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DE LA RECHERCHE À L'INDUSTRIE

# Non-uniform meshes in gyrokinetic simulations

NumKin – 07/11/2022

Emily Bourne, V. Grandgirard, Y. Munschy, P. Leleux, C. Kruse, K. Kormann

- ▶ GYSELA code developed at IRFM/CEA since 2001 - strong collaboration between physicists, mathematicians and computer scientists
- ▶ **5D gyrokinetic code** based on a backward semi-lagrangian scheme used **to study plasma turbulence in tokamaks**
- ▶ Requires state-of-the-art development on HPCs
  - Hybrid MPI/OpenMP parallelism
  - Optimized for up to 750,000 cores

<https://gyselax.github.io>

### Intensive use of petascale resources

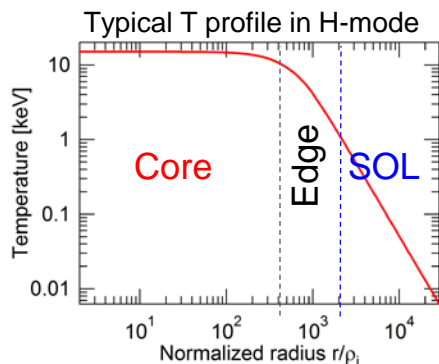
- ▶ **> 100s of millions of hours / year**
  - (GENCI + PRACE + HPC Fusion resources)

#### 1 simulation:

- **100 billion points** (5D mesh: 3D space + 2D velocity)
- **> 8 million hours** (20 days / 18 432 cores),

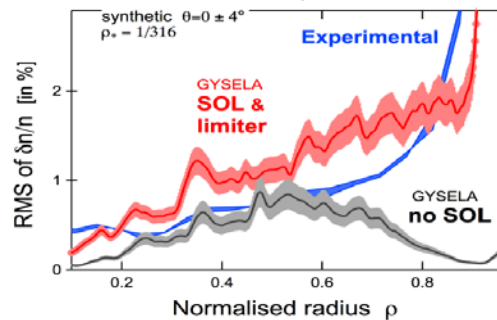
**Exascale needed** for ITER plasma turbulence simulation with electromagnetic effects

► Strong temperature gradients in Scrape-Off Layer (SOL)

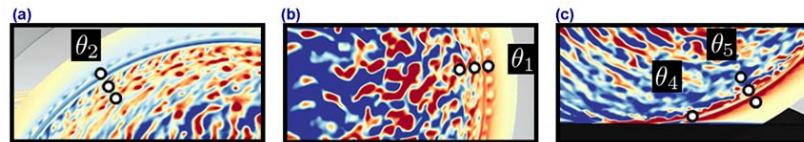
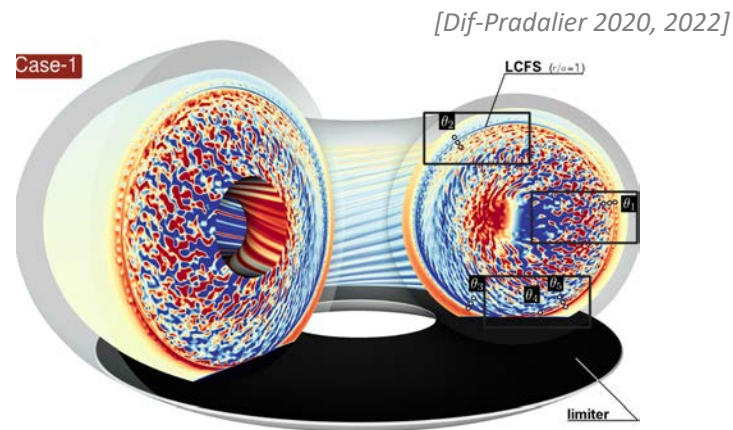


► More accurate results when modelling SOL

[Caschera PhD (2018), Dif-Pradalier (2018)]



► Smaller structures in edge-region



1 – Vlasov-Poisson Simulations on Non-Uniform Points:  
A reduced dimension case study

2 – 2D Poisson Solvers for Non-Uniform Points

**GYSELA****5D Vlasov Solver**

$$B_{\parallel s}^* \frac{\partial F_s}{\partial t} + \nabla \cdot \left( \frac{dx_G}{dt} B_{\parallel s}^* F_s \right) + \frac{\partial}{\partial v_{G\parallel}} \left( \frac{dv_{G\parallel}}{dt} B_{\parallel s}^* F_s \right) \\ = C(F_s) + S + K_{buff}(F_s) + D_{buff}(F_s)$$

- Backward semi-Lagrangian Advection on cubic splines
- Penalisation for walls
- Collision operator

**3D Poisson Solver**

$$\frac{e}{T_{e,eq}} (\phi - \langle \phi \rangle) - \frac{1}{n_{e0}} \sum_s Z_s \nabla_{\perp} \cdot \left( \frac{n_{s,eq}}{B\Omega_s} \nabla_{\perp} \phi \right) \\ = \frac{1}{n_{e0}} \sum_s Z_s \int J_0 \cdot (F_s - F_{s,eq}) d^3v$$

- Finite Differences in r
- Fourier Transform in  $\theta, \varphi$

**VOICE****2D Vlasov Solver**

$$\partial_t f_s(t, x, v) + v \partial_x f_s(t, x, v) - \frac{q_s}{m_s} \partial_x \phi(t, x) \partial_v f_s(t, x, v) \\ = C_{ss}(t, x, v) + S_{s,w_1} + S_{s,w_2} + S_{s,k}$$

- Backward semi-Lagrangian Advection on arbitrary degree splines
- Penalisation for walls
- Collision operator

**1D Poisson Solver**

$$\partial_x^2 \phi(t, x) = - \frac{\rho_q(t, x)}{\epsilon_0}$$

- Finite Elements

- Sheath physics
- Kinetic electrons and ions
- Penalisation describes the wall

### ► Vlasov Equation

$$\partial_t f_s(t, x, v) + v \partial_x f_s(t, x, v) - \frac{q_s}{m_s} \partial_x \phi(t, x) \partial_v f_s(t, x, v) = S_s(t, x, v) + C_{ss}(t, x, v)$$

