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Non-uniform meshes in gyrokinetic simulations

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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

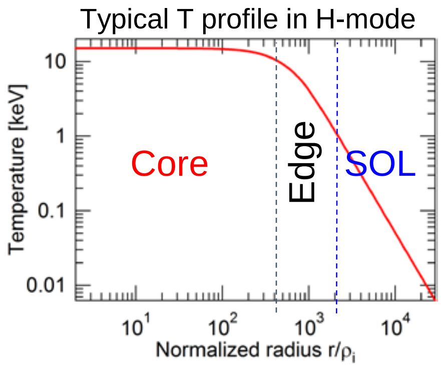
Intensive use of petascale resources

- > 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),

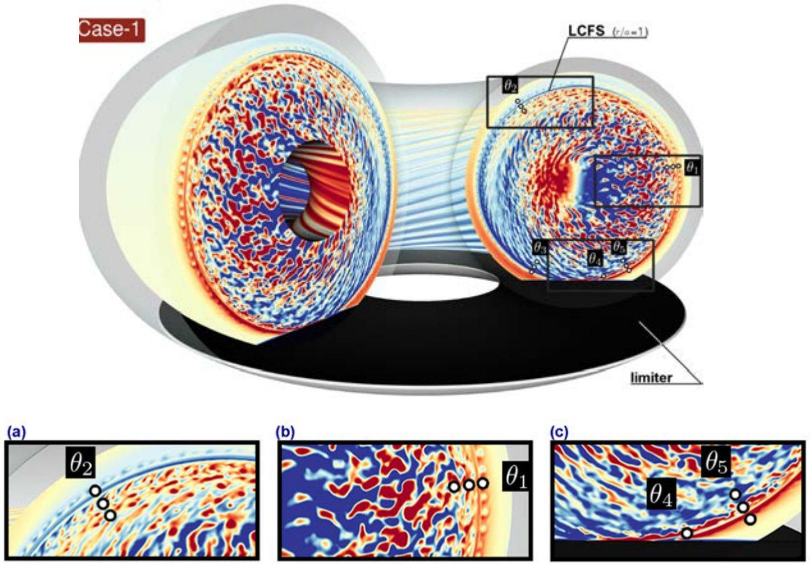
Exascale needed for ITER plasma turbulence simulation with electromagnetic effects

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



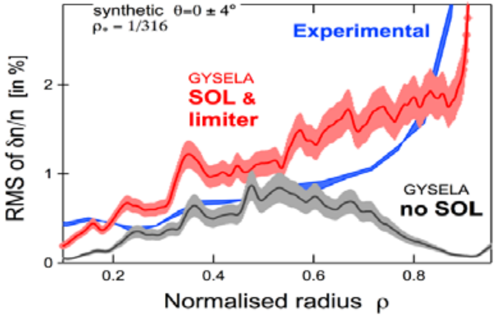
- Smaller structures in edge-region

[Dif-Pradalier 2020, 2022]



- More accurate results when modelling SOL

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



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

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

- 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 θ, φ

VOICE

2D Vlasov Solver

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

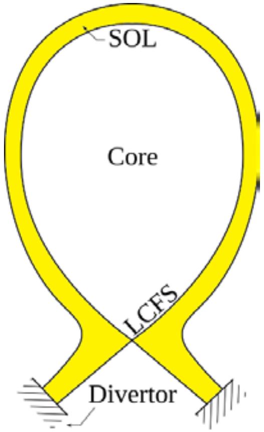
- Backward semi-Lagrangian Advection on arbitrary degree splines
- Penalisation for walls
- Collision operator

