sim \left(\frac{L_{\text{turb}}}{L_{\text{transp}}}\right)^3 (N_v \sim 10)^2 \sim 10^{14} \text{ phase-space grid points in 5D}$$

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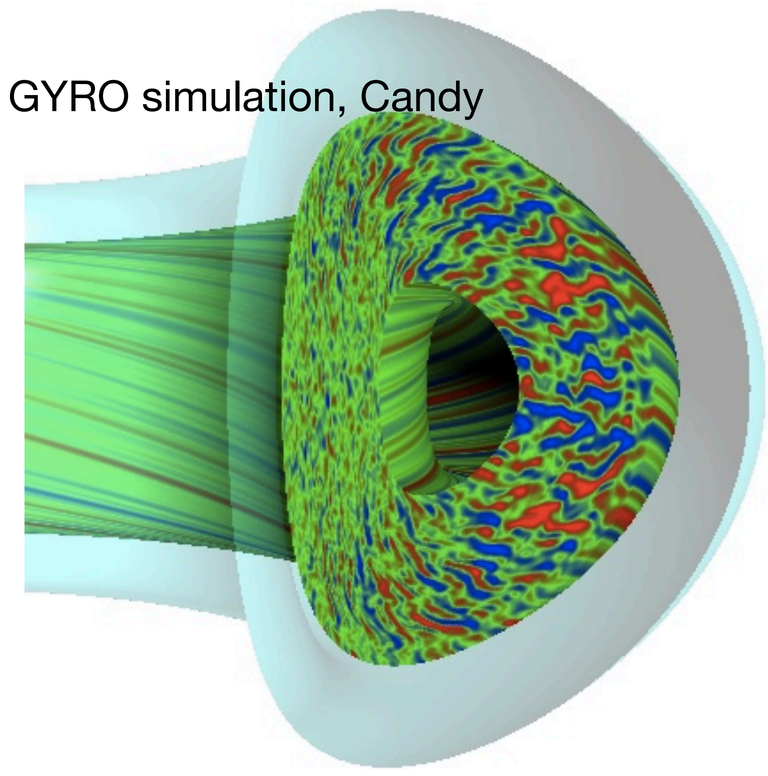

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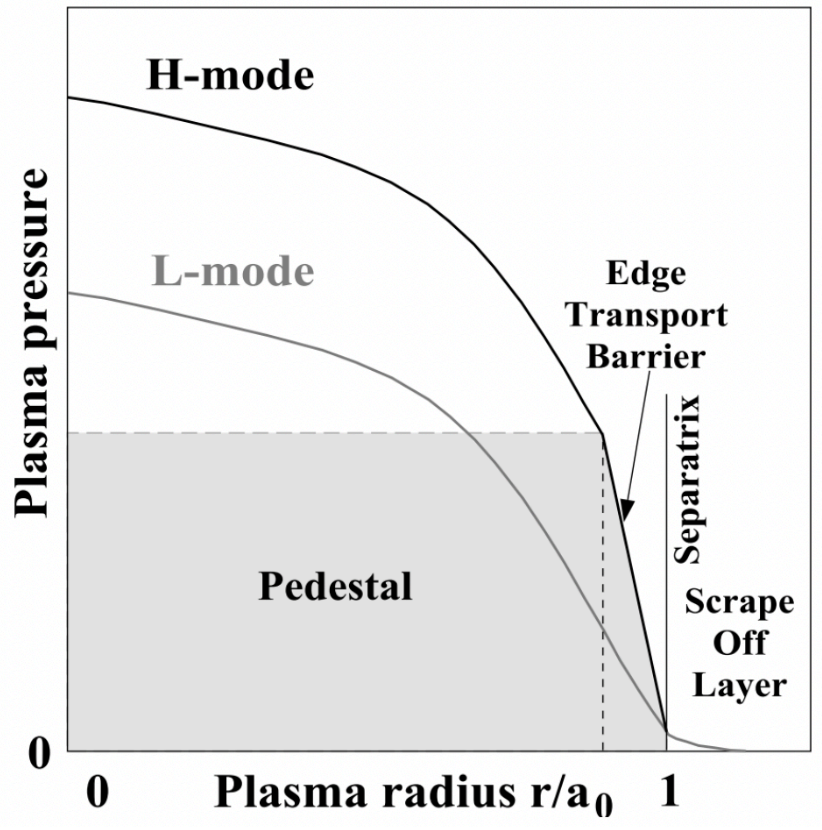

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$$\mathrm{NFLOP} \sim \mathcal{O}(N^2)\left(\frac{\tau_{\mathrm{turb}}}{\tau_{\mathrm{transp}}}\right) \sim 10^{33}\text{, which would require } 10^{15}\ \mathrm{s} \text{ on an exascale computer}$$

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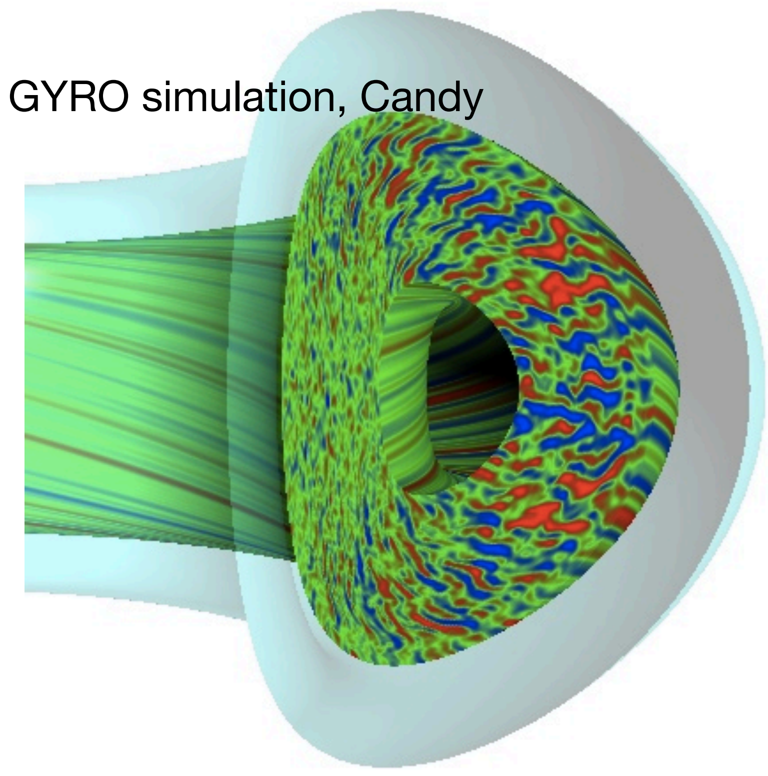

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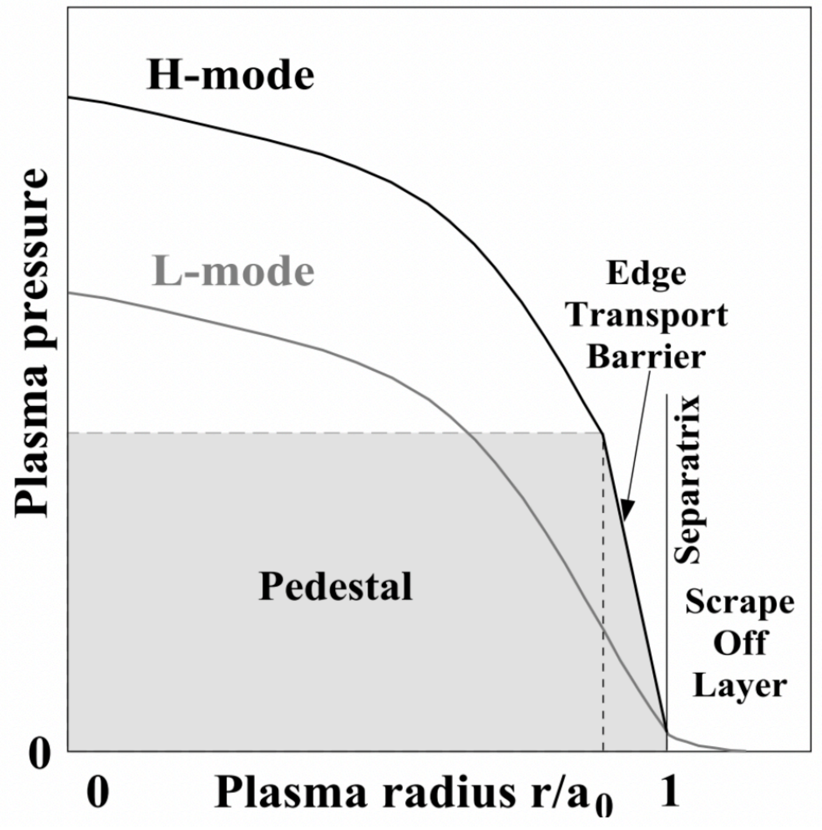


small-scale turbulence **slowly-varying background profiles**

- Extreme temperatures require a **kinetic** description (instead of fluid), which means solving a PDE in 5D (3x+2v, after averaging over fast gyromotion to get **gyrokinetics**)
- Modeling this range of scales with a brute-force 5D+time discretization would then require

$$N \sim \left(\frac{L_\mathrm{turb}}{L_\mathrm{transp}}\right)^3 (N_v \sim 10)^2 \sim 10^{14} \text{ phase-space grid points in 5D}$$

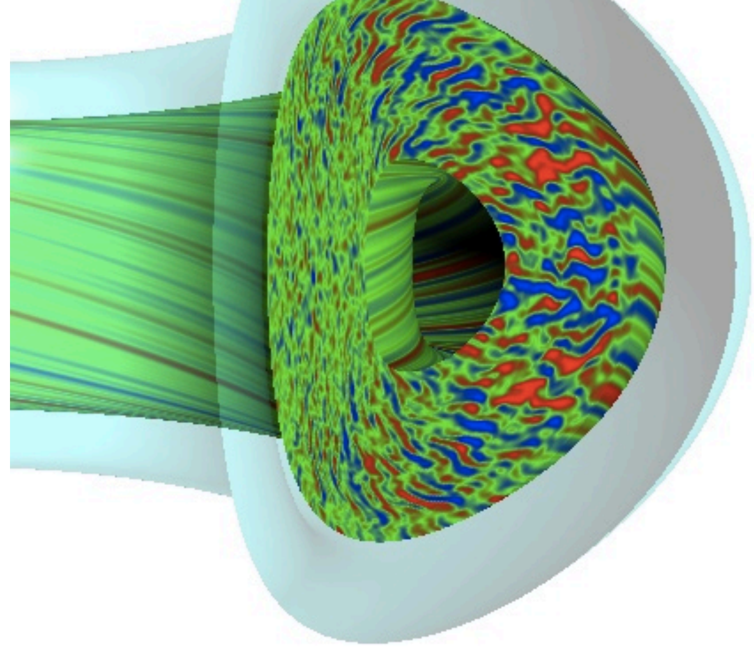
$$\mathrm{NFLOP} \sim \mathcal{O}(N^2)\left(\frac{\tau_\mathrm{turb}}{\tau_\mathrm{transp}}\right) \sim 10^{33}, \text{ which would require } 10^{15}\ \mathrm{s} \text{ on an exascale computer}$$

- These problems require **intense computational resources**, but also **clever multi-scale numerical algorithms and theory** to enable tractable calculations

Fusion is hard; *modeling* a fusion plasma is hard, too

- A fusion reactor has an **enormous range of scales**. In the core, we have **turbulence at micro-scales** and background **profile evolution (transport) at macro-scales**, separated by several orders of magnitude

GYRO simulation, Candy



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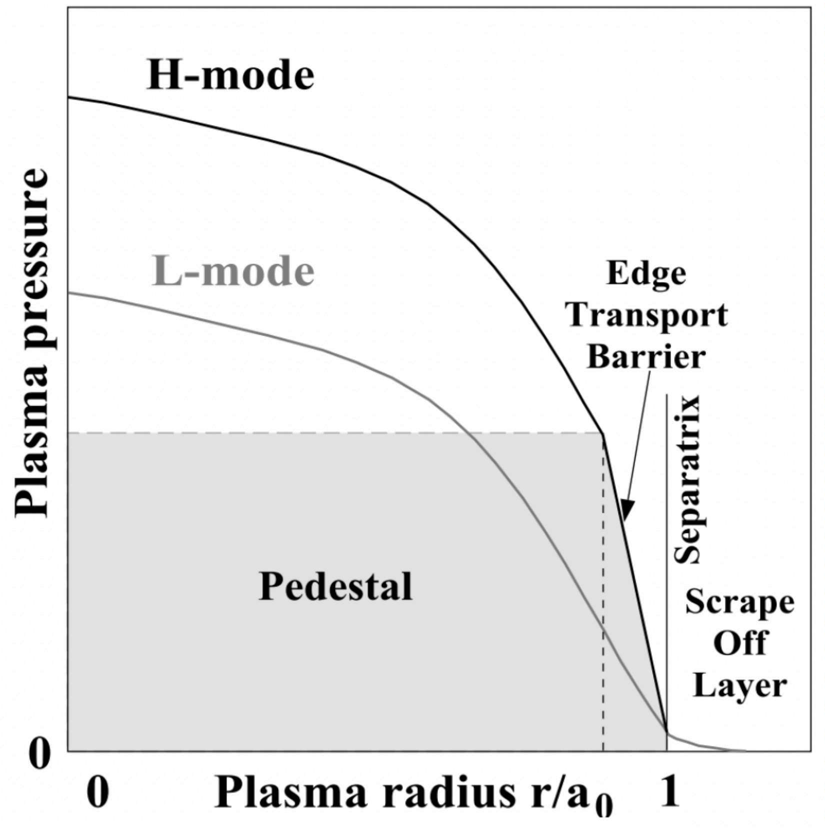

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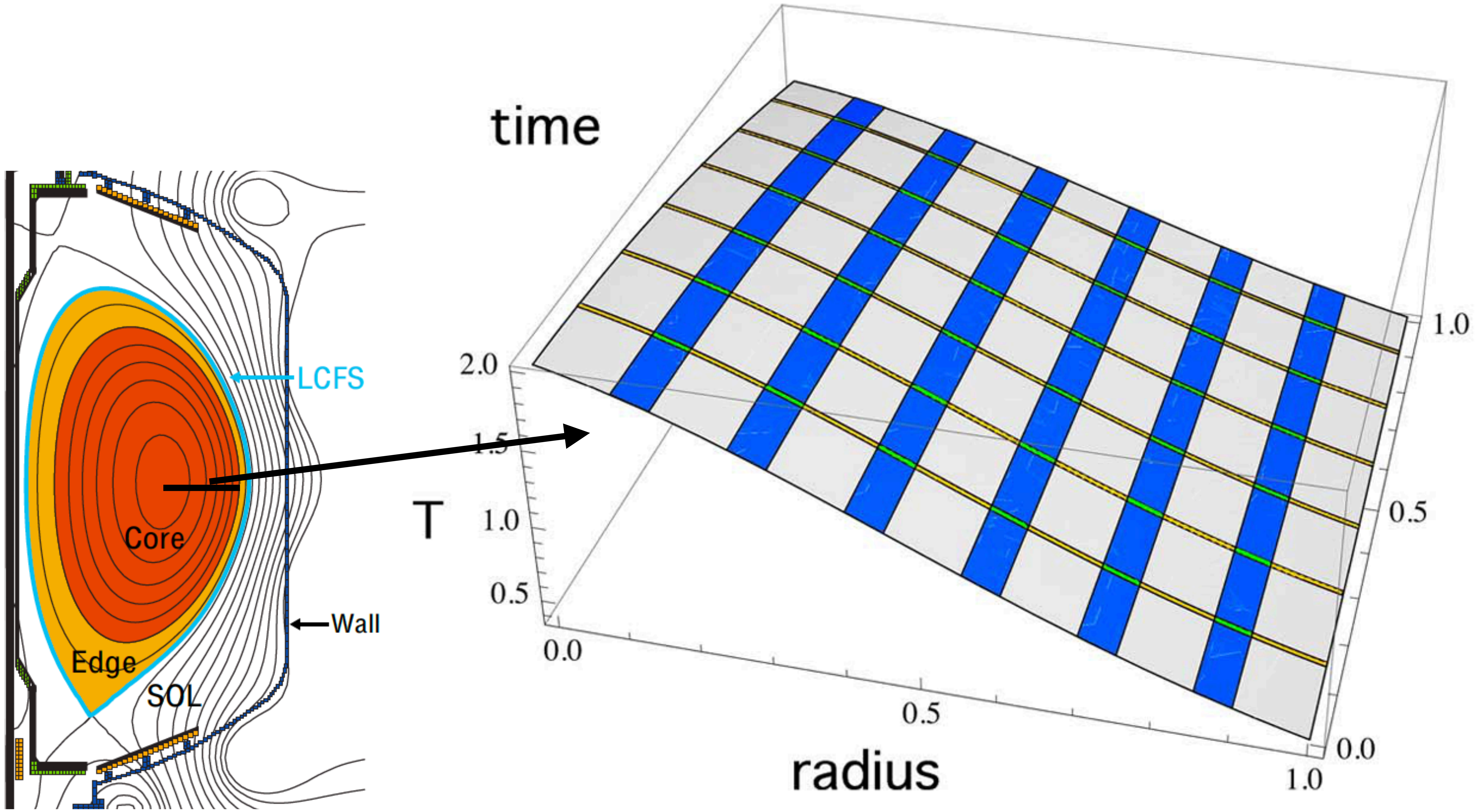
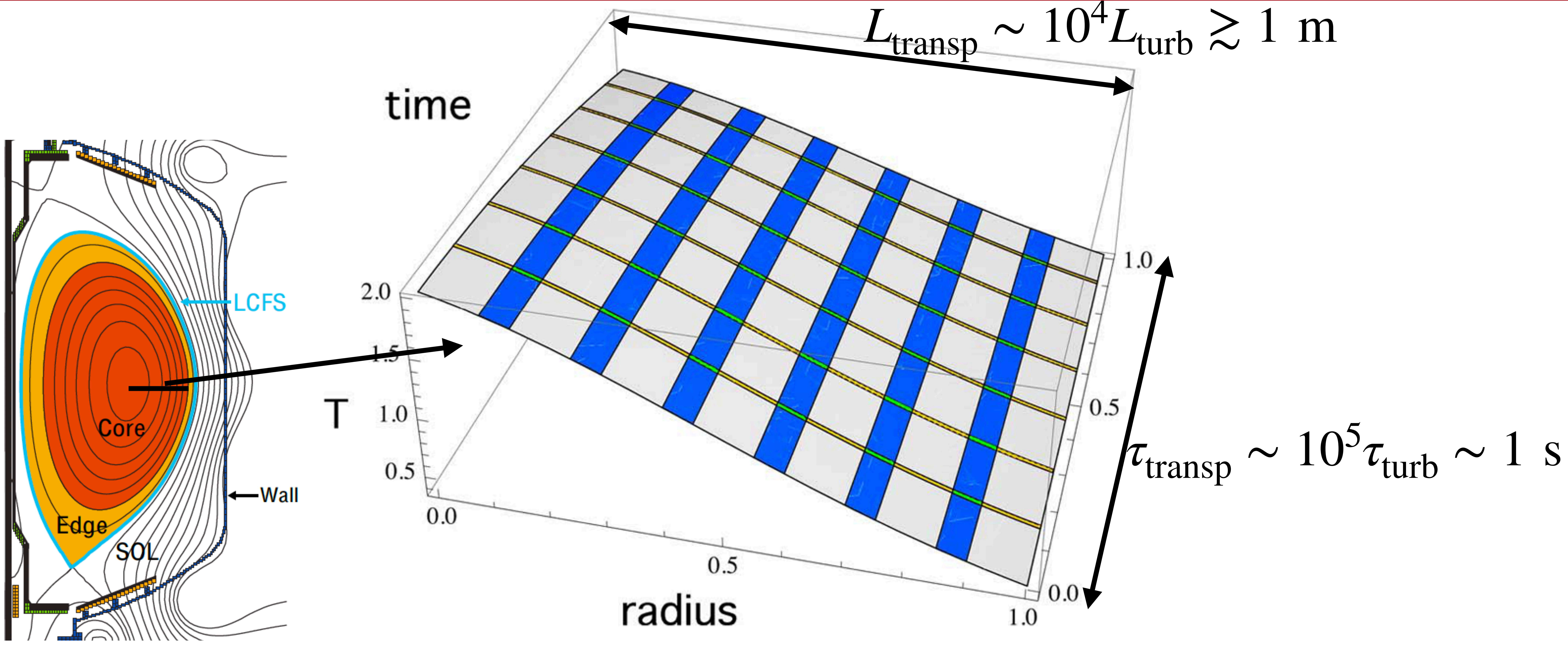
- These problems require **intense computational resources**, but also **clever multi-scale numerical algorithms and theory** to enable tractable calculations
- In **optimization** context, $\mathcal{O}(10^3)$ or more such calculations may be needed, so need additional acceleration to make tractable

Savings from using a multi-scale approach



Savings from using a multi-scale approach

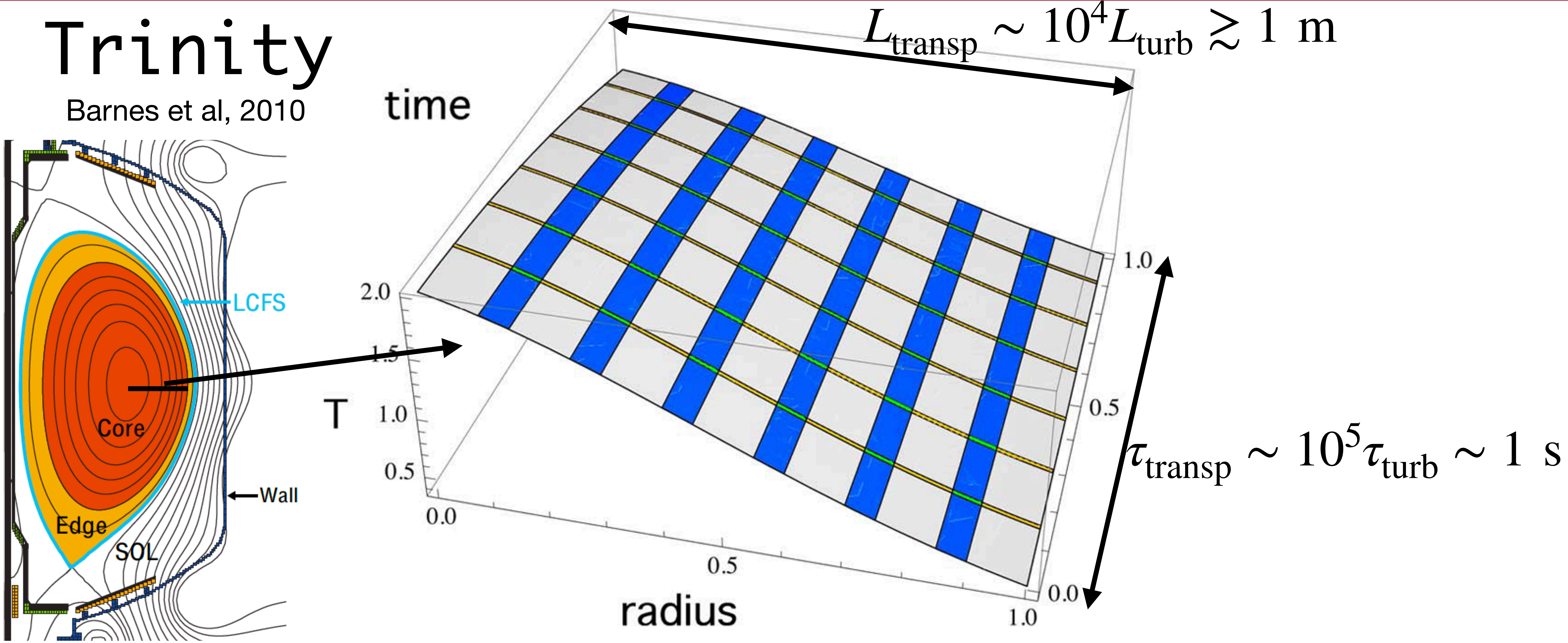


- Brute-force approach: fine space-time mesh for entire domain, with $\Delta x \sim L_{\text{turb}}$ and $\Delta t \sim \tau_{\text{turb}}$