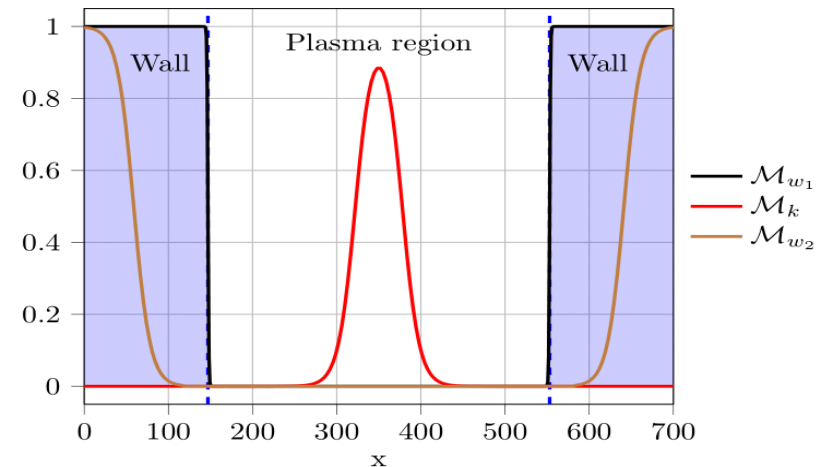
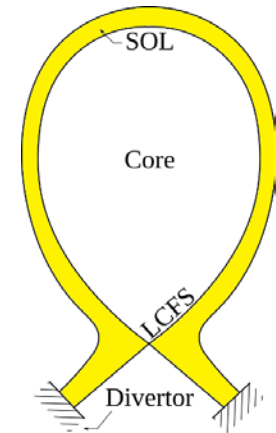
### ► Poisson Equation

$$\partial_x^2 \phi(t, x) = -\frac{\rho_q(t, x)}{\epsilon_0}$$

### ► Sources

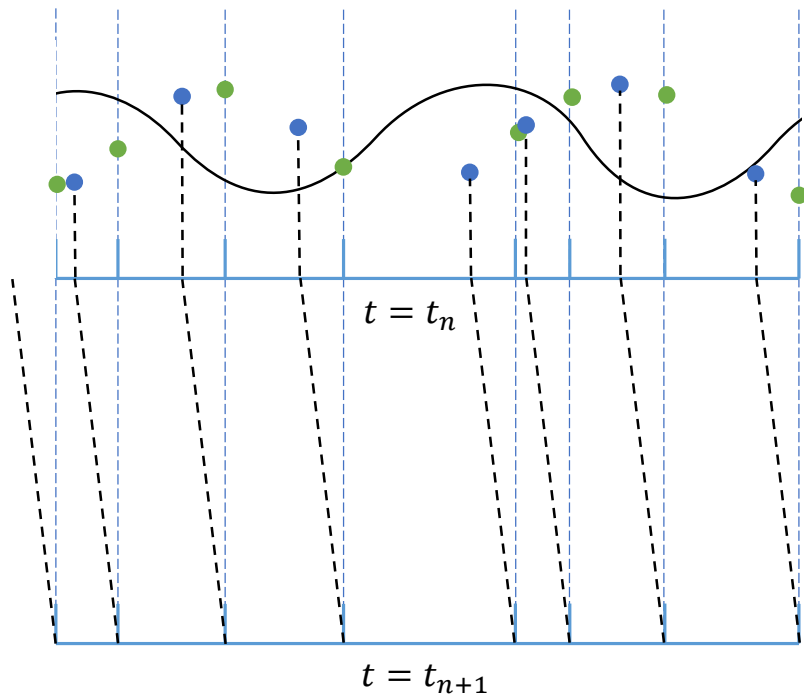
$$S_s(t, x, v) = S_{s,w_1} + S_{s,w_2} + S_{s,k}$$

- Particle sink
- Momentum/Energy sink
- Kinetic source



<sup>1</sup>E. Bourne, Y. Munsch et al, submitted 2022

<sup>2</sup>Y. Munsch, E. Bourne et al, submitted 2022



- The semi-Lagrangian method is a method for solving an advection equation

$$\partial_t F(x) + v(x) \cdot \nabla F(x) = 0$$

- It uses the fact that an advection is a translation

### Method Steps

- Find the spline interpolation of the function
  - » Requires non-uniform splines
- Find feet of the characteristics
- Approximate the value at the feet of the characteristics
  - » Requires a binary search to find spline cell
- Update the values
- Handle boundary conditions



- ▶ Newton-Cotes methods are optimised for equidistant points
- ▶ Spline representation can be used to calculate a quadrature scheme

$$\sum_i b_j(x_i)q_i = \int b_j(x)dx \quad \forall j$$

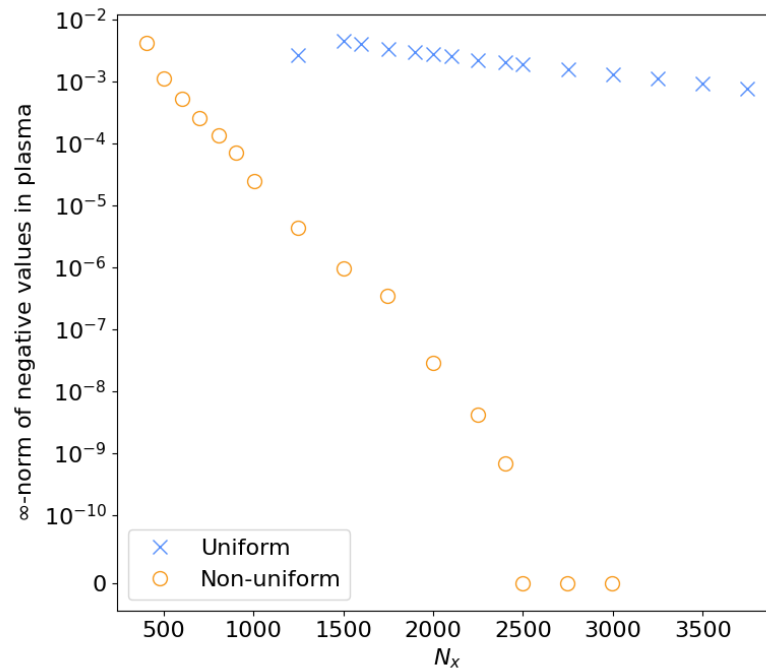
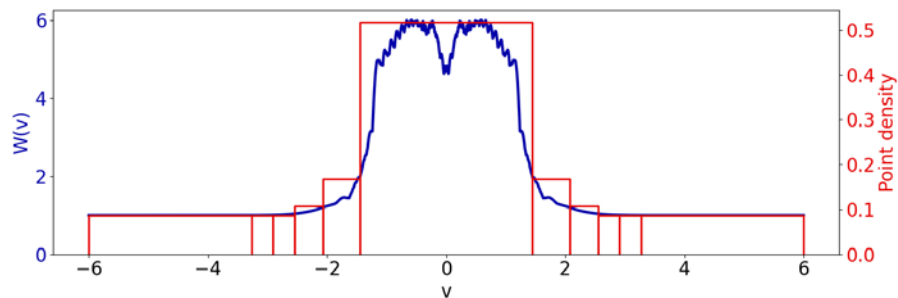
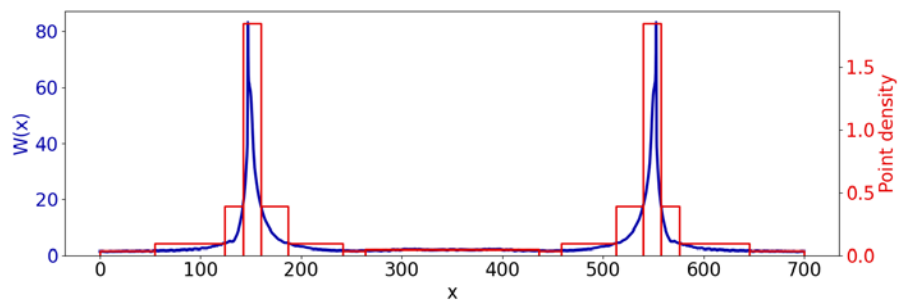
- ▶ Boundary conditions must be chosen such that no additional values are required
  - Greville interpolation points with knots at boundary
    - Same number of interpolation points and basis splines
  - Natural boundary condition = Schoenberg's "best" quadrature (well conditioned calculation described in [Bourne et al, submitted 2022])
    - Largest derivatives set to 0 at boundaries
    - Quadrature order is equal to number of free derivatives at boundary