1D Poisson Solver

$$\partial_x^2\phi(t,x) = -\frac{\rho_q(t,x)}{\varepsilon_0}$$

- Finite Elements

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



Vlasov Equation

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

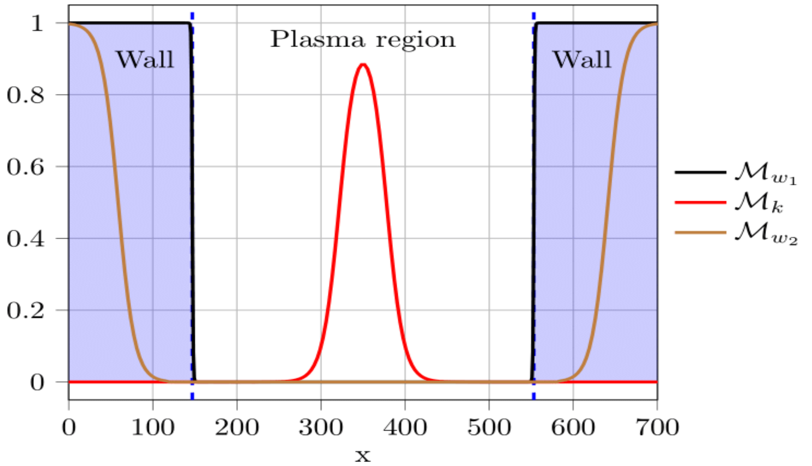
Poisson Equation

$$\partial_x^2\phi(t,x) = -\frac{\rho_q(t,x)}{\varepsilon_0}$$

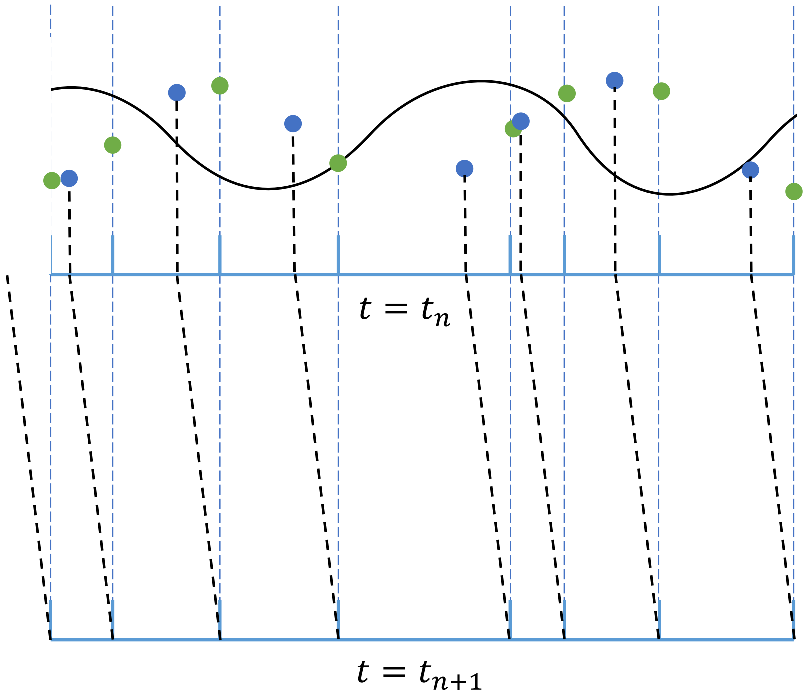
Sources

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

- Particle sink
- Momentum/Energy sink
- Kinetic source



[1]E. Bourne, Y. Munschy et al, submitted *2022*
[2]Y. Munschy, 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

Non-Uniform Quadrature from Splines

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

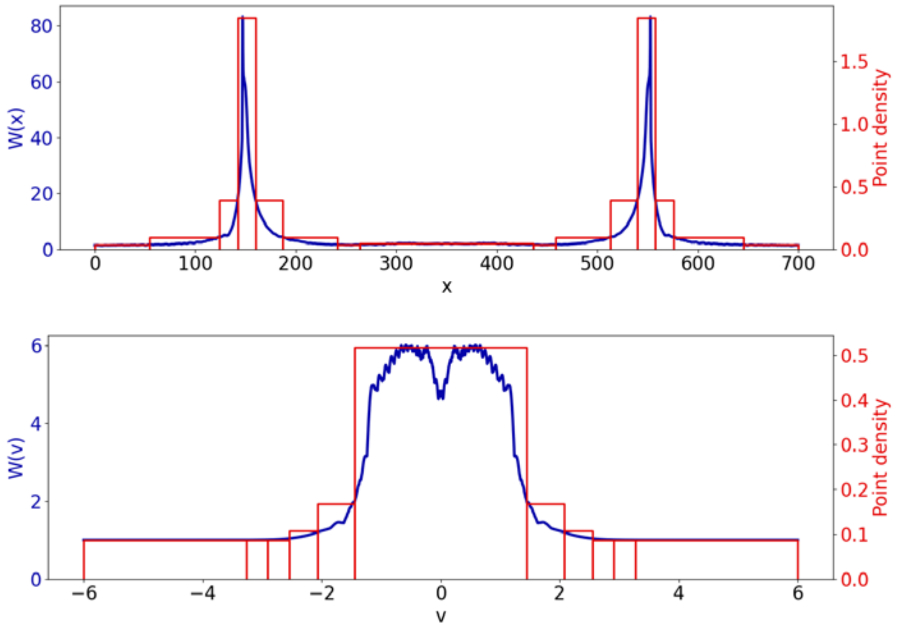
$$\sum_i b_j(x_i)q_i = \int b_j(x)dx \qquad \forall\, j$$

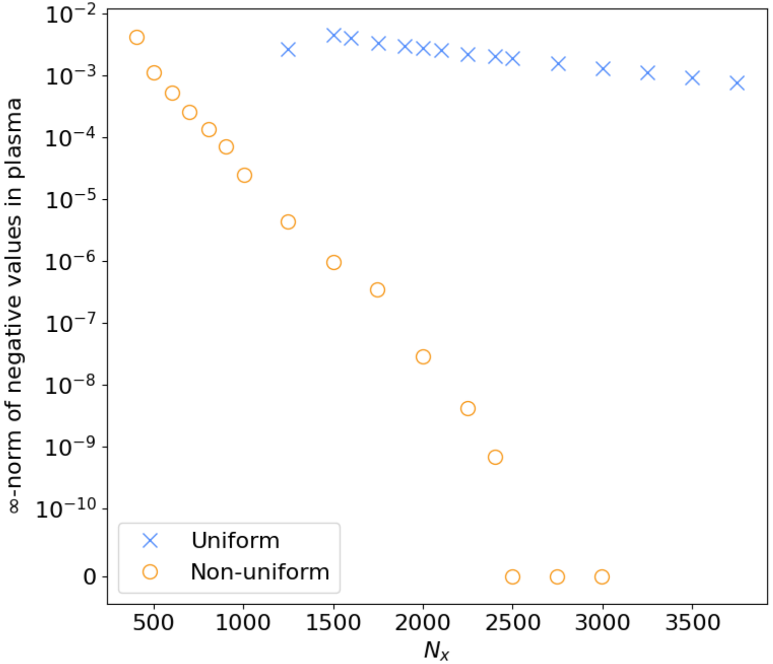
- Boundary conditions must be chosen such that no additional values are required
  - Greville interpolation points with knots at boundary
    - Same number of interpolation points and basis splines
  - Natural boundary condition = Schoenberg's "best" quadrature
    (well conditioned calculation described 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. Munschy et al, submitted 2022]*
- Wider simulations would be more realistic but require even more points

- Points are spaced proportionally to a weight function:

