Accuracy and scalability of incompressible inductionless MHD codes applied to fusion technologies

4th Fusion HPC Workshop

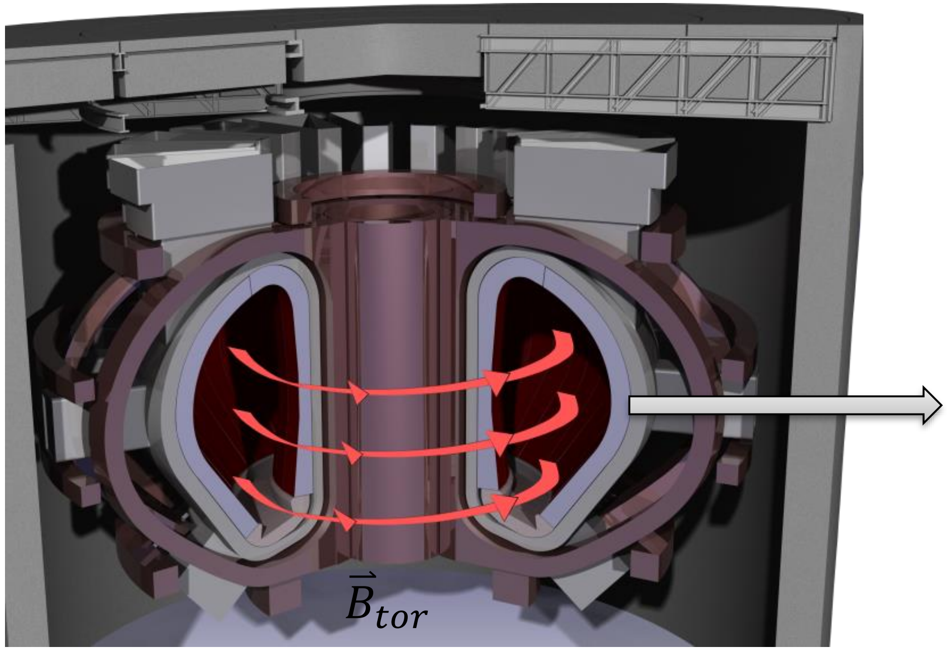
F. R. Urgorri[1], G. G. Fonfría[1], J. Príncipe[2], F. Verdugo[3] and S. Badía[4]
[1]Fusion Technologies Division National Fusion Laboratory CIEMAT
[2]International Centre for Numerical Methods in Engineering
[3]Vrije Universiteit Amsterdam
[4]Monash University

Outline

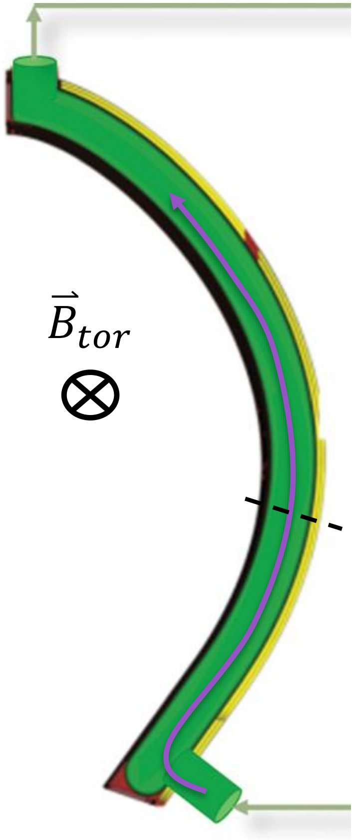
- The inductionless MHD problem in fusion breeding blankets
- The need of HPC for simulating MHD flows in fusion conditions
- The *φ*-formulation and the charge conservation issue
- Commercial platforms: ANSYS-Fluent
- The j/φ-formulation and the monolithic approach: GridapMHD
- Conclusions

The inductionless MHD problem in fusion breeding blankets

- The MHD phenomenon in breeding blankets arises as a result of the movement of a fluid electrical conductor (PbLi) inside the B-field used for the magnetic confinement



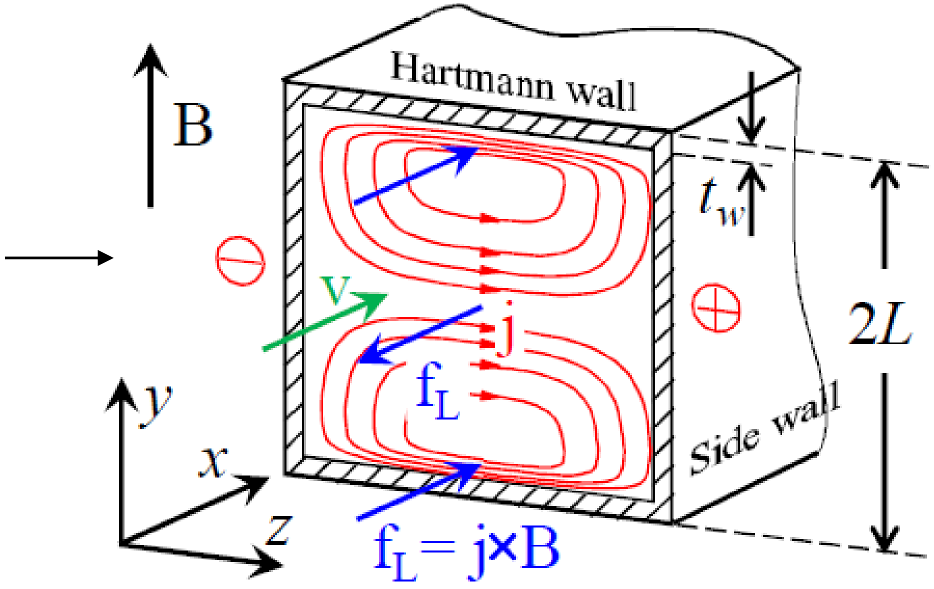
DEMO with DCLL blanket. Courtesy of Dr. I. Fernández-Berceruelo



D. Rapisarda et al 2021 Nucl. Fusion 61 115001.

Induced currents due to the moving conductor

$$\vec{j} \sim \sigma(\vec{u} \times \vec{B})$$



C. Mistrangelo, WPB5 PbLi Technologies and TER meeting

The inductionless MHD problem in fusion breeding blankets

- From the mathematical perspective, the Lorentz force is added as a source term to the **incompressible Navier-Stokes equation** (momentum continuity):

$$\frac{1}{N}(\partial_t \hat{u} - (\hat{u} \cdot \nabla)\hat{u}) = \frac{1}{Ha^2}\nabla^2 \hat{u} - \nabla \hat{p} + \underline{\hat{j} \times \hat{B}_0}$$

Interaction parameter:
Ratio Lorentz forces-inertia

$$N = \frac{B_0^2 \sigma L}{\rho u_0}$$

$$Ha = B_0 L \sqrt{\frac{\sigma}{\eta}}$$

Hartmann number:
Ratio Lorentz-viscous forces

The inductionless MHD problem in fusion breeding blankets

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- In the so-called **inductionless regime**, the magnetic field is independent of the flow and only the electric is influenced by the flow dynamics:

$$\hat{j} = -\nabla\hat{\varphi} + \hat{u}\times\hat{B}_0$$

Generalized Ohm's law

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$$\hat{j} = -\nabla \hat{\varphi} + \hat{u} \times \hat{B}_0$$

- Charge and mass conservation closed the system of equations:

$$\nabla \cdot \hat{u} = 0 \qquad \nabla \cdot \hat{j} = 0$$

- J/φ formulation: System with 8 equations and 8 variables: $\hat{u}, \hat{p}, \hat{j}, \hat{\varphi}$

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The need of HPC for simulating MHD flows in fusion conditions

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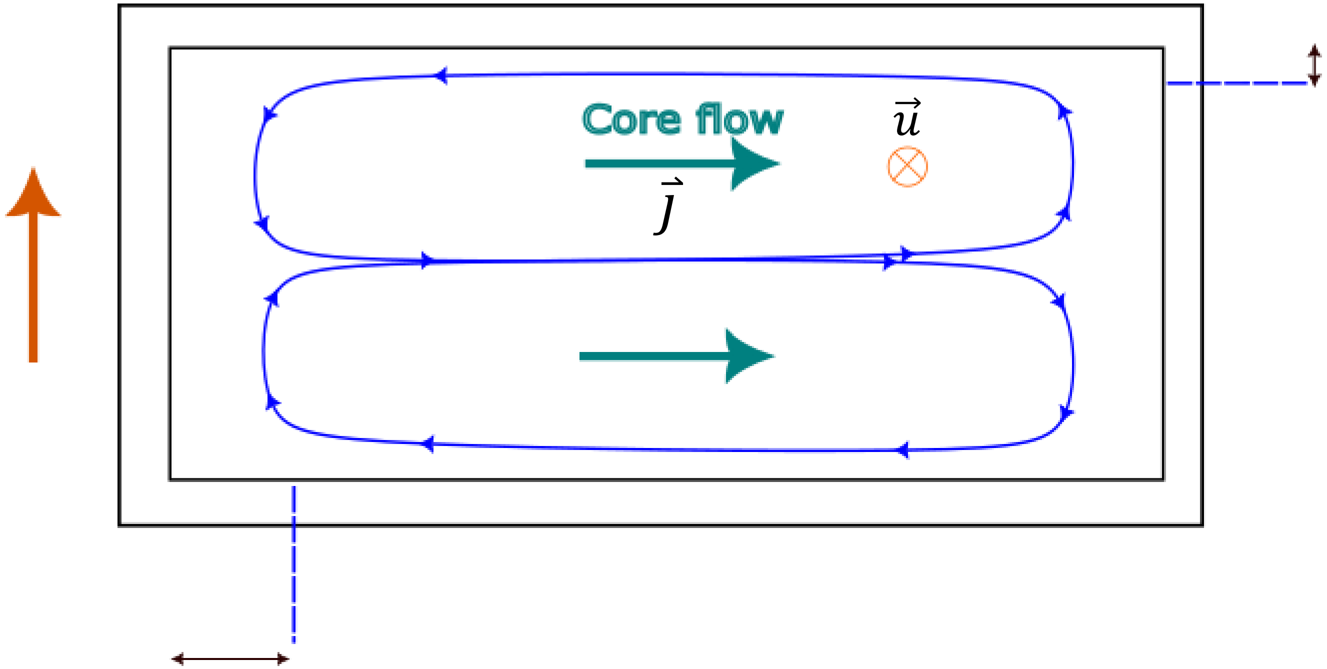
- Fusion breeding blankets are characterized by very high Hartmann numbers ($Ha{\sim}10^4$)
- The Lorentz force opposes the flow motion in the majority of the cross section (core flow)
- Viscous forces are therefore negligible in most of the channel cross-section but in the very thin boundary layers

External, high magnetic field $\vec{B}_0$



Hartmann boundary layers $\delta{\sim}L/Ha$

Side boundary layers $\delta{\sim}L/Ha^{0.5}$

Ohm's law

$$\vec{j} = \sigma(-\nabla\varphi + \vec{u} \times \vec{B}_0)$$

Lorentz force

$$f_L = \vec{j} \times \vec{B}_0$$

The need of HPC for simulating MHD flows in fusion conditions

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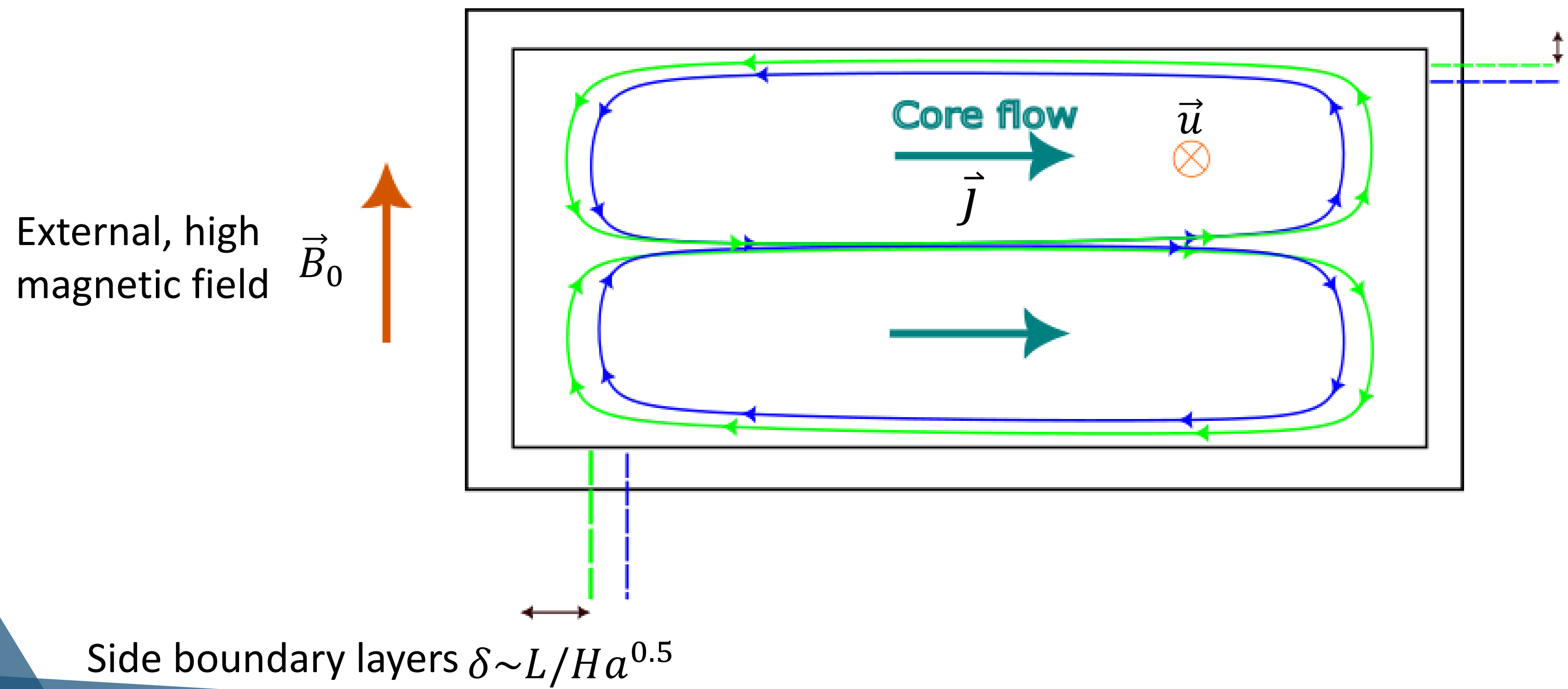

