Simulation and validation of MHD benchmark problems using ALMA

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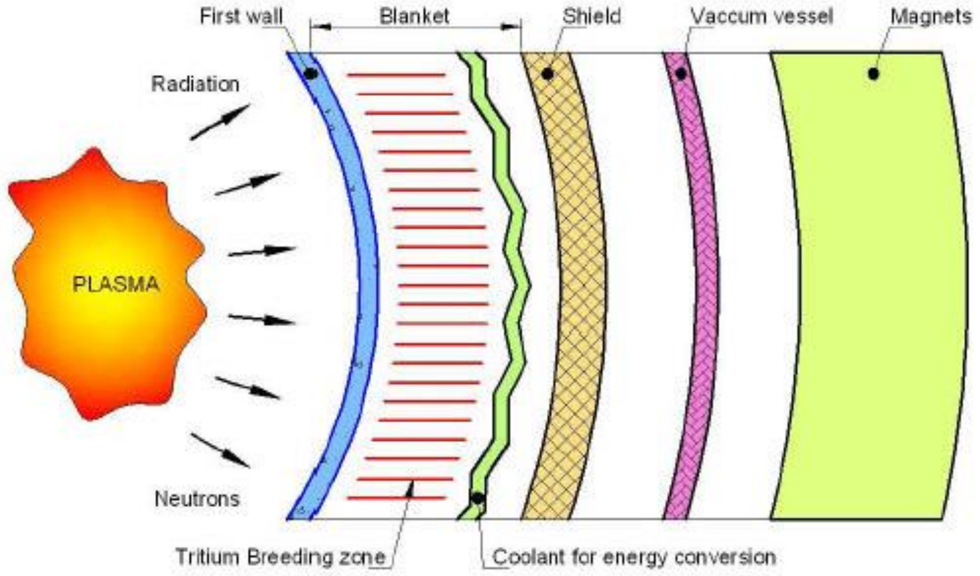
Need for simulation of liquid metal (e.g. PbLi) flows in fusion reactors

Design of liquid metal blankets

- **Blankets and integrated first wall is an important component separating the vacuum vessel and plasma.**
- **Blankets perform 3 main functions**
  - Protect the magnets and the vacuum vessel from neutron radiation
  - Produce tritium necessary for continued fusion reaction
  - Convert neutron energy to heat and transport it away from the vessel
- **Design of fusion blankets is a challenge**