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





[1]E. Bourne, Y. Munschy et al, submitted *2022*

Non-Uniform Splines reach better conservation errors faster

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

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

- Density

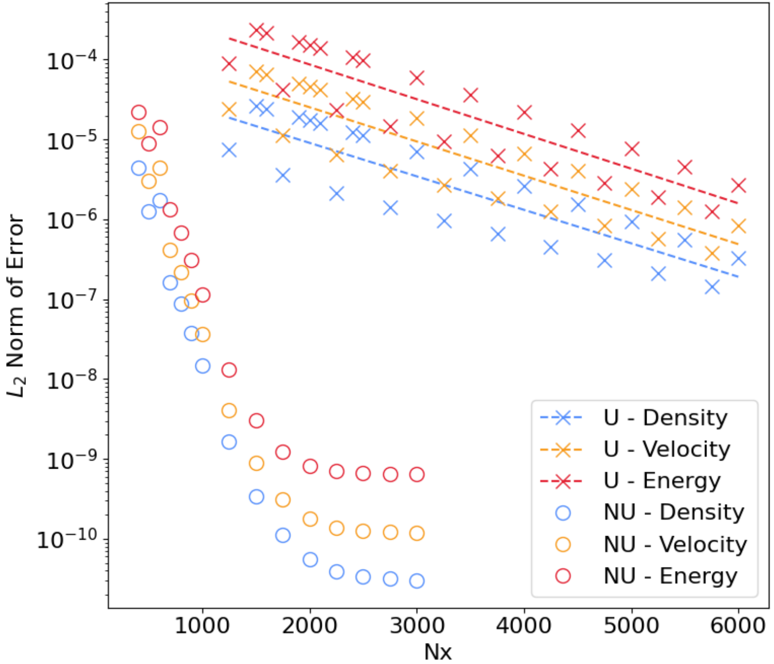
$$\partial_t n_s(t,x) + \frac{1}{\sqrt{m_s}} \partial_x \Gamma_s(t,x) = \int S_s(t,x,v_s) + C_{ss}(t,x,v_s)dv_s$$

- Velocity

$$\partial_t \Gamma_s(t,x) + \frac{1}{\sqrt{m_s}}\left(\partial_x \Pi_s(t,x) + q_s \partial_x \phi(t,x) n_s(t,x)\right) = \int v_s S_{s(t,x,v_s)} + v_s C_{ss}(t,x,v_s)dv_s$$

- Energy

$$\partial_t \Pi_{s(t,x)} + 2\frac{1}{\sqrt{m_s}}\left(\partial_x Q_{s(t,x)} + q_s \partial_x \phi(t,x)\Gamma_s\right) = \int v_s^2 S_{s(t,x,v_s)} + v_s^2 C_{ss}(t,x,v_s)dv_s$$

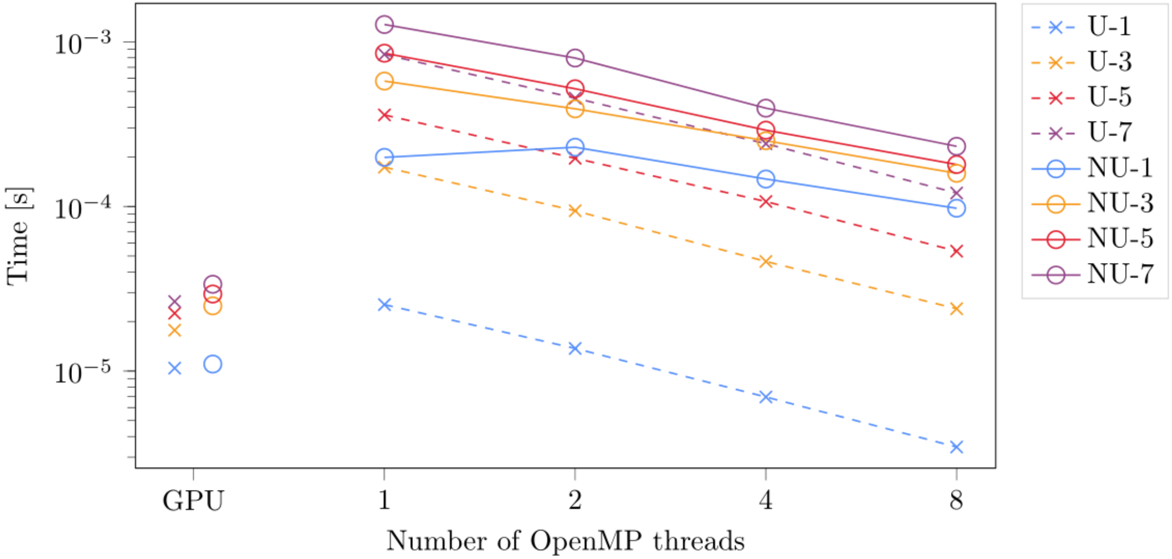


[1]E. Bourne, Y. Munschy et al, submitted *2022*

GPUs are crucial to make non-uniform splines competitive

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

(U-1 = Uniform splines of degree 1)



[1]E. Bourne, Y. Munschy et al, submitted *2022*

- 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

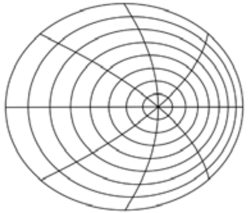
[1] E. Bourne, Y. Munschy et al, submitted *2022*

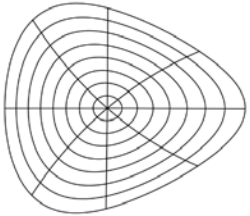
FDM/FFT

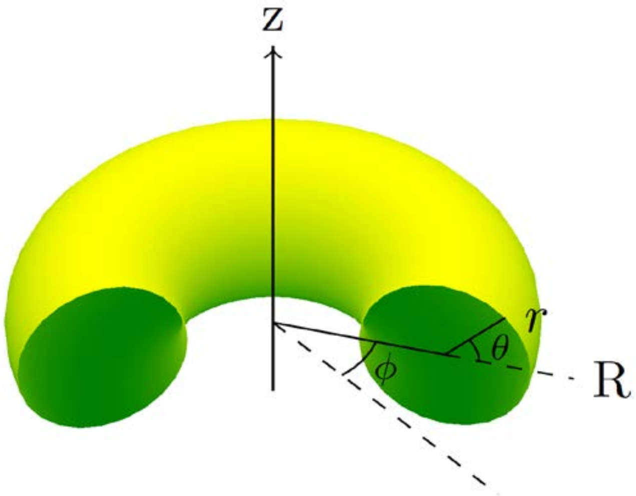
- Solves the equation:

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

- 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
- ~4^{th} order
- Matrix free

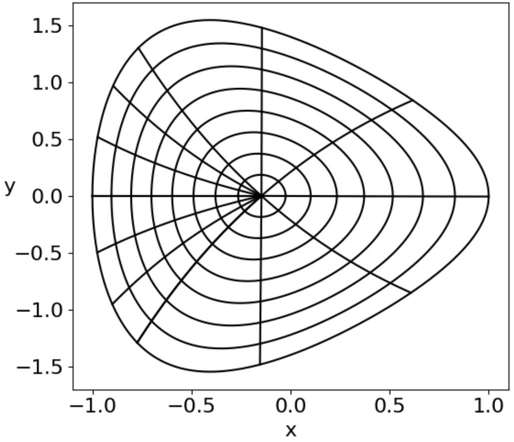
Common Problem

$$-\frac{1}{n_{e_0}}\sum_s Z_s \nabla_\perp \cdot \left(\frac{n_{s,eq}}{B\Omega_s}\nabla_\perp \phi\right) + \frac{e}{T_{e,eq}}(\phi - \langle\phi\rangle)$$

$$= \frac{1}{n_{e_0}}\sum_s Z_s \int J_0 \cdot (\bar{F}_s - \bar{F}_{s,eq}) d^3 v$$

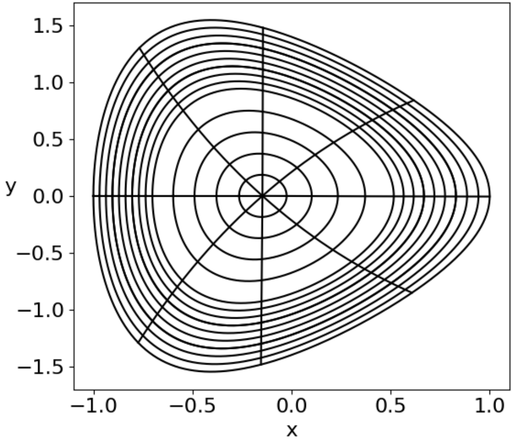
$$\langle\phi\rangle = \frac{\int \phi R J d\theta d\phi}{\int RJ d\theta d\phi}$$

[1]E. Bourne, P. Leleux et al, submitted *2022*



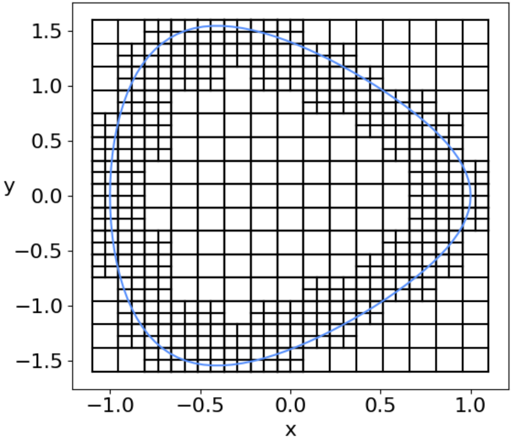
Poloidal refinement
(Spline FEM / GmgPolar)

+ 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

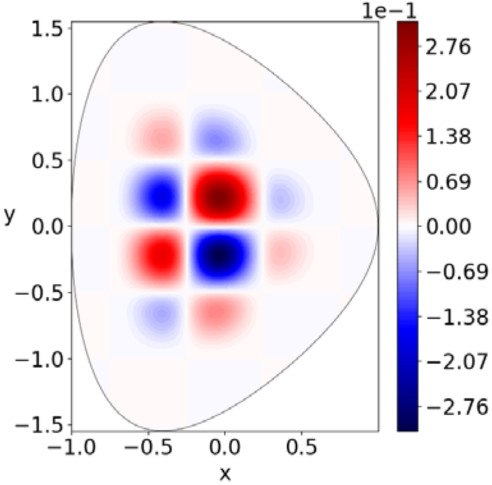
[1]E. Bourne, P. Leleux et al, submitted *2022*

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

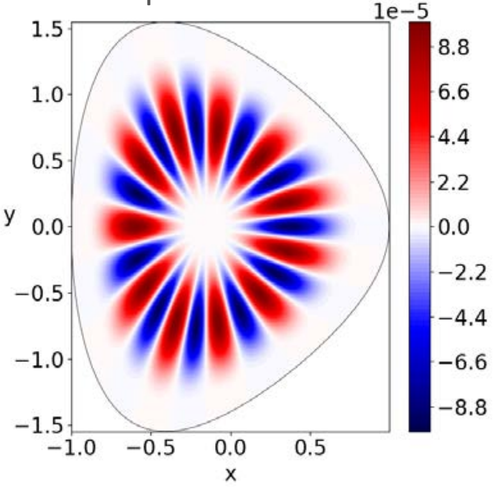
$$\alpha(r) = \exp\left(-\tanh\left(\frac{r - r_p}{\delta_r}\right)\right)$$