- ▶ Penalisation confines the plasma
- ▶ Lack of refinement leads to negative values which are problematic for physical interpretations
- ▶ Steep gradients at wall
- ▶ Tends towards an equilibrium  
*[Y. Munsch et al, submitted 2022]*
- ▶ Wider simulations would be more realistic but require even more points



- Points are spaced proportionally to a weight function:

$$W(x) = \sqrt{1 + \alpha^2 \left( \max_{t,v} \partial_x f(t, x, v) \right)^2}$$



<sup>1</sup>E. Bourne, Y. Munsch et al, submitted 2022

$$n_{s(t,x)} = \int f_s(t, x, v_s) dv_s \quad \Pi_{s(t,x)} = \int v_s^2 f_s(t, x, v_s) dv_s$$

$$\Gamma_{s(t,x)} = \int v_s f_s(t, x, v_s) dv_s \quad Q_{s(t,x)} = \int \frac{1}{2} v_s^3 f_s(t, x, v_s) dv_s$$

► Density

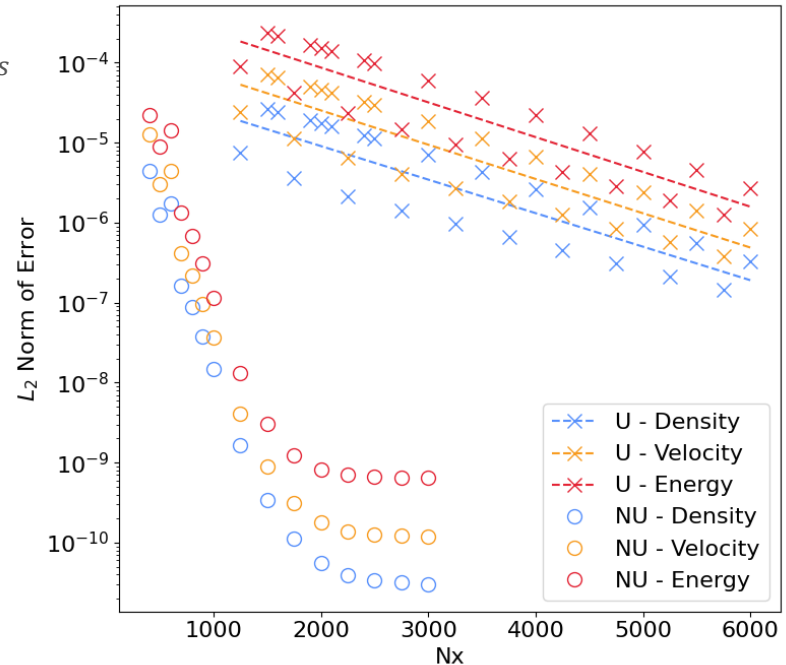
$$\begin{aligned} \partial_t n_s(t, x) + \frac{1}{\sqrt{m_s}} \partial_x \Gamma_s(t, x) \\ = \int S_s(t, x, v_s) + C_{ss}(t, x, v_s) dv_s \end{aligned}$$

► Velocity

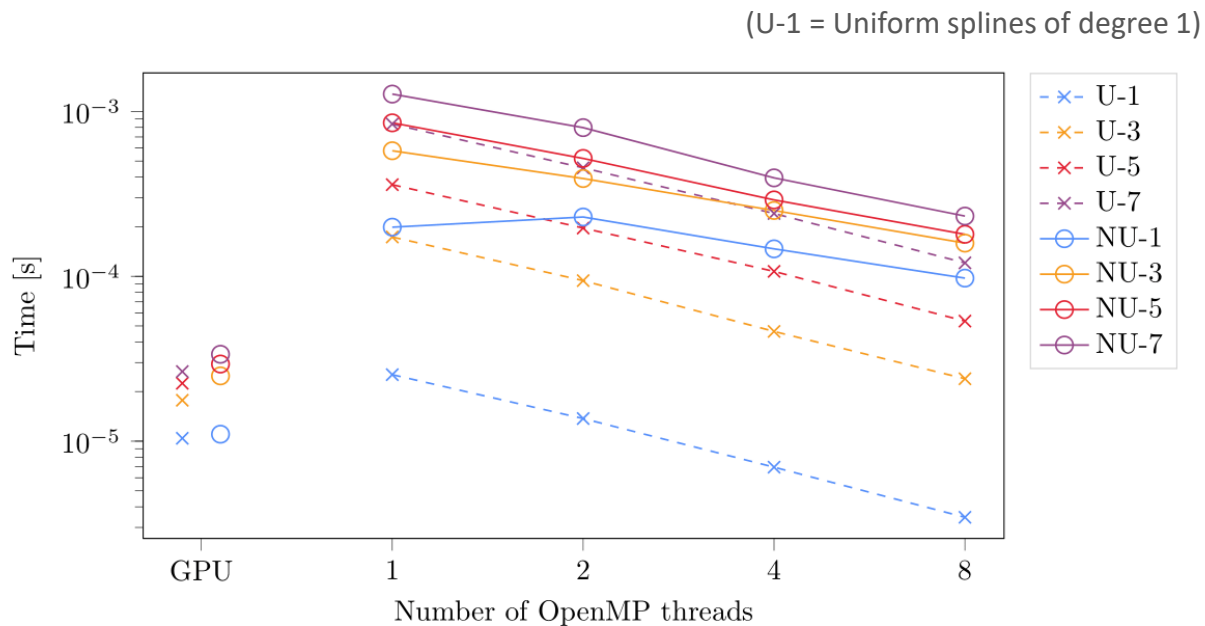
$$\begin{aligned} \partial_t \Gamma_s(t, x) + \frac{1}{\sqrt{m_s}} (\partial_x \Pi_s(t, x) + q_s \partial_x \phi(t, x) n_s(t, x)) \\ = \int v_s S_s(t, x, v_s) + v_s C_{ss}(t, x, v_s) dv_s \end{aligned}$$

► Energy

$$\begin{aligned} \partial_t \Pi_s(t, x) + 2 \frac{1}{\sqrt{m_s}} (\partial_x Q_s(t, x) + q_s \partial_x \phi(t, x) \Gamma_s) \\ = \int v_s^2 S_s(t, x, v_s) + v_s^2 C_{ss}(t, x, v_s) dv_s \end{aligned}$$