Savings from using a multi-scale approach

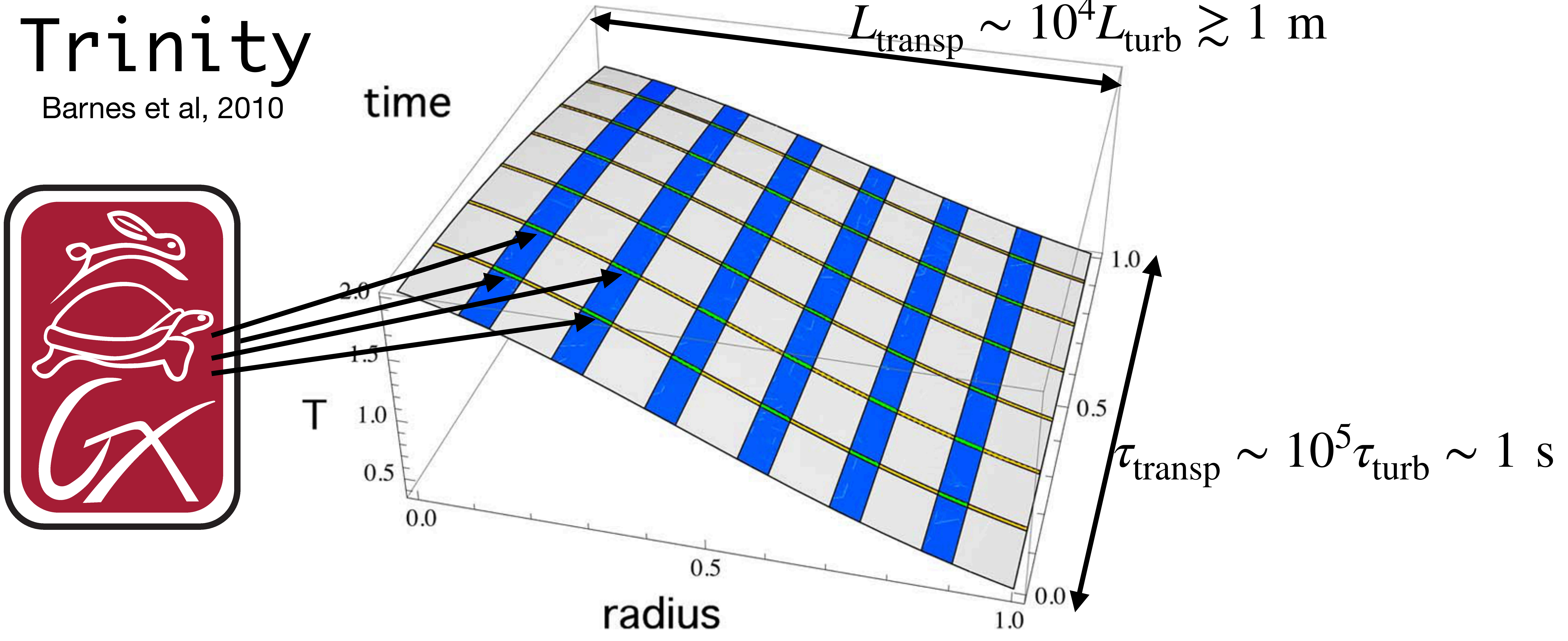
Trinity

Barnes et al, 2010



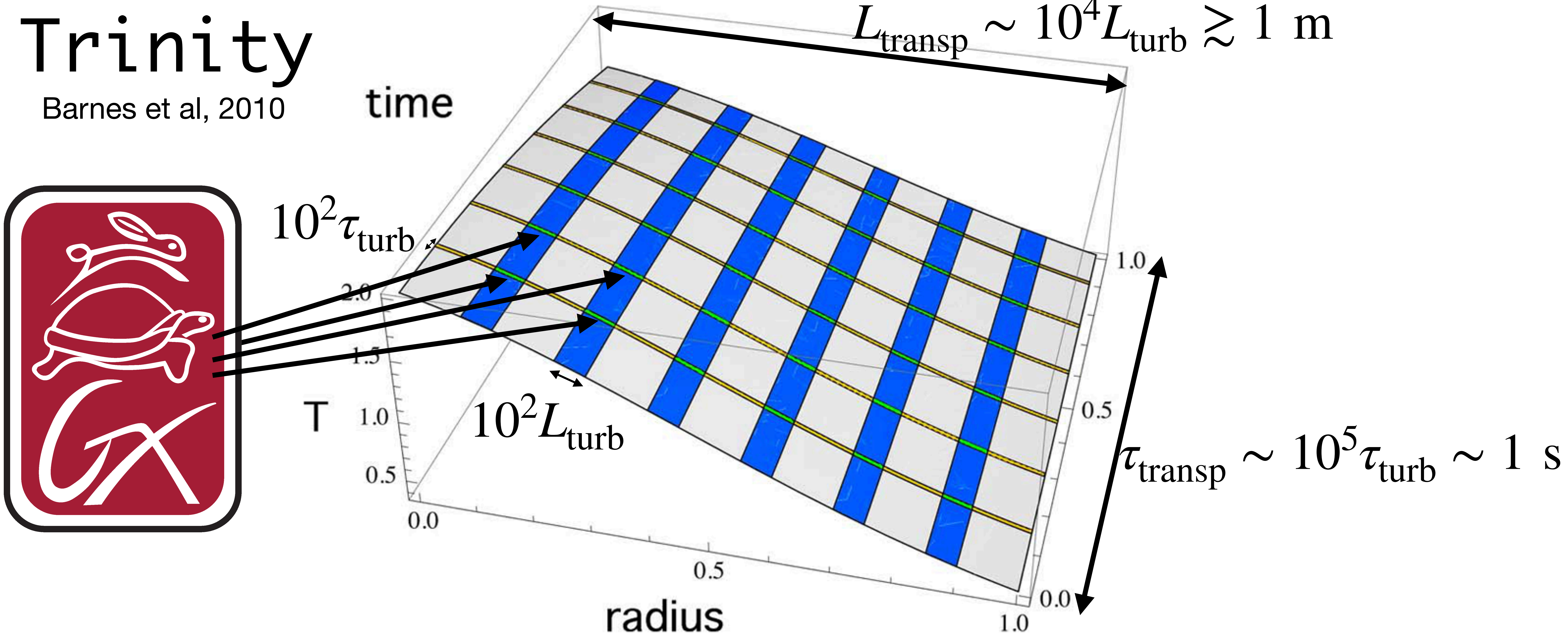
- Brute-force approach: fine space-time mesh for entire domain, with $\Delta x \sim L_{\mathrm{turb}}$ and $\Delta t \sim \tau_{\mathrm{turb}}$
- Trinity **multi-scale** approach (Barnes et al, 2010):

Savings from using a multi-scale approach



- Brute-force approach: fine space-time mesh for entire domain, with $\Delta x \sim L_{\rm turb}$ and $\Delta t \sim \tau_{\rm turb}$
- `Trinity` **multi-scale** approach (Barnes et al, 2010):
  - Can "zoom in" with small regions of fine grid (for turbulence) embedded in coarse grid (for slow profile evolution), in both space and time, dramatically reducing the domain over which a fine space-time mesh is needed

Savings from using a multi-scale approach



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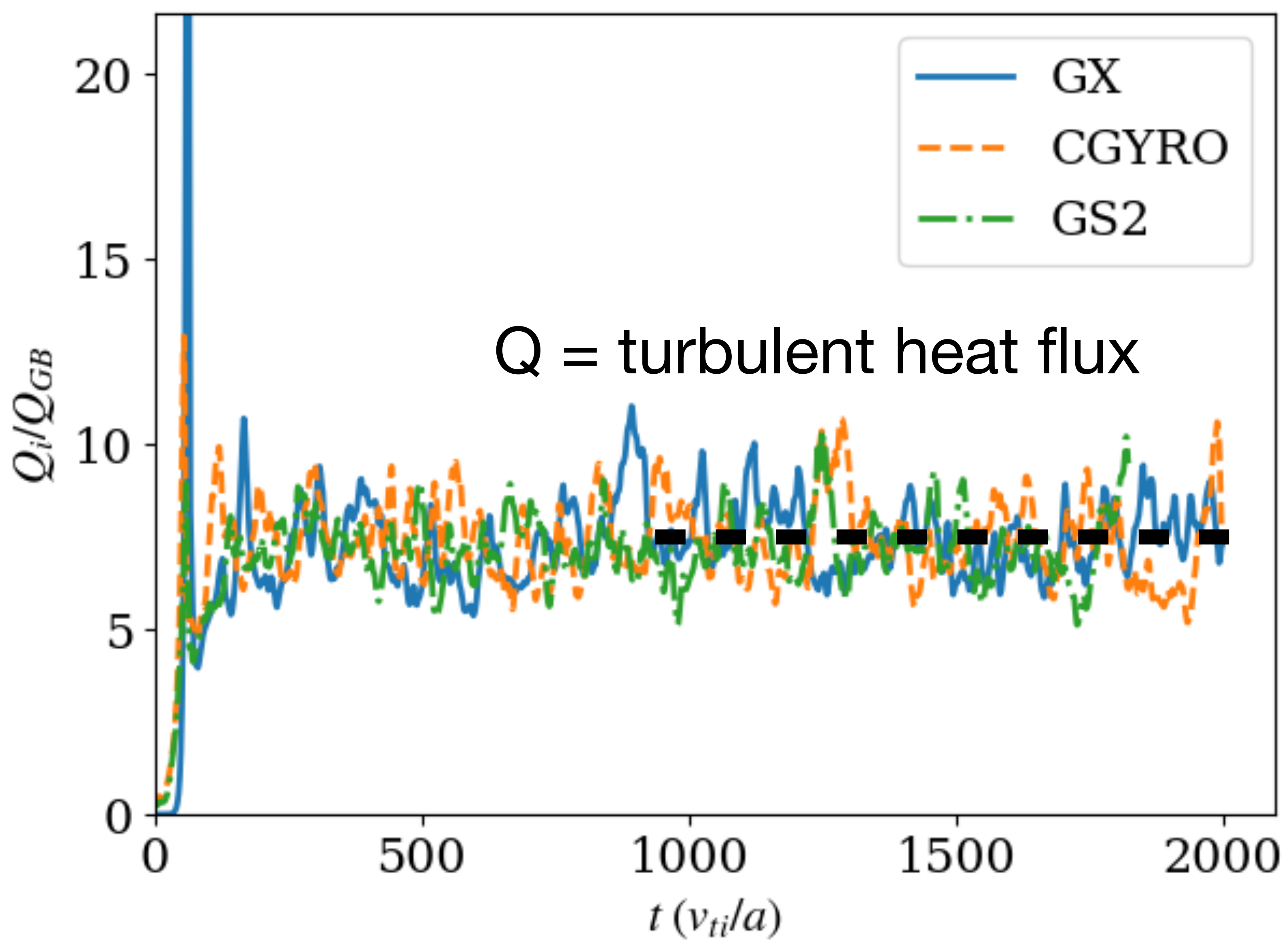
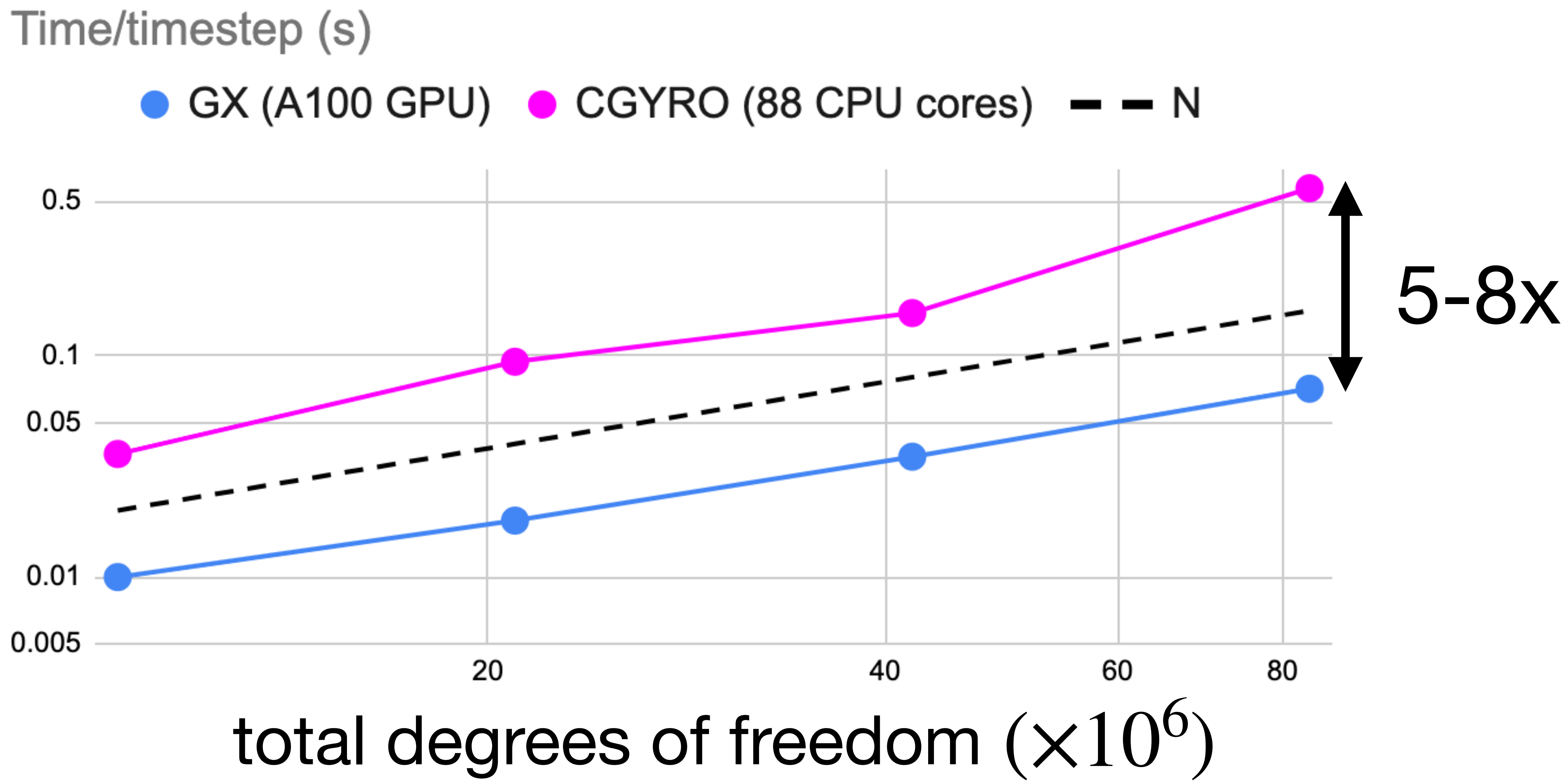
GX: a GPU-native pseudo-spectral kinetic turbulence code

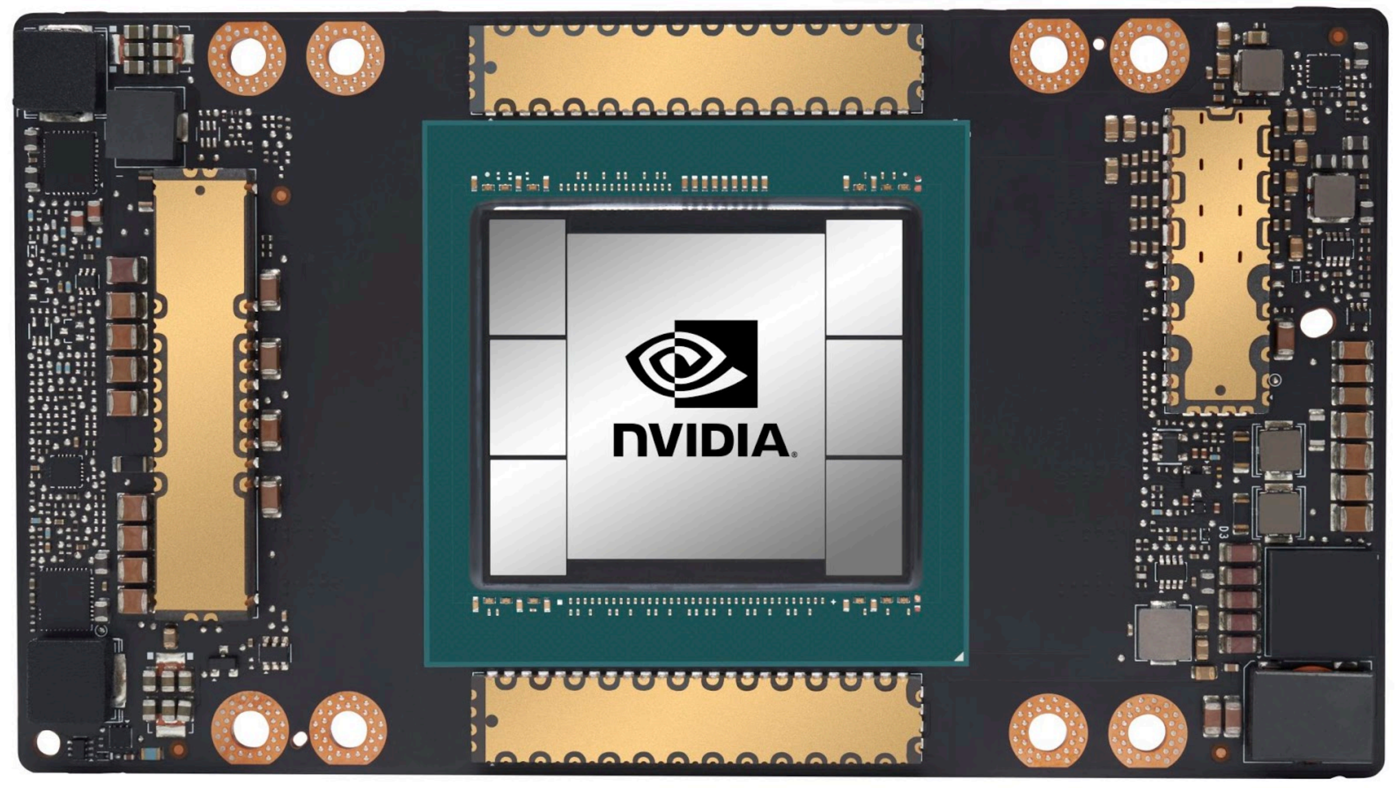
- GX models micro-scale turbulent fluctuations, which drive heat and particle losses in the reactor
  - Solves a nonlinear PDE in 5D+time
- Uses pseudo-spectral (Fourier-Hermite-Laguerre) methods
  - Ideal for GPUs (compute intensity is mostly in fast transforms and tensor operations)
- Designed and implemented directly in CUDA/C





Cyclone base case, adiabatic electrons

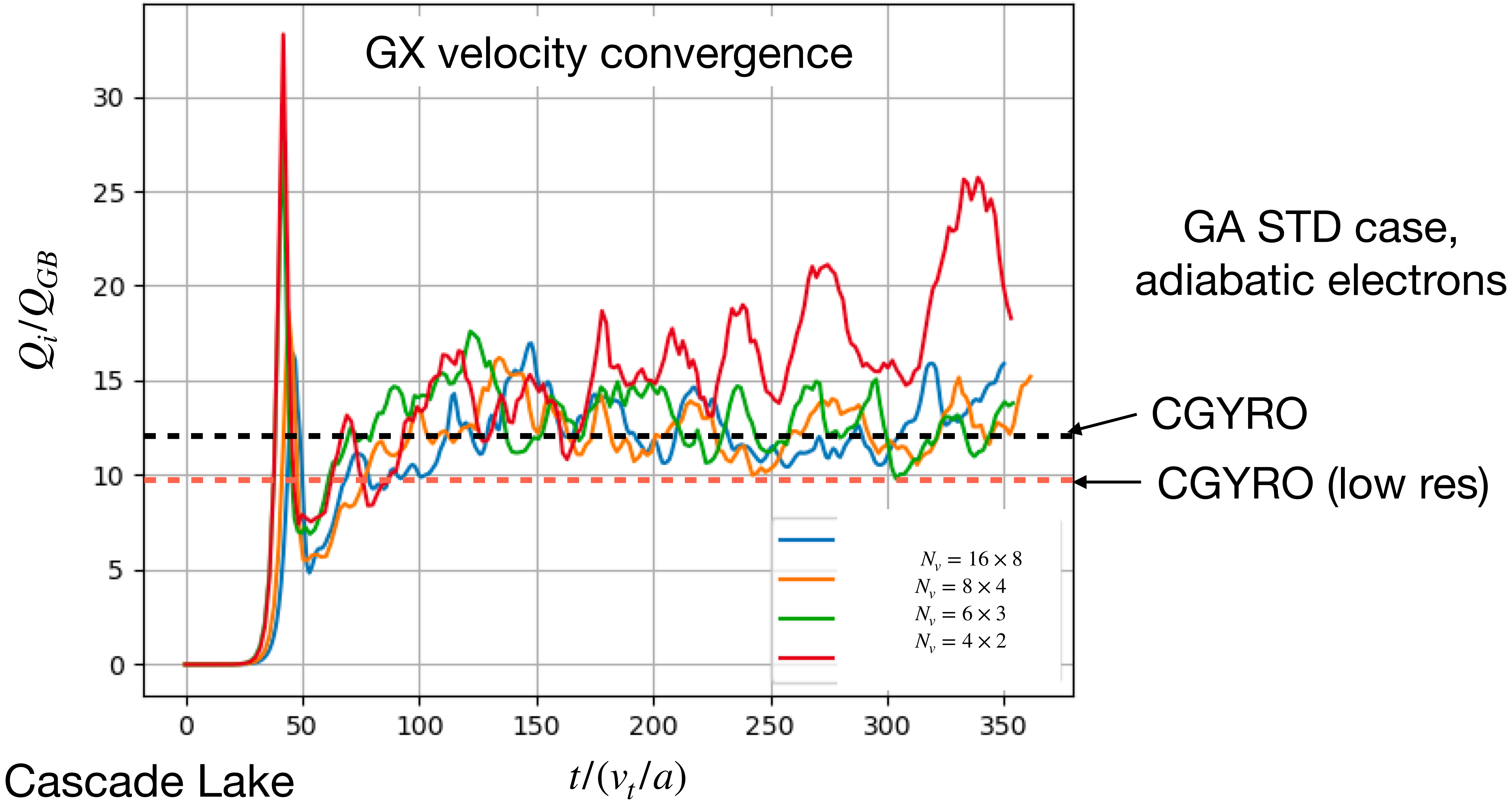
https://gx.readthedocs.io
https://bitbucket.org/gyrokinetics/gx



Combining algorithmic and hardware improvements

- GX's velocity basis appears to have **better convergence properties**, making GX still accurate even with 7x less velocity resolution than CGYRO
- **Combination of algorithmic and hardware** improvements makes GX **10-15x faster** than CGYRO on 256 cores!

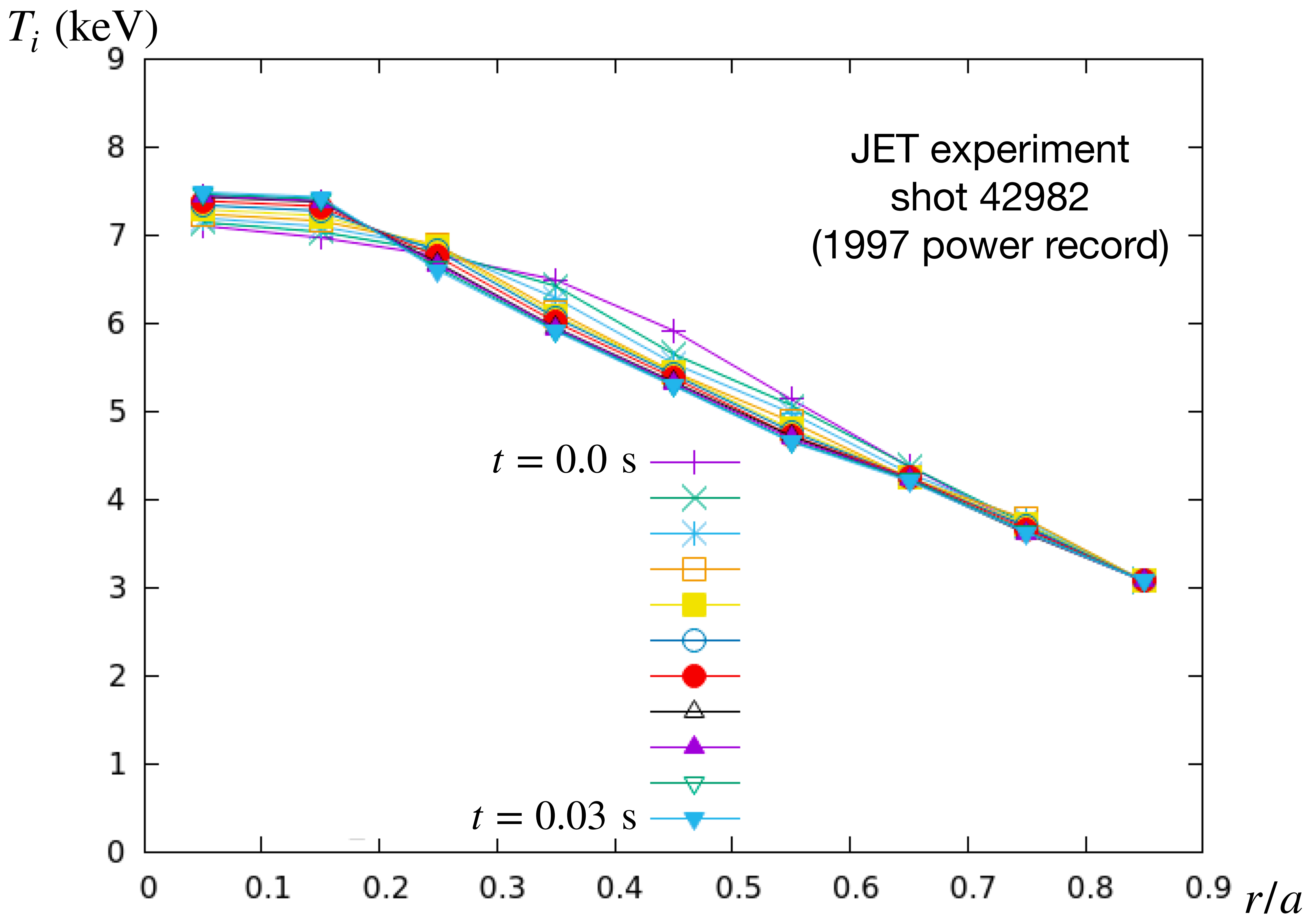
	GX (1 A100 GPU)		CGYRO (256 CPU cores†)	
Velocity resolution	Heat flux	Simulation time	Heat flux	Simulation time
16 x 8	12.5	17.5 min	12.1	31 min ~ 8000 CPU-min
8 x 4	12.3	3 min	9.8	9.5 min ~ 2400 CPU-
6 x 3	12.8	2.3 min	—	—
4 x 2	17.5	1.6 min	—	—



†CPU = 2.9 GHz Intel Cascade Lake

Preliminary GX + Trinity simulation

- The speed of GX makes once-daunting coupled turbulence-transport simulations manageable



8 radial cells

16 GX instances (2 per cell for a Jacobian calculation)

10 timesteps, 18 total evaluations (including intermediate Newton iterations)