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

Cartesian solution not aligned with coordinate system

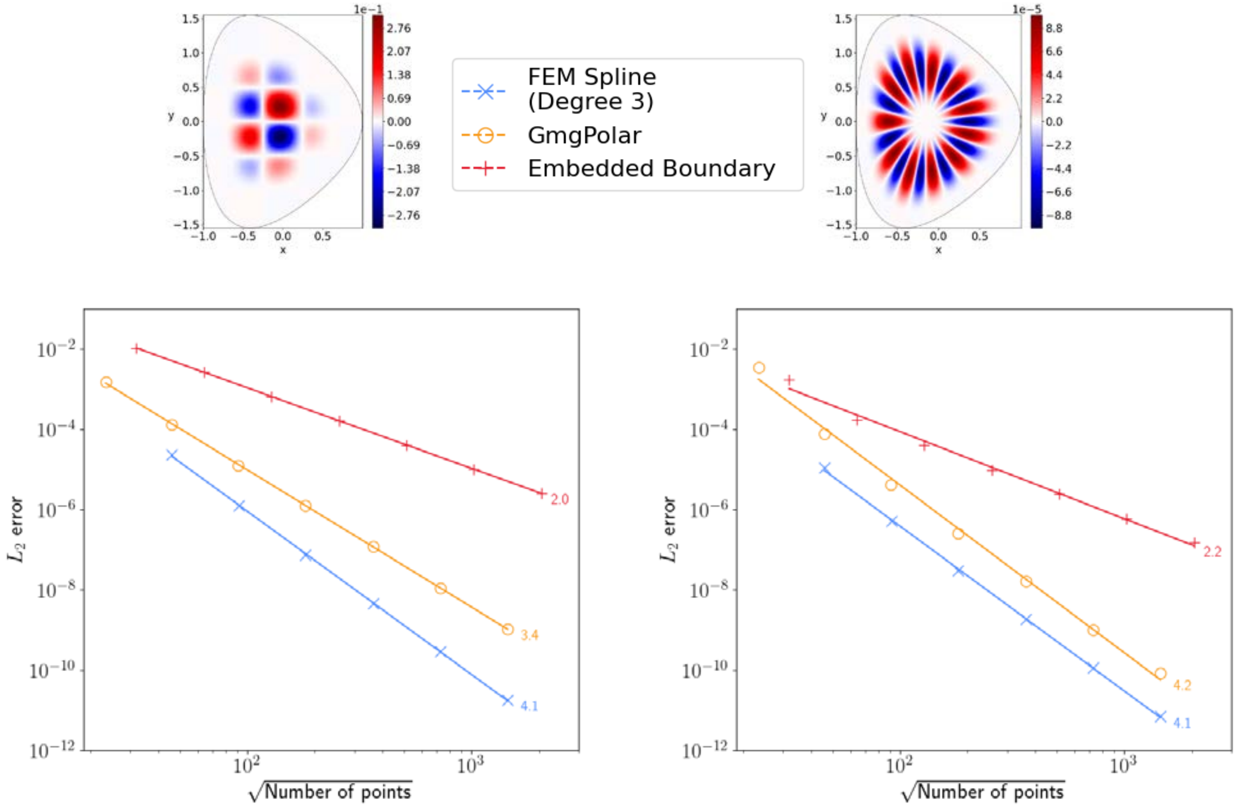


Solution aligned with curvilinear coordinates (used as initial perturbation in GYSELA)



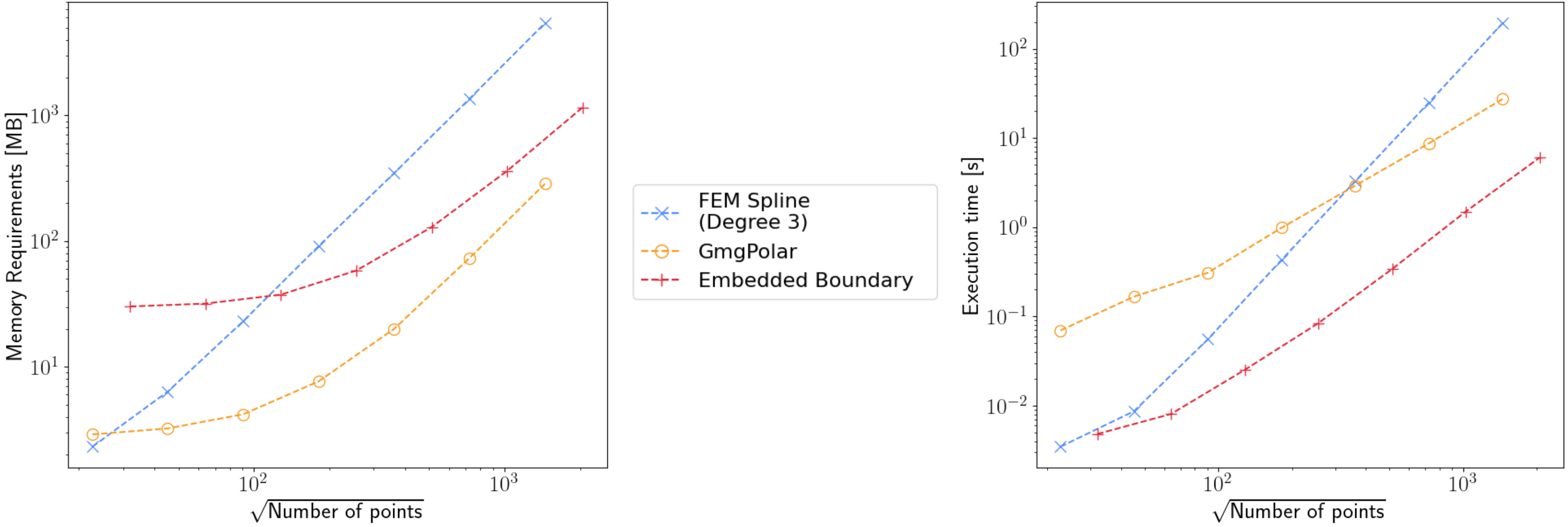
[1]E. Bourne, P. Leleux et al, submitted *2022*