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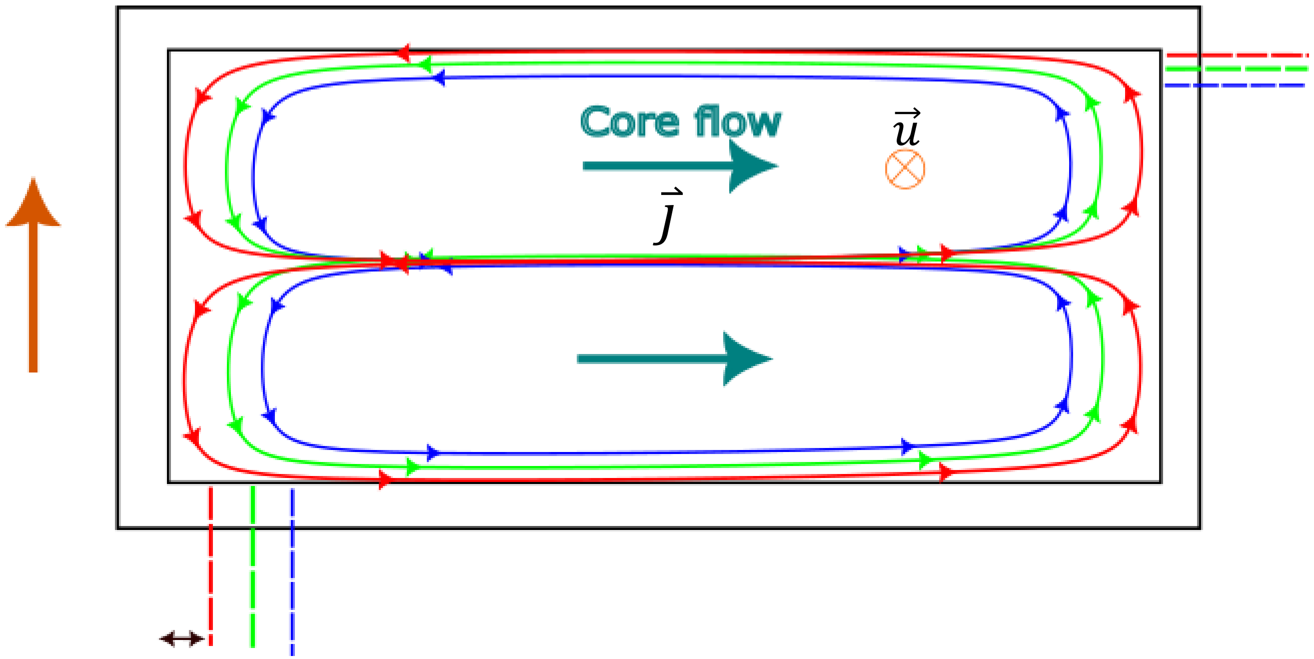

Hartmann boundary layers $\delta \sim L/Ha$

Ohm's law

$$\vec{j} = \sigma(-\nabla\varphi + \vec{u} \times \vec{B}_0)$$

Lorentz force

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Side boundary layers $\delta \sim L/Ha^{0.5}$

The need of HPC for simulating MHD flows in fusion conditions

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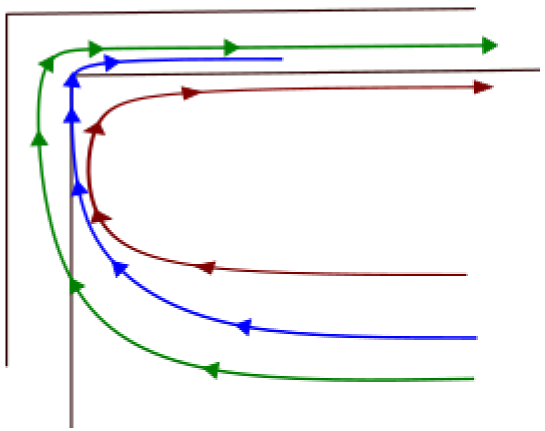
- The pressure in insulated channels is mostly caused by viscous friction in the very thin Hartmann boundary layers.
- In conducting-walls channels, electric currents can penetrate into the wall. Computing the fraction that goes through fluid and solid is crucial for accurately computing pressure drop associated to the Lorentz force.



Sketch of the electric currents near the corner of a channel

$$\nabla p_{EM}\left[\frac{Pa}{m}\right] = -\frac{1}{S}\int_S \left(\vec{j}\times\vec{B}_0\right)\cdot d\vec{s}$$

- Very high mesh resolution are needed next to the boundary layers and other 3D elements of the domain
- Time resolution will be also a constrain if the transient period want to be computed or in terms of stability for explicit solvers

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The φ-formulation and the charge conservation issue

- By far the most common method employed to solve the MHD problem is the **Finite Volume Method (FMV)**
- The complete mathematical MHD inductionless problem:

$$\frac{1}{N}(\partial_t \hat{u} - (\hat{u}\cdot\nabla)\hat{u}) = \frac{1}{Ha^2}\nabla^2\hat{u} - \nabla\hat{p} + \hat{j}\times\hat{B}_0$$ → Momentum continuity

$$\nabla\cdot\hat{u} = 0$$ → Mass conservation

$$\hat{j} = -\nabla\hat{\varphi} + \hat{u}\times\hat{B}_0$$ → Ohm's law

$$\nabla\cdot\hat{j} = 0$$ → Charge conservation

The φ-formulation and the charge conservation issue

- The most usual procedure to solve the inductionless set of equations is combining charge conservation and the Ohm's law

$$\frac{1}{N}(\partial_t \hat{u} - (\hat{u} \cdot \nabla)\hat{u}) = \frac{1}{Ha^2}\nabla^2 \hat{u} - \nabla \hat{p} + \hat{j} \times \hat{B}_0$$ → Momentum continuity

$$\nabla \cdot \hat{u} = 0$$ → Mass conservation

$$-\nabla^2 \hat{\varphi} + \nabla \cdot \left(\hat{u} \times \hat{B}_0\right) = 0$$ → Poisson equation for the electrical potential

- φ-formulation: 5 equations and 5 variables: $\hat{u}, \hat{p}, \hat{\varphi}$

The φ-formulation and the charge conservation issue

- The most usual procedure to solve the inductionless set of equations is combining charge conservation and the Ohm's law

$$\frac{1}{N}\left(\partial_t \hat{u} - (\hat{u}\cdot\nabla)\hat{u}\right) = \frac{1}{Ha^2}\nabla^2\hat{u} - \nabla\hat{p} + \hat{j}\times\hat{B}_0$$

→ Momentum continuity

$$\nabla\cdot\hat{u} = 0$$

→ Mass conservation

$$-\nabla^2\hat{\varphi} + \nabla\cdot\left(\hat{u}\times\hat{B}_0\right) = 0$$

→ Poisson equation for the electrical potential

$$\hat{j} = -\nabla\hat{\varphi} + \hat{u}\times\hat{B}_0$$

Staggered scheme

1. Poisson equation for electric potential
2. Computation of the current density
3. SIMPLE-like scheme for p-u coupling

⇒ Charge is not necessarily conserved at discrete level

The φ-formulation and the charge conservation issue

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- Charge conservation issues arises when reconstructing the electric current and computing the Lorentz force
- At high Hartmann number the truncation errors of the Poisson's equation finite differences can accumulate when computing the current density and the Lorentz force
- **Core velocity equation** in a fully developed flow at high Hartmann: $\nabla \hat{p} = \hat{j} \times \hat{B}_0$

$$\hat{j} = -\nabla\hat{\varphi} + \left(\hat{u}_c \times \hat{B}_0\right) = \begin{pmatrix} -\partial_x\hat{\varphi} \\ -\partial_y\hat{\varphi} \\ -\partial_z\hat{\varphi} + u_c \end{pmatrix}$$

$$\hat{u}_c = u_c\hat{x}$$

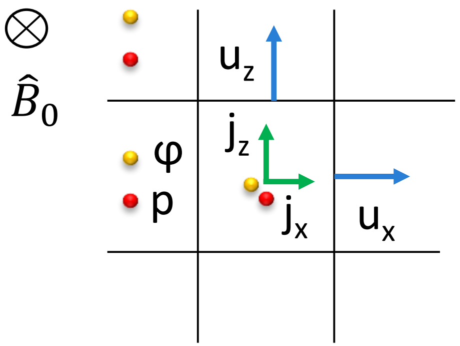
$$\hat{B}_0 = \hat{y}$$

$$\hat{j} \times \hat{B}_0 = -\nabla\hat{\varphi} \times \hat{B}_0 + \left(\hat{u}_c \times \hat{B}_0\right) \times \hat{B}_0 = \underbrace{\begin{pmatrix} \partial_z\hat{\varphi} - u_c \\ 0 \\ -\partial_x\hat{\varphi} \end{pmatrix}}$$

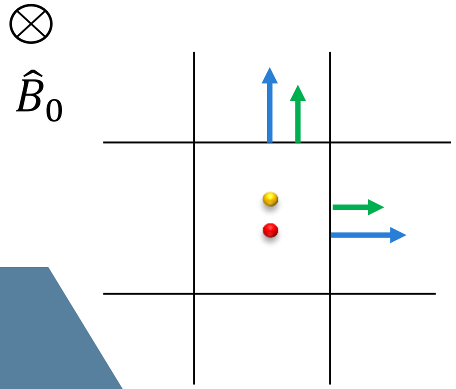
The Lorentz force (and the current) is obtained from differentiating two nearly identical numbers

The φ-formulation and the charge conservation issue

- Interpolation of current density can also lead to errors:



Sketches of a 2D staggered mesh



- Option 1: Reconstruct the current directly in the cell center

$$\hat{j}_c = -(\nabla\varphi)_c + \hat{u}_c \times \hat{B}_0$$

E.g. $(\nabla\varphi)_c \sim \frac{1}{V}\sum_1^{n_f} \varphi_f s_f \hat{n}$

$$f_L = \hat{j}_c \times \hat{B}_0 = -(\nabla\varphi)_c \times \hat{B}_0 + (\hat{u}_c \times \hat{B}_0) \times \hat{B}_0$$

- Option 2: Reconstruct in the face and interpolate the center value

$$\hat{j}_f = -(\nabla\varphi)_f + \hat{u}_f \times \hat{B}_0$$

E.g. $(\nabla\varphi)_f \sim \frac{1}{\Delta x_i}(\varphi_{c(i+1)} - \varphi_{c(i)})$

$$f_L = \hat{j}_c \times \hat{B}_0 \sim \frac{\sum_1^{n_f} J_f |s_f| \hat{n}}{\sum_1^{n_f} s_f} \times \hat{B}_0$$

The φ-formulation and the charge conservation issue

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- In conclusion, despite there are numerical schemes more advanced than others, there are mesh-size and mesh-quality limitations inherent to the φ-formulation staggered scheme
- The numerical stability criterion can be more strict than the spatial resolution required which is already quite demanding for high Hartmann numbers (E.g. [1] for uniform hexahedral ordinary staggered mesh)
- The numerical errors and instabilities sources are more frequent for meshes with high aspect ratio and/or high skewness. This are the kind of meshes required for fusion technology applications.
- The problem is much higher than standard hydrodynamics: highly scalable codes are needed in HPC clusters to solve real MHD problems in fusion applications