- ▶ Backward semi-Lagrangian advection on non-uniform splines is slower than uniform splines
- ▶ The cost difference is much smaller on a GPU



- ▶ Non-uniform knots reduce the memory requirements by 89%
- ▶ Non-uniform simulations run 5.5 times faster than uniform simulations providing equivalent results on GPUs
- ▶ Non-uniform points allow simulations on much larger domains with more realistic (steeper) walls

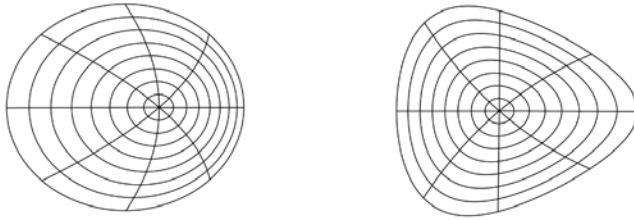
## FDM/FFT

► Solves the equation:

$$\checkmark \quad \frac{e}{T_{e,eq}} (\phi - \langle \phi \rangle) - \frac{1}{n_{e0}} \sum_s Z_s \nabla_{\perp} \cdot \left( \frac{n_{s,eq}}{B \Omega_s} \nabla_{\perp} \phi \right) = \frac{1}{n_{e0}} \sum_s Z_s \int J_0 \cdot (F_s - F_{s,eq}) d^3 v$$

► Handles complex geometry

✗



!

► Easy refinement

✓

► Fast

✓

► Good parallelisation

✓

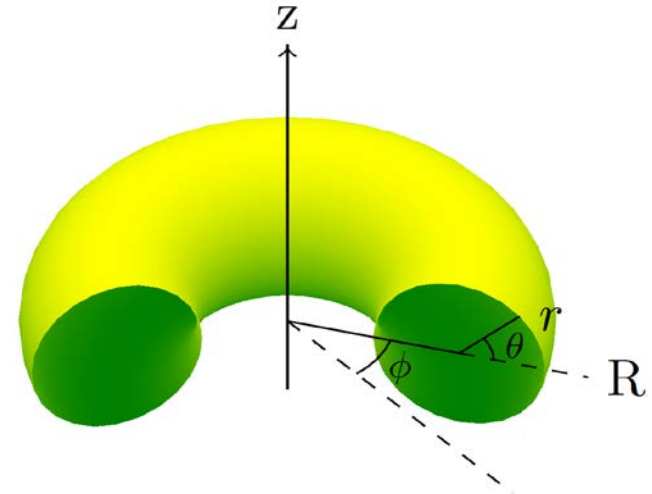
► Accurate

✓

► Low memory footprint

!

► Good representation of the boundary



### ► Spline FEM Solver (IPP)

[Zoni, Güçlü 2019]

- Finite Element Method
- Conjugate Gradient solver
- Curvilinear coordinates
- Arbitrary order
- $C^1$  polar splines

### ► Embedded Boundary Solver (IPP)

[Zhang, Weiqun 2019]

- Finite Volume Method
- Multi-grid solver
- Cartesian coordinates
- Second order
- Uses AMReX library

### ► GmgPolar Solver (CERFACS)

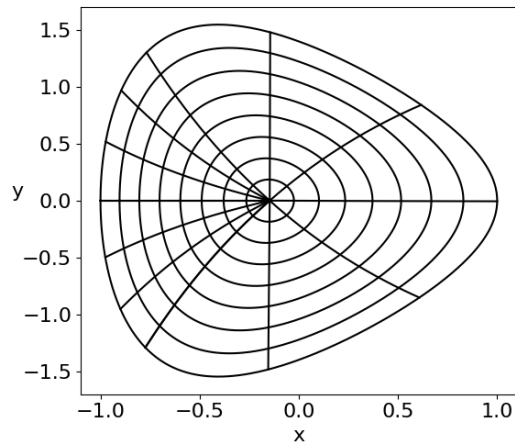
[Kühn, Kruse 2022]

- Finite Difference Method
- Multi-grid solver
- Curvilinear coordinates
- $\sim 4^{\text{th}}$  order
- Matrix free

### ► Common Problem

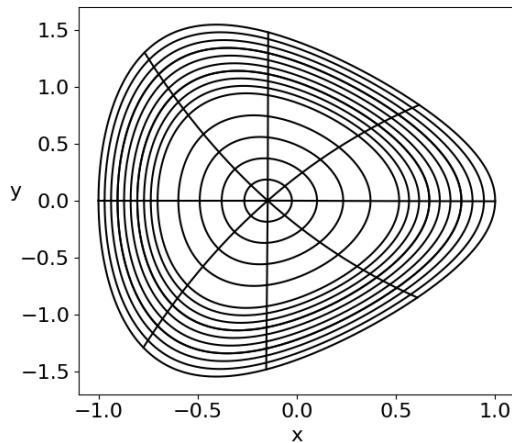
$$\begin{aligned}
 & -\frac{1}{n_{e0}} \sum_s Z_s \nabla_{\perp} \cdot \left( \frac{n_{s,eq}}{B\Omega_s} \nabla_{\perp} \phi \right) + \frac{e}{T_{e,eq}} (\phi - \langle \phi \rangle) \\
 & = \frac{1}{n_{e0}} \sum_s Z_s \int J_0 \cdot (\bar{F}_s - \bar{F}_{s,eq}) d^3v \quad \langle \phi \rangle = \frac{\int \phi R J d\theta d\phi}{\int R J d\theta d\phi}
 \end{aligned}$$





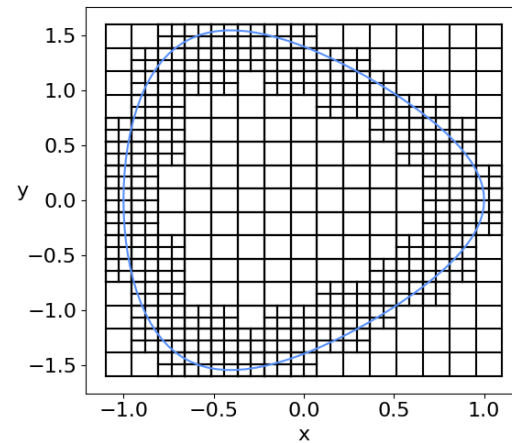
Poloidal refinement  
(Spline FEM / GmgPolar)

+ Handles anisotropy



Radial refinement  
(Spline FEM / GmgPolar)

+ Easy to refine in target area  
- Doesn't handle poloidally  
small objects



Refinement with Patches  
(Embedded Boundary)