- 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



[1]E. Bourne, P. Leleux et al, submitted *2022*

AMReX is highly optimised but matrix-free GmgPolar has low memory



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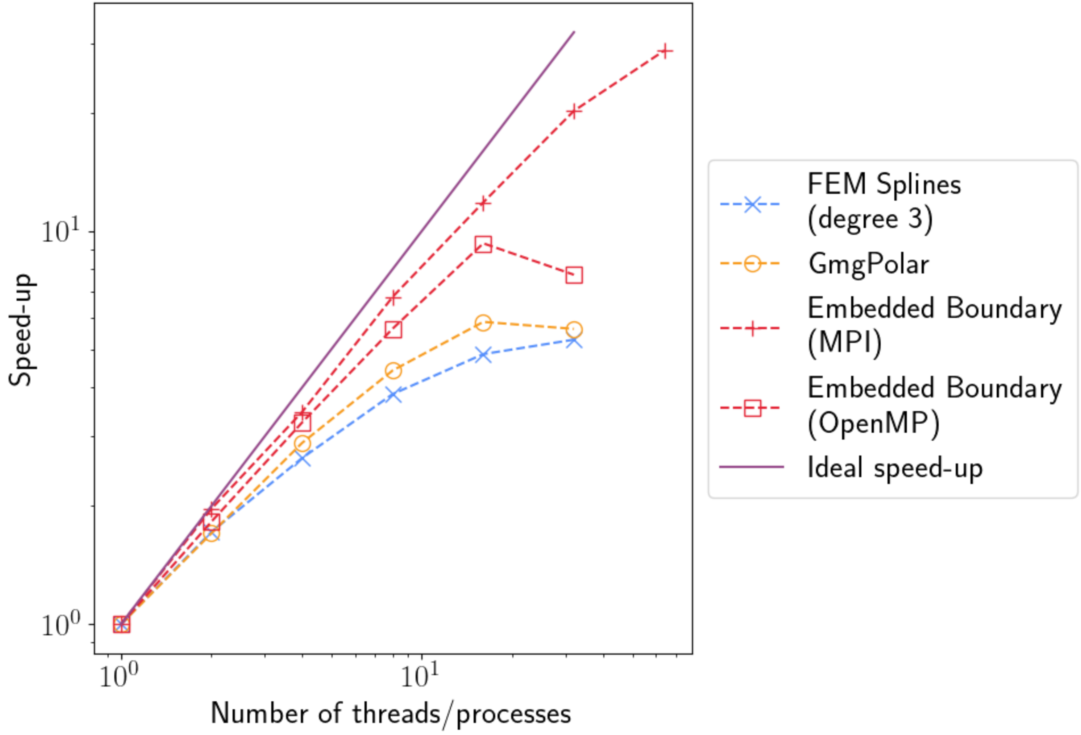


[1]E. Bourne, P. Leleux et al, submitted *2022*

Spline FEM Solver (IPP)

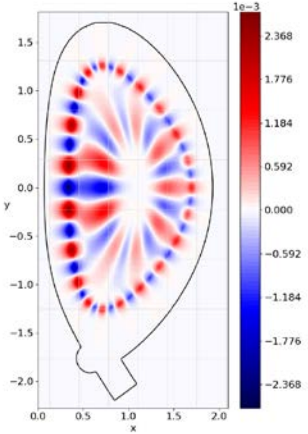
- \+ Highly accurate
- – Weaker performance for large problems
- – Does not handle the flux-surface average
- – Refinement must preserve tensor-product mesh

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

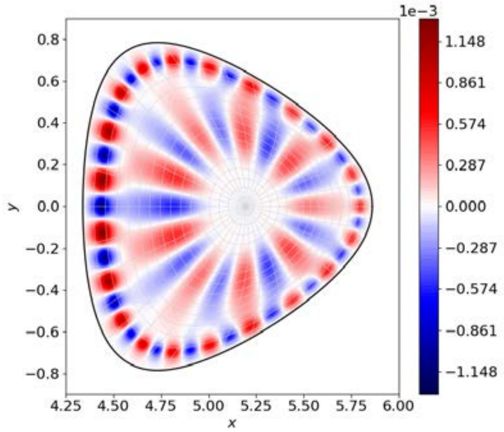


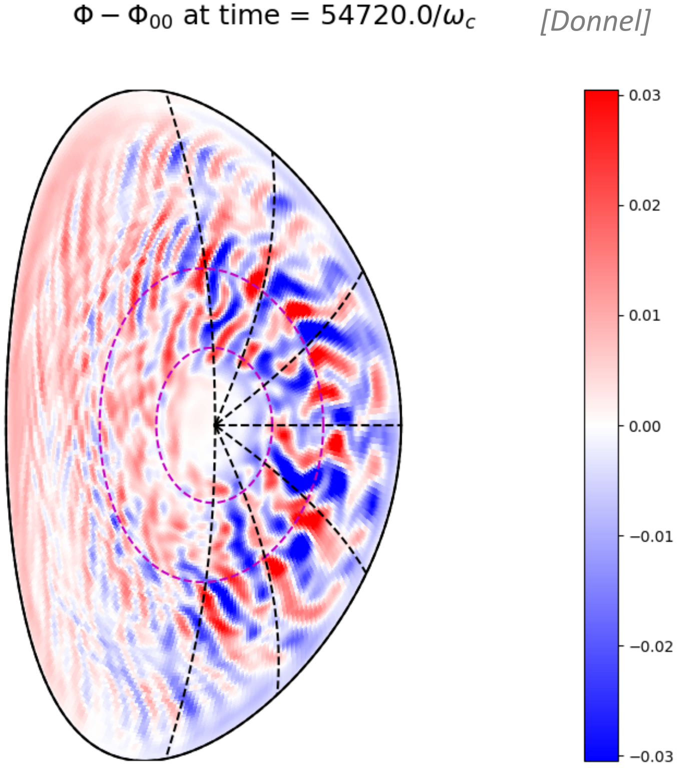
[1]E. Bourne, P. Leleux et al, submitted *2022*