[1]L. Leboucher (1999). Monotone Scheme and Boundary Conditions for Finite Volume Simulation of Magnetohydrodynamic Internal Flows at High Hartmann Number. Journal of Computational Physics 150(1):181-198

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Commercial Platforms: Ansys-Fluent

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- ANSYS-Fluent is a commercial simulation platform based on the finite volume method
- It features a MHD module build using its customization capabilities

PROS	CONS
Versatility	Use protected by a license
Compatible with the rest of ANSYS tools: • ICEM for mesh generator • Ensight for post-process	The source code is not available to the user
Soft learning curve	The parallelization capabilities depends on the license
Includes many modules allowing multiphysics analyses • Multiphase flows • Turbulence (including LES) • Heat and mass transport • Buoyant flows	There is limited customization options in the MHD module
Implicit scheme for the transient solver	The MHD module employs the option 1 for the current reconstruction
The MHD module has been validated for moderate Hartmann numbers	The validation only applies to hexahedral meshes

Numerical experimentation with Ansys-Fluent

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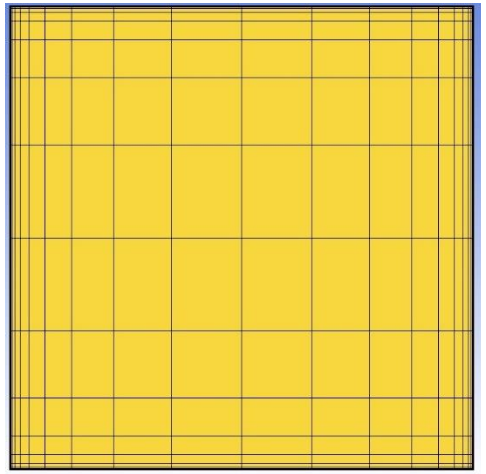
- Simple 3D problem of a square section channel with conducting walls

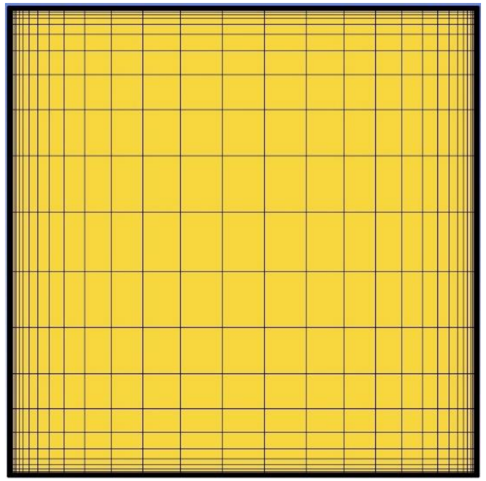
$$Ha = 10^3, \qquad N = 10^6 \ (Re = 1), \qquad C_w = 10^{-2}$$

- Different meshes have been employed with different time steps:

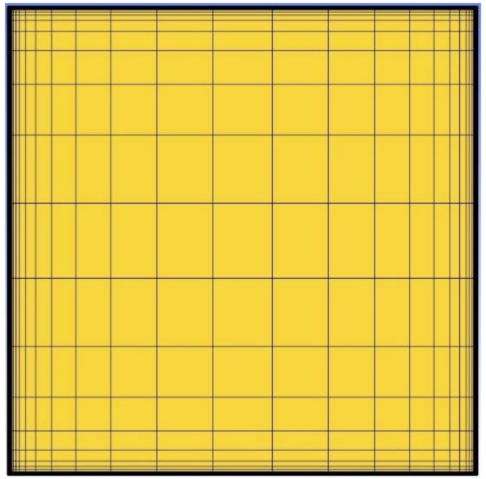
$$\frac{Dt}{\tau_u} = 10^{-2}, 5 \cdot 10^{-3}, 10^{-3}$$



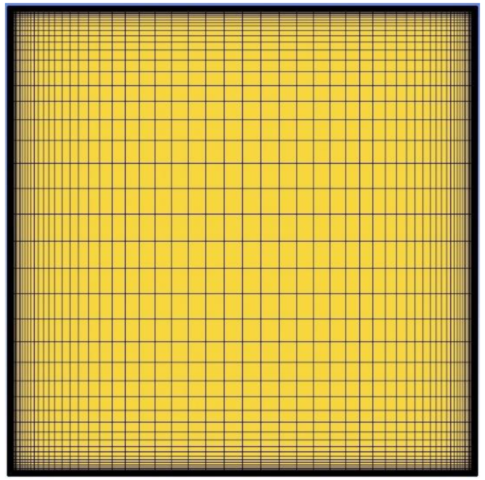
Coarse: 25x25x50



Medium: 38x38x75

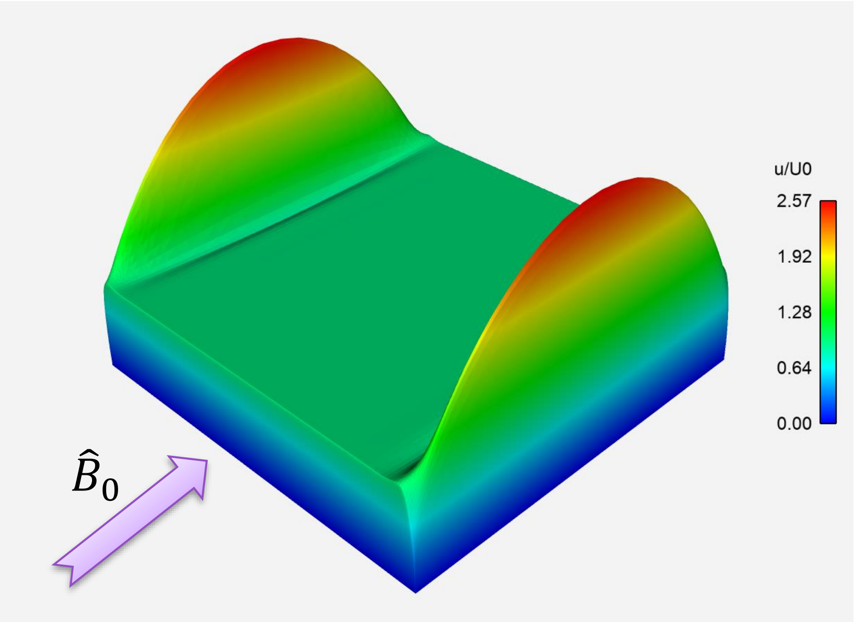


Medium_EB: 38x38x75



Fine: 75x75x100

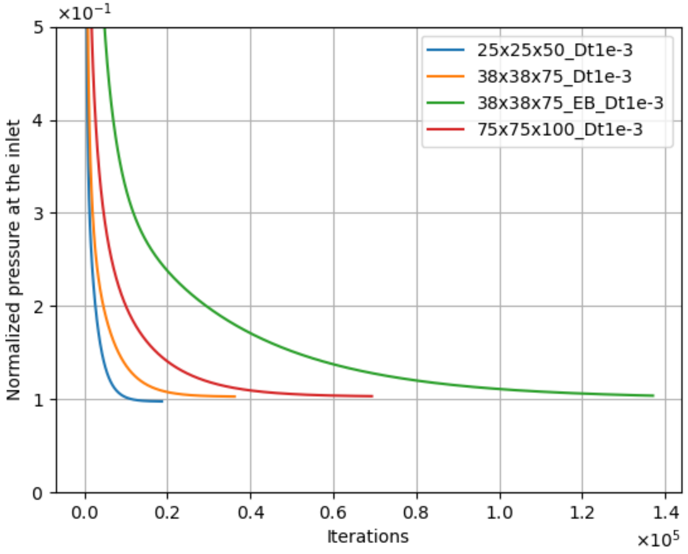
- The solution of this kind of flows is well known:
  - The flow becomes fully developed with very small developing lengths (suppression of inertia)
  - The induced currents are contained in the cross-sectional plane
  - The flow exhibits an M-shaped profile. The intensity of the jets depends on *Ha* and C_w
  - The dimension less pressure drop is linear and depends only on *Ha* and C_w

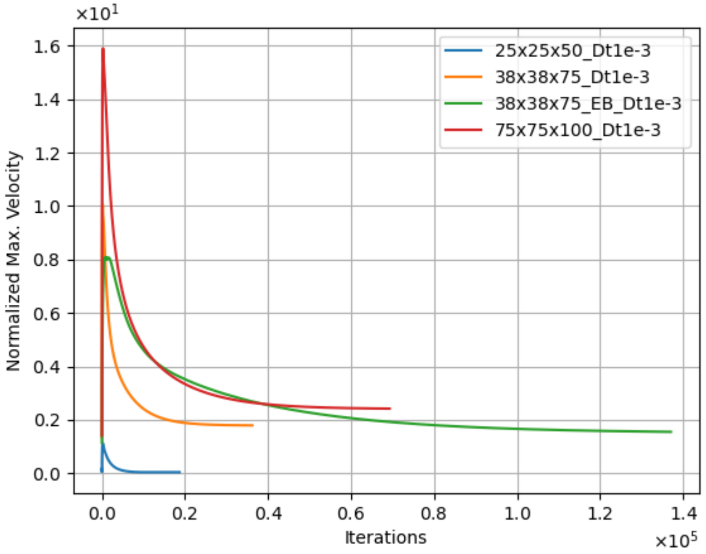


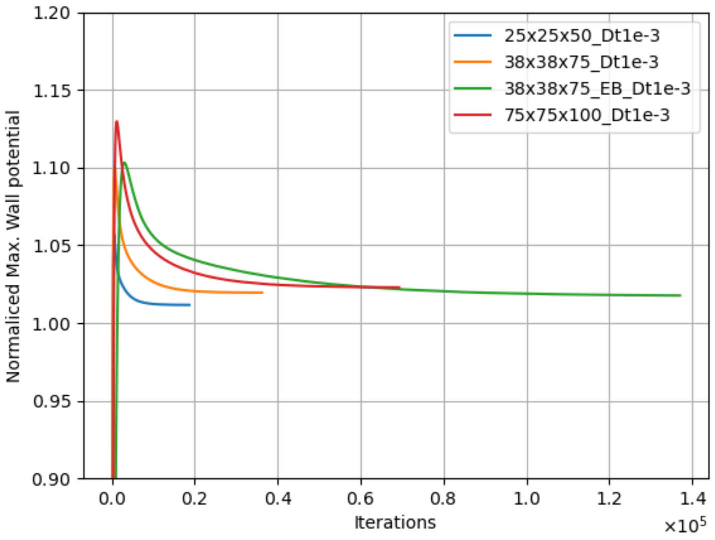
Velocity profile obtained with a fully developed (2D) model

Ansys-Fluent: convergence

- The convergence is slow and it requires several iterations to reach the solution
- Increasing the mesh size increases the necessary number of iterations
- A too aggressive bunching towards the walls slow down the simulations and do not increase the accuracy







Ansys-Fluent accuracy: Pressure gradient

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- Pressure drop is in well agreement with fully developed (2D) calculations for medium and fine meshes

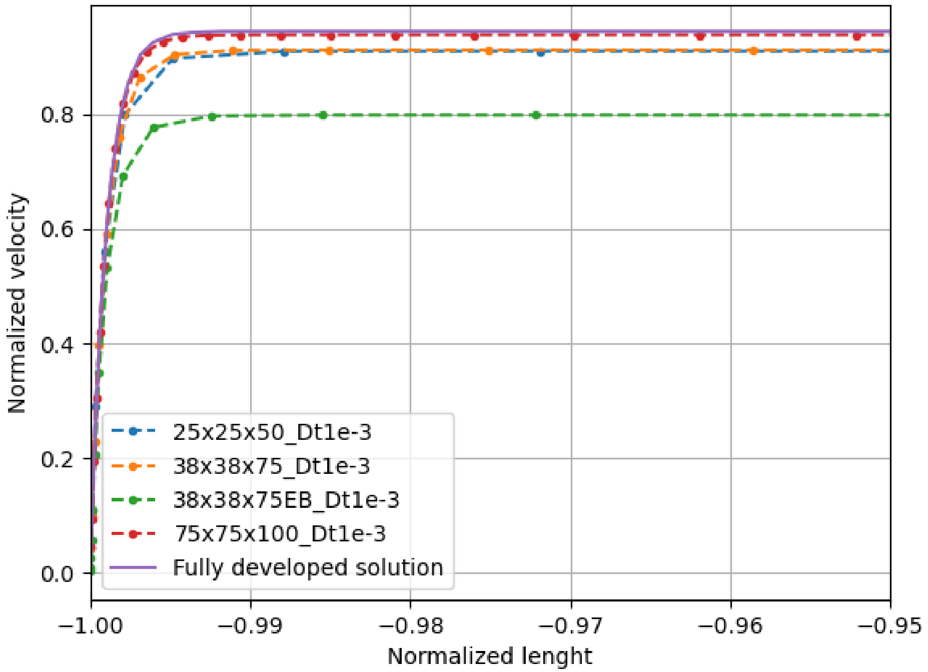
Normalized pressure drop and deviation with respect to the Fully Developed (FD) solution