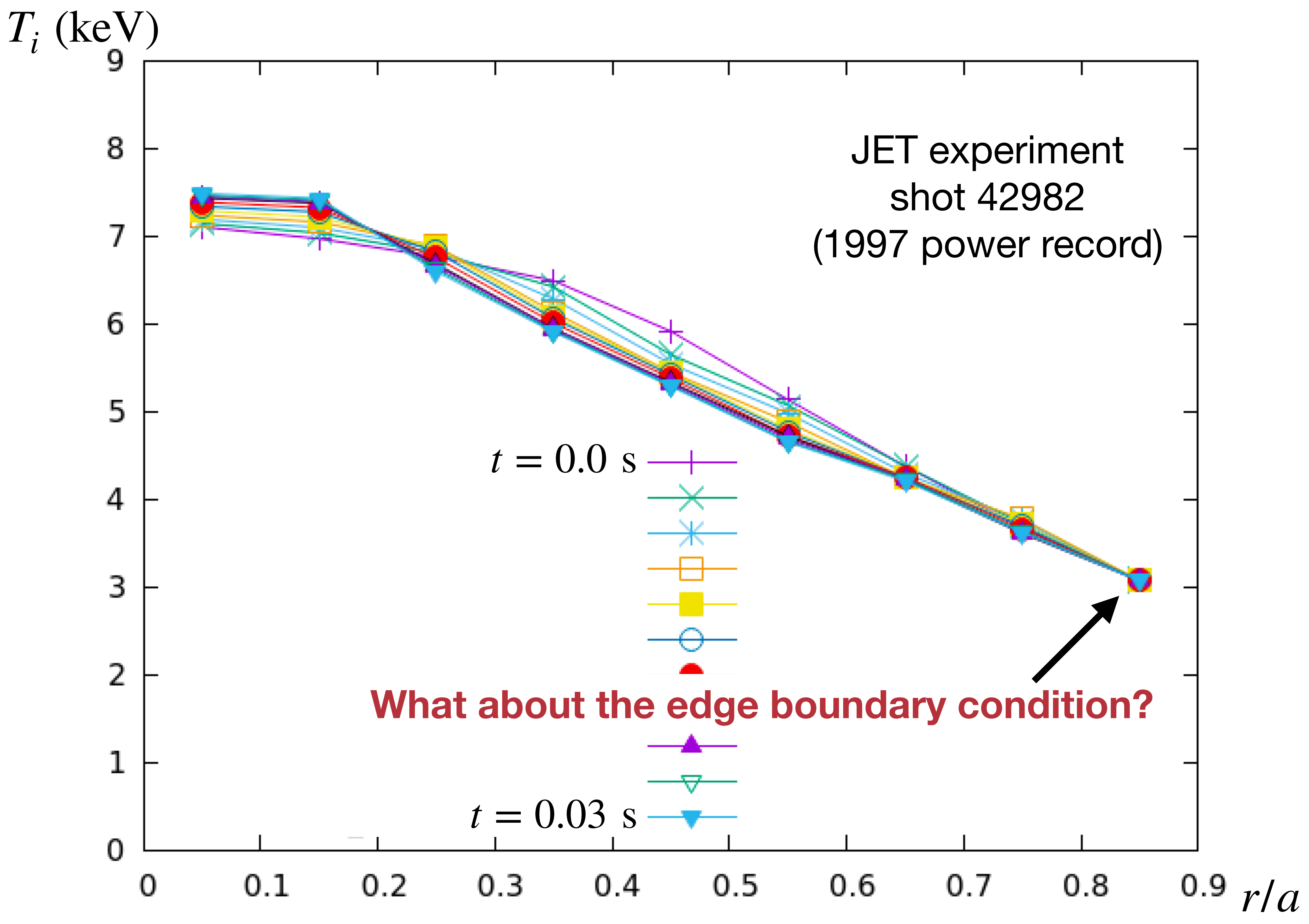
18 x 16 = 288 nonlinear turbulence evaluations

~2 hours total on 16 GPUs (V100)
(would be ~70% faster on A100)

(Might have taken CGYRO+Trinity ~12 hours on ~4000 cores)

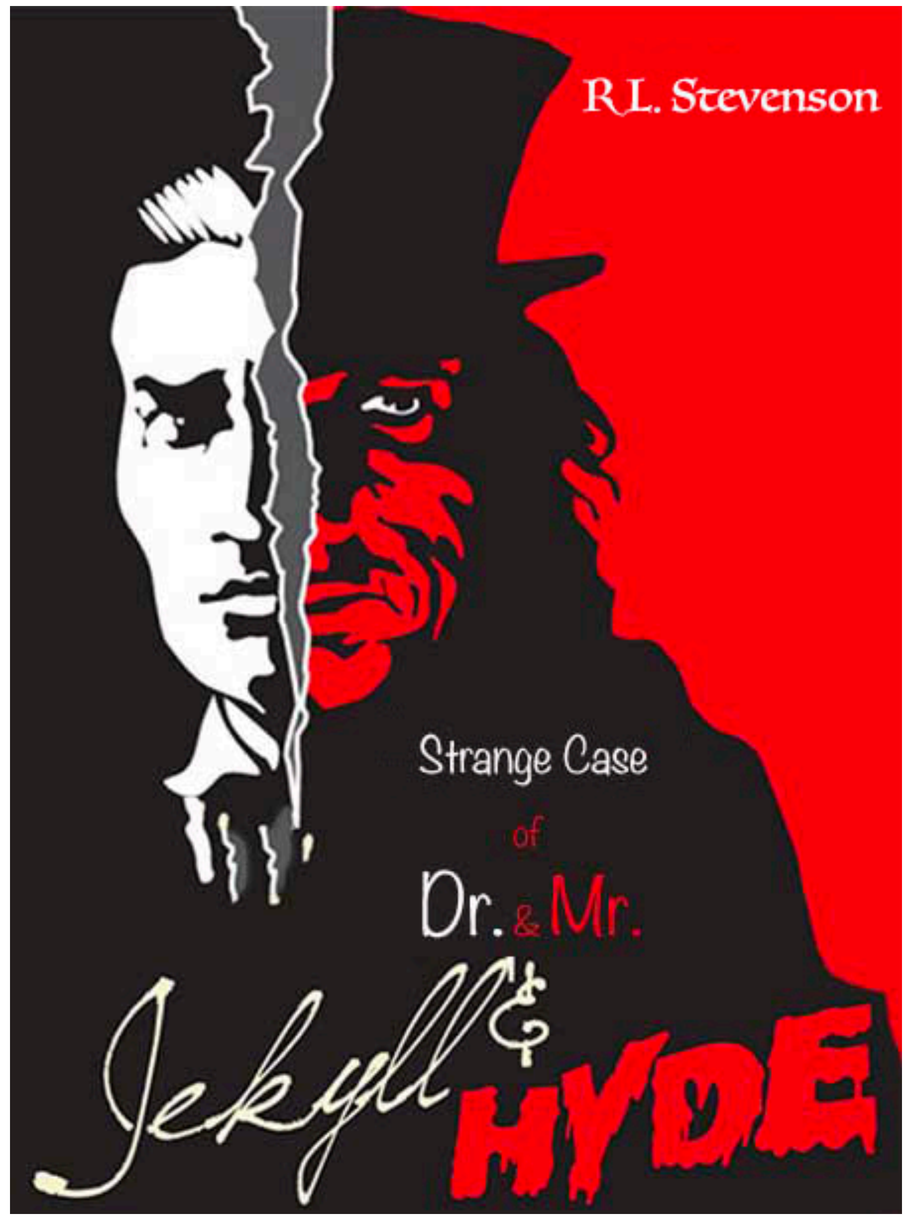
GX+Trinity transport model can be used to predict and optimize core profiles for future fusion experiments!

Thinking on the edge



Gkeyll: a gyrokinetic model for the boundary

- Modeling boundary requires specialized kinetic turbulence codes; can't use multi-scale approach from core
- Gkeyll is specialized for modeling kinetic turbulence in the tokamak boundary
  - Handles arbitrarily large fluctuations, special boundary conditions where plasma interacts with walls
- Energy-conserving discontinuous Galerkin (DG) discretization scheme for Hamiltonian systems (like GK)
- **Central contribution of my thesis work:** Novel scheme that models electromagnetic interactions between kinetic plasma turbulence and the confining magnetic field in tokamak boundary for the first time
- Massively-parallel implementation scales efficiently to ~1000 CPU cores; GPU implementation in progress!



https://github.com/ammarhakim/gkyl/

https://gkyl.readthedocs.io

https://gkyl.readthedocs.io/en/latest/gkyl/pubs.html

The discontinuous Galerkin method

- We use the **discontinuous Galerkin** (DG) method in Gkeyll
  - Class of finite-element methods with discontinuous basis functions to represent solution in each cell
  - Highly local, highly parallelizable, allows high-order accuracy, enforces local conservation laws
  - Can use limiters for stability (as in FV)

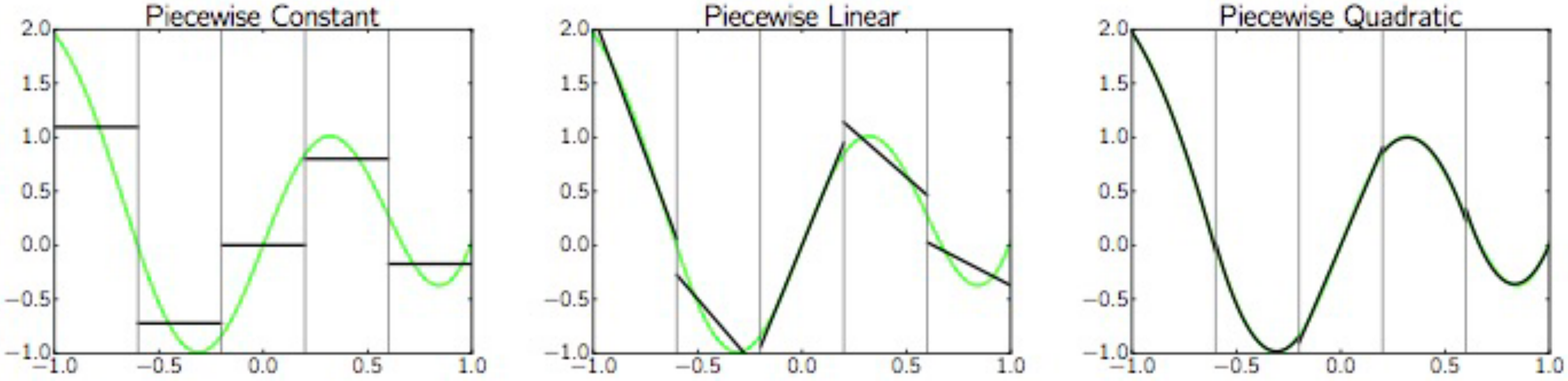


Figure: The best L_2 fit of $x^4 + \sin(5x)$ (green) using piecewise constant (left), linear (center), and quadratic (right) polynomials.

Orthonormal modal DG

- Our system can be expressed as a hyperbolic conservation law: $\frac{\partial f}{\partial t} + \nabla_{\vec{Z}} \cdot \left(\vec{\alpha} f\right) = 0$
- *Modal* expansion of solution in each cell: $f(\vec{Z},t) = \sum_{k}^{N_b} f_k(t) w_k(\vec{Z})$
- Fundamental DG operations can be expressed as tensor products, e.g. volume term:

$$\int_{C_m} d\vec{Z}\ f\vec{\alpha}\cdot\nabla w_i = \sum_{j,k} \underbrace{\left(\int_{C_m} d\vec{Z}\ w_j w_k \nabla w_i\right)}_{\overleftrightarrow{T}_{ijk}} \cdot \vec{\alpha}_j f_k$$

- Naively, this requires $\mathcal{O}(N_b^3)$ operations, same as quadrature (without aliasing)
- But if we choose basis functions to be *orthonormal*, $\overleftrightarrow{T}_{ijk}$ is sparse!
  - We use “Serendipity” Legendre polynomials as our orthonormal basis functions
- Use a computer algebra system (Maxima) to compute sparse tensor products *analytically* and generate solver kernels

Computer-generated DG kernels

$$\mathtt{out}_i = \sum_{j,k} \overleftrightarrow{T}_{ijk} \cdot \overrightarrow{\alpha}_j f_k \quad \Rightarrow$$

```
out[1] += 0.3061862178478971*(alphax[9]*f[9]+alphax[7]*f[7]+alphax[4]*f[4]+alphax[3]*f[3]+alphax[1]*f[1]
out[2] += 0.3061862178478971*(alphay[16]*f[16]+alphay[12]*f[12]+alphay[9]*f[9]+alphay[8]*f[8]+alphay[7]*
out[3] += 0.3061862178478971*(alphaz[1]*f[1]+alphaz[0]*f[0]);
out[4] += 0.3061862178478971*(alphav[26]*f[26]+alphav[23]*f[23]+alphav[19]*f[19]+alphav[18]*f[18]+alphav
out[6] += 0.3061862178478971*(alphax[9]*f[17]+(alphay[8]+alphax[7])*f[16]+f[8]*alphay[16]+alphay[5]*f[12
out[7] += 0.3061862178478971*(alphax[9]*f[18]+alphax[4]*f[11]+alphax[1]*f[7]+f[1]*alphax[7]+alphax[0]*f[
out[8] += 0.3061862178478971*(alphay[12]*f[21]+alphay[9]*f[18]+alphay[6]*f[16]+f[6]*alphay[16]+alphay[5]
out[9] += 0.3061862178478971*(alphav[19]*f[26]+f[19]*alphav[26]+alphav[15]*f[23]+f[15]*alphav[23]+(alpha
out[10] += 0.3061862178478971*(alphav[23]*f[28]+(alphav[18]+alphay[16])*f[26]+f[18]*alphav[26]+alphav[15
out[11] += 0.3061862178478971*(alphav[23]*f[29]+alphav[17]*f[26]+f[17]*alphav[26]+alphav[15]*f[25]+alpha
out[12] += 0.3061862178478971*(alphax[9]*f[23]+alphax[7]*f[21]+alphax[4]*f[15]+alphax[3]*f[14]+alphax[1]
out[13] += 0.3061862178478971*(alphay[16]*f[27]+alphay[9]*f[23]+alphay[8]*f[22]+alphay[7]*f[21]+alphay[6
out[14] += 0.3061862178478971*(alphaz[1]*f[12]+alphaz[0]*f[5]);
out[15] += 0.3061862178478971*(alphav[26]*f[31]+alphav[19]*f[30]+alphav[18]*f[29]+alphav[17]*f[28]+alpha
out[16] += 0.3061862178478971*(alphax[9]*f[26]+alphay[5]*f[21]+alphax[4]*f[19]+alphay[4]*f[18]+(alphay[2
out[17] += 0.3061862178478971*(alphav[15]*f[28]+(alphav[11]+alphay[8]+alphax[7])*f[26]+f[11]*alphav[26]+
out[18] += 0.3061862178478971*(alphav[15]*f[29]+alphav[10]*f[26]+f[10]*alphav[26]+alphav[23]*f[25]+alpha
out[19] += 0.3061862178478971*(alphav[23]*f[31]+alphav[15]*f[30]+alphay[12]*f[29]+alphav[12]*f[27]+(alph
out[20] += 0.3061862178478971*(alphax[9]*f[28]+(alphay[8]+alphax[7])*f[27]+alphax[4]*f[24]+alphay[4]*f[2
out[21] += 0.3061862178478971*(alphax[9]*f[29]+alphax[4]*f[25]+alphax[1]*f[21]+alphax[0]*f[14]+(alphax[7
out[22] += 0.3061862178478971*(alphay[9]*f[29]+alphay[6]*f[27]+alphay[4]*f[25]+alphay[2]*f[22]+alphay[1]
out[23] += 0.3061862178478971*(alphav[19]*f[31]+alphav[26]*f[30]+(alphav[11]+alphax[7])*f[29]+alphav[10]
out[24] += 0.3061862178478971*((alphav[18]+alphay[16])*f[31]+(alphav[11]+alphay[8])*f[30]+(alphav[26]+al
out[25] += 0.3061862178478971*(alphav[17]*f[31]+alphav[10]*f[30]+alphav[9]*f[29]+alphav[26]*f[28]+alphav
out[26] += 0.3061862178478971*(alphav[15]*f[31]+alphav[23]*f[30]+alphay[5]*f[29]+alphav[5]*f[27]+(alphav
out[27] += 0.3061862178478971*(alphax[9]*f[31]+alphax[4]*f[30]+alphay[4]*f[29]+(alphay[2]+alphax[1])*f[2
out[28] += 0.3061862178478971*((alphav[11]+alphay[8]+alphax[7])*f[31]+(alphav[18]+alphay[16]+alphax[3])*
out[29] += 0.3061862178478971*(alphav[10]*f[31]+alphav[17]*f[30]+(alphav[4]+alphax[1])*f[29]+alphav[19]*
out[30] += 0.3061862178478971*((alphav[9]+alphay[6])*f[31]+(alphav[4]+alphay[2])*f[30]+(alphav[17]+alpha
out[31] += 0.3061862178478971*((alphav[4]+alphay[2]+alphax[1])*f[31]+(alphav[9]+alphay[6]+alphax[0])*f[3
```

Computer-generated DG kernels

$$\mathtt{out}_i = \sum_{j,k} \overleftrightarrow{T}_{ijk} \cdot \overrightarrow{\alpha}_j f_k \quad \rightarrow$$

```
out[1] += 0.3061862178478971*(alphax[9]*f[9]+alphax[7]*f[7]+alphax[4]*f[4]+alphax[3]*f[3]+alphax[1]*f[1]
out[2] += 0.3061862178478971*(alphay[16]*f[16]+alphay[12]*f[12]+alphay[9]*f[9]+alphay[8]*f[8]+alphay[7]*
out[3] += 0.3061862178478971*(alphaz[1]*f[1]+alphaz[0]*f[0]);
out[4] += 0.3061862178478971*(alphav[26]*f[26]+alphav[23]*f[23]+alphav[19]*f[19]+alphav[18]*f[18]+alphav
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out[7] += 0.3061862178478971*(alphax[9]*f[18]+alphax[4]*f[11]+alphax[1]*f[7]+f[1]*alphax[7]+alphax[0]*f[
out[8] += 0.3061862178478971*(alphay[12]*f[21]+alphay[9]*f[18]+alphay[6]*f[16]+f[6]*alphay[16]+alphay[5]
out[9] += 0.3061862178478971*(alphav[19]*f[26]+f[19]*alphav[26]+alphav[15]*f[23]+f[15]*alphav[23]+(alpha
out[10] += 0.3061862178478971*(alphav[23]*f[28]+(alphav[18]+alphay[16])*f[26]+f[18]*alphav[26]+alphav[15
out[11] += 0.3061862178478971*(alphav[23]*f[29]+alphav[17]*f[26]+f[17]*alphav[26]+alphav[15]*f[25]+alpha
out[12] += 0.3061862178478971*(alphax[9]*f[23]+alphax[7]*f[21]+alphax[4]*f[15]+alphax[3]*f[14]+alphax[1]
out[13] += 0.3061862178478971*(alphay[16]*f[27]+alphay[9]*f[23]+alphay[8]*f[22]+alphay[7]*f[21]+alphay[6
out[14] += 0.3061862178478971*(alphaz[1]*f[12]+alphaz[0]*f[5]);
out[15] += 0.3061862178478971*(alphav[26]*f[31]+alphav[19]*f[30]+alphav[18]*f[29]+alphav[17]*f[28]+alpha
out[16] += 0.3061862178478971*(alphax[9]*f[26]+alphay[5]*f[21]+alphax[4]*f[19]+alphay[4]*f[18]+(alphay[2
out[17] += 0.3061862178478971*(alphav[15]*f[28]+(alphav[11]+alphay[8]+alphax[7])*f[26]+f[11]*alphav[26]+
out[18] += 0.3061862178478971*(alphav[15]*f[29]+alphav[10]*f[26]+f[10]*alphav[26]+alphav[23]*f[25]+alpha
out[19] += 0.3061862178478971*(alphav[23]*f[31]+alphav[15]*f[30]+alphay[12]*f[29]+alphav[12]*f[27]+(alph
out[20] += 0.3061862178478971*(alphax[9]*f[28]+(alphay[8]+alphax[7])*f[27]+alphax[4]*f[24]+alphay[4]*f[2
out[21] += 0.3061862178478971*(alphax[9]*f[29]+alphax[4]*f[25]+alphax[1]*f[21]+alphax[0]*f[14]+(alphax[7
out[22] += 0.3061862178478971*(alphay[9]*f[29]+alphay[6]*f[27]+alphay[4]*f[25]+alphay[2]*f[22]+alphay[1]
out[23] += 0.3061862178478971*(alphav[19]*f[31]+alphav[26]*f[30]+(alphav[11]+alphax[7])*f[29]+alphav[10]
out[24] += 0.3061862178478971*((alphav[18]+alphay[16])*f[31]+(alphav[11]+alphay[8])*f[30]+(alphav[26]+al
out[25] += 0.3061862178478971*(alphav[17]*f[31]+alphav[10]*f[30]+alphav[9]*f[29]+alphav[26]*f[28]+alphav
out[26] += 0.3061862178478971*(alphav[15]*f[31]+alphav[23]*f[30]+alphay[5]*f[29]+alphav[5]*f[27]+(alphav
out[27] += 0.3061862178478971*(alphax[9]*f[31]+alphax[4]*f[30]+alphay[4]*f[29]+(alphay[2]+alphax[1])*f[2
out[28] += 0.3061862178478971*((alphav[11]+alphay[8]+alphax[7])*f[31]+(alphav[18]+alphay[16]+alphax[3])*
out[29] += 0.3061862178478971*(alphav[10]*f[31]+alphav[17]*f[30]+(alphav[4]+alphax[1])*f[29]+alphav[19]*
out[30] += 0.3061862178478971*((alphav[9]+alphay[6])*f[31]+(alphav[4]+alphay[2])*f[30]+(alphav[17]+alpha
out[31] += 0.3061862178478971*((alphav[4]+alphay[2]+alphax[1])*f[31]+(alphav[9]+alphay[6]+alphax[0])*f[3
```

- Maxima generates thousands of lines of machine-written C code… no loops!
  - Takes advantage of significant sparsity in tensor contractions

Computer-generated DG kernels

5D piecewise linear basis = 32 basis functions

$$\mathtt{out}_i = \sum_{j,k} \overleftrightarrow{T}_{ijk} \cdot \overrightarrow{\alpha}_j f_k$$

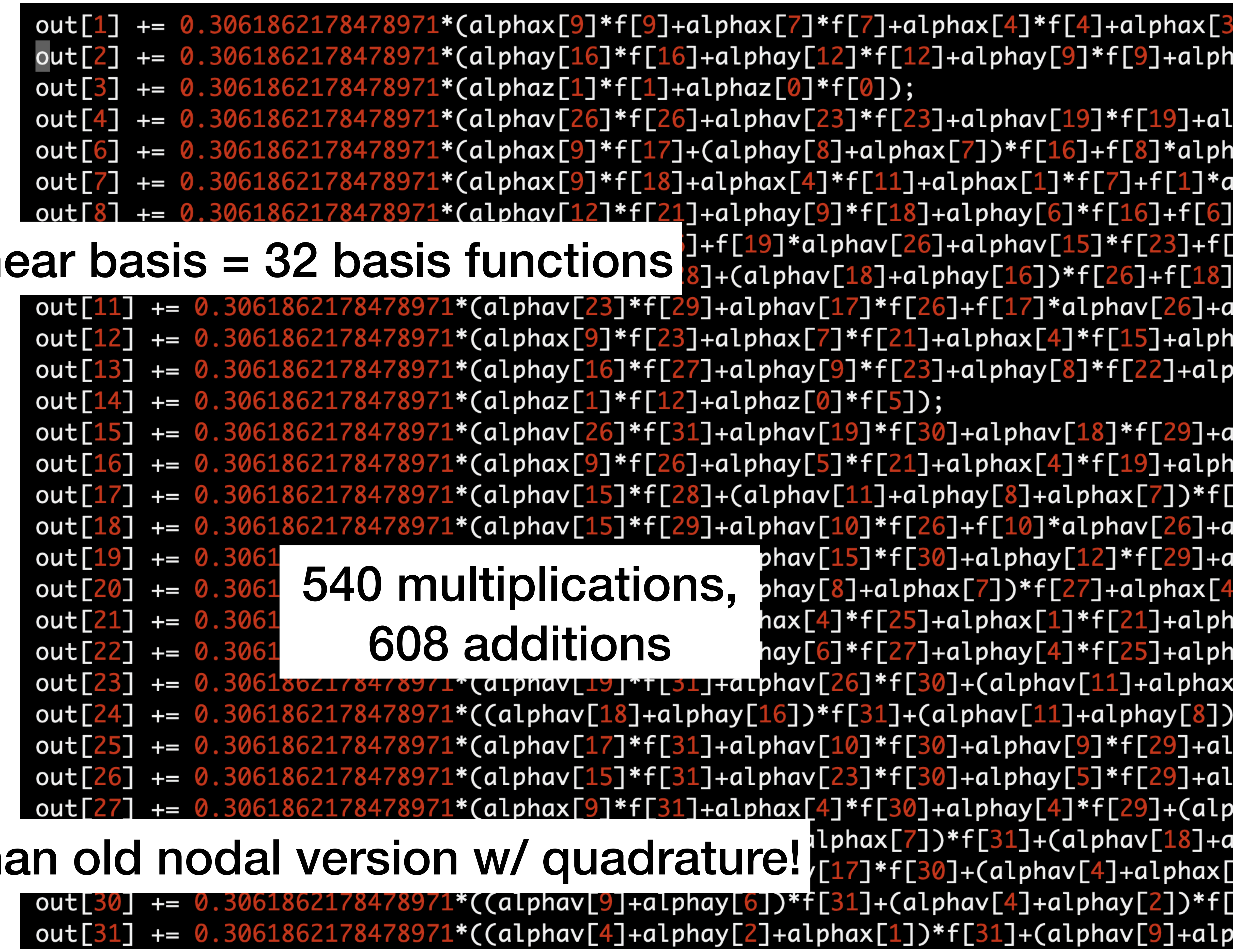
163,840 multiplications,
98,304 additions

```
out[1] += 0.3061862178478971*(alphax[9]*f[9]+alphax[7]*f[7]+alphax[4]*f[4]+alphax[3]*f[3]+alphax[1]*f[1]
out[2] += 0.3061862178478971*(alphay[16]*f[16]+alphay[12]*f[12]+alphay[9]*f[9]+alphay[8]*f[8]+alphay[7]*
out[3] += 0.3061862178478971*(alphaz[1]*f[1]+alphaz[0]*f[0]);
out[4] += 0.3061862178478971*(alphav[26]*f[26]+alphav[23]*f[23]+alphav[19]*f[19]+alphav[18]*f[18]+alphav
out[6] += 0.3061862178478971*(alphax[9]*f[17]+(alphay[8]+alphax[7])*f[16]+f[8]*alphay[16]+alphay[5]*f[12
out[7] += 0.3061862178478971*(alphax[9]*f[18]+alphax[4]*f[11]+alphax[1]*f[7]+f[1]*alphax[7]+alphax[0]*f[
out[8] += 0.3061862178478971*(alphay[12]*f[21]+alphay[9]*f[18]+alphay[6]*f[16]+f[6]*alphay[16]+alphay[5]
]+f[19]*alphav[26]+alphav[15]*f[23]+f[15]*alphav[23]+(alpha
8]+(alphav[18]+alphay[16])*f[26]+f[18]*alphav[26]+alphav[15
out[11] += 0.3061862178478971*(alphav[23]*f[29]+alphav[17]*f[26]+f[17]*alphav[26]+alphav[15]*f[25]+alpha
out[12] += 0.3061862178478971*(alphax[9]*f[23]+alphax[7]*f[21]+alphax[4]*f[15]+alphax[3]*f[14]+alphax[1]
out[13] += 0.3061862178478971*(alphay[16]*f[27]+alphay[9]*f[23]+alphay[8]*f[22]+alphay[7]*f[21]+alphay[6
out[14] += 0.3061862178478971*(alphaz[1]*f[12]+alphaz[0]*f[5]);
out[15] += 0.3061862178478971*(alphav[26]*f[31]+alphav[19]*f[30]+alphav[18]*f[29]+alphav[17]*f[28]+alpha
out[16] += 0.3061862178478971*(alphax[9]*f[26]+alphay[5]*f[21]+alphax[4]*f[19]+alphay[4]*f[18]+(alphay[2
out[17] += 0.3061862178478971*(alphav[15]*f[28]+(alphav[11]+alphay[8]+alphax[7])*f[26]+f[11]*alphav[26]+
out[18] += 0.3061862178478971*(alphav[15]*f[29]+alphav[10]*f[26]+f[10]*alphav[26]+alphav[23]*f[25]+alpha
out[19] += 0.3061 phav[15]*f[30]+alphay[12]*f[29]+alphav[12]*f[27]+(alph
out[20] += 0.3061 phay[8]+alphax[7])*f[27]+alphax[4]*f[24]+alphay[4]*f[2
out[21] += 0.3061 hax[4]*f[25]+alphax[1]*f[21]+alphax[0]*f[14]+(alphax[7
out[22] += 0.3061 hay[6]*f[27]+alphay[4]*f[25]+alphay[2]*f[22]+alphay[1]
out[23] += 0.3061862178478971*(alphav[19]*f[31]+alphav[26]*f[30]+(alphav[11]+alphax[7])*f[29]+alphav[10]
out[24] += 0.3061862178478971*((alphav[18]+alphay[16])*f[31]+(alphav[11]+alphay[8])*f[30]+(alphav[26]+al
out[25] += 0.3061862178478971*(alphav[17]*f[31]+alphav[10]*f[30]+alphav[9]*f[29]+alphav[26]*f[28]+alphav
out[26] += 0.3061862178478971*(alphav[15]*f[31]+alphav[23]*f[30]+alphay[5]*f[29]+alphav[5]*f[27]+(alphav
out[27] += 0.3061862178478971*(alphax[9]*f[31]+alphax[4]*f[30]+alphay[4]*f[29]+(alphay[2]+alphax[1])*f[2
out[28] += 0.3061862178478971*((alphav[11]+alphay[8]+alphax[7])*f[31]+(alphav[18]+alphay[16]+alphax[3])*
out[29] += 0.3061862178478971*(alphav[10]*f[31]+alphav[17]*f[30]+(alphav[4]+alphax[1])*f[29]+alphav[19]*
out[30] += 0.3061862178478971*((alphav[9]+alphay[6])*f[31]+(alphav[4]+alphay[2])*f[30]+(alphav[17]+alpha
out[31] += 0.3061862178478971*((alphav[4]+alphay[2]+alphax[1])*f[31]+(alphav[9]+alphay[6]+alphax[0])*f[3
```

540 multiplications,
608 additions

- Maxima generates thousands of lines of machine-written C code… no loops!
  - Takes advantage of significant sparsity in tensor contractions

Computer-generated DG kernels



5D piecewise linear basis = 32 basis functions

$$\mathtt{out}_i = \sum_{j,k} \overleftrightarrow{T}_{ijk} \cdot \overrightarrow{\alpha}_j f_k \quad \Rightarrow$$

163,840 multiplications,
98,304 additions

540 multiplications,
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Code is ~30x faster than old nodal version w/ quadrature!