- Culham Geometry has been implemented in GYSELA

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

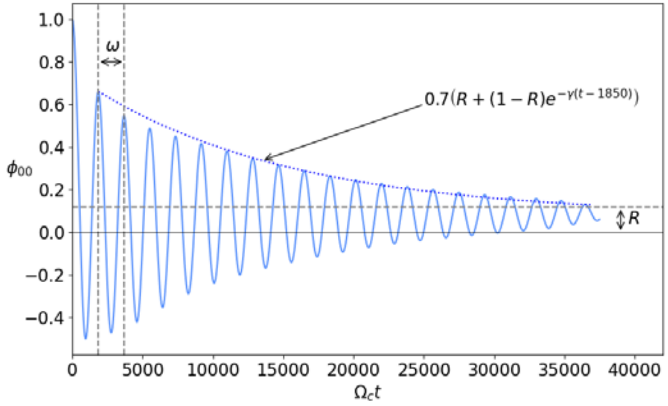
- The Spline FEM Solver has also been implemented using an iterative method to handle the flux-surface average

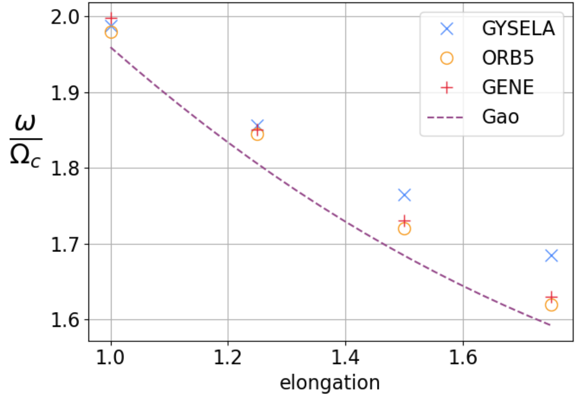




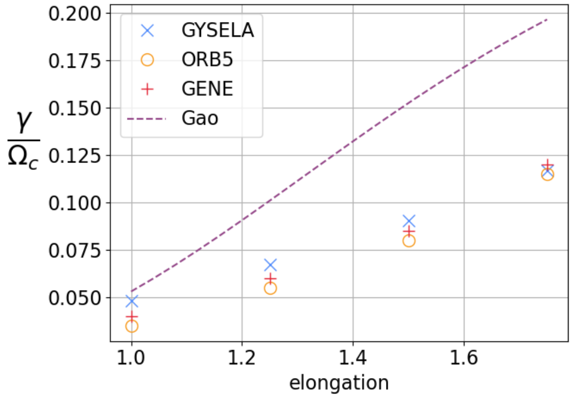
[Donnel]

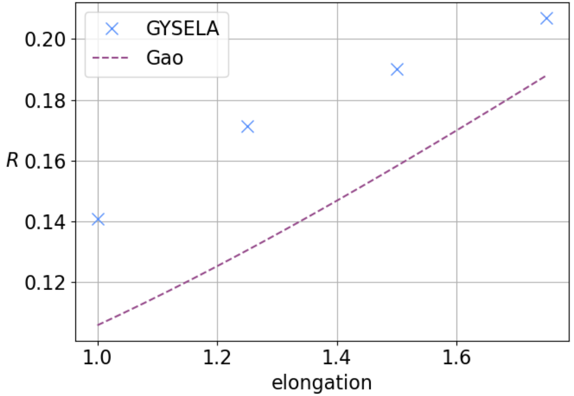
Geodesic Acoustic Mode (GAM) test





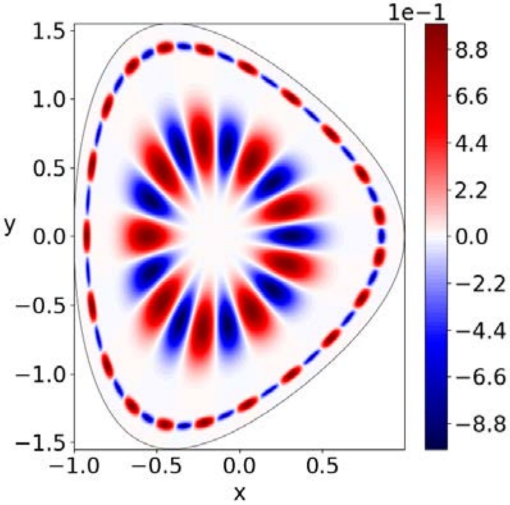
- Results agree with other codes and follow trend predicted by theory