Case id	Pressure gradient (kp)	Deviation from FD (%)
FD solution	1.024E-02	--
25x25x50_Dt1e-3	9.736E-03	4.90
38x38x75EB_Dt1e-3	1.133E-02	9.62
38x38x75_Dt1e-3	1.031E-02	0.71
75x75x100_Dt1e-3	1.034E-02	0.98

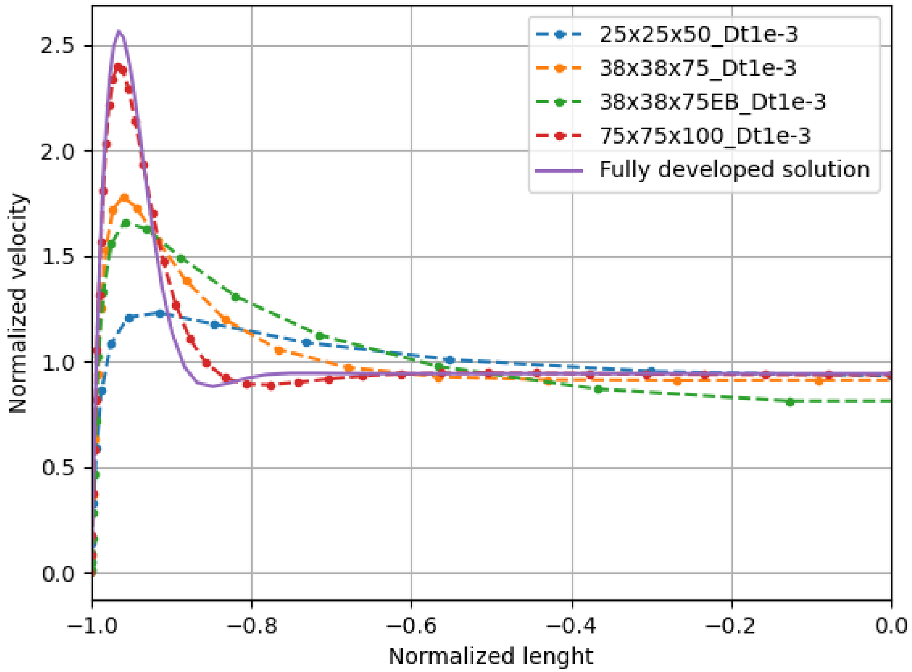
Ansys-Fluent accuracy: Velocity

- The boundary layers are not well reproduced by the medium and coarse meshes
- Specially critical is the situation in the Side BL:
  - Significant impact on heat and mass transfer through the channel walls
  - Moderate-weak impact on the pressure drop gradient

Hartmann Boundary Layer

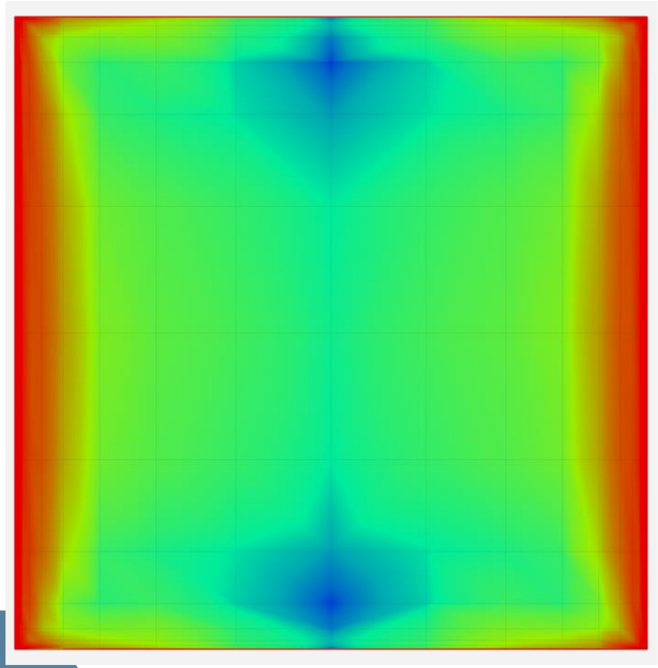


Side Boundary Layer



Ansys-Fluent accuracy: Electric charge

- The lack of accuracy next to the velocity has its origin in the charge conservation issue
- Charge is not preserved at discrete level and the deviation is maximal next to the boundary layer



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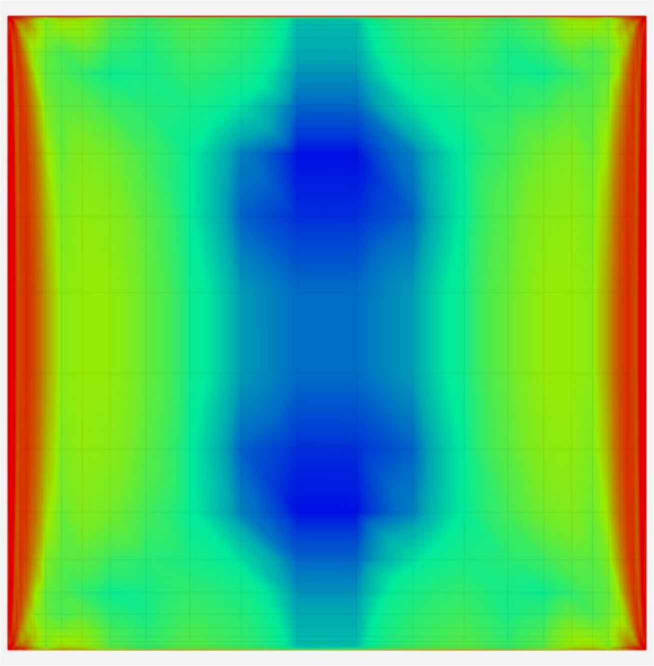

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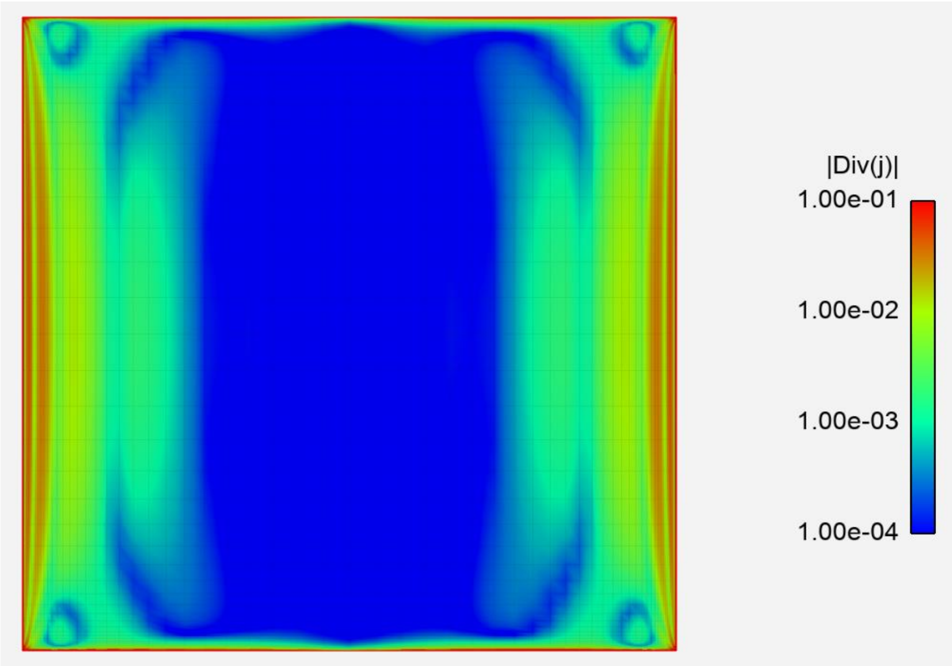
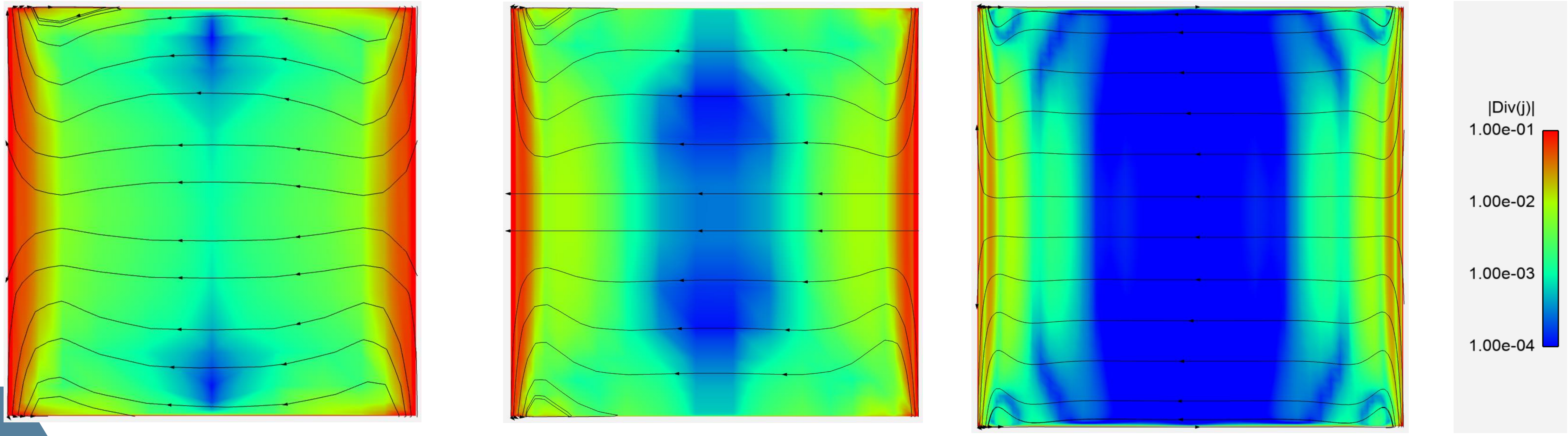


Fine: 75x75x100

Ansys-Fluent accuracy: Electric charge

- Charge is well conserved globally
- When charge is not conserved locally, the shape of the currents is significantly modified and the solution becomes unphysical