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Computer-generated DG kernels

```
out[1] += 0.3061862178478971*(alphax[9]*f[9]+alphax[7]*f[7]+alphax[4]*f[4]+alphax[3]*f[3]+alphax[1]*f[1]
out[2] += 0.3061862178478971*(alphay[16]*f[16]+alphay[12]*f[12]+alphay[9]*f[9]+alph
out[3] += 0.3061862178478971*(alphaz[1]*f[1]+alphaz[0]*f[0]);
out[4] += 0.3061862178478971*(alphav[26]*f[26]+alphav[23]*f[23]+alphav[19]*f[19]+al
out[6] += 0.3061862178478971*(alphax[9]*f[17]+(alphay[8]+alphax[7])*f[16]+f[8]*alph
out[7] += 0.3061862178478971*(alphax[9]*f[18]+alphax[4]*f[11]+alphax[1]*f[7]+f[1]*a
out[8] += 0.3061862178478971*(alphay[12]*f[21]+alphay[9]*f[18]+alphay[6]*f[16]+f[6]
]+f[19]*alphav[26]+alphav[15]*f[23]+f[
8]+(alphav[18]+alphay[16])*f[26]+f[18]
out[11] += 0.3061862178478971*(alphav[23]*f[29]+alphav[17]*f[26]+f[17]*alphav[26]+a
out[12] += 0.3061862178478971*(alphax[9]*f[23]+alphax[7]*f[21]+alphax[4]*f[15]+alph
out[13] += 0.3061862178478971*(alphay[16]*f[27]+alphay[9]*f[23]+alphay[8]*f[22]+alp
out[14] += 0.3061862178478971*(alphaz[1]*f[12]+alphaz[0]*f[5]);
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out[16] += 0.3061862178478971*(alphax[9]*f[26]+alphay[5]*f[21]+alphax[4]*f[19]+alph
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out[19] += 0.3061                phav[15]*f[30]+alphay[12]*f[29]+alphav[12]*f[27]+(alph
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out[26] += 0.3061862178478971*(alphav[15]*f[31]+alphav[23]*f[30]+alphay[5]*f[29]+alphav[5]*f[27]+(alphav
out[27] += 0.3061862178478971*(alphax[9]*f[31]+alphax[4]*f[30]+alphay[4]*f[29]+(alphay[2]+alphax[1])*f[2
lphax[7])*f[31]+(alphav[18]+alphay[16]+alphax[3])*
[17]*f[30]+(alphav[4]+alphax[1])*f[29]+alphav[19]*
out[30] += 0.3061862178478971*((alphav[9]+alphay[6])*f[31]+(alphav[4]+alphay[2])*f[30]+(alphav[17]+alpha
out[31] += 0.3061862178478971*((alphav[4]+alphay[2]+alphax[1])*f[31]+(alphav[9]+alphay[6]+alphax[0])*f[3
```

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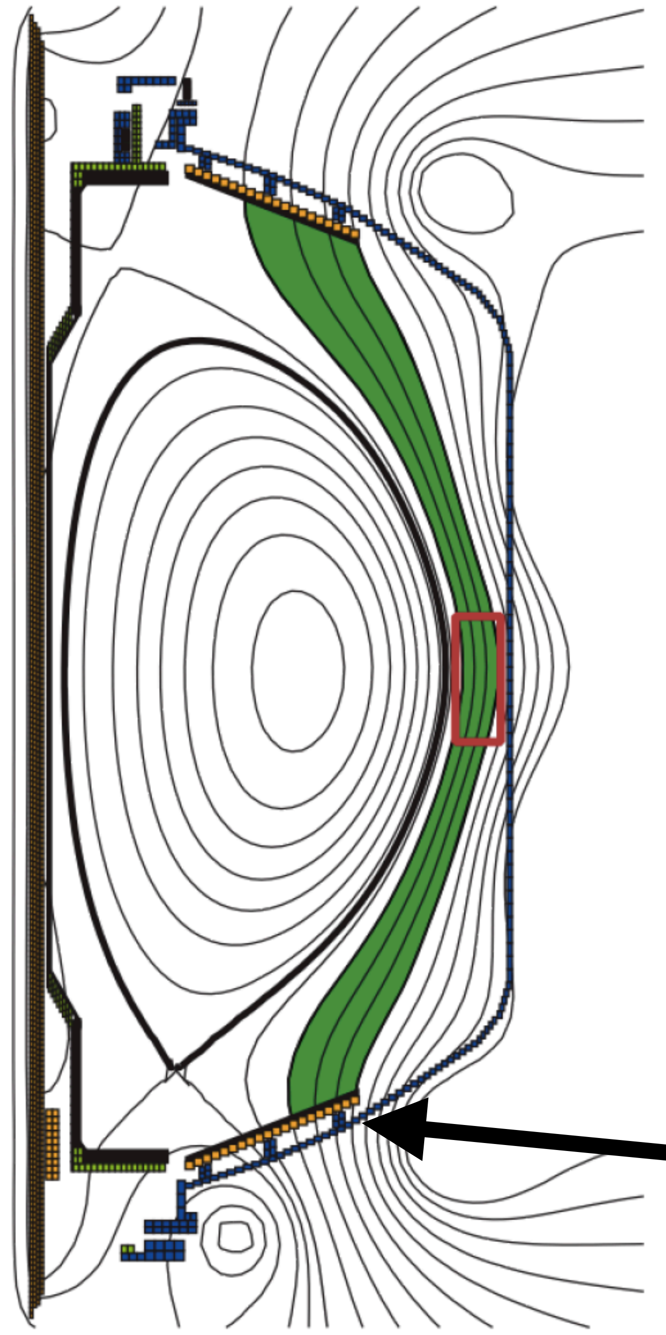
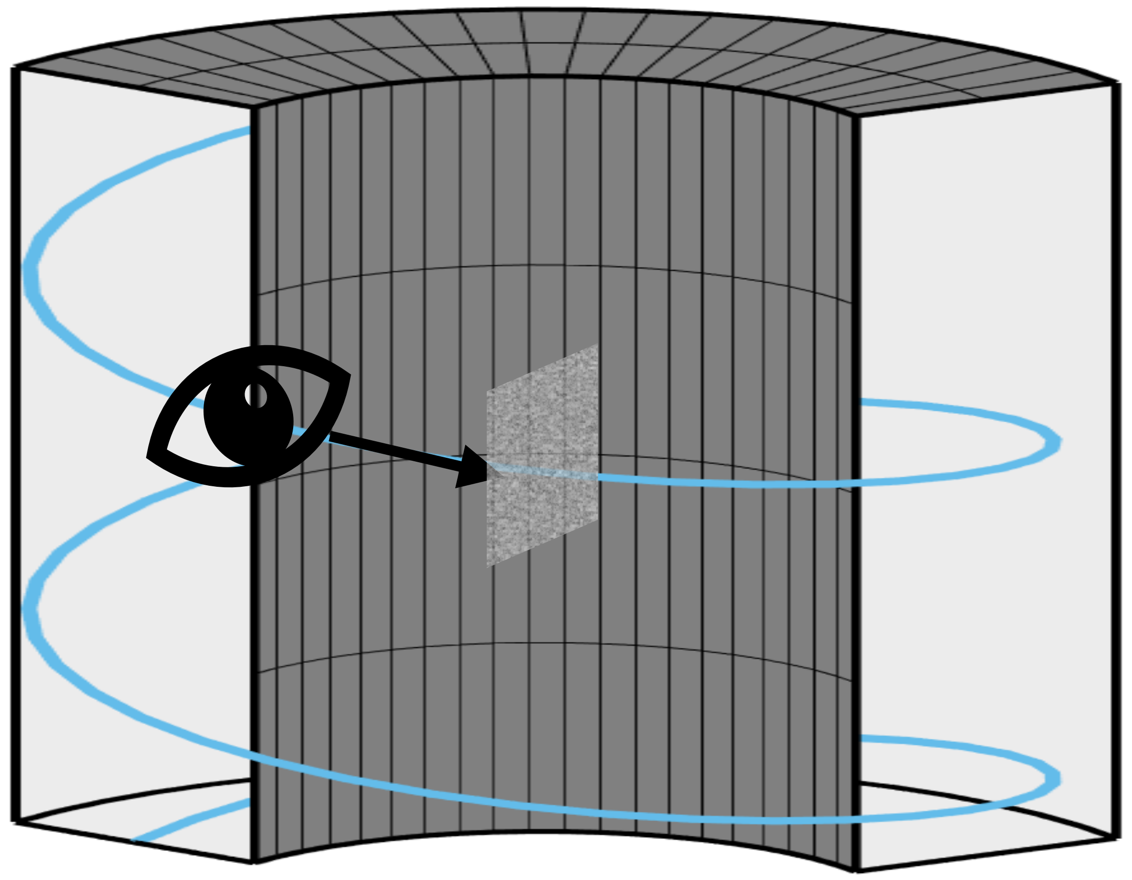
Code is ~30x faster than old nodal version w/ quadrature!

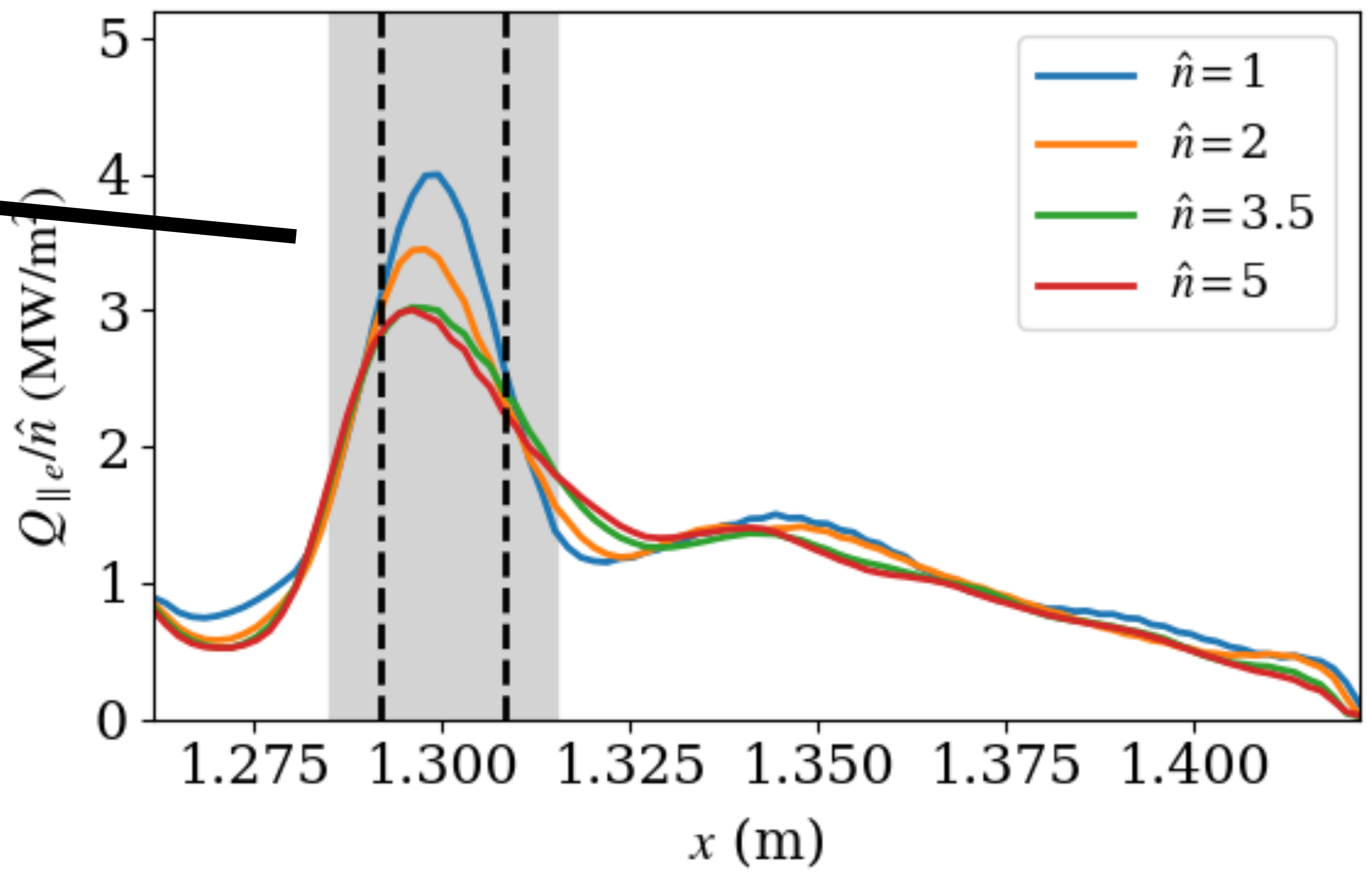
- Maxima generates thousands of lines of machine-written C code… no loops!
  - Takes advantage of significant sparsity in tensor contractions
- High arithmetic intensity is ideal for modern computing architectures
  - GPU version of Gkeyll nearly finished!

Blobby turbulence in the tokamak boundary

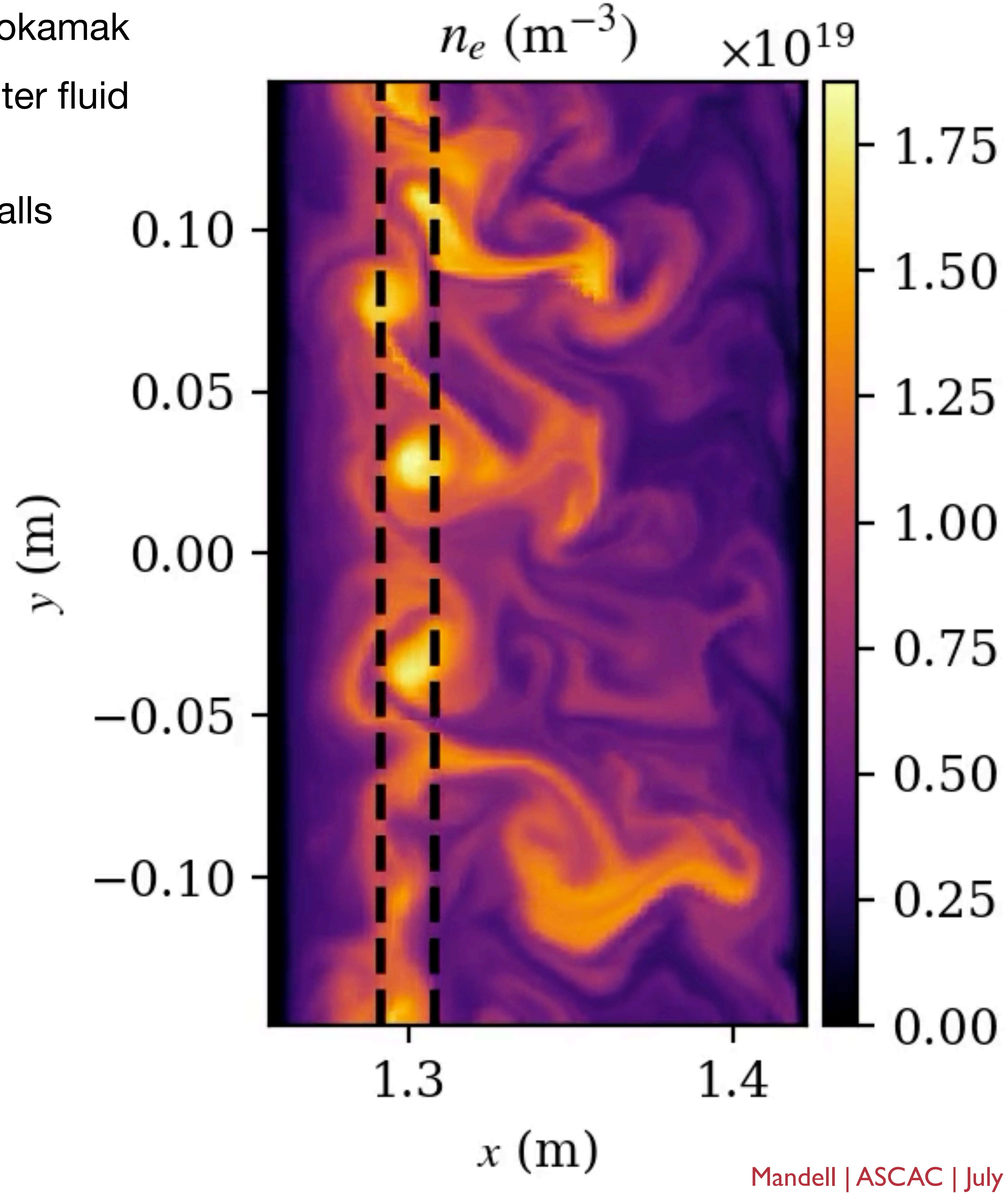
- Blobs of plasma propagate radially outwards in boundary region of tokamak
- Similar to Rayleigh-Taylor instability of heavy fluid falling through lighter fluid (flipped on its side)
- Turbulence can spread out heat flux “footprint” on device material walls







heat “footprint” on walls



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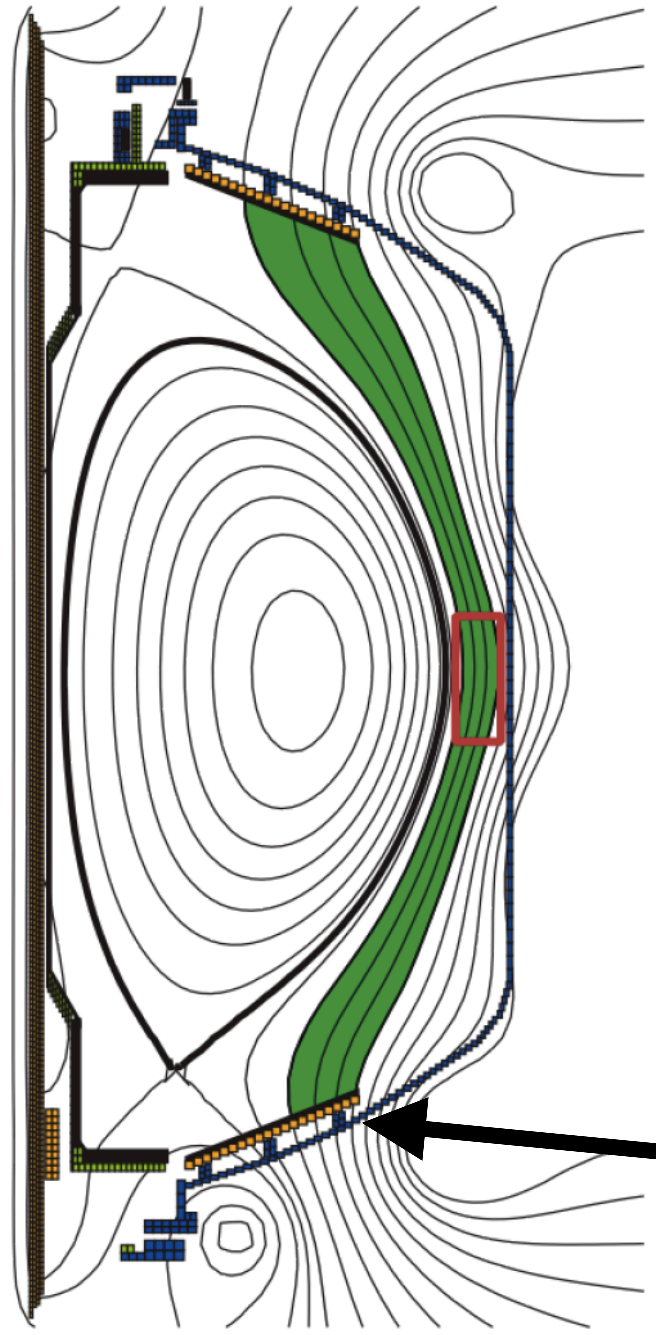