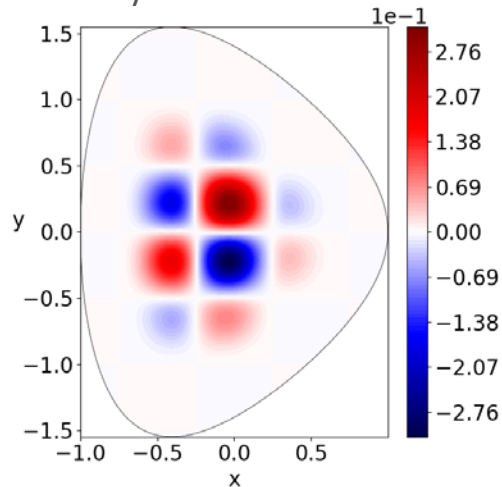
+ Good for handling small objects  
- Difficult to find required patches  
- Lots of patches to handle

$$-\nabla \cdot (\alpha \nabla u) + \beta u = f$$

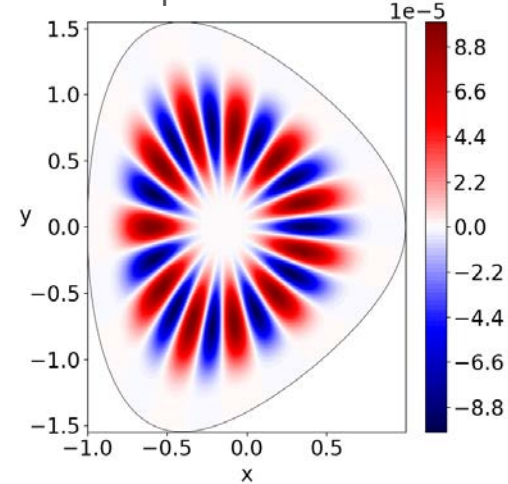
$$\alpha(r) = \exp\left(-\tanh\left(\frac{r - r_p}{\delta_r}\right)\right)$$

$$\beta(r) = \exp\left(\tanh\left(\frac{r - r_p}{\delta_r}\right)\right)$$

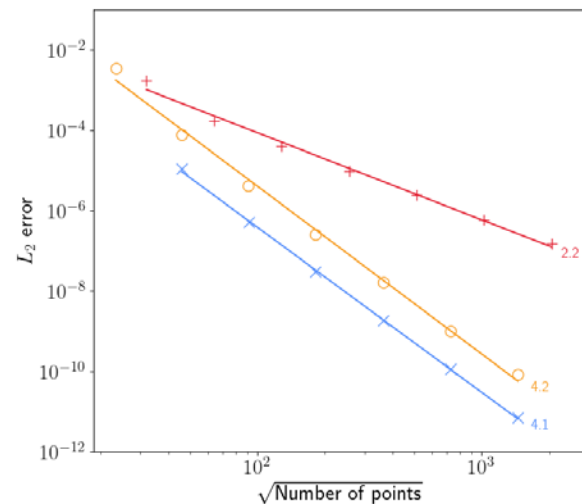
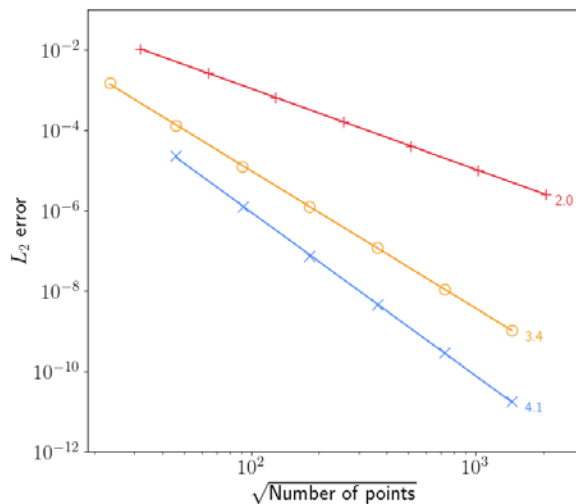
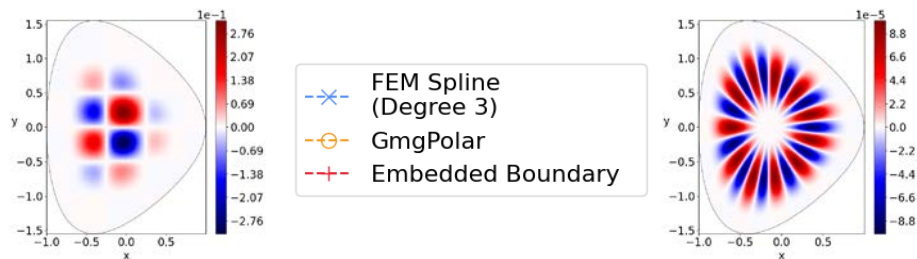
Cartesian solution not aligned with coordinate system

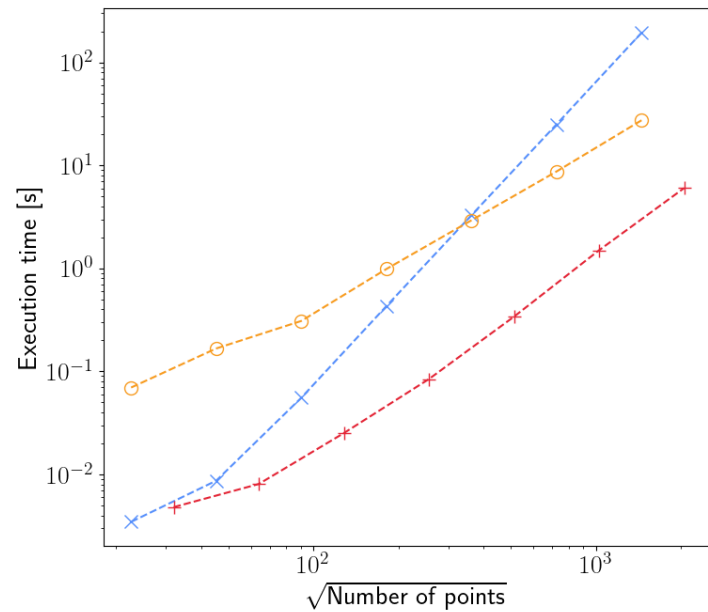
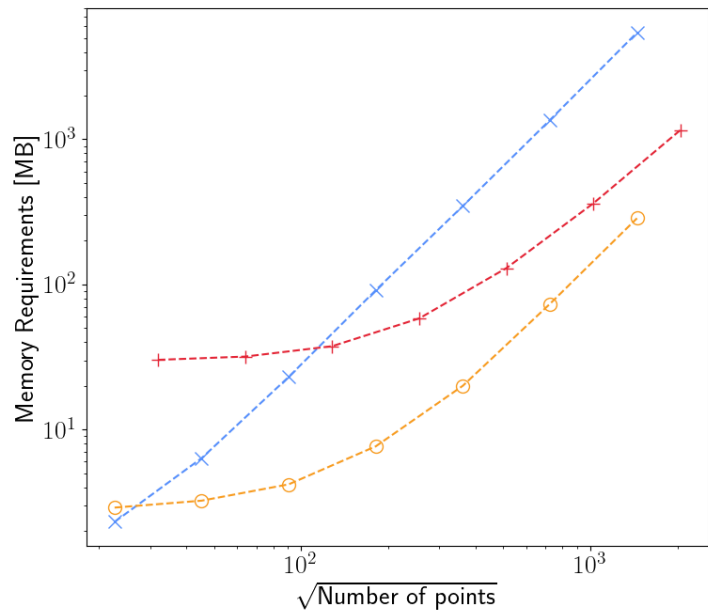