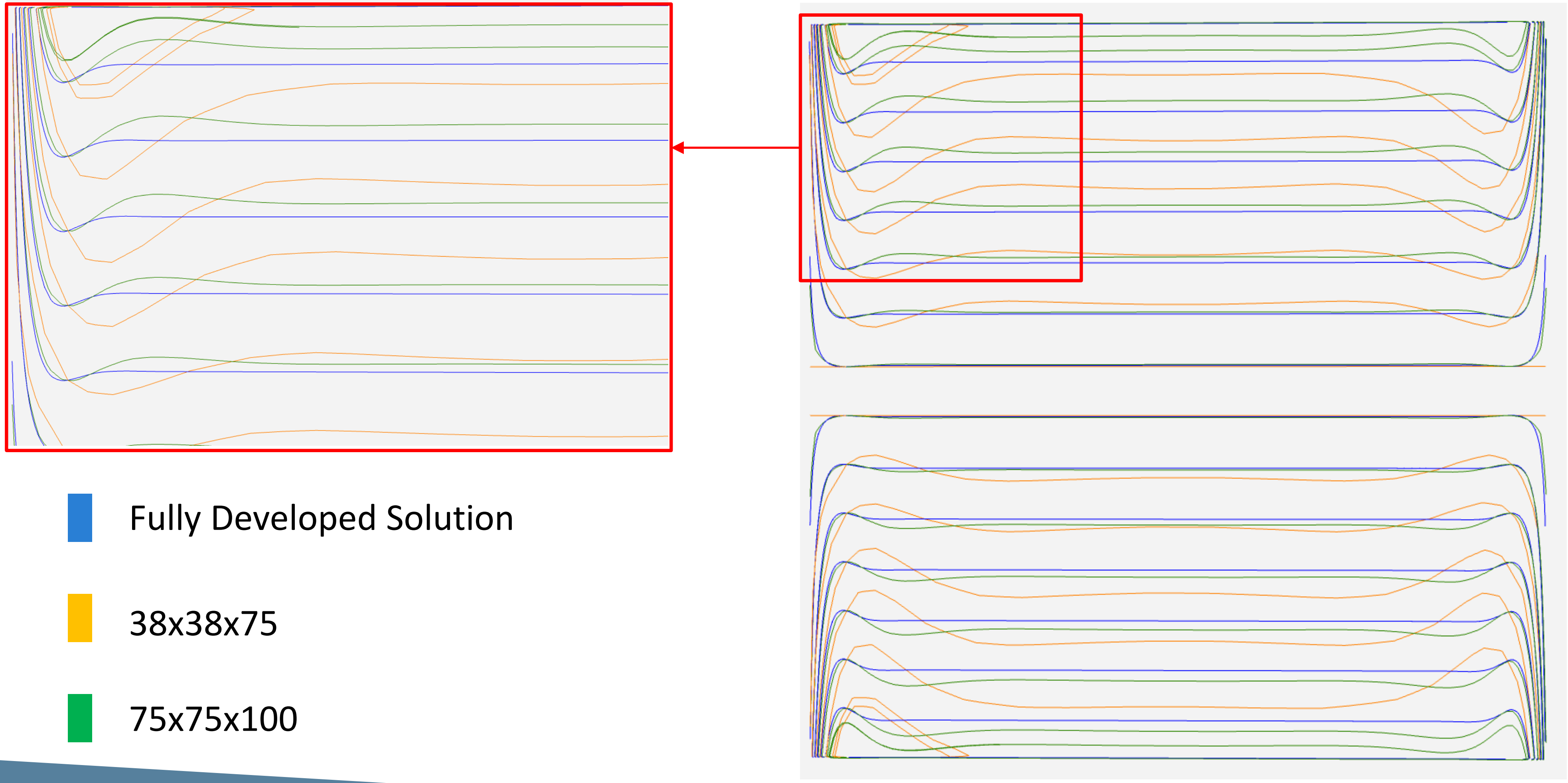
Coarse: 25x25x50

Medium: 38x38x75

Fine: 75x75x100

Ansys-Fluent accuracy: Electric charge

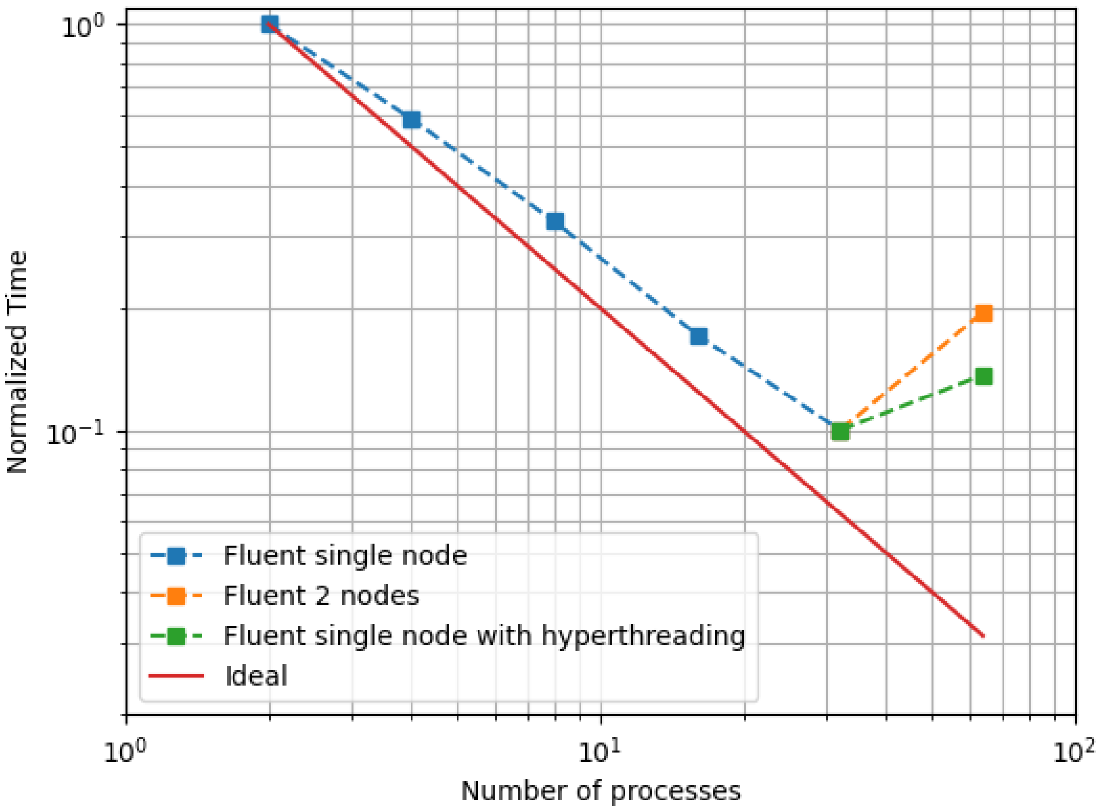
- The differences on the current curvature explain the different thickness of the side boundary layer



- Fully Developed Solution
- 38x38x75
- 75x75x100

Ansys-Fluent: Strong scaling

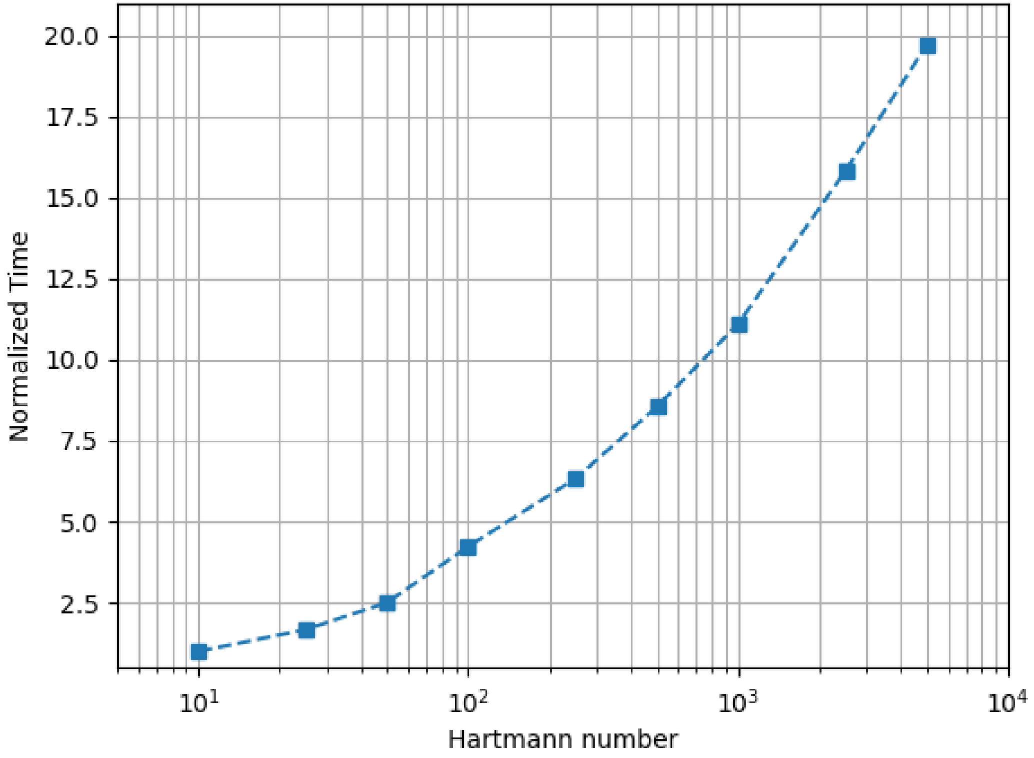
- A strong scaling exercise has been performed with a mesh of 75x75x50 and Ha = 1000



- Good scaling while working in a single node (up to 36 processors in this case)
- Poor performance when going to 2 nodes due to the time lost in the communications

Ansys Fluent: Hartmann Scaling

- Another scaling exercise has been performed varying the Hartmann number while fixing the mesh size (75x75x50) and the rest of the conditions (C_w = 0.01, Re=1)



The solving time <u>grows with $Ha^{0.3}$</u>

Both the time needed per iteration and the total number of iterations grows with Hartmann:

- Small increment in the time per iteration
- Significant increment in the total number of iterations to fulfil the same convergence criterion

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The j/φ-formulation and the monolithic approach

- The fundamental issue associated to the staggered approach of the φ-formulation will always be present
- As an alternative it is possible to solve the problem in the J/φ-formulation (8 equations) with a monolithic approach

$$\frac{1}{N}(\partial_t \hat{u} - (\hat{u} \cdot \nabla)\hat{u}) = \frac{1}{Ha^2}\nabla^2 \hat{u} - \nabla \hat{p} + \hat{j} \times \hat{B}_0$$ → Momentum continuity

$$\nabla \cdot \hat{u} = 0$$ → Mass conservation

$$\hat{j} = -\nabla \hat{\varphi} + \hat{u} \times \hat{B}_0$$ → Ohm's law

$$\nabla \cdot \hat{j} = 0$$ → Charge conservation

- By solving all the equations simultaneously, <u>charge conservation is guaranteed at discrete level</u>

GridapMHD

- In the framework of the EUROfusion Breeding Blanket Work Package, the CIMNE institute is developing GridapMHD (https://github.com/gridapapps/GridapMHD.jl).
- The opensource GridapMHD code is built using the tools provided in the Gridap[1] finite element library.
- The formulation is the one introduced by Li et al.[2] It is a divergence-conforming and inf-sup stable formulation:

$$V_u^h = \{\mathbf{v} \in H^1(\Omega)^d : \mathbf{v}|_K \in Q_2(K)^{\mathbf{d}}, \forall K \in \mathcal{T}_h\},$$
$$V_p^h = \{q \in L^2(\Omega) : q|_K \in P_1(K), \forall K \in \mathcal{T}_h\},$$

The velocity elements are one order higher than pressure to satisfy inf-sup condition

$$V_j^h = \{\mathbf{k} \in H(\mathrm{div};\Omega) : \mathbf{k}|_K \in RT_1, \forall K \in \mathcal{T}_h\},$$

→ Raviart-Thomas polynomial space of order 1

$$V_\varphi^h = \{\psi \in L^2(\Omega) : \psi|_K \in Q_1(K), \forall K \in \mathcal{T}_h\},$$

$$RT_k = Q_{(k+1,k,k)} \times Q_{(k,k+1,k)} \times Q_{(k,k,k+1)}$$

($\mathcal{T}_h$ is a hexa-mesh of the domain Ω)

(Valid for a hexa-mesh)

CIMNE EXCELENCIA SEVERO OCHOA

[1]F. Verdugo and S. Badia (2022). The software design of Gridap: A Finite Element package based on the Julia JIT compiler. Computer Physics Communications, 276:108341

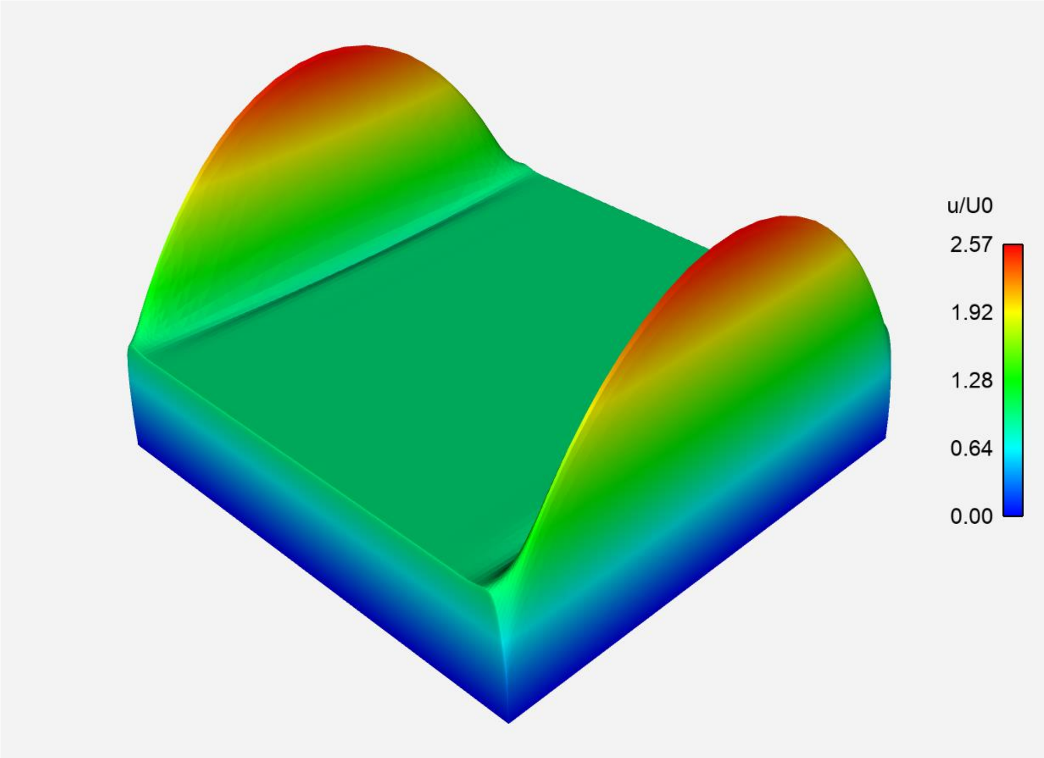
[2]Li et al., (2019). A Charge-Conservative Finite Element Method for Inductionless MHD Equations. Part I: Convergence. SIAM Journal on Scientific Computing 41(4), B796-B815