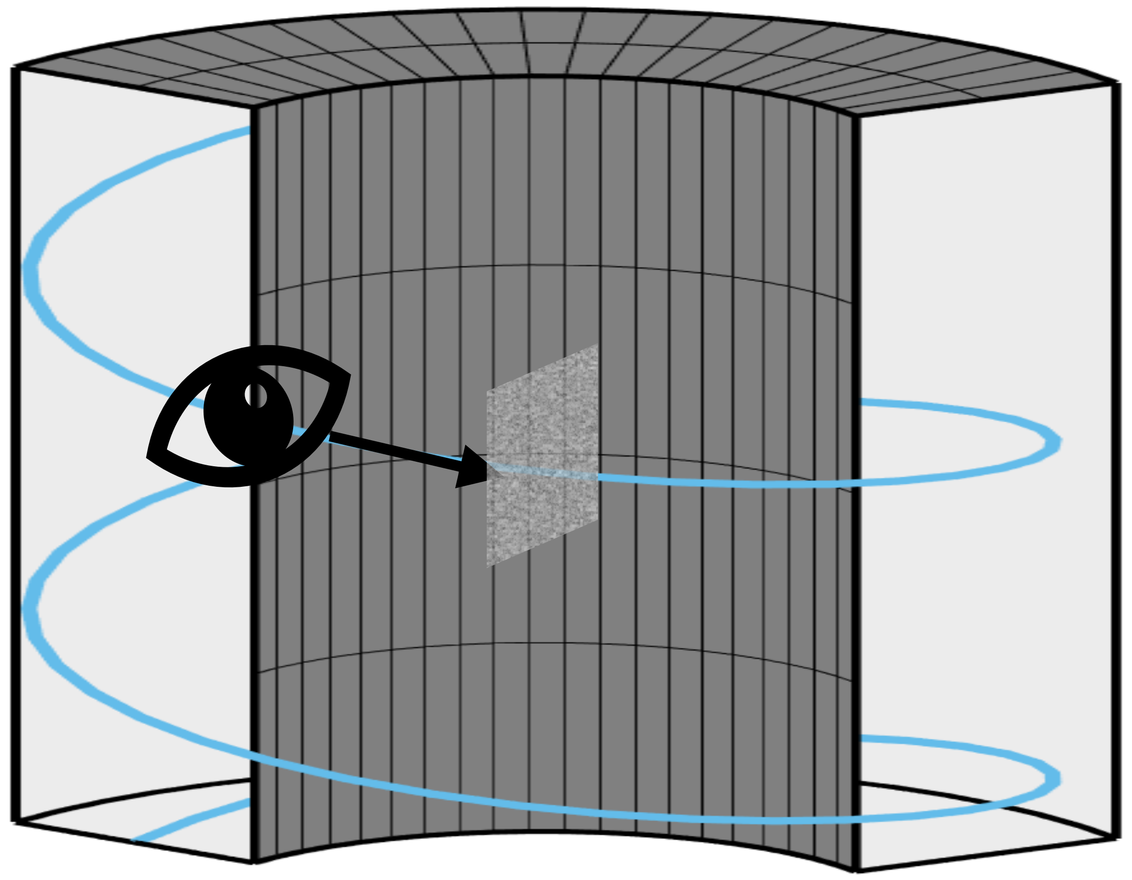

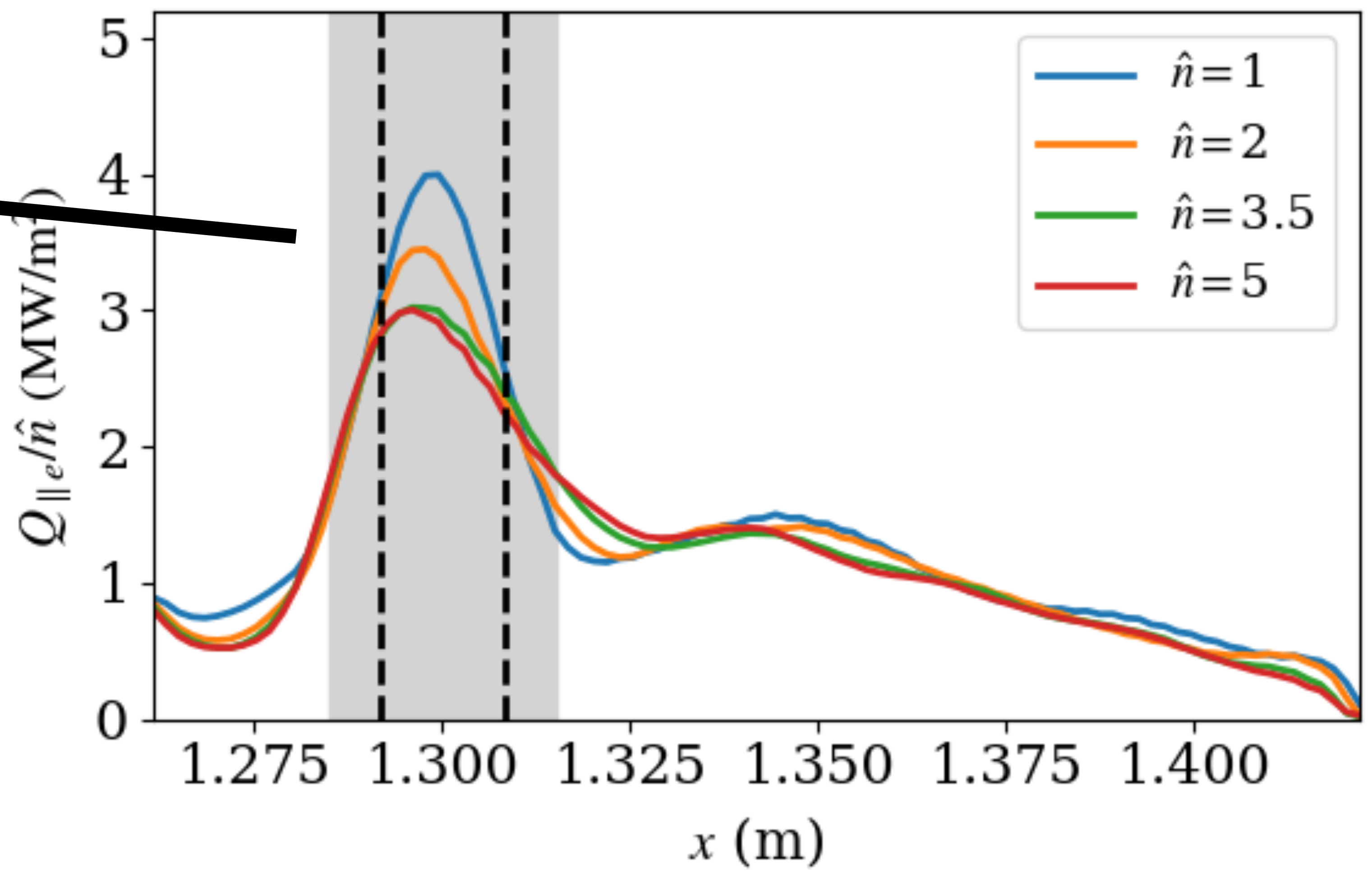

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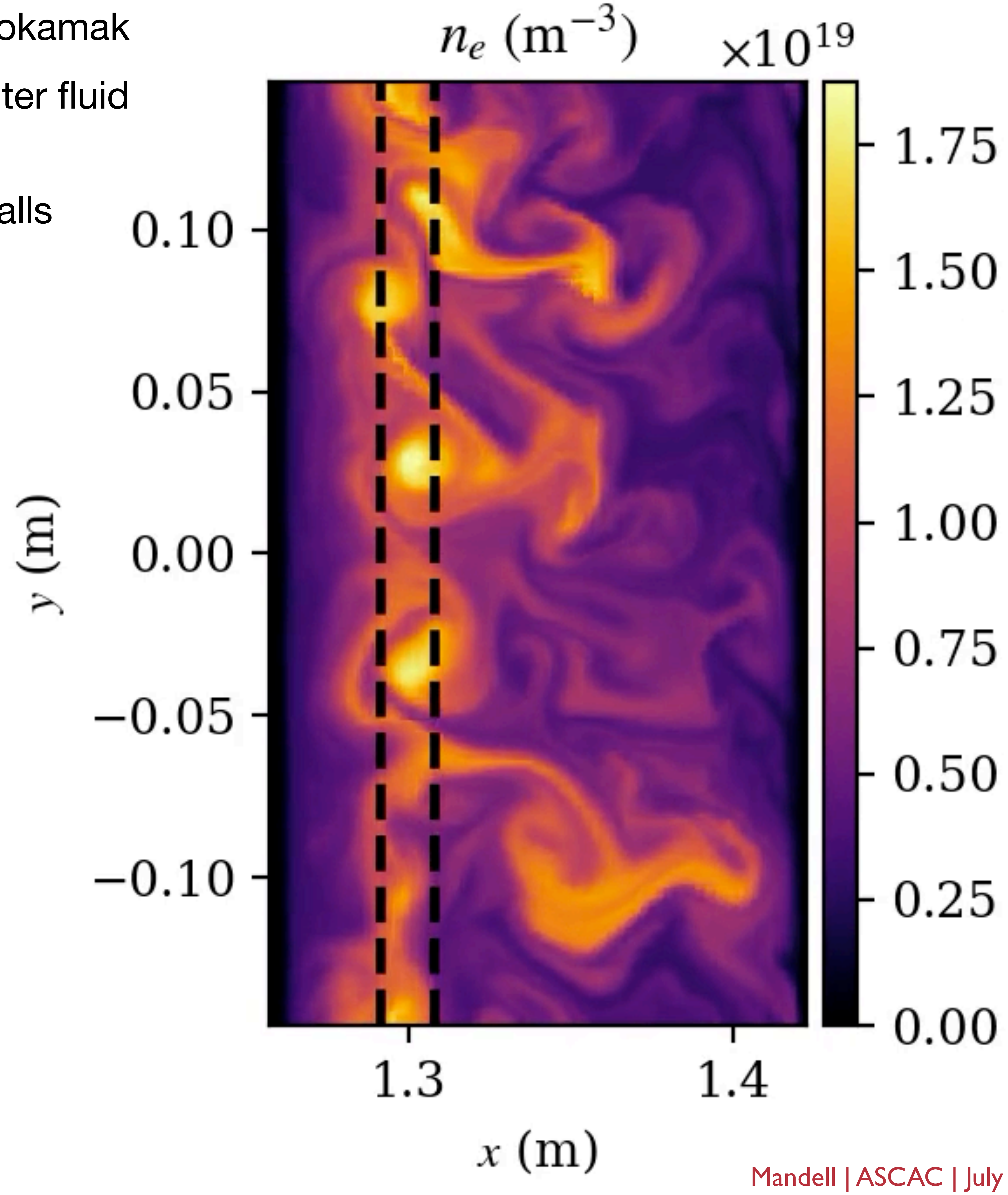
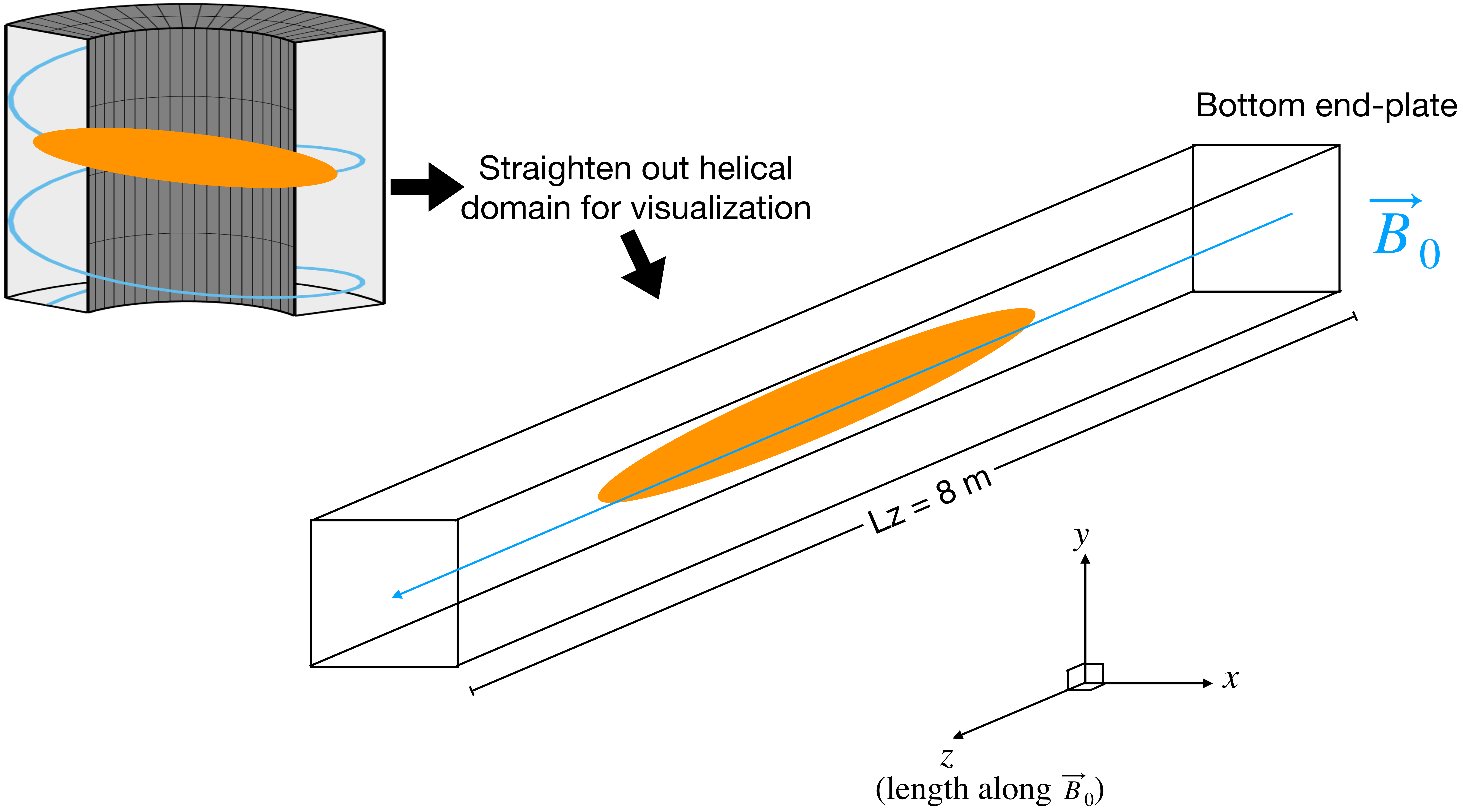
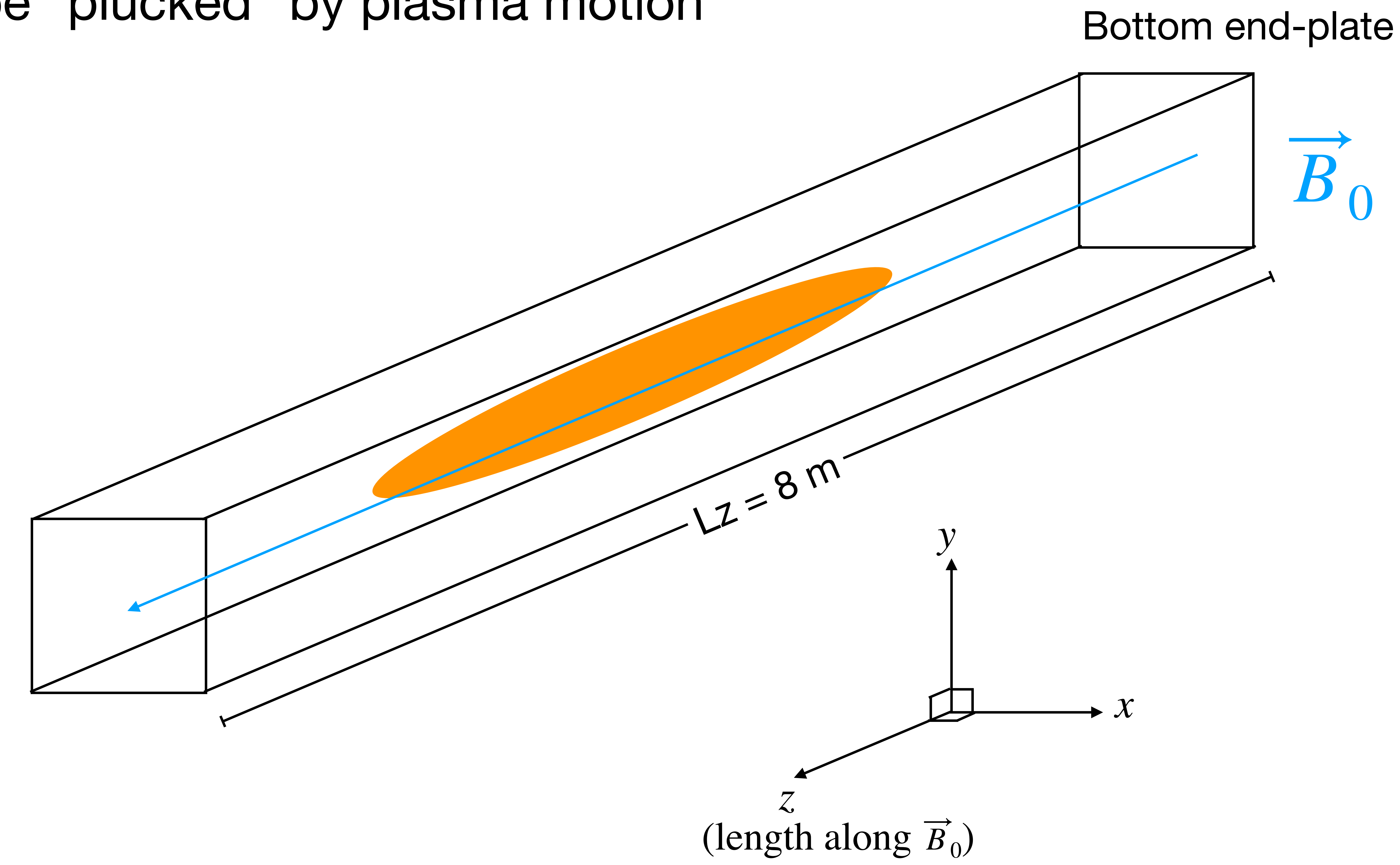


Interaction between magnetic field lines and plasma



Interaction between magnetic field lines and plasma

- Magnetic field lines in plasma behave like taut strings
- The field lines can be "plucked" by plasma motion



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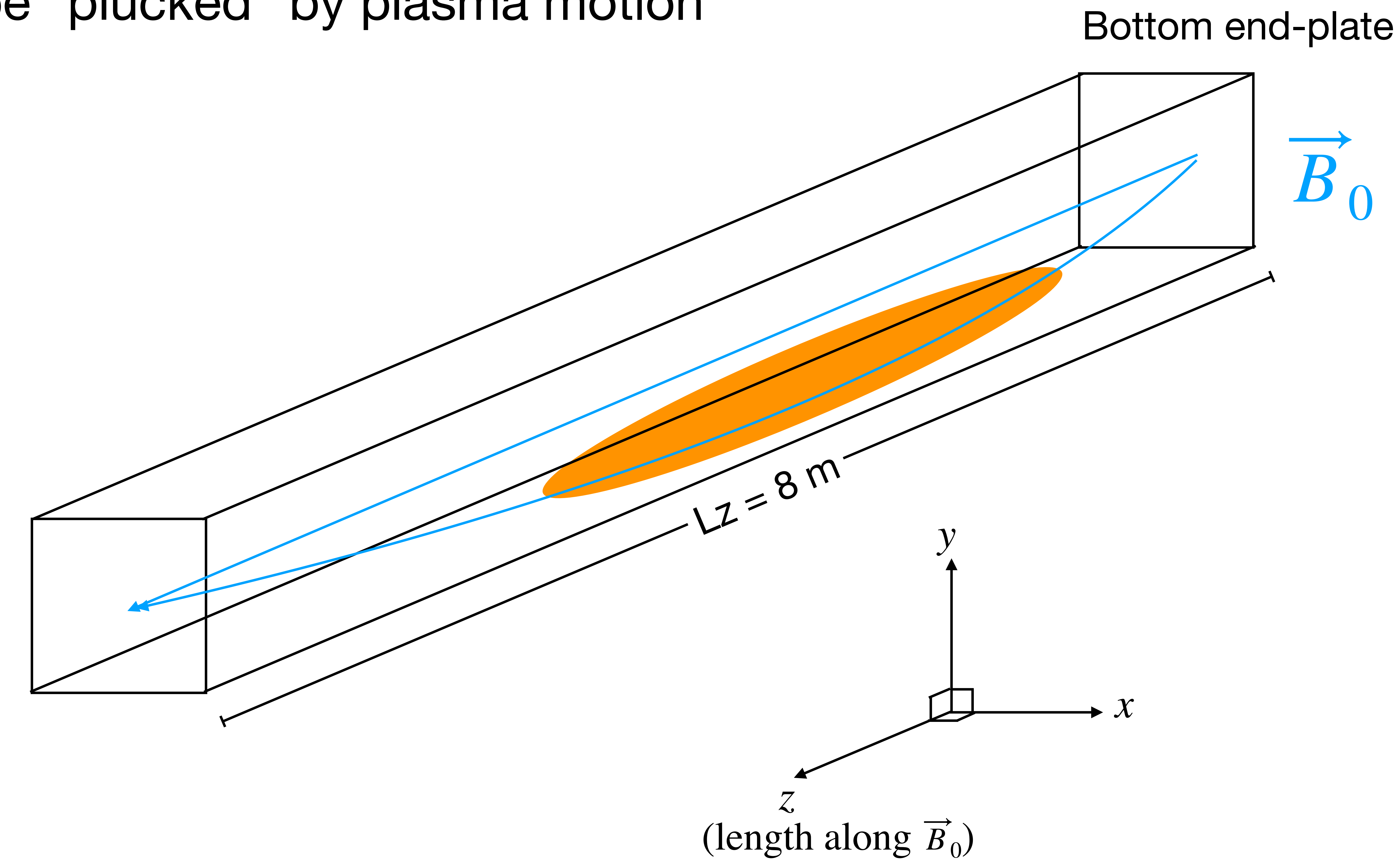

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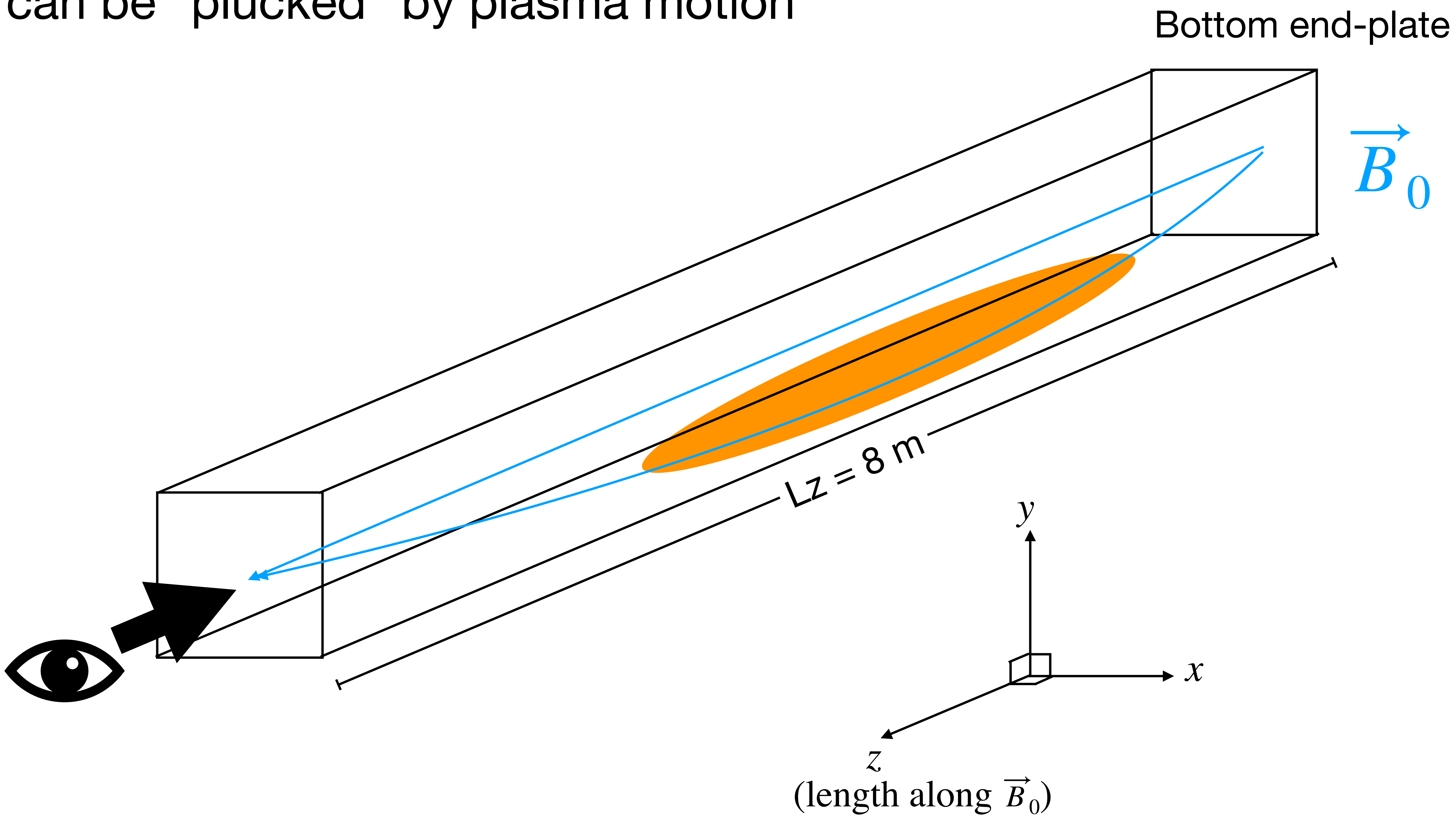