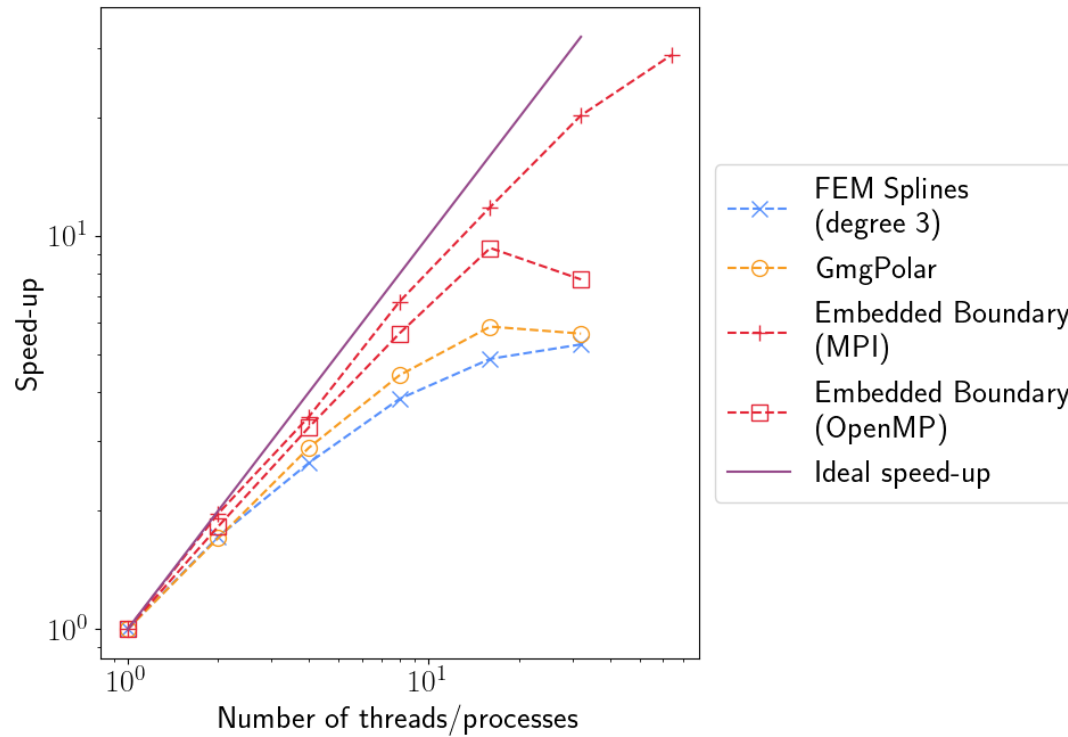
Solution aligned with curvilinear coordinates  
(used as initial perturbation in GYSELA)



- ▶ Spline FEM solver is most accurate
- ▶ The singular point is a source of imprecision for the GmgPolar solver
- ▶ The lower order of the Embedded Boundary solver makes it much less accurate







### ► Spline FEM Solver (IPP)

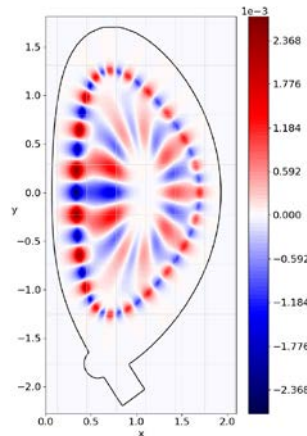
- + Highly accurate
- Weaker performance for large problems
- Does not handle the flux-surface average
- Refinement must preserve tensor-product mesh

### ► Embedded Boundary Solver (IPP)

- Not very accurate
- Does not handle the flux-surface average
- Difficult refinement
- + Good performance
- + Possible to solve problems with complex boundary conditions

### ► GmgPolar Solver (CERFACS)

- + Good accuracy
- + Good performance
- Does not handle the flux-surface average
- Refinement must preserve tensor-product mesh

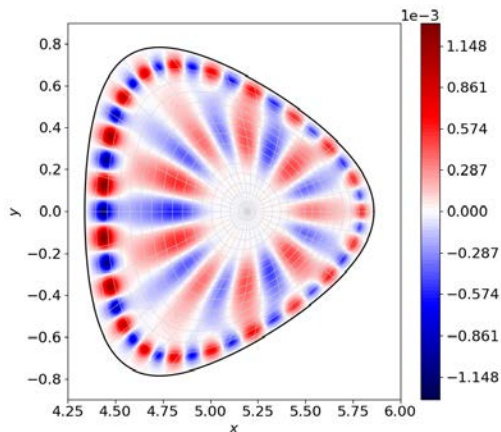


- Culham Geometry has been implemented in GYSELA

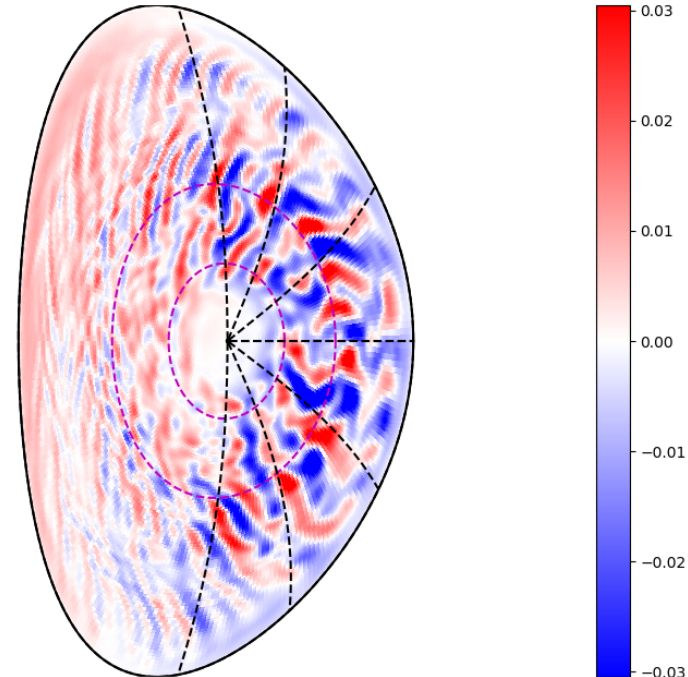
$$x(r, \theta) = r \cos \theta - E(r) \cos \theta + T(r) \cos 2\theta - P(r) \cos \theta + \delta(r) + R_0$$

$$y(r, \theta) = r \sin \theta + E(r) \sin \theta - T(r) \sin 2\theta - P(r) \sin \theta$$

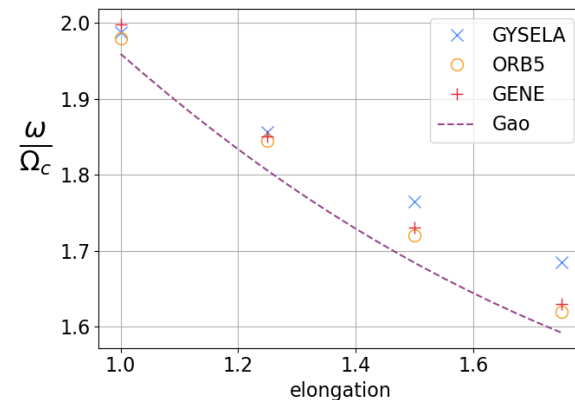
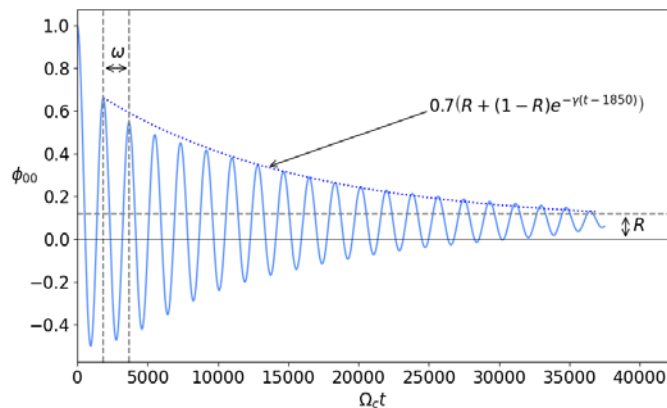
- The Spline FEM Solver has also been implemented using an iterative method to handle the flux-surface average



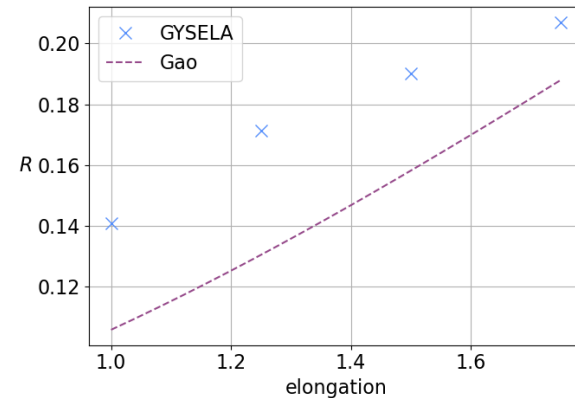
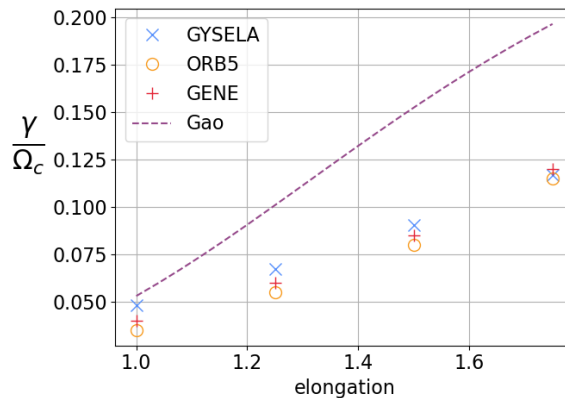
$\Phi - \Phi_{00}$  at time = 54720.0/ $\omega_c$  [Donnel]



## ► Geodesic Acoustic Mode (GAM) test



- Results agree with other codes and follow trend predicted by theory



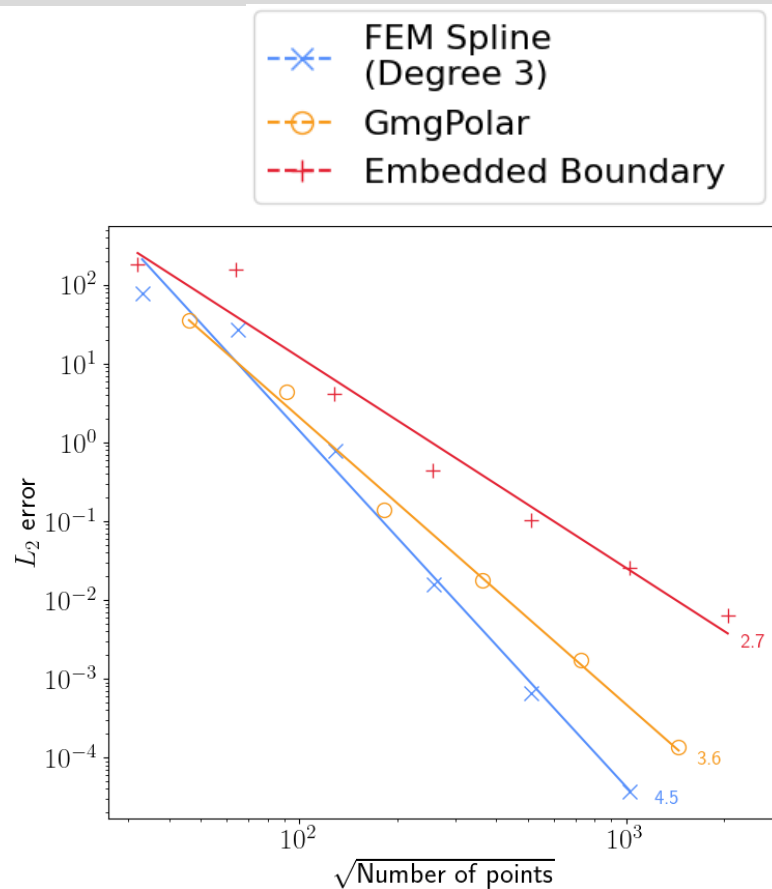
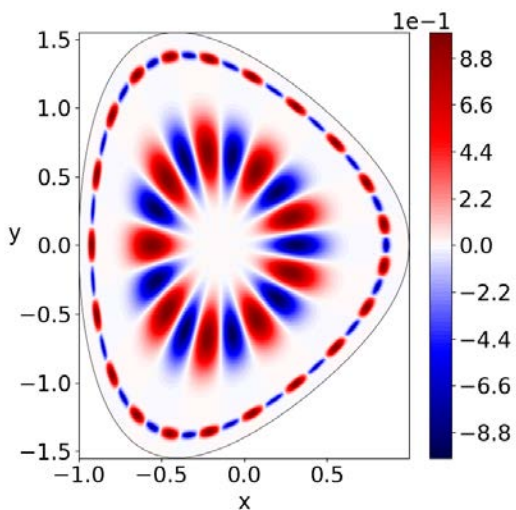