GridapMHD

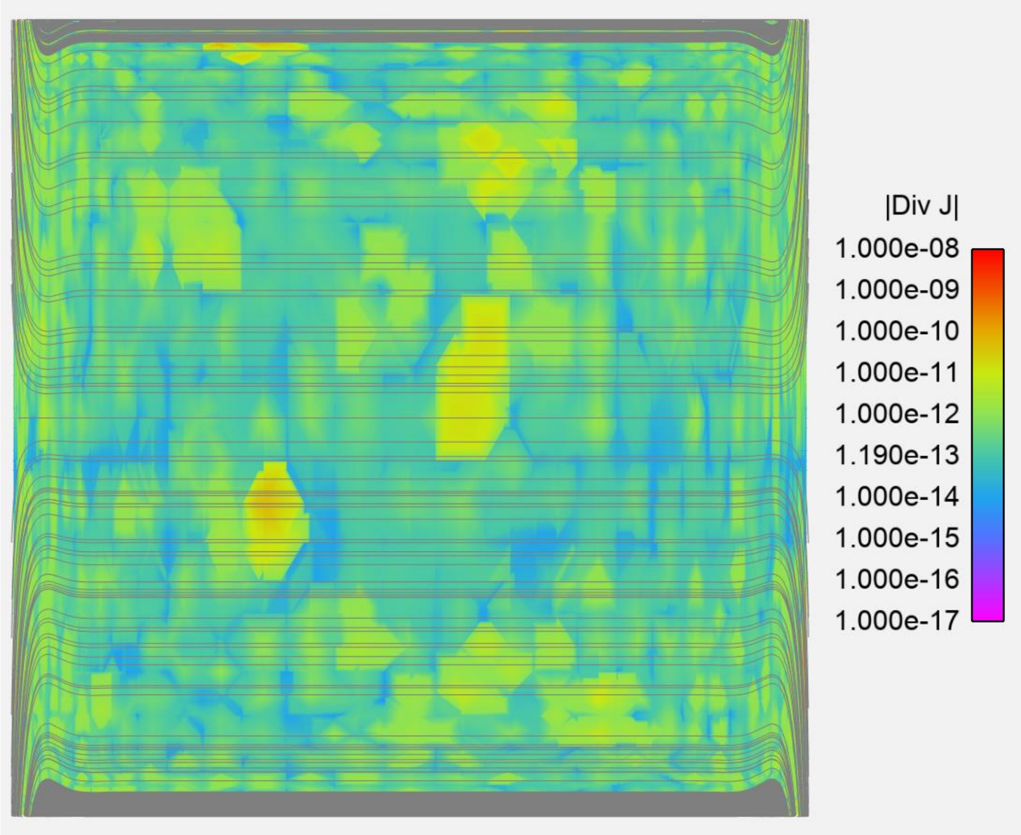
- GridapMHD is currently under development.
  - The code have been validated for 2D cases against the Hunt and Shercliff analytical solutions at high Hartmann number
  - We are in the process of validating the code in 3D geometries against experimental data in the literature.

- In its current state, the code is prepared to solve with a monolithic approach steady-state MHD problems using iterative procedure (Newton-Raphson) for the non-linear problem and a direct solver for the linear problem in each iteration.
- The solver for the linear problem is taken from the external PETSc library: MUMPS
  - This direct solver provides robustness but it is not very efficient

- The divergence-conforming formulation together with the monolithic approach ensures charge conservation at discrete level.



Fully developed flow computed with GridapMHD

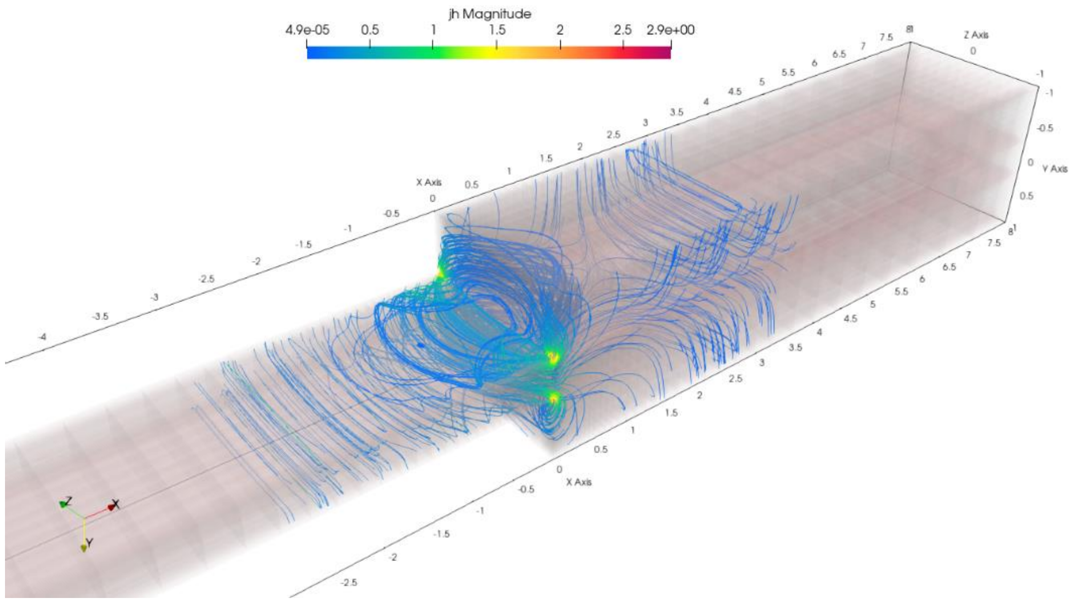


Cross-sectional electric currents computed with GridapMHD

GridapMHD

- The price to be paid is an enormous amount of degrees of freedom witch means the direct solver very costly in terms of memory
- Ej. 3D flow: Abrupt expansion in the direction of the magnetic field (Ha = 100)

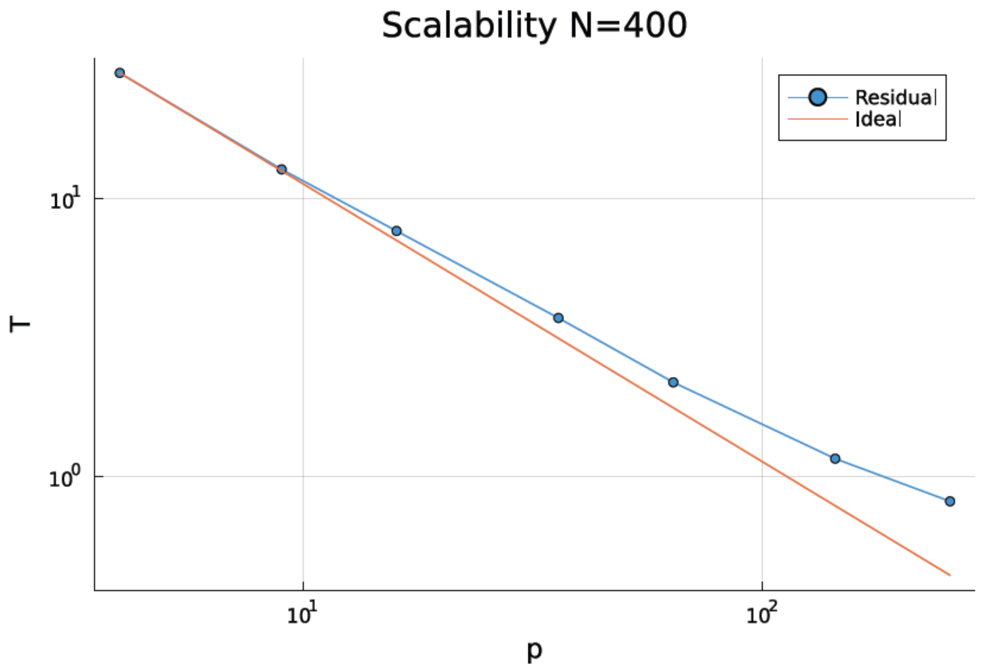
- Relatively small mesh required: **56 160** hexa-cells
  - DOF for velocity: 1 295 892
  - DOF for pressure: 224 640
  - DOF for electric current: 1 363 872
  - DOF for electric potential: 449 280
  - Total DOF of the problem: **3 333 684**

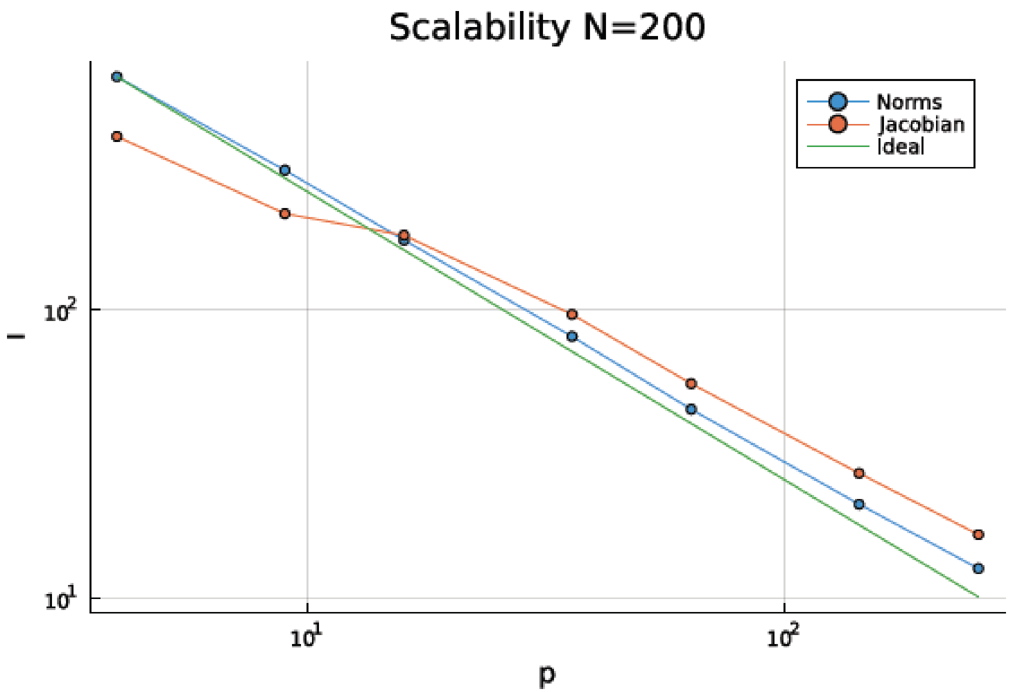


Electric currents near the expansion computed with GridapMHD

GridapMHD: Strong scaling

- The strong scalability of GridapMHD has been tested by simulating a well known 2D flow (Hunt flow) with a uniform mesh
- The test shows a good scalability in the computation of the residual, the norms and the jacobian

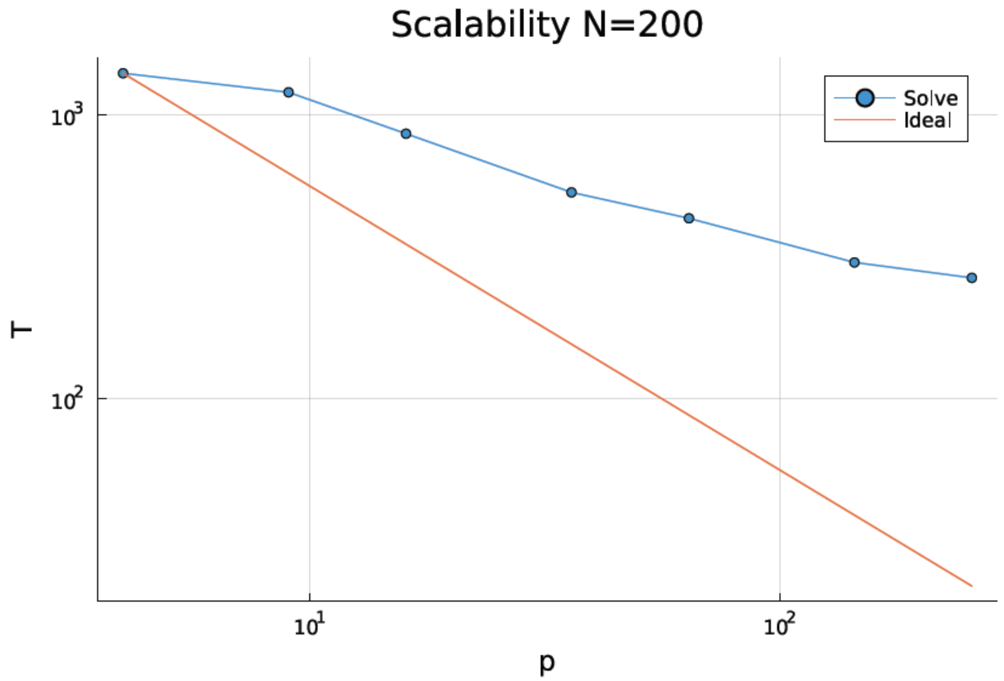




Strong scalability test. T is the wall clock time measured in seconds and p is the number of processors