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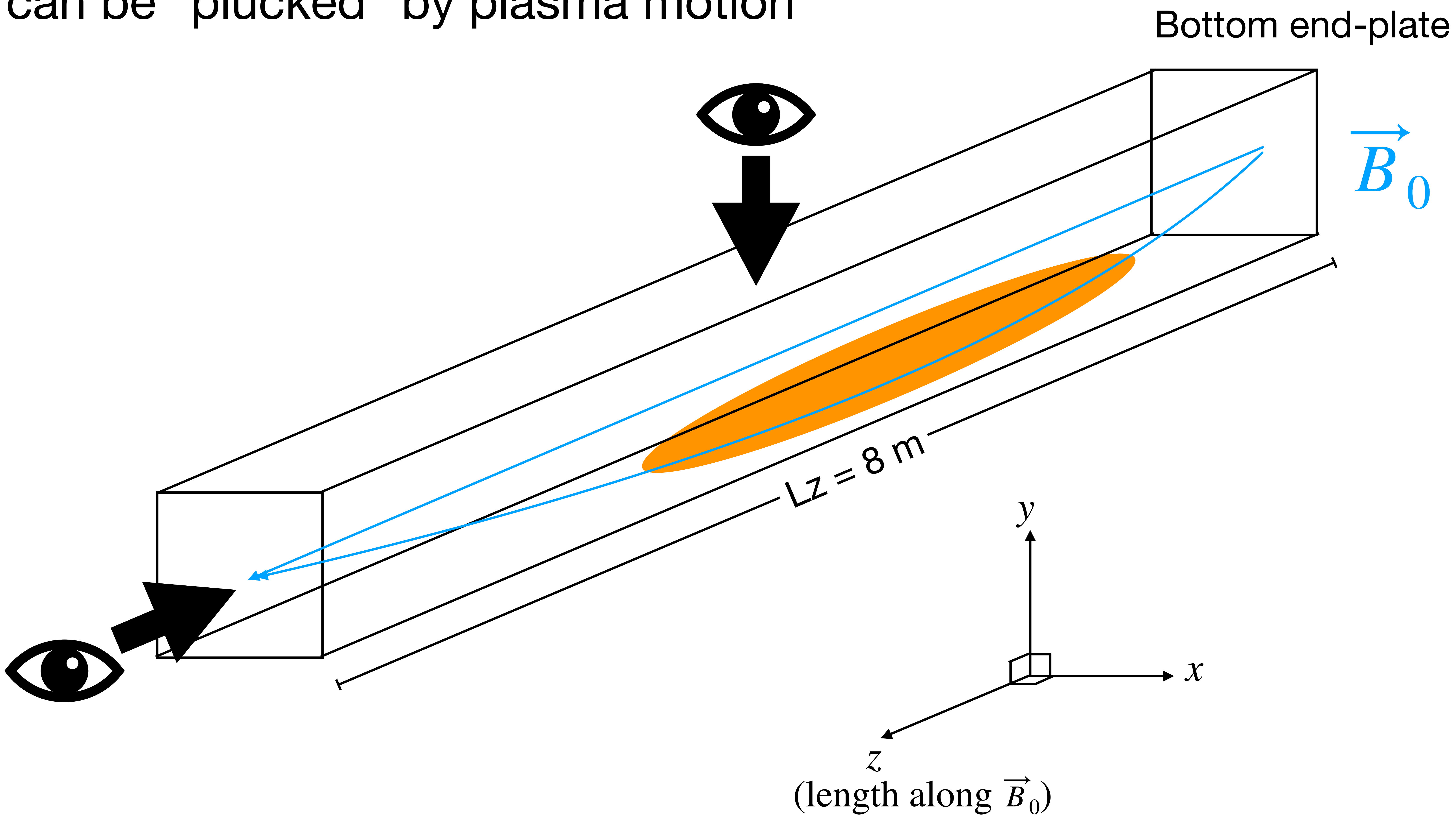
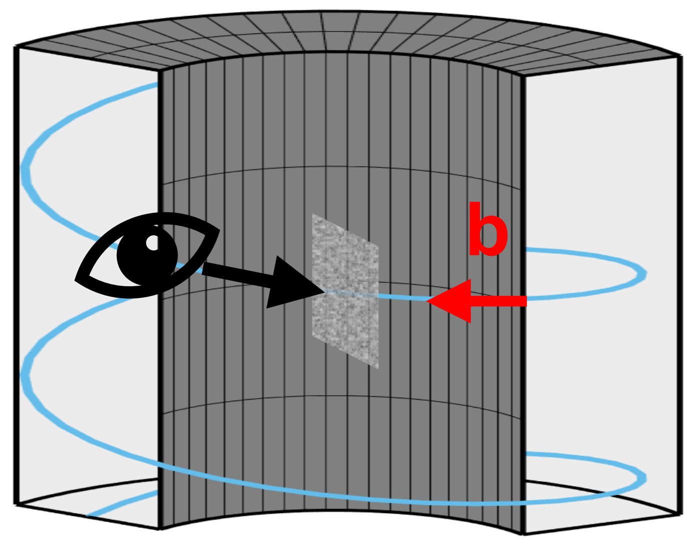
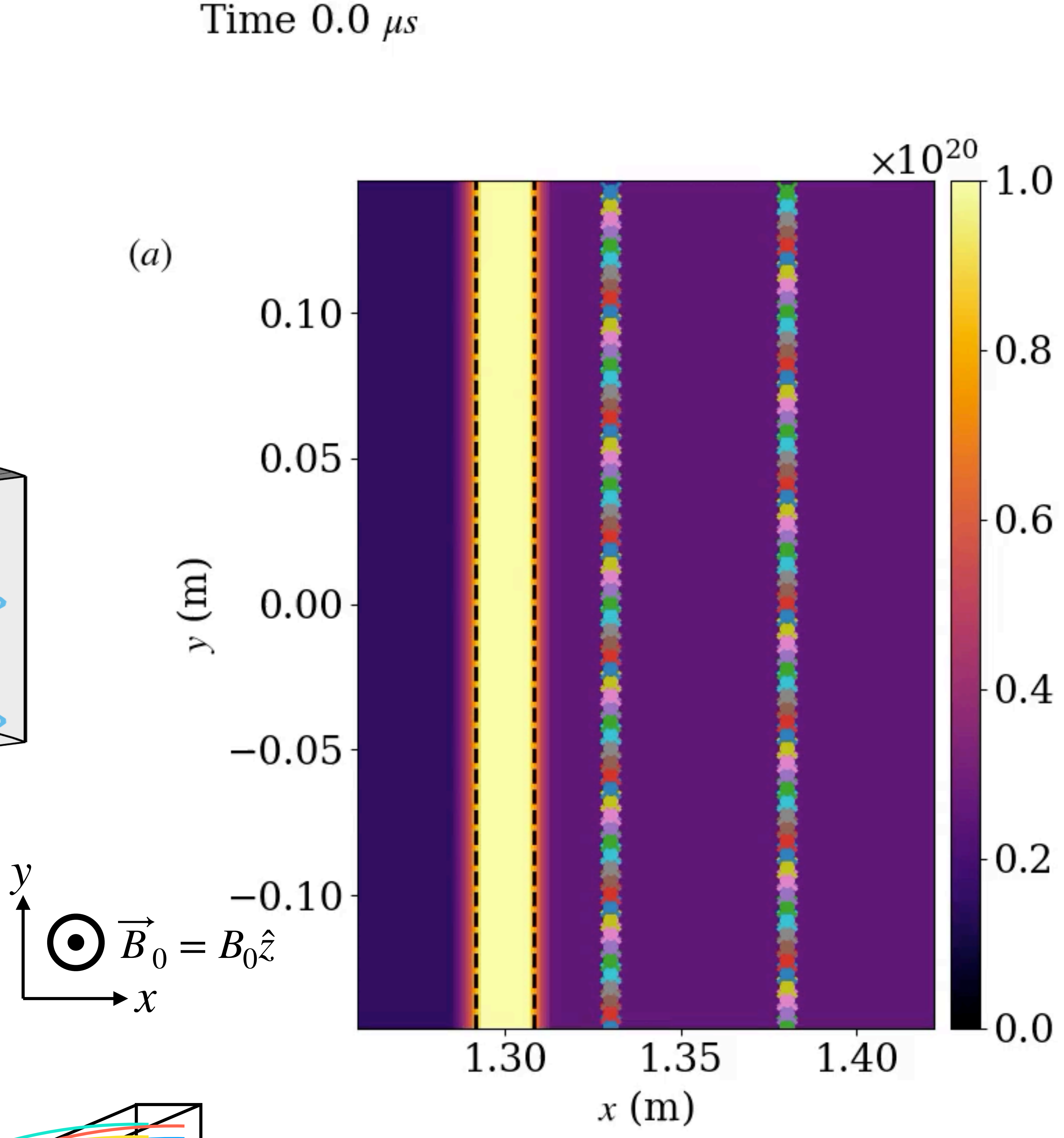
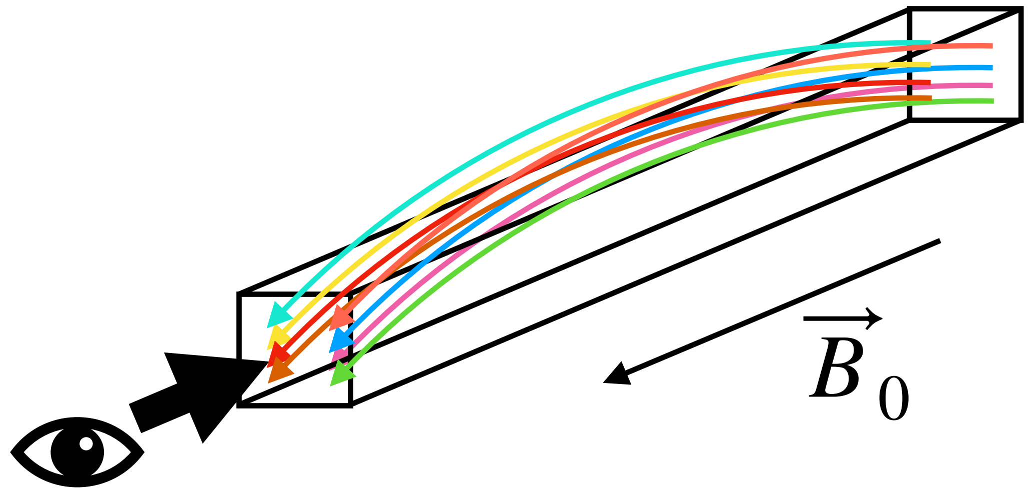
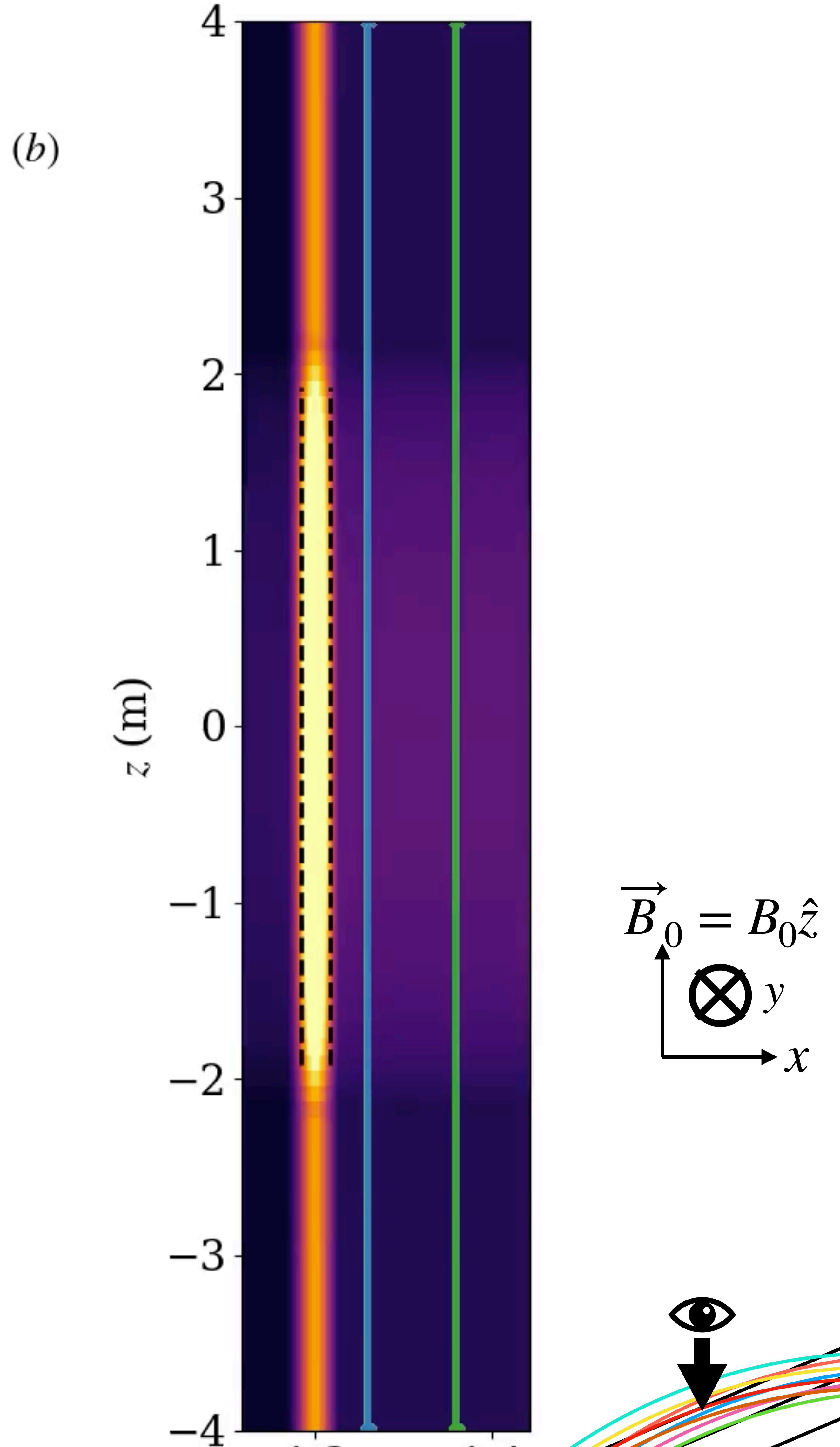


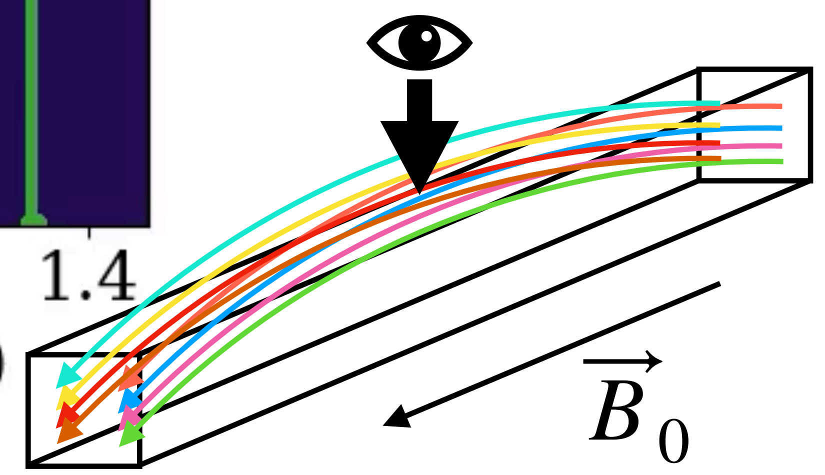
Visualizing Gkeyll's first-of-a-kind electromagnetic capabilities





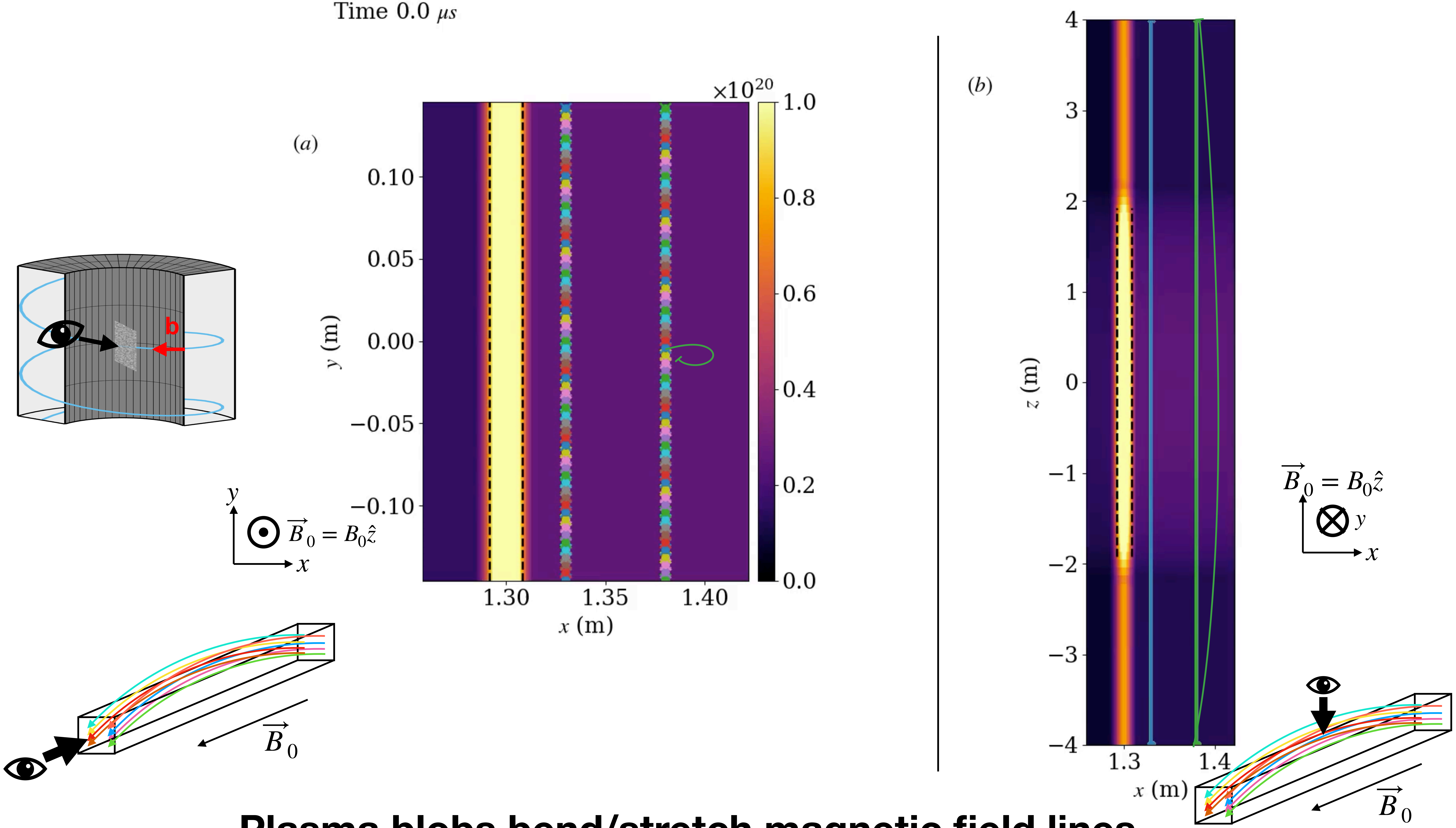






Plasma blobs bend/stretch magnetic field lines

Visualizing Gkeyll's first-of-a-kind electromagnetic capabilities



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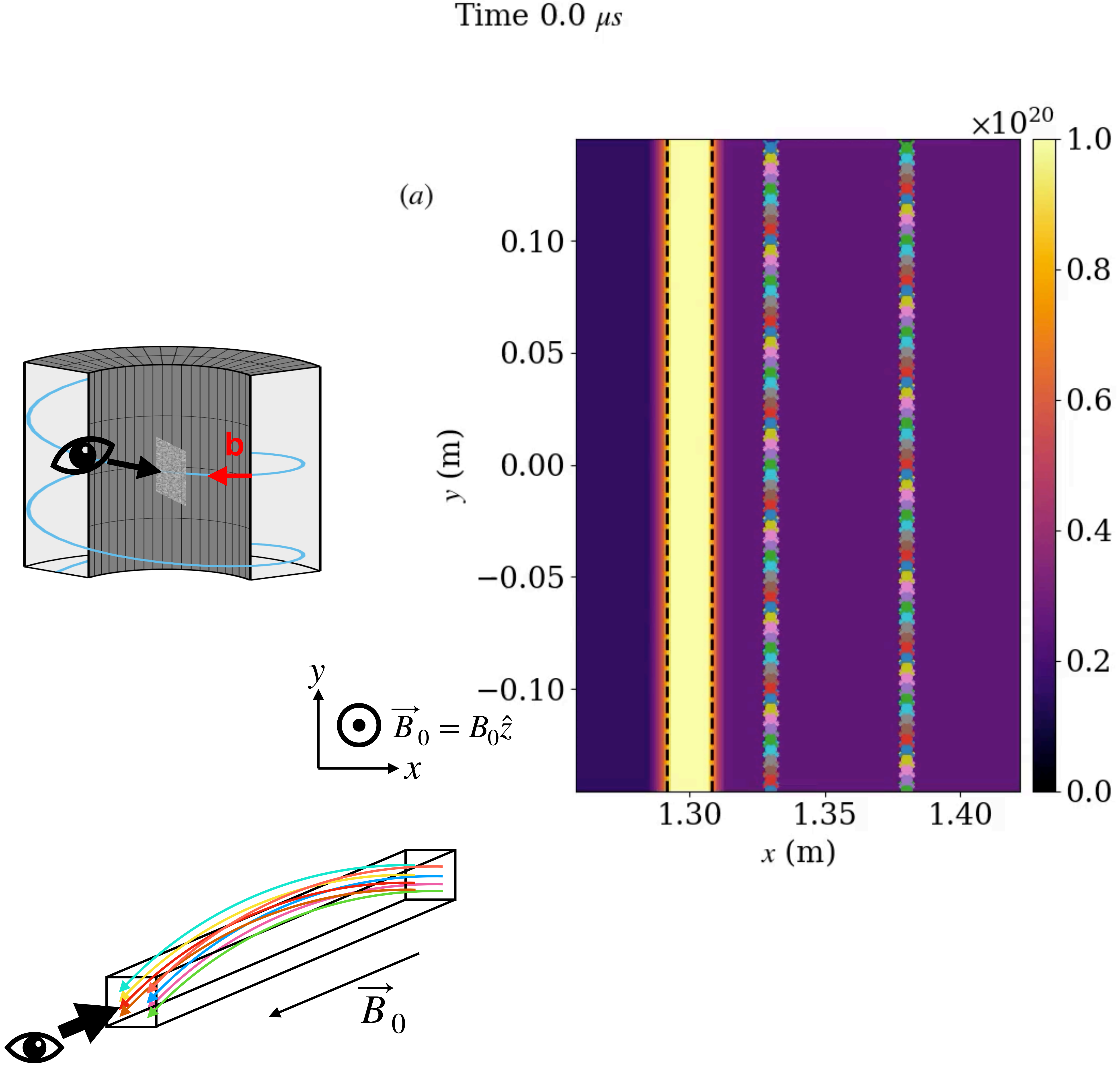
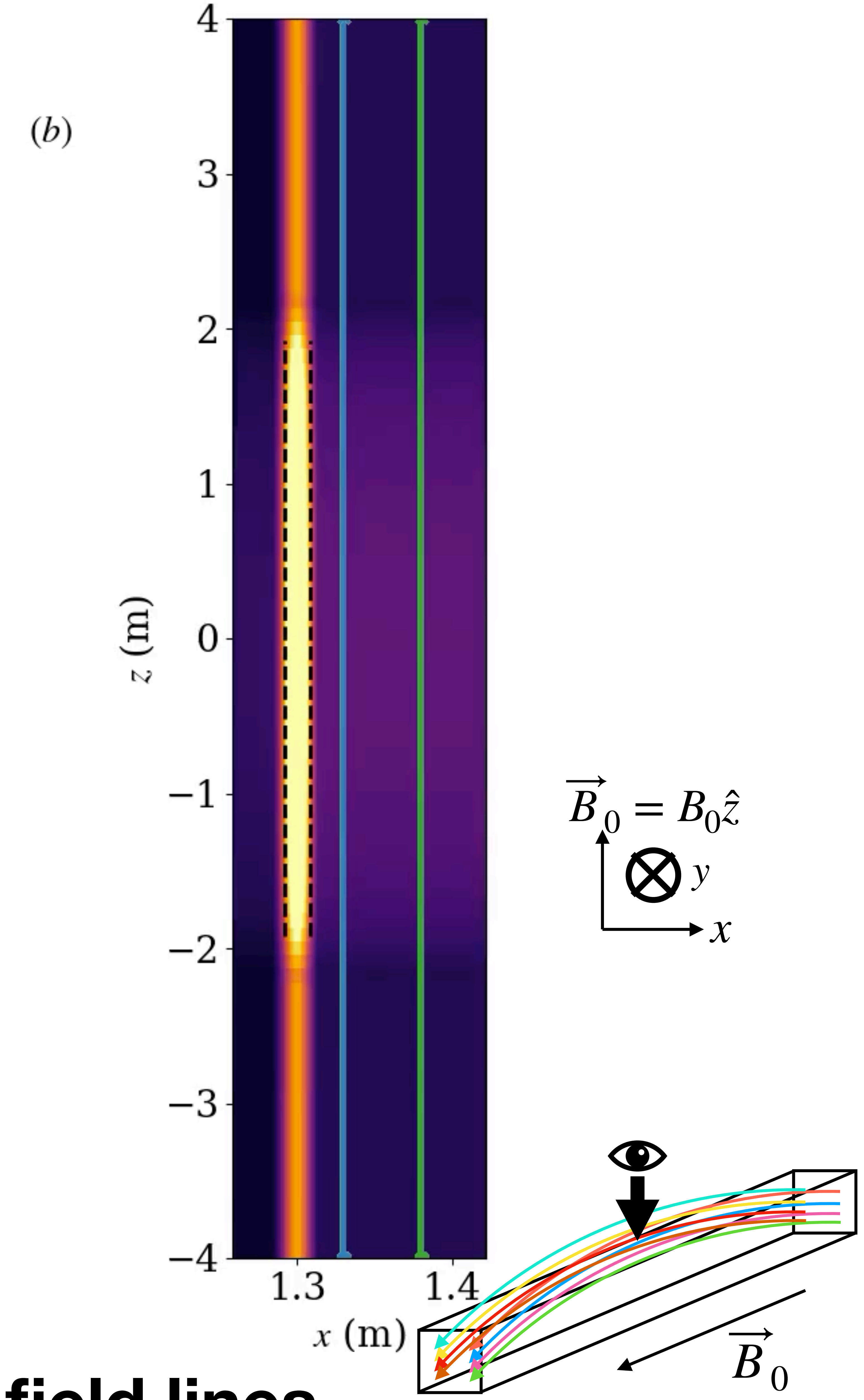
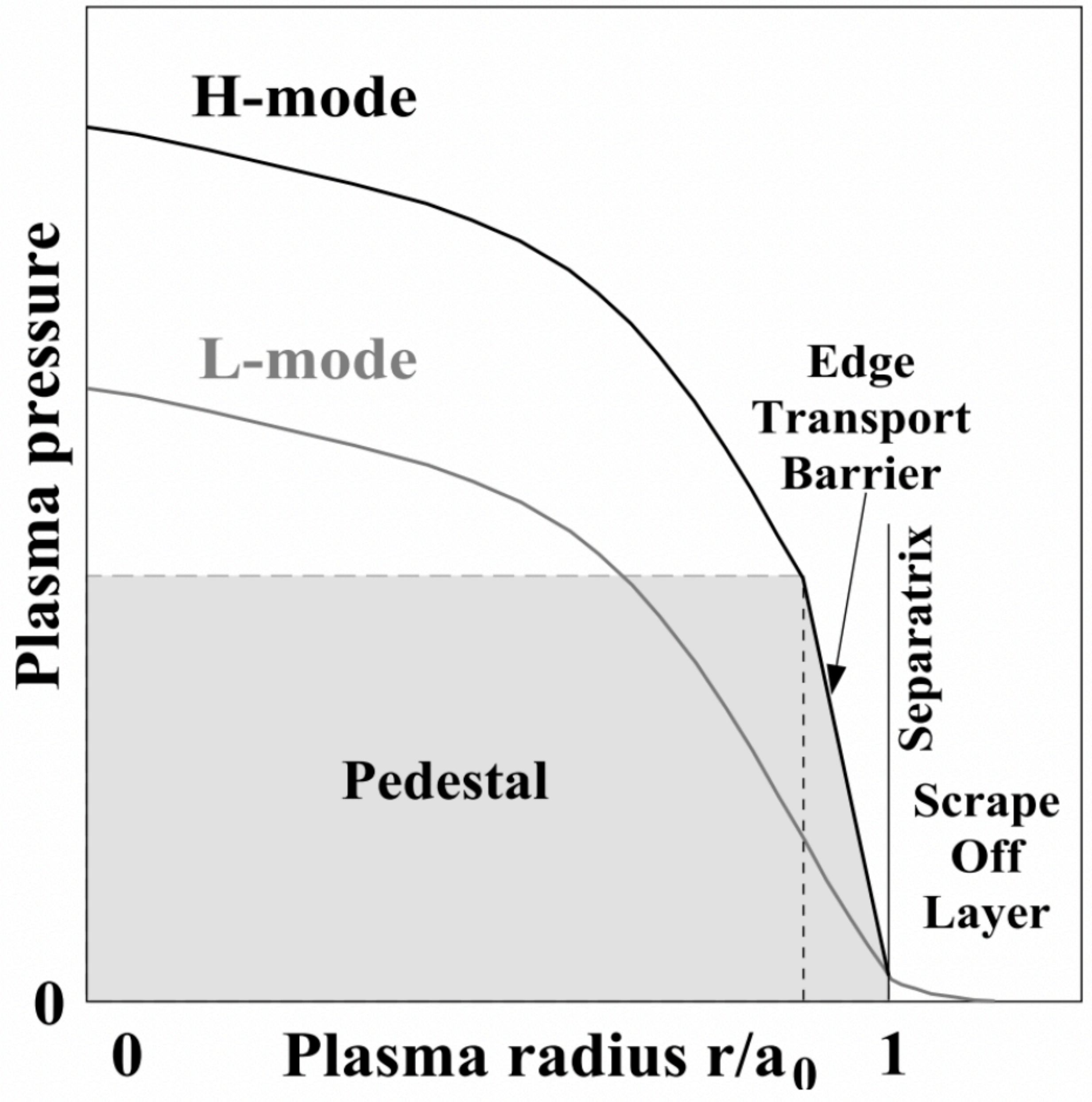