**Thank you for your attention**

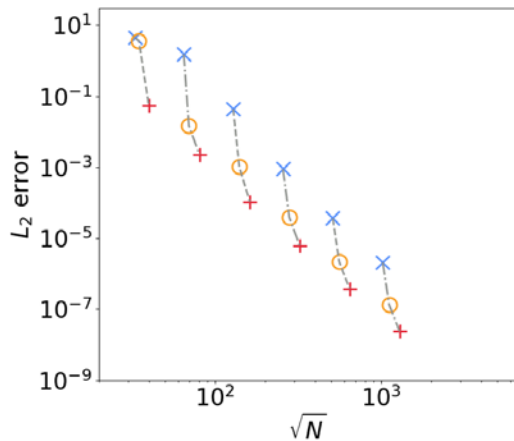


- At least  $500^2$  points are required for an error. But using more than  $2000^2$  points is too costly for the machine where the tests were run

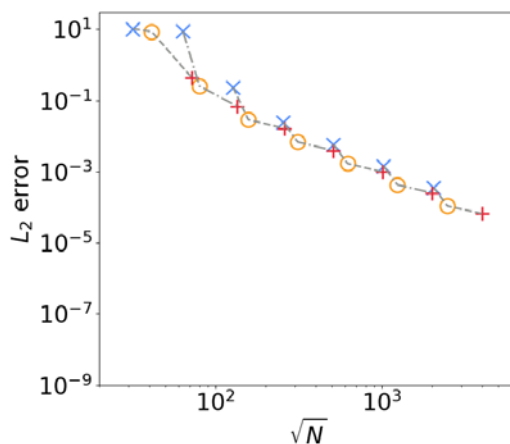


- ▶ Lack of poloidal refinement in the poloidal direction hampers Spline FEM and GmgPolar convergence
- ▶ Overlarge patches and low convergence order hampers Embedded Boundary convergence

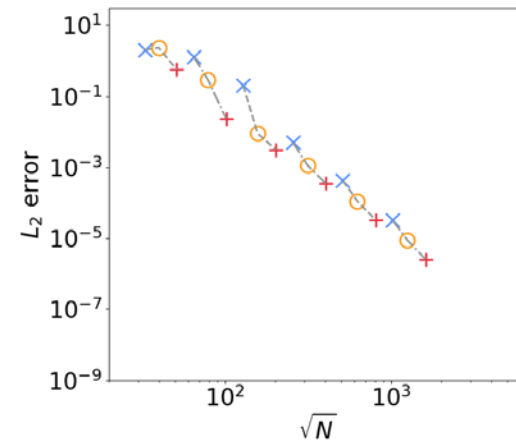
Spline FEM Solver



Embedded Boundary Solver

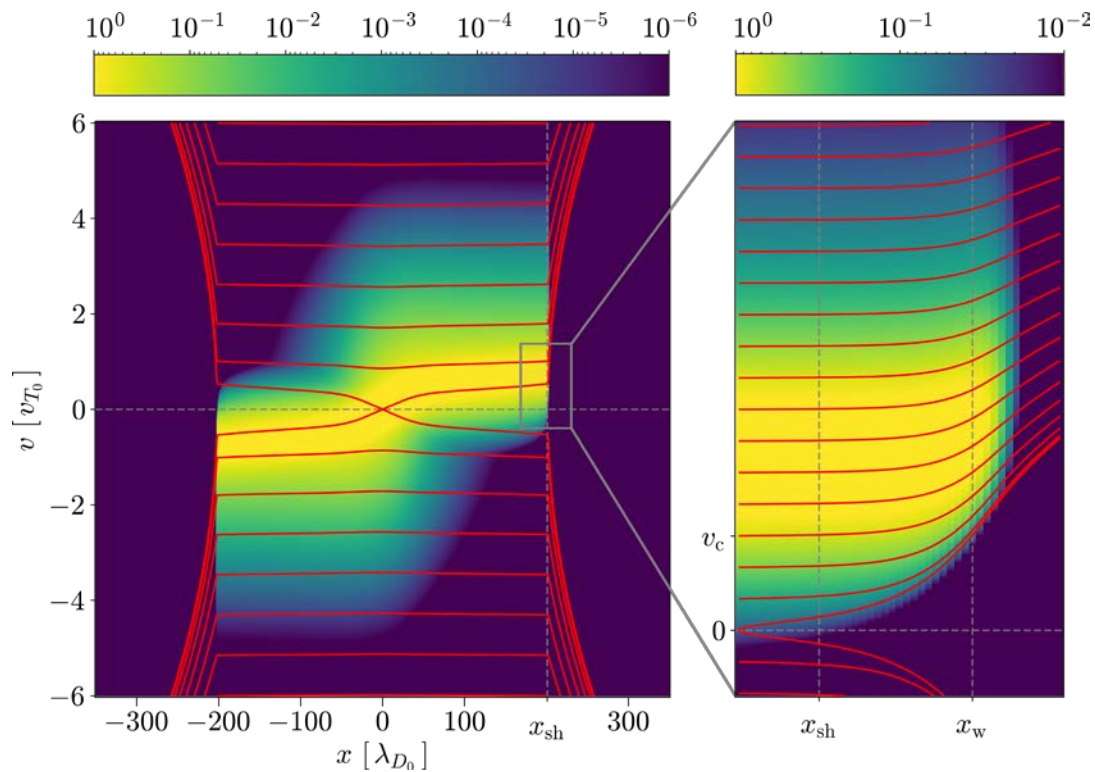


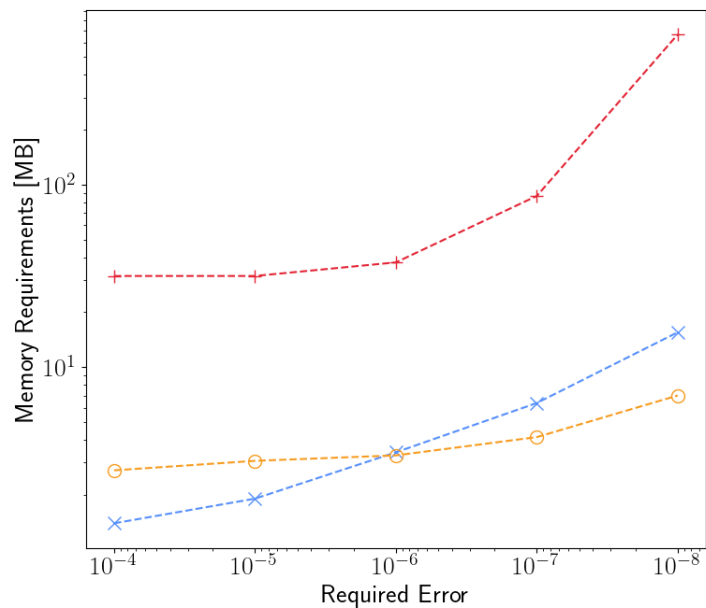
GmgPolar Solver



× No refinement    ○ 1 refinement    + 2 refinements

- ▶ VOICE equilibrium for ions
- ▶ Red lines show the trajectory of the particles
  - Trajectories in the wall are nonsensical as all ions in the wall are absorbed





—x— FEM Spline (Degree 3)  
—o— GmgPolar  
—+— Embedded Boundary