GridapMHD: Strong scaling

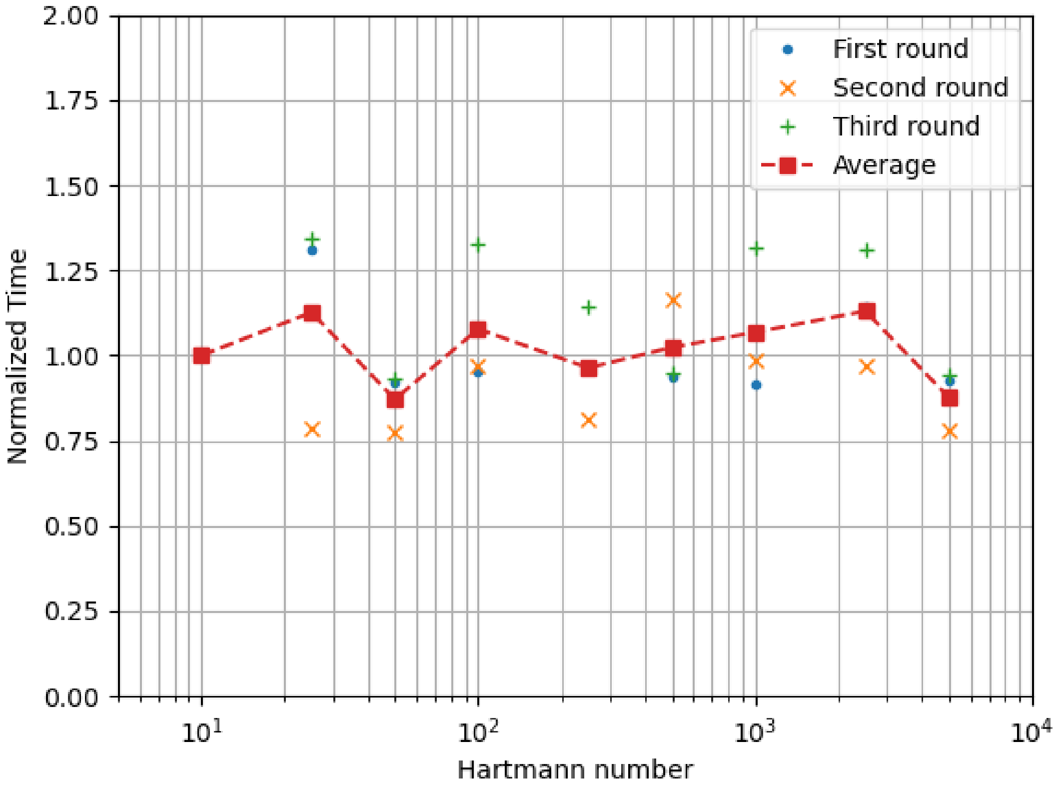
- The strong scalability of GridapMHD has been tested by simulating a well known 2D flow (Hunt flow) with a uniform mesh
- The MUMPS solver present a poor scalability even with few processors
- New solvers are being developed based on iterative methods with block preconditioners



Strong scalability test. T is the wall clock time measured in seconds and p is the number of processors

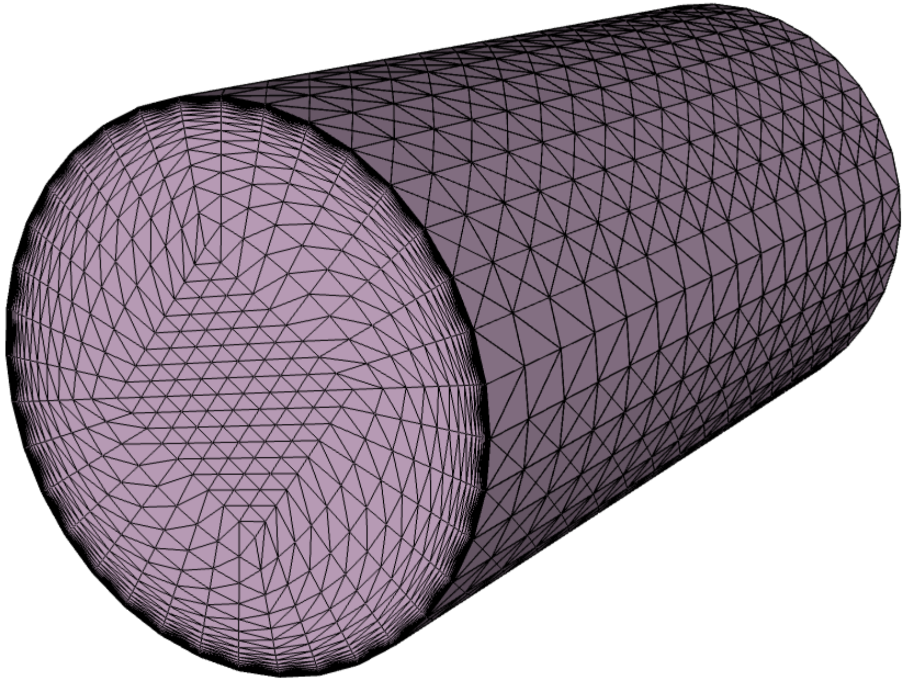
GridapMHD: Hartmann scaling

- Similar scaling exercise than the one performed with Fluent (Ha = 1000, Re =1, $C_w = 10^{-2}$)
- The monolithic approach has an extra advantage. For a given mesh size, the solving time is Hartmann independent

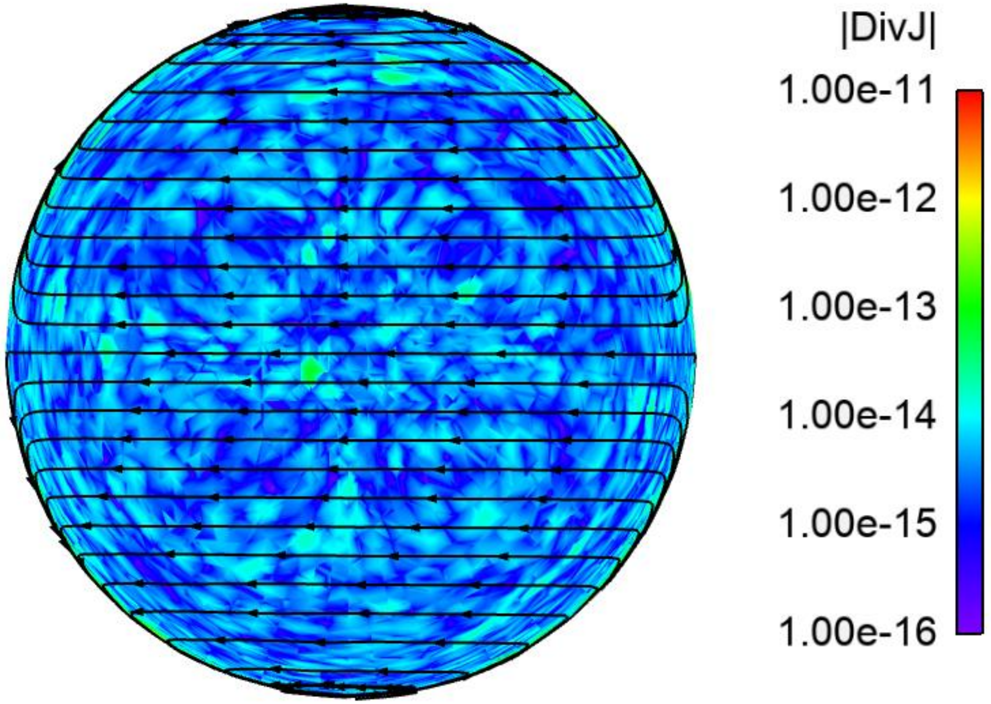


Performance with tetrahedral meshes

- The monolithic scheme allows using meshes of simplexes without important requirements to the skewness or high aspect ratio
- Insulated pipe with *Ha*=500 and *Re*=1



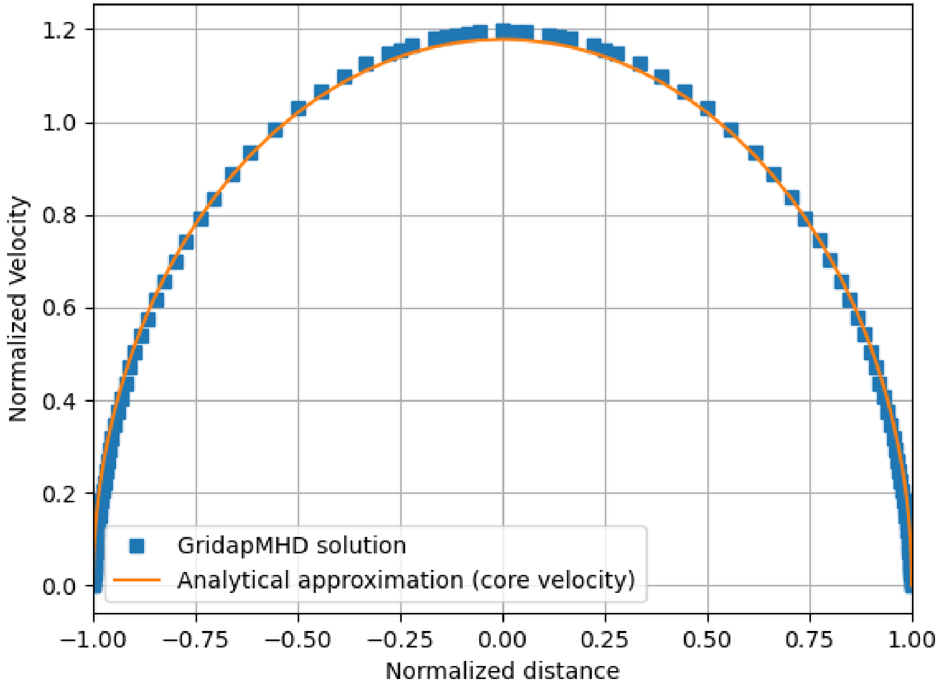
Tetrahedral mesh



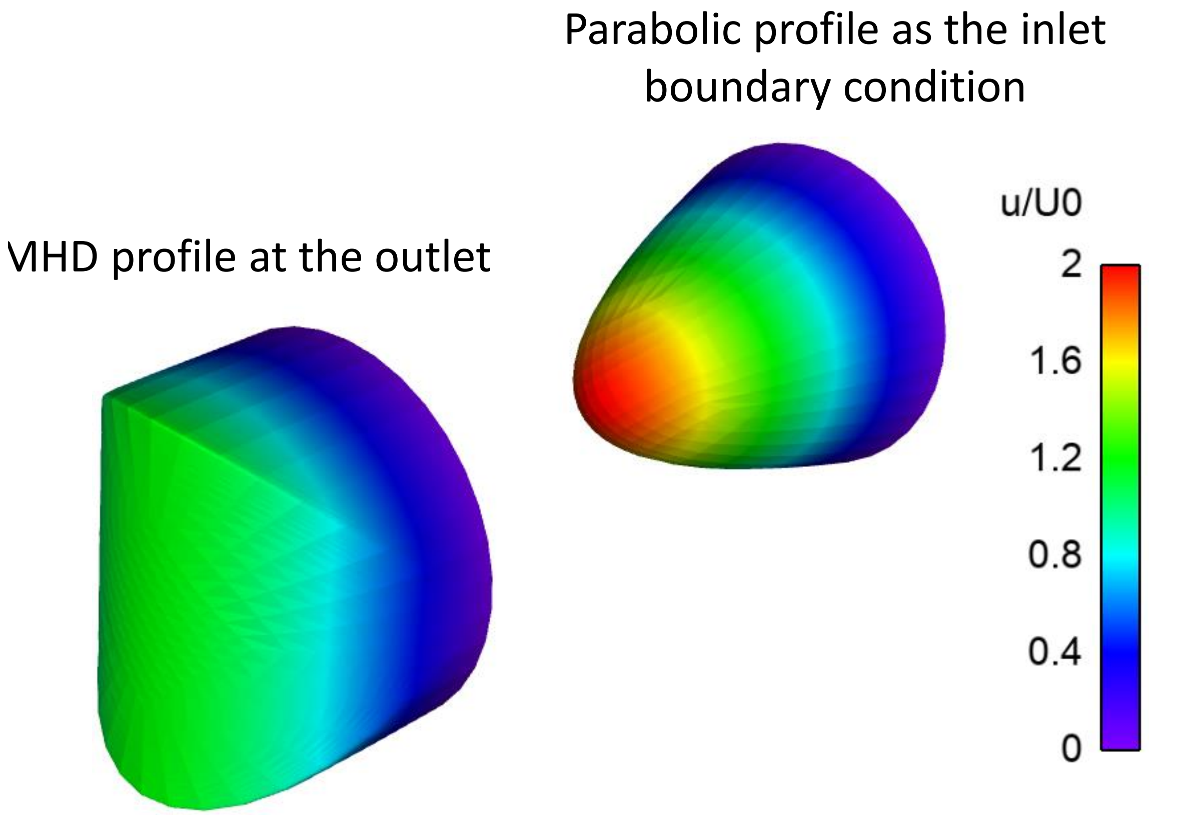
Divergence and stream lines of the electric currents