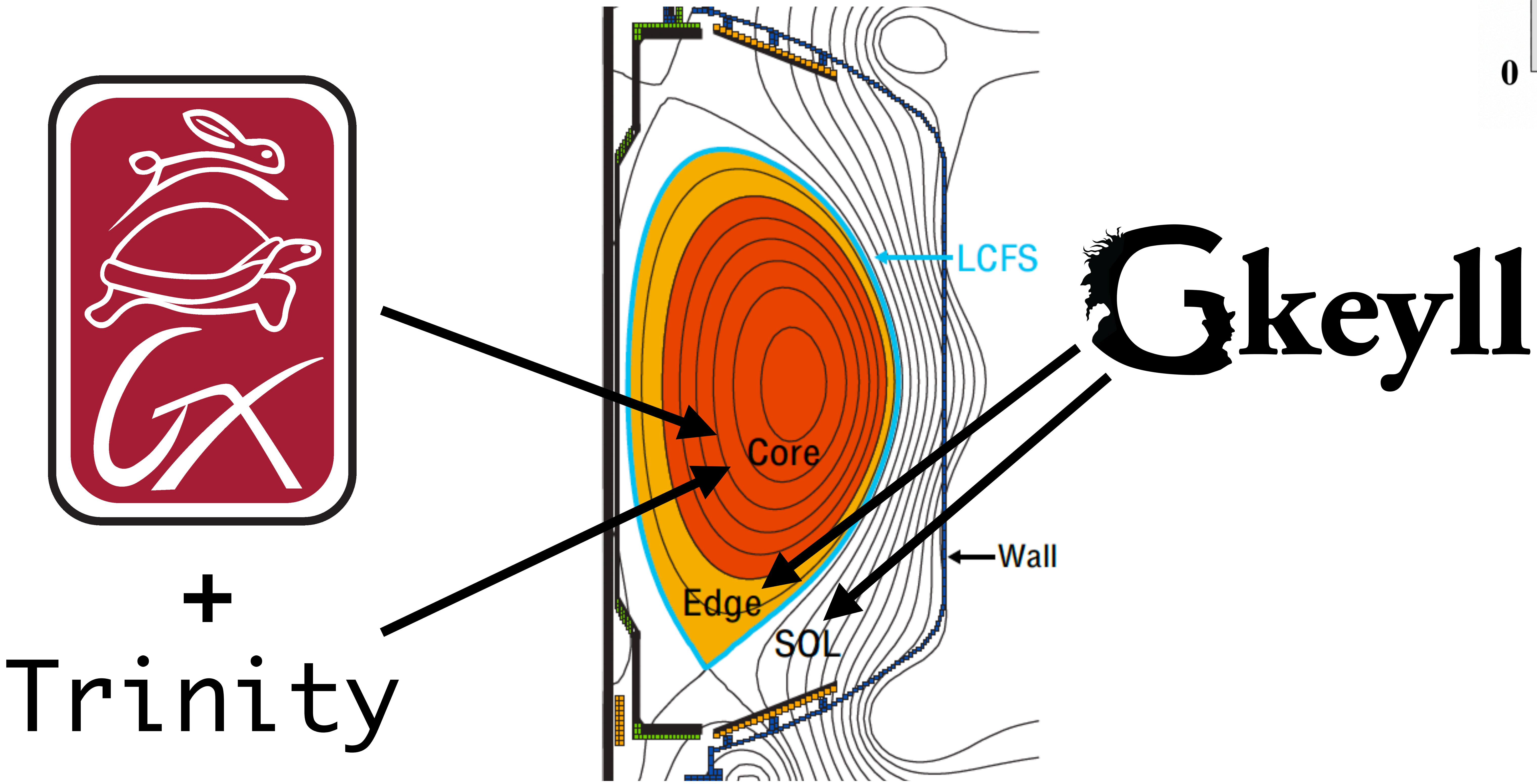


Plasma blobs bend/stretch magnetic field lines

A whole-device transport model

- Using GX+Trinity in the core and Gkeyll in the boundary, we have a whole-device transport model
  - Will be able to directly study impact of changes in core confinement on boundary exhaust
  - Will be able to directly study impact of boundary exhaust solutions (like detachment) on core confinement
  - As we add more physics to the models, we can achieve true **predict-first modeling capability**





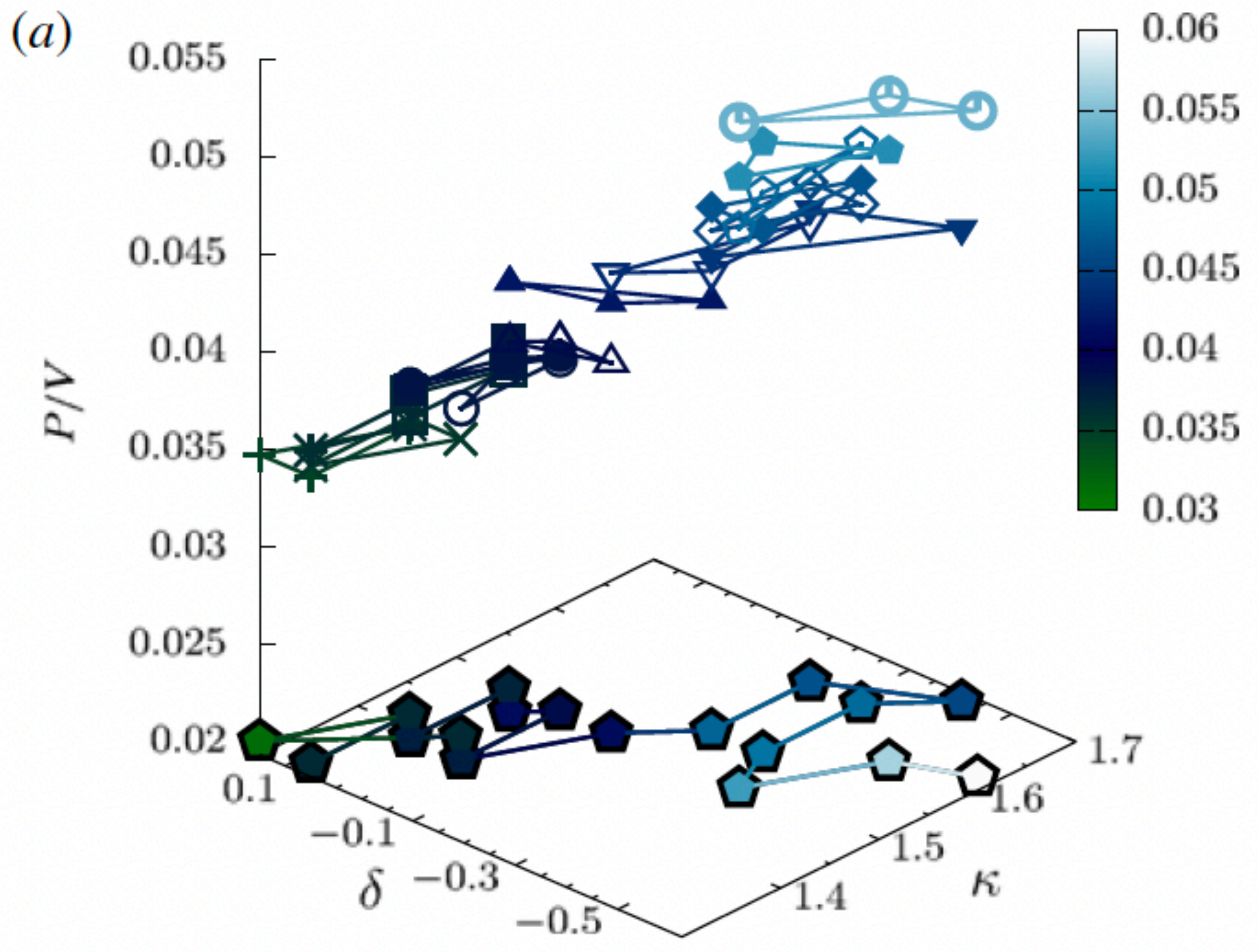
The goal: whole-device transport optimization

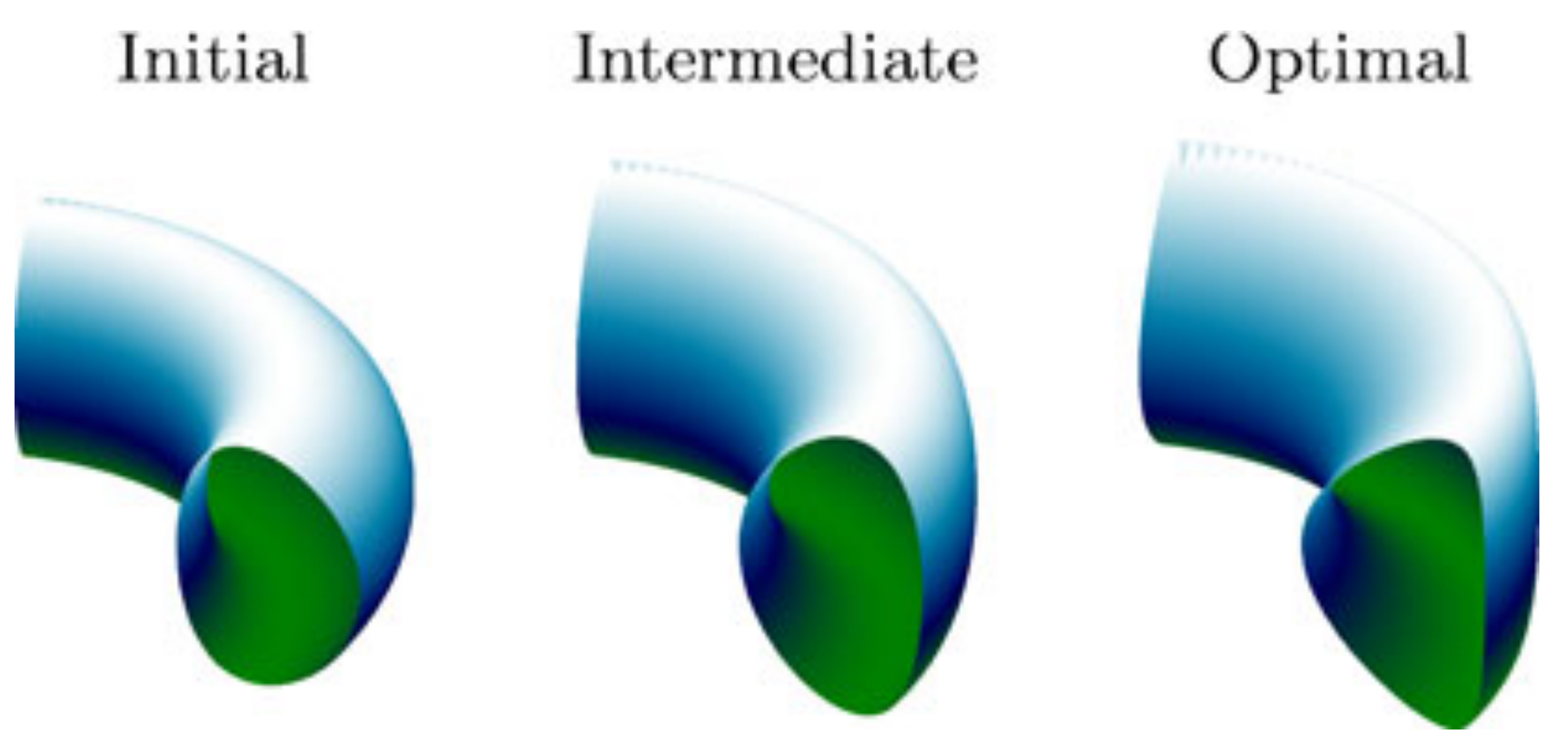
The goal: whole-device transport optimization

- Can we do **optimization at exascale?**
  - Need to ensure that a whole-device model calculation is sub-exascale (petascale?)
    - Requires both algorithmic advancements and effective use of latest hardware, like GPUs
  - Each whole-device calculation can compute key figures of merit to be optimized for a fusion reactor design
    - Total fusion power, energy confinement time, heat load to walls, etc
  - In a tokamak core, there are ~20 shaping parameters that could be varied simultaneously; in the boundary, could start with a few candidate divertor configurations
  - Parallel optimization algorithm could run O(10)-O(100) shapes simultaneously
  - Can use a hierarchy of models of varying speed and accuracy (incl. machine learning models) to progressively narrow design space
  - Could also build in economic (e.g. cost) and safety/environmental factors (e.g. minimize tritium onsite)

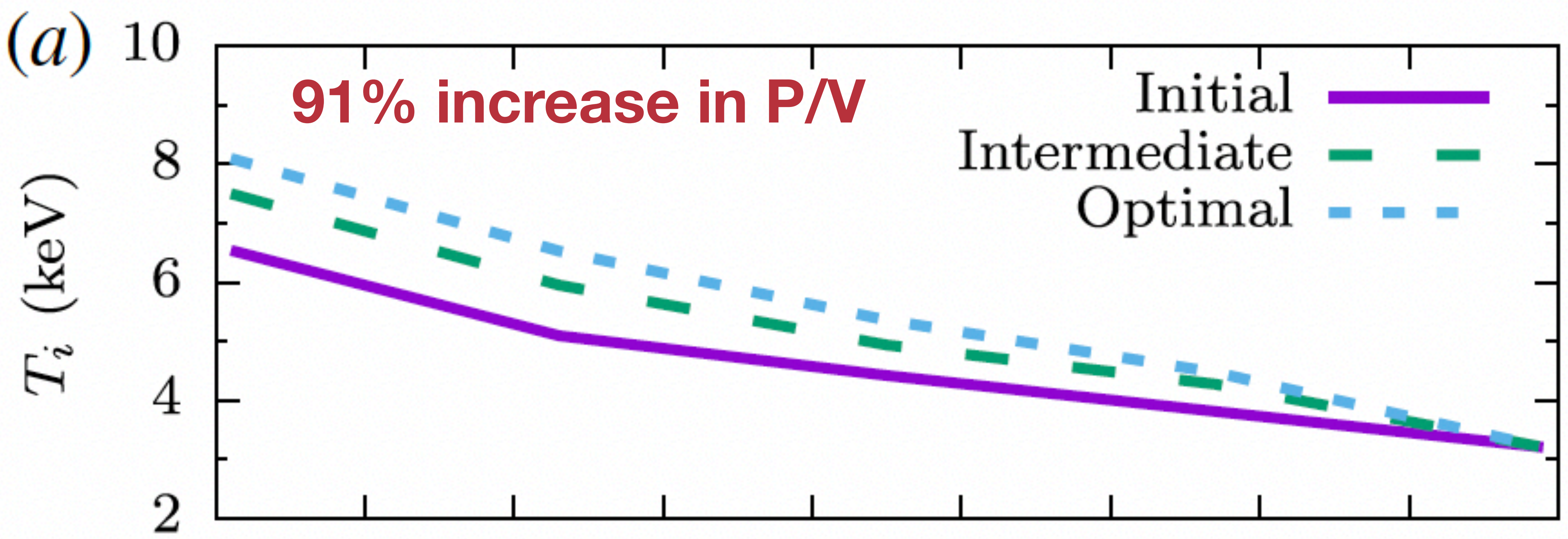
Transport optimization is possible!

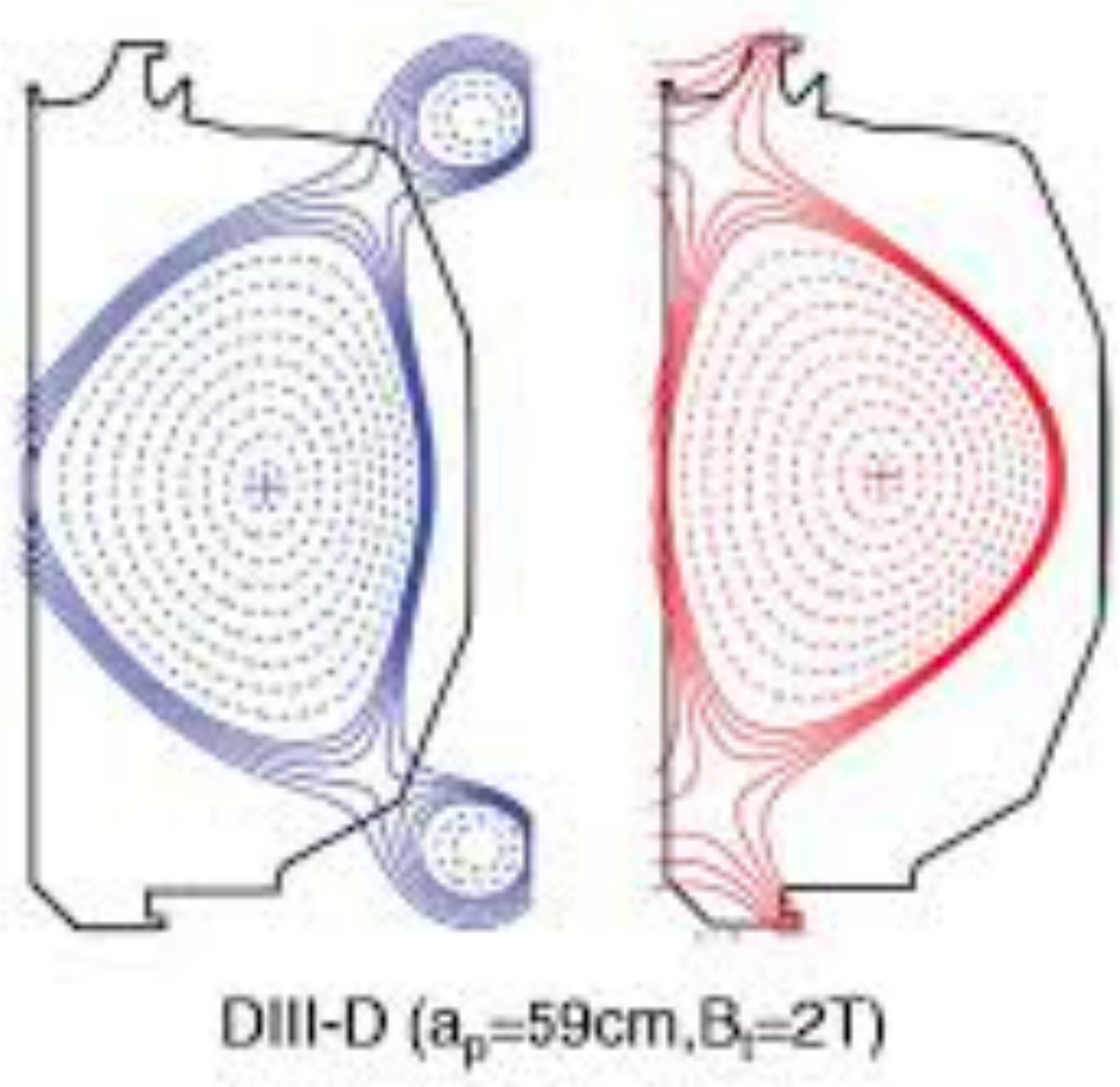
- Preliminary design study (**Highcock, Mandell, Barnes, Dorland (2018)**) found **negative triangularity** to be optimal in core
  - Used a lower-fidelity precursor to GX, coupled to Trinity
  - **18 shape design evaluations = 8680 nonlinear calculations = 3000 GPU node hours**
  - **91% improvement in fusion power per unit volume from going to negative triangularity**
  - Consistent with recent DIII-D experimental results showing confinement improvement with negative triangularity





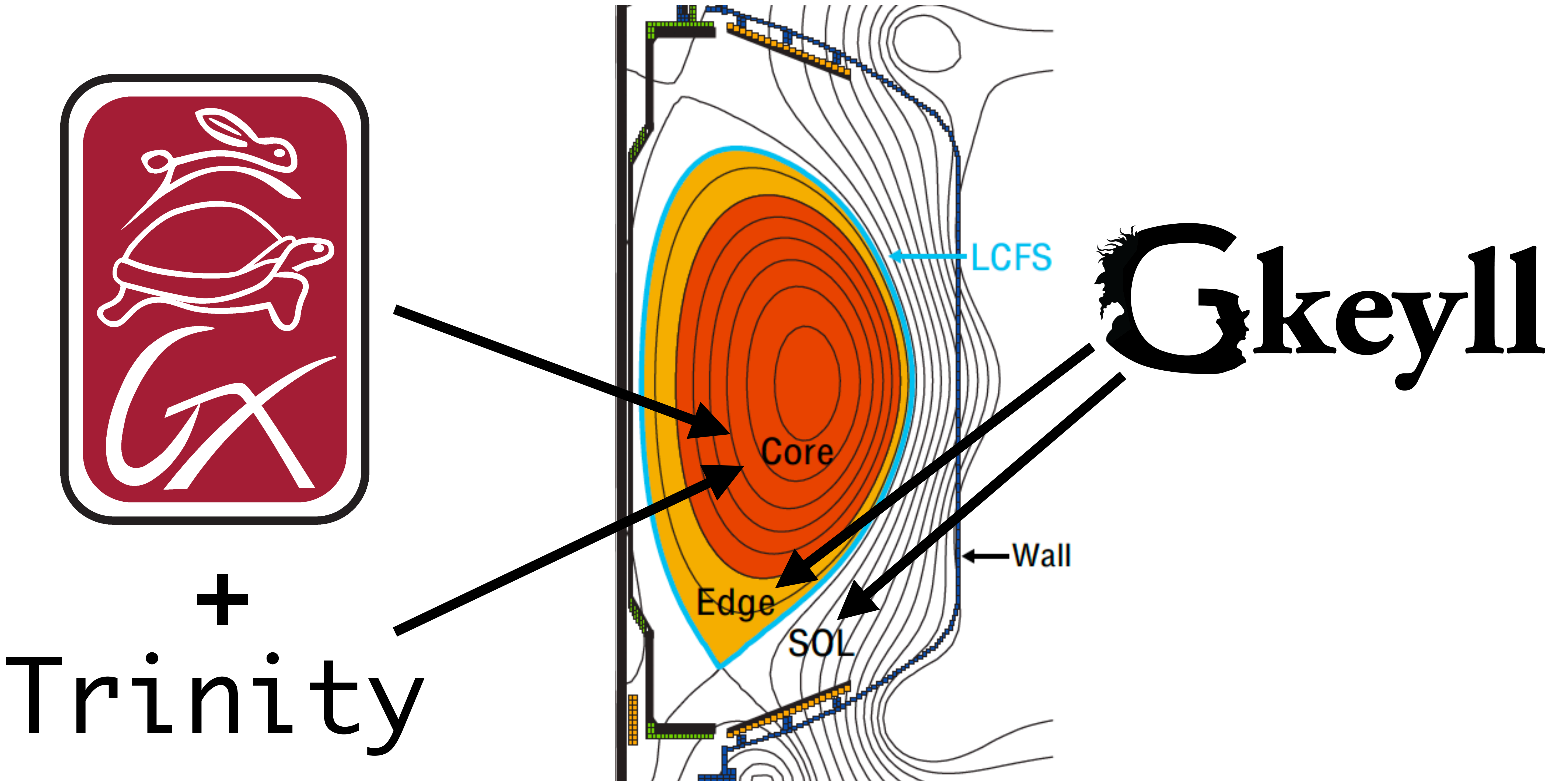
Highcock, Mandell, Barnes, Dorland (2018)





Summary

- I have presented a whole-device framework for modeling turbulence and transport in fusion reactors
  - **GX** models **core turbulence** with **spectral methods** on **GPUs**, and couples to a transport solver like **Trinity** to form a **multi-scale core transport model**
  - **Gkeyll** models **boundary turbulence** with **discontinuous Galerkin methods** and a first-of-a-kind **kinetic** scheme that includes **magnetic fluctuations**
- A number of key advances have been made, spanning theory, algorithms, and hardware
- Still work to do, but we can achieve game-changing **whole-device transport modeling and optimization** to **design better fusion reactors**



Acknowledgements

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Massachusetts Institute of Technology

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PPPL Princeton Plasma Physics Laboratory

Princeton University

GX group:

- **William Dorland**
- Ian Abel
- Nate Barbour
- Braden Buck
- Sarah Fischer
- Rahul Gaur
- Patrick Kim
- Matt Landreman
- Tony Qian
- … and others!

Gkeyll group:

- **Ammar Hakim**
- **Greg Hammett**
- Tess Bernard
- Petr Cagas
- Mana Francisquez
- Jimmy Juno
- … and others!

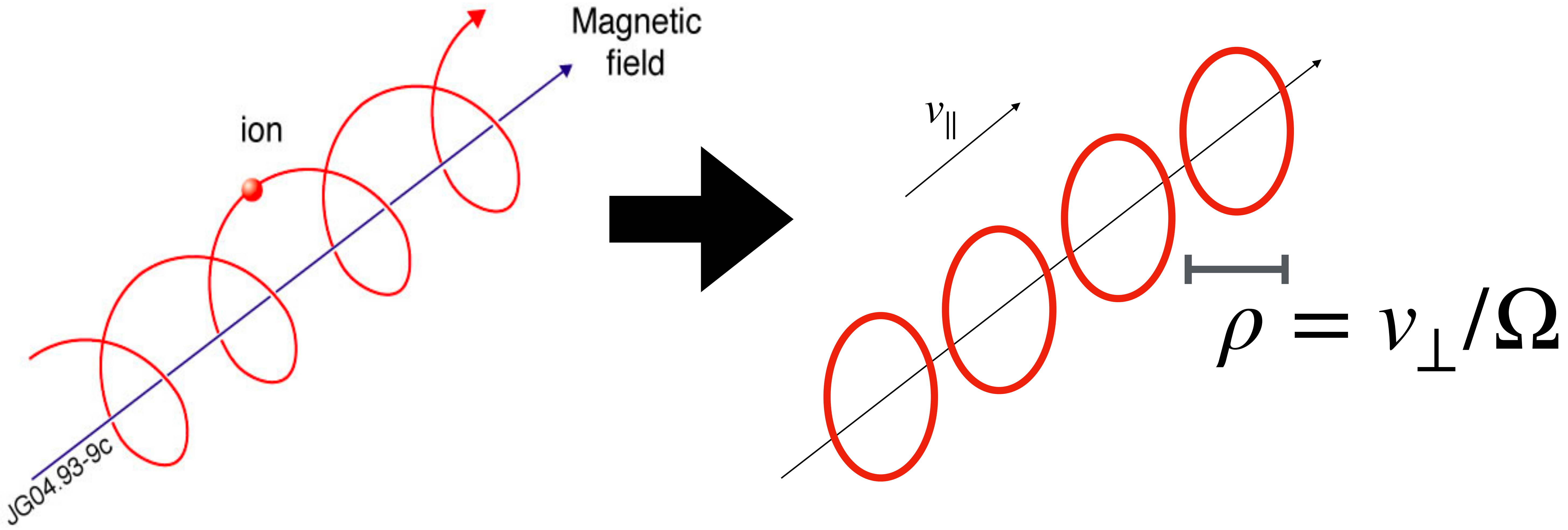
https://github.com/ammarhakim/gkyl/

https://gkyl.readthedocs.io/

Backup

Modeling turbulence in fusion plasmas

- Turbulence in a fusion plasma (both core and boundary) is well-described by **gyrokinetics**
  - A kinetic description (where particle positions *and* velocities are tracked) is necessary because fusion plasmas are very collisionless
  - A naive kinetic description would involve a 6D phase space, tracking PDF $f(x, y, z, v_x, v_y, v_z)$
    - E.g. Vlasov-Boltzmann-Maxwell system
  - We can reduce the dimensionality by one velocity dimension by averaging out the high frequency particle gyration, tracking PDF $f(x, y, z, v_{||}, v_\perp)$
    - Effectively a transformation from discrete charged particles → rings of charge
    - Still a 5D nonlinear PDE!