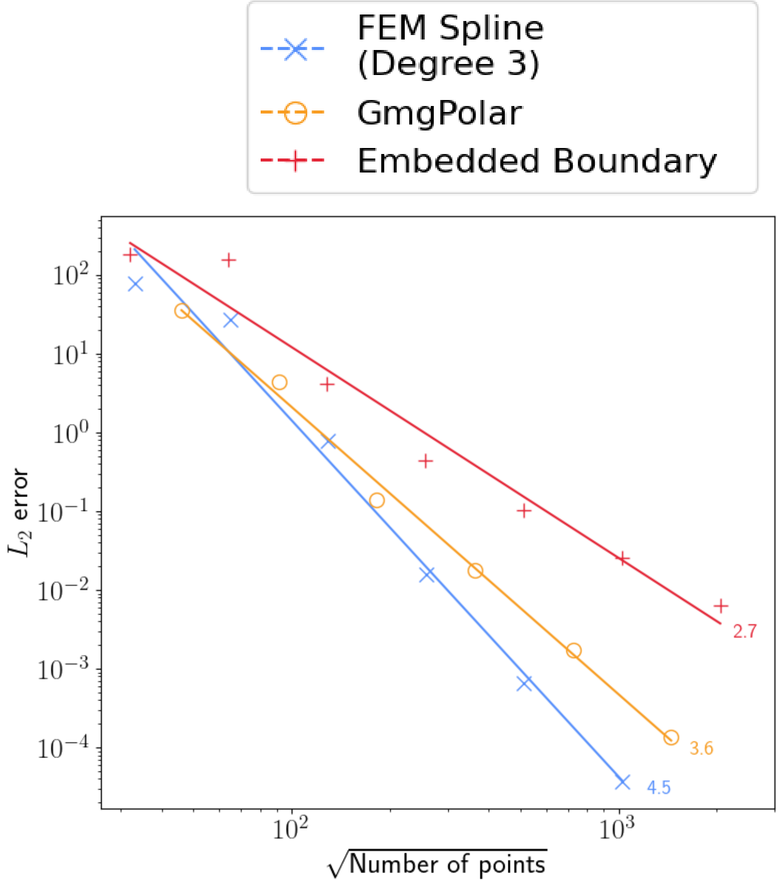




Thank you for your attention

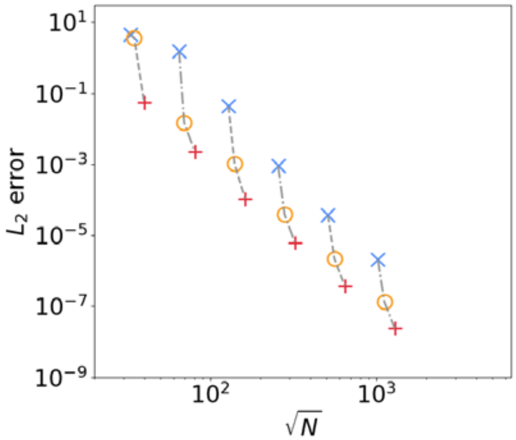
- At least 500^2 points are required for an error. But using more than 2000^2 points is too costly for the machine where the tests were run



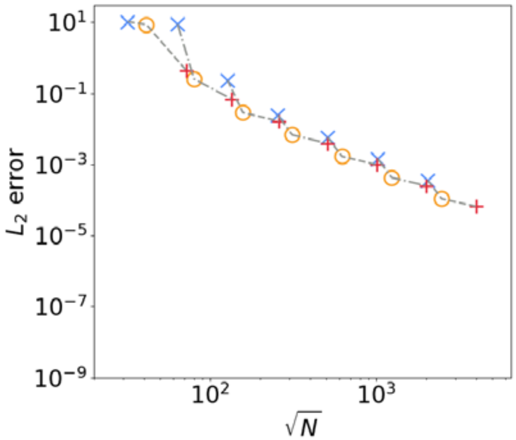


- Lack of poloidal refinement in the poloidal direction hampers Spline FEM and GmgPolar convergence
- Overlarge patches and low convergence order hampers Embedded Boundary convergence

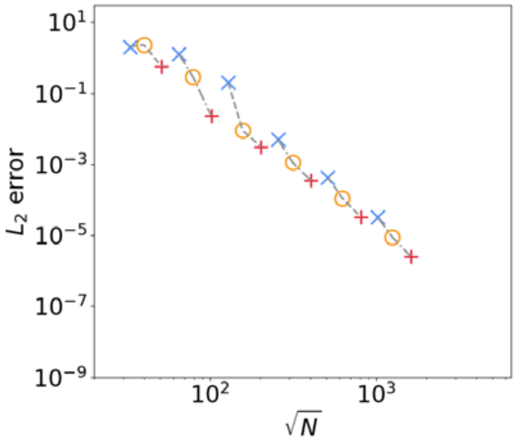
Spline FEM Solver



Embedded Boundary Solver

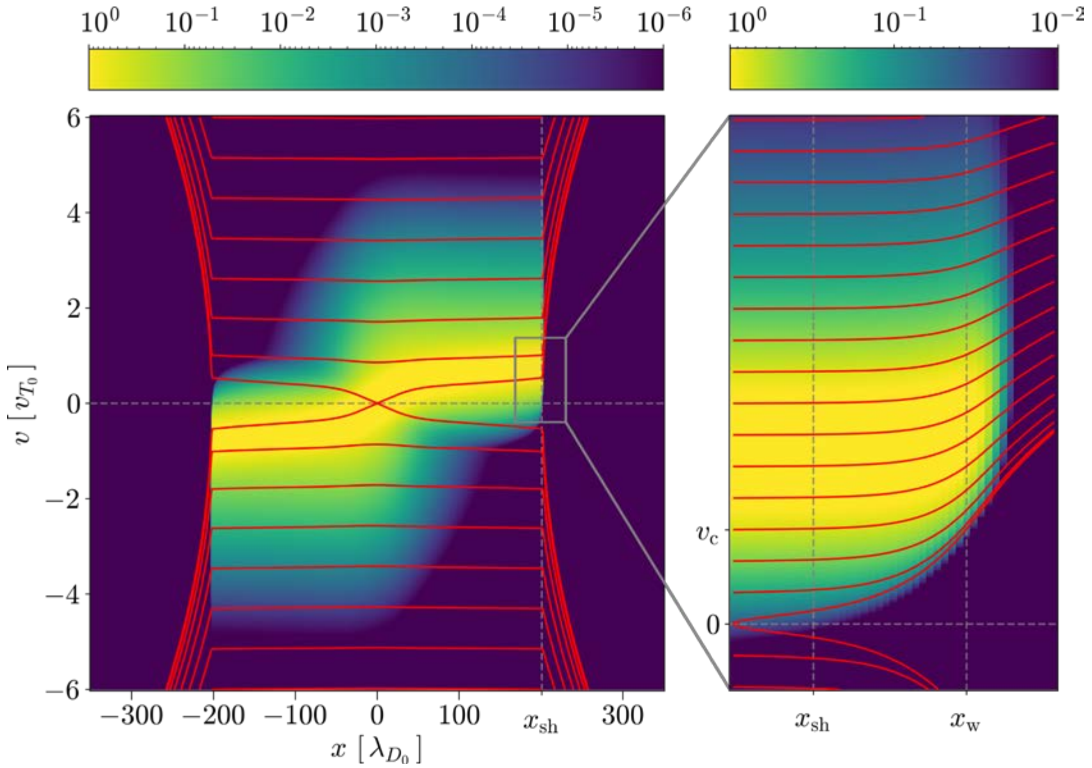


GmgPolar Solver



× 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



FEM Spline Solver is Performant if the Required Error Determines the Number of Points