Performance with tetrahedral meshes

- The monolithic scheme allows using meshes of simplexes without important requirements to the skewness or high aspect ratio



MHD velocity profile across a line perpendicular to the B-field



Velocity profile at the inlet and outlet of an insulated pipe with Ha=500

Conclusions

- The simulation of MHD flows relevant for fusion technologies applications is still a big computational challenge
- Charge conservation imposes strong limitations on the mesh size and quality (skewness and aspect ratio). They can be higher than the required spatial resolution
- The accuracy and scalability of two different codes has been tested in this work under control conditions:
  - ANSYS-Fluent
  - GridapMHD

Conclusions

	ANSYS-Fluent	GridapMHD
Numerical method	Finite Volume Method	Finite Element Method
MHD formulation	φ-formulation	J/φ-formulation
Solving scheme	Pseudo-transient staggered scheme with reconstruction of the current at the cell center	Monolithic steady state.
Transient scheme	Implicit	Under development
Charge conservation	Mesh dependent	Guaranteed at discrete level
Strong scaling	Good in a single node. Poor otherwise	Poor because of the direct solver
Hartmann scaling	Solving time grows with $Ha^{0.3}$	Hartman independent
Unstructured meshes	Possible but difficult to preserve accuracy	Possible
Memory consumption	Not a problem	Very high due to high nº dofs

Accuracy and scalability of incompressible inductionless MHD codes applied to fusion technologies

Fernando.roca@ciemat.es

www.ciemat.es

The need of HPC for simulating MHD flows in fusion conditions

Laboratorio Nacional de Fusión Ciemat

Simulation of an MHD flow in a fusion breeding blanket

- Large mesh sizes (millions of cells for 3D geometries using FVM)
- Transient simulations with small time steps

The time scale is given by the magnetic damping time

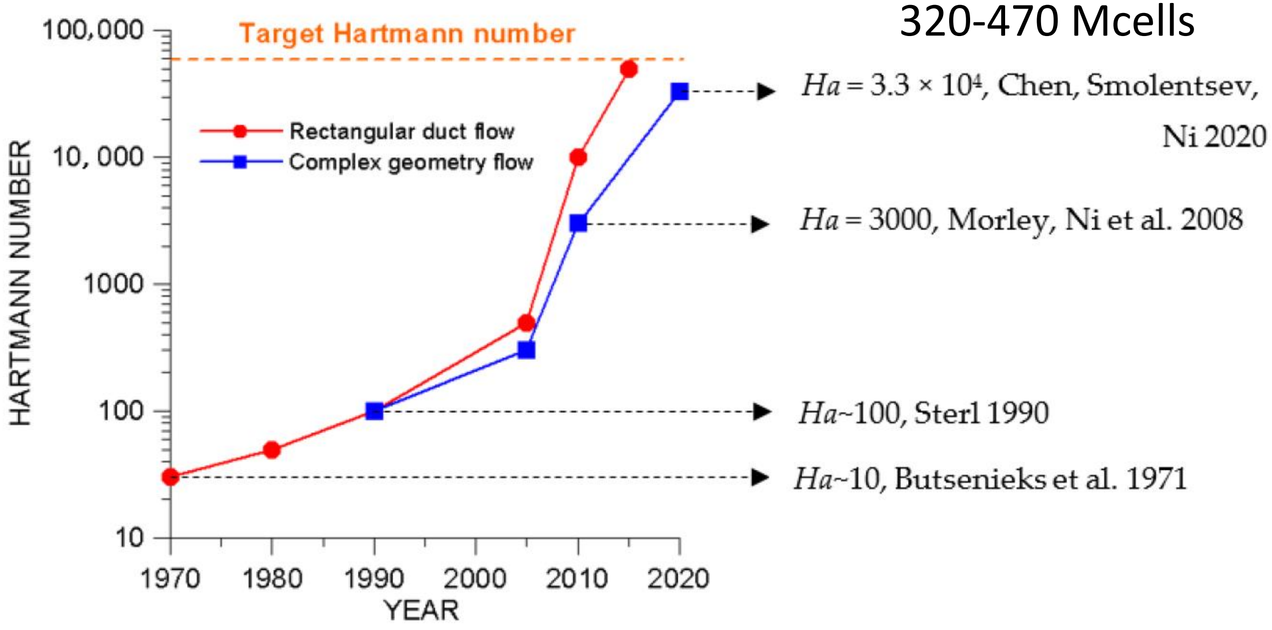
$$\tau_B = \frac{\rho}{\sigma B_0^2} \sim 10^{-4} - 10^{-5}$$

Stability condition in terms of the magnetic Courant number

$$C_{rm} \coloneqq \frac{\sigma B_0^2}{\rho} \Delta t = N C_r < 0.2$$

- Highly scalable codes are needed in HPC clusters to solve real MHD problems in fusion applications

320-470 Mcells



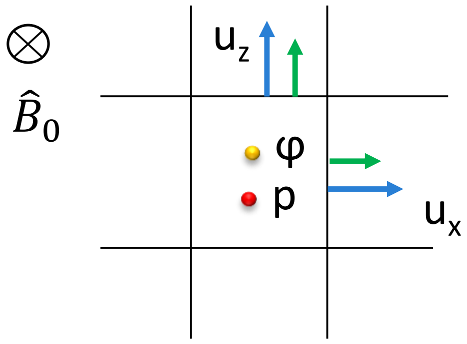
S. Smolentsev 2021 Fluids, 6(3), 110

- Option 2 is the preferred one for most of specialized MHD codes

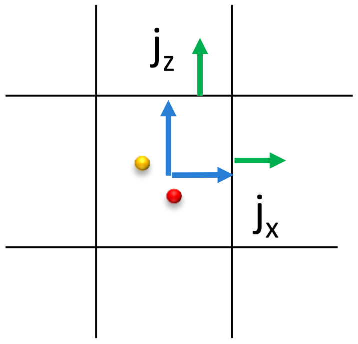
$$f_L = \hat{j}_c \times \hat{B}_0 = -(\nabla\varphi)_c \times \hat{B}_0 + (\hat{u}_c \times \hat{B}_0) \times \hat{B}_0$$

$$\nabla\varphi \times \hat{B}_0 = B_0 \begin{pmatrix} -\partial_z\varphi \\ 0 \\ \partial_x\varphi \end{pmatrix} \qquad (\hat{u} \times \hat{B}_0) = B_0 \begin{pmatrix} -u_z \\ 0 \\ u_x \end{pmatrix}$$

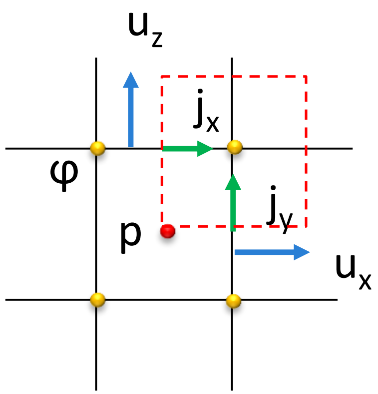
- This option can lead to instabilities in an ordinary staggered mesh due to the presence of fluxes which are parallel to the control volume



Sketch of a 2D staggered mesh



Sketch of a 2D collocated mesh[1]



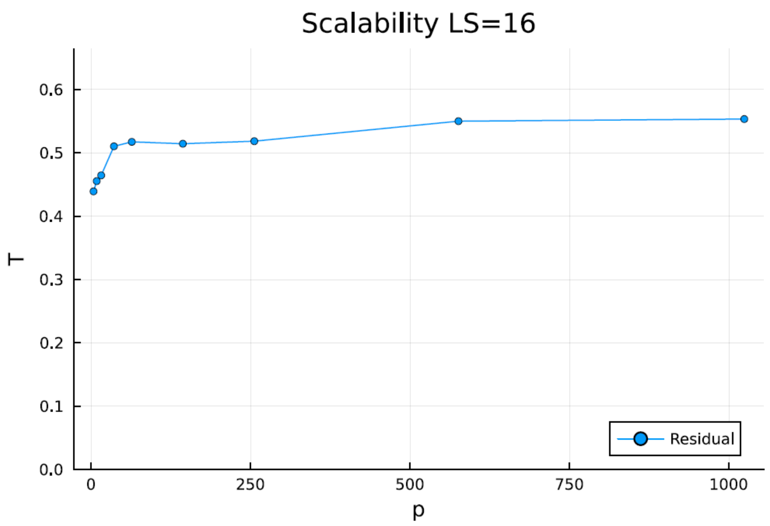
Sketch of a 2D fully staggered mesh[2]

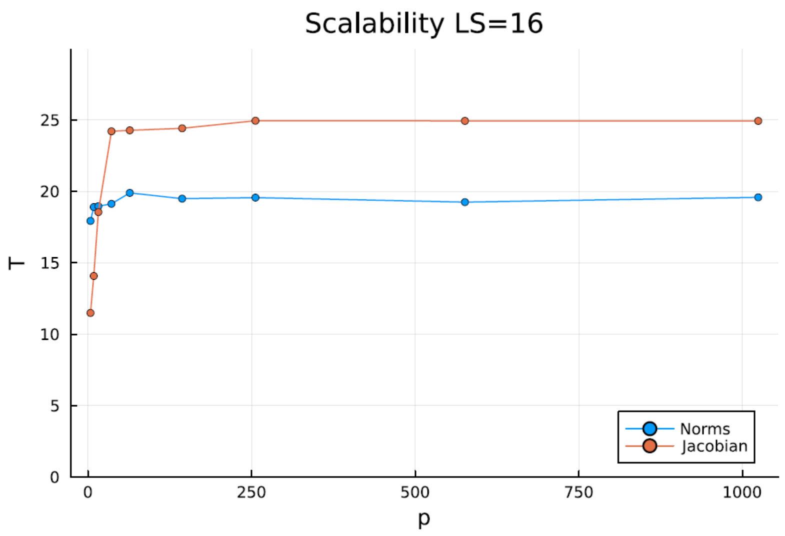
[1]M.J. Ni et al (2007). A current density conservative scheme for incompressible MHD flows at a low magnetic Reynolds number. Part II: On an arbitrary collocated mesh. Journal of Computational Physics 227(1):205-228

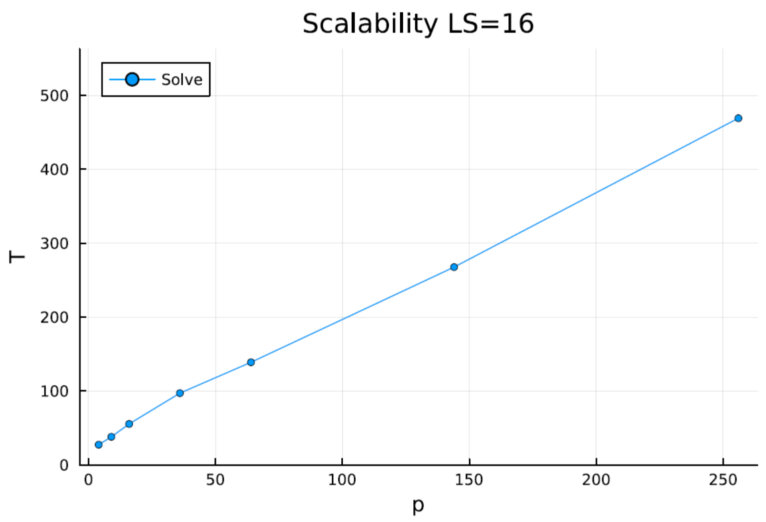
[2]L. Leboucher (1999). Monotone Scheme and Boundary Conditions for Finite Volume Simulation of Magnetohydrodynamic Internal Flows at High Hartmann Number. Journal of Computational Physics 150(1):181-198

GridapMHD: weak scaling

- A weak scaling test has been also performed starting with a local problem size of 16x16x3
- The same behavior is observed than in the strong scalability test:







Weak scalability test. T is the wall clock time measured in seconds and p is the number of processors