Typical turbulence scale length
~ ion gyroradius ρ_i

DG for general Hamiltonian system

$$\frac{\partial f}{\partial t} = \{H, f\}$$

Define phase-space velocity $\vec{\alpha} = \{\vec{Z}, H\}$, write in conservative form as

$$\frac{\partial f}{\partial t} + \nabla_{\vec{Z}} \cdot \left(\vec{\alpha} f\right) = 0$$

DG weak form:

- divide global phase-space domain into cells
- multiply GK eq. by a test function w_i and integrate (by parts) over cell C_m

$$\int_{C_m} d\vec{Z}\ w_i \frac{\partial f}{\partial t} + \oint_{\partial C_m} dS\ w_i^- \widehat{f \vec{\alpha} \cdot \vec{n}} - \int_{C_m} d\vec{Z}\ f \vec{\alpha} \cdot \nabla_{\vec{Z}} w_i = 0$$

- Particle conservation by taking $w = 1$
- Energy conservation by taking $w = H$, requires H to be continuous!

DG for full-f gyrokinetics

- GK is a Hamiltonian system, with $H = \frac{1}{2}mv_\parallel^2 + \frac{1}{2}mv_\perp^2 + q\phi$, and a non-canonical Poisson bracket:

$$\{F,G\} = \frac{\vec{B}^*}{mB_\parallel^*} \cdot \left(\nabla F \frac{\partial G}{\partial v_\parallel} - \frac{\partial F}{\partial v_\parallel}\nabla G\right) - \frac{\hat{b}}{qB_\parallel^*} \times \nabla F \cdot \nabla G$$

- Same DG weak form, recall $\vec{\alpha} = \{\vec{Z}, H\}$:

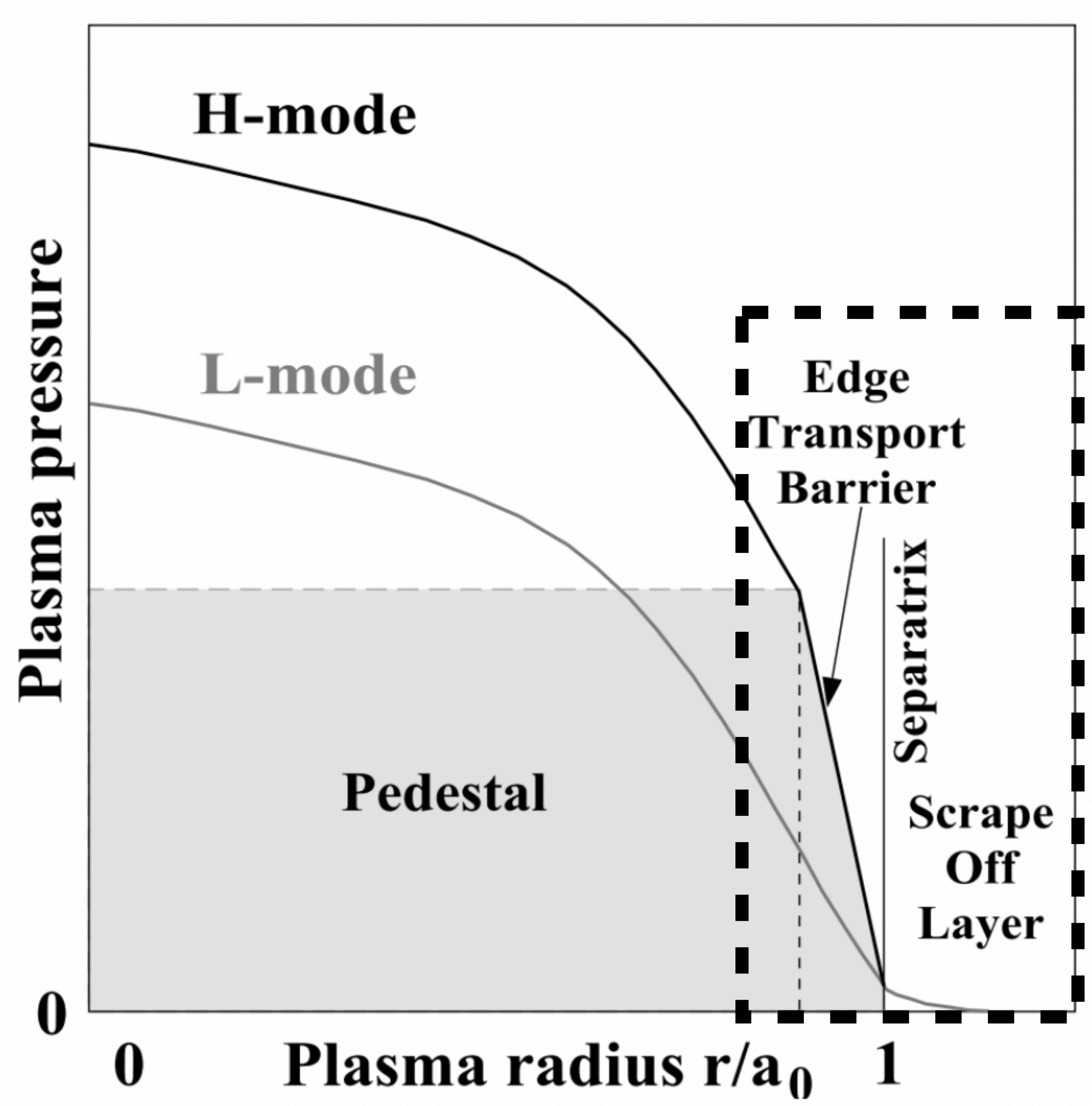
$$\int_{C_m} d\vec{Z}\; w_i \frac{\partial f}{\partial t} + \oint_{\partial C_m} dS\; w_i^- \widehat{f\vec{\alpha}\cdot\vec{n}} - \int_{C_m} d\vec{Z}\; f\vec{\alpha}\cdot\nabla_{\vec{Z}} w_i = 0$$

- Implicit conservation laws via integrals:
  - particle conservation $\int d\vec{Z}\, \frac{\partial f}{\partial t} = 0$ by taking $w = 1$
  - energy conservation $\int d\vec{Z}\, H\frac{\partial f}{\partial t} = 0$ by taking $w = H$, requires H continuous
  - since H must be continuous, ϕ must be continuous — use standard FEM for Poisson eq.
  - conservation laws require integrals to be computed exactly! (i.e. no aliasing errors)
  - exact integration with numerical quadrature $\sim \mathcal{O}(N_q N_b) \sim \mathcal{O}(N_b^3)$

The edge boundary condition is crucial to reactor performance

The edge boundary condition is crucial to reactor performance

- In most of today's fusion experiments, achieving good performance requires "high-confinement-mode" (H-mode)
  - H-mode occurs when a transport barrier forms at the edge of the core, enabling a steep-gradient region that lifts up the pressure profile in the core (as if it were standing on a "pedestal")



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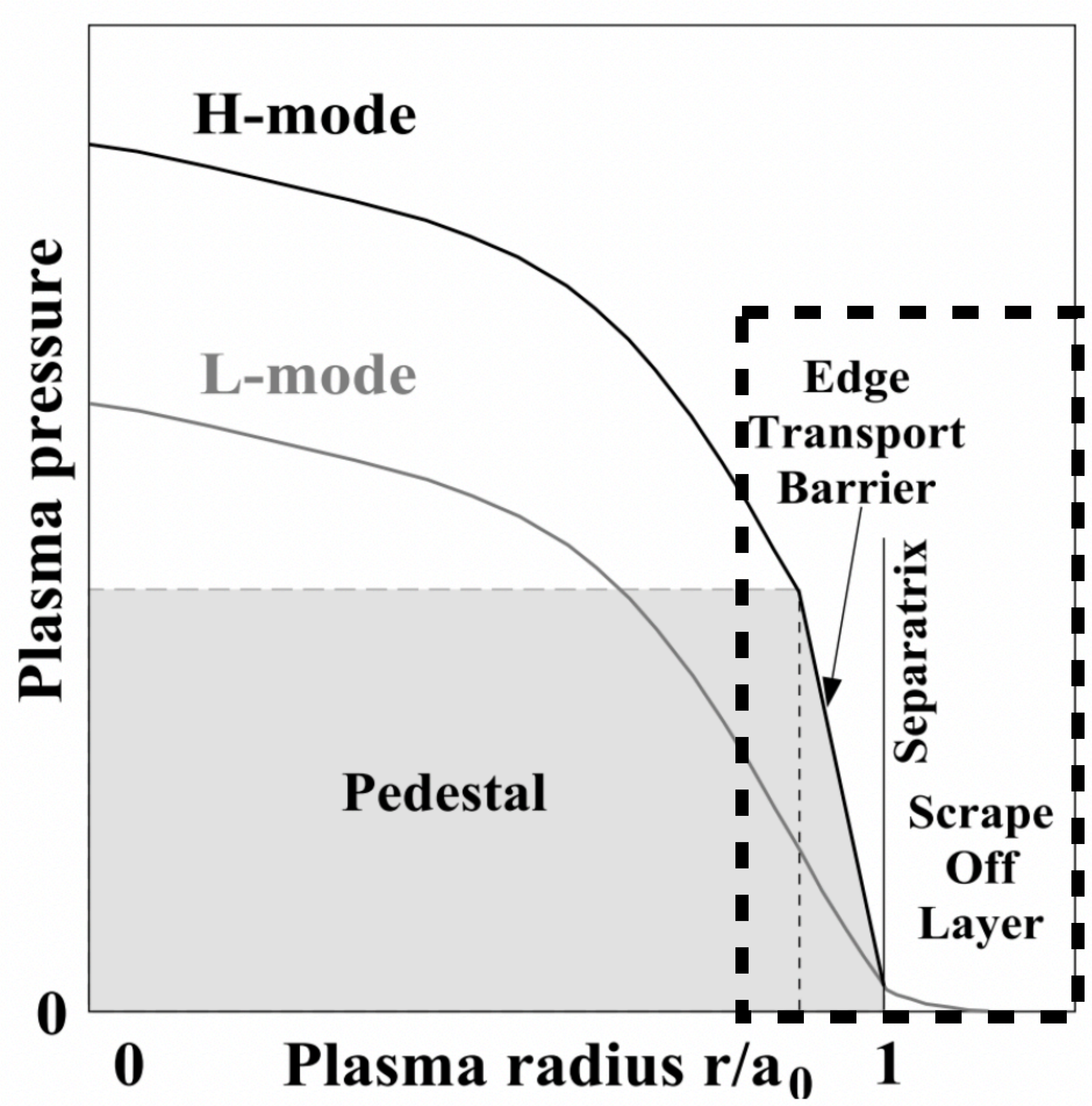

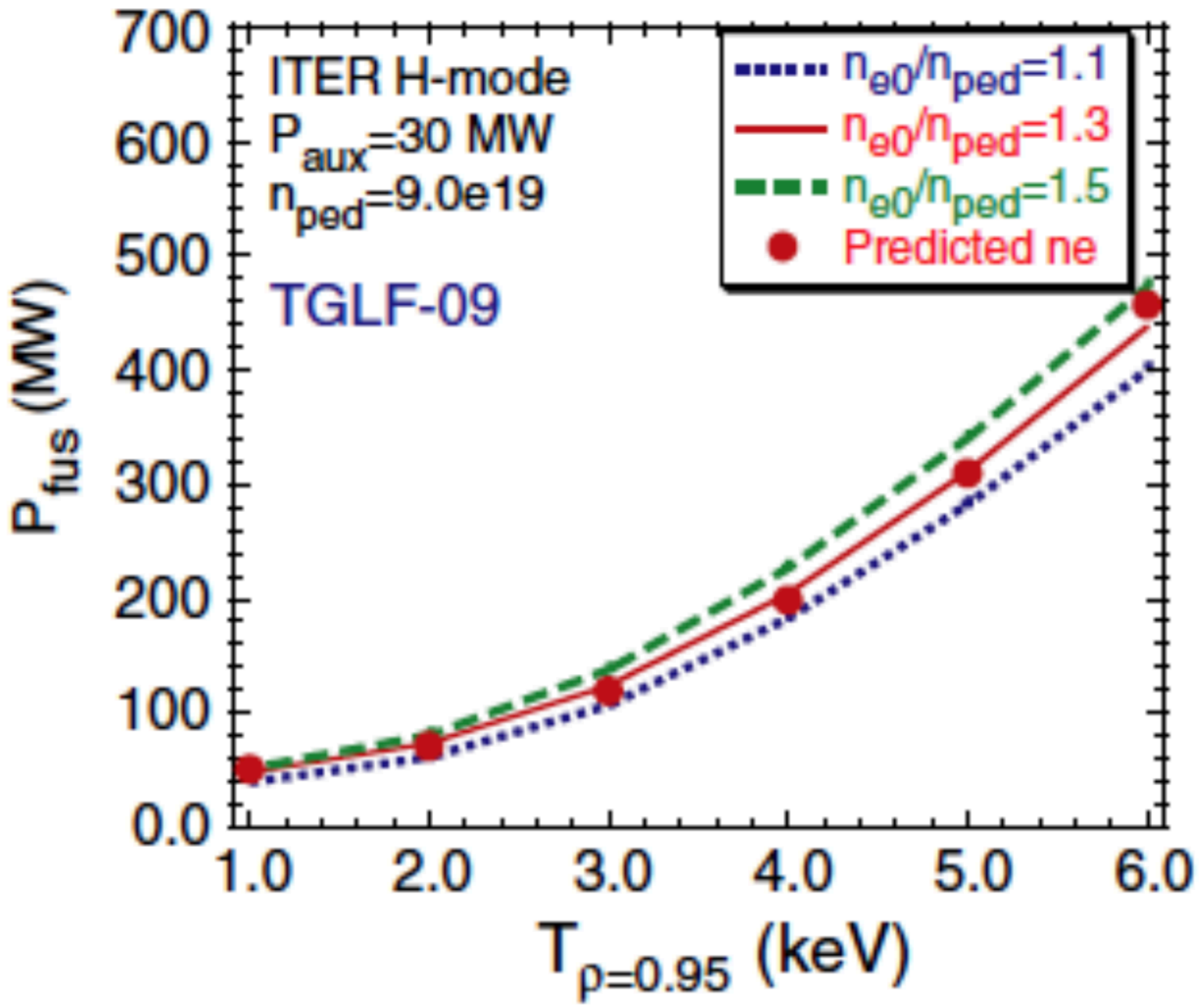

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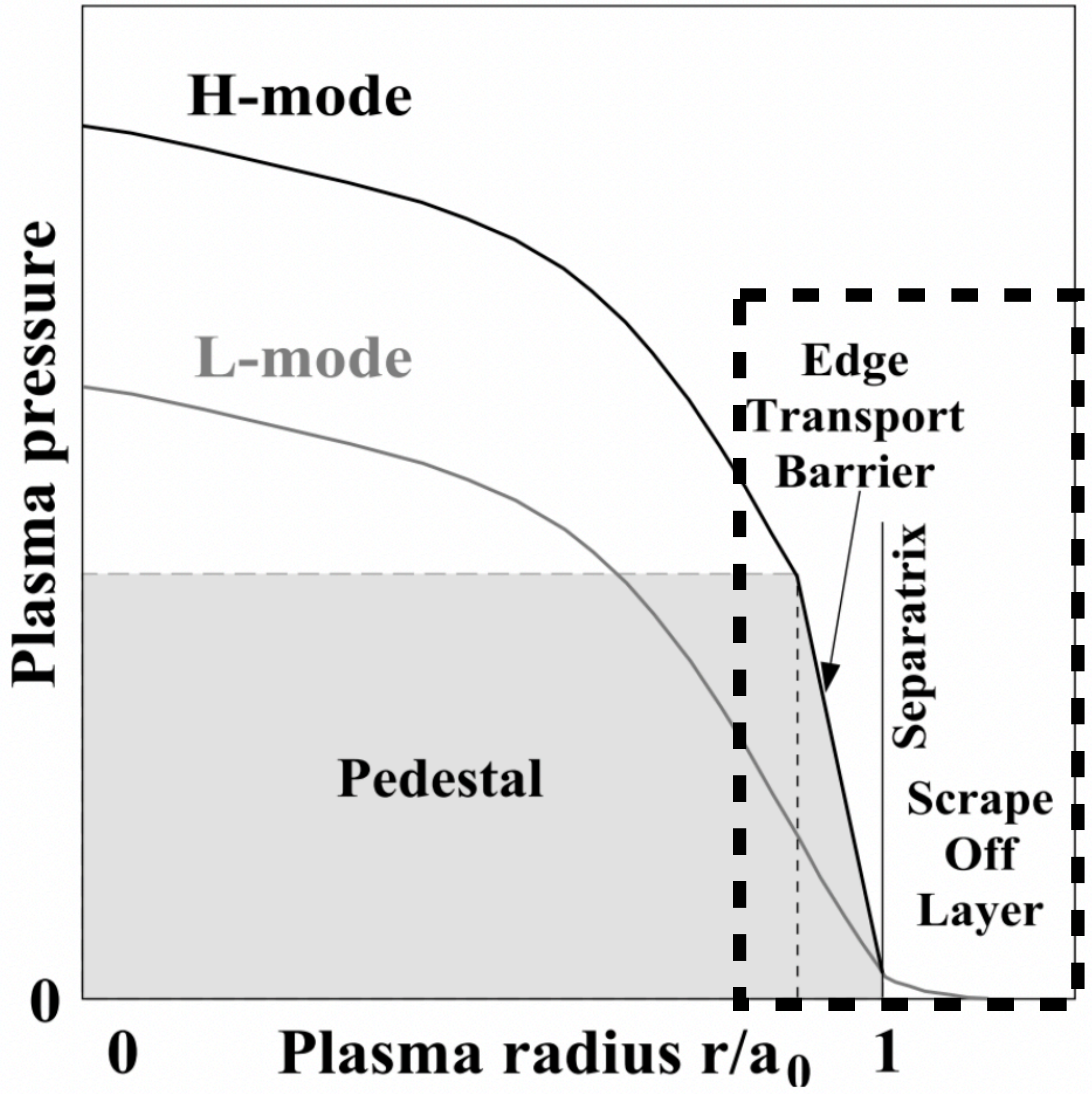
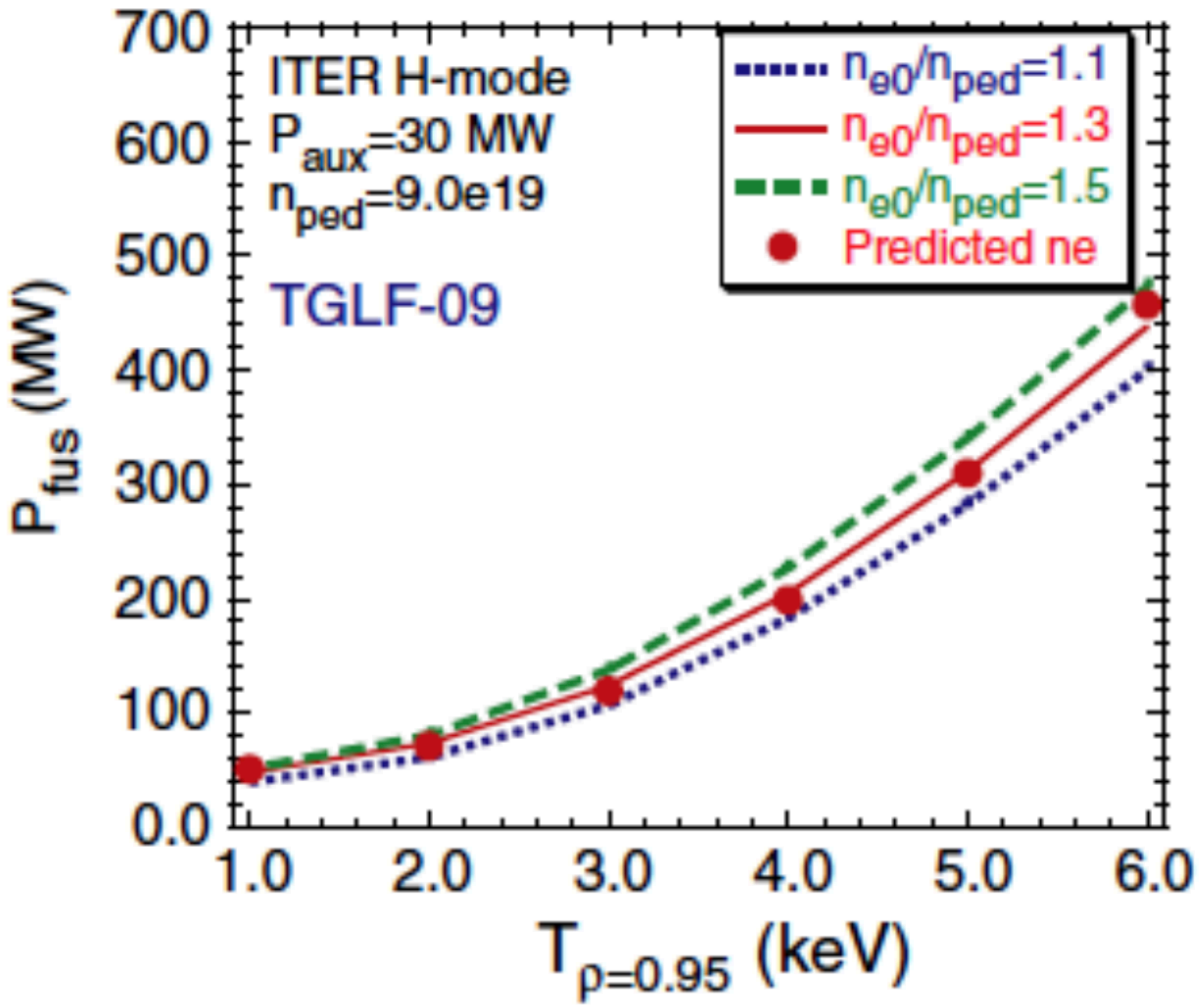
    - H-mode occurs when a transport barrier forms at the edge of the core, enabling a steep-gradient region that lifts up the pressure profile in the core (as if it were standing on a "pedestal")
- **Need to be able to confidently predict/optimize edge boundary condition (pedestal temperature) of reactor designs**





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The boundary heat exhaust problem is a potential show-stopper

- Heat exhausted in boundary could damage divertor plates if heat flux width is too narrow
  - Major problem at reactor scale (~500 MW)
- Turbulence in the boundary could help by broadening the width of the heat flux channel
- **Need first-principles kinetic models to model/optimize turbulent broadening of boundary heat flux**
- Modeling boundary requires specialized kinetic turbulence codes; can't use multi-scale approach from core
  - Boundary plasma has large-amplitude fluctuations, open field lines, plasma-wall interactions, X-point geometry, neutral/atomic physics, etc

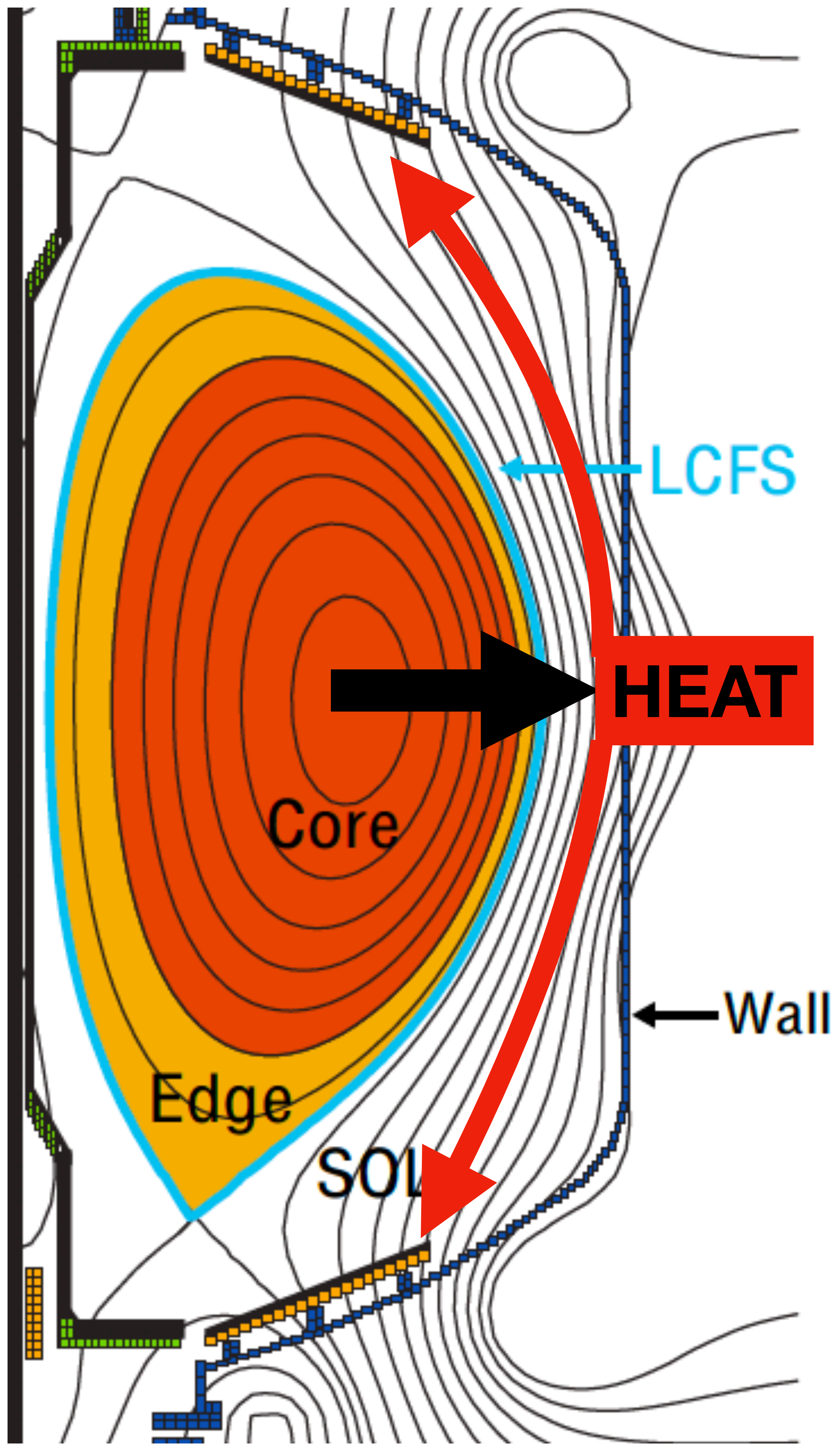

Figure adapted from Stoltzfus-Dueck (2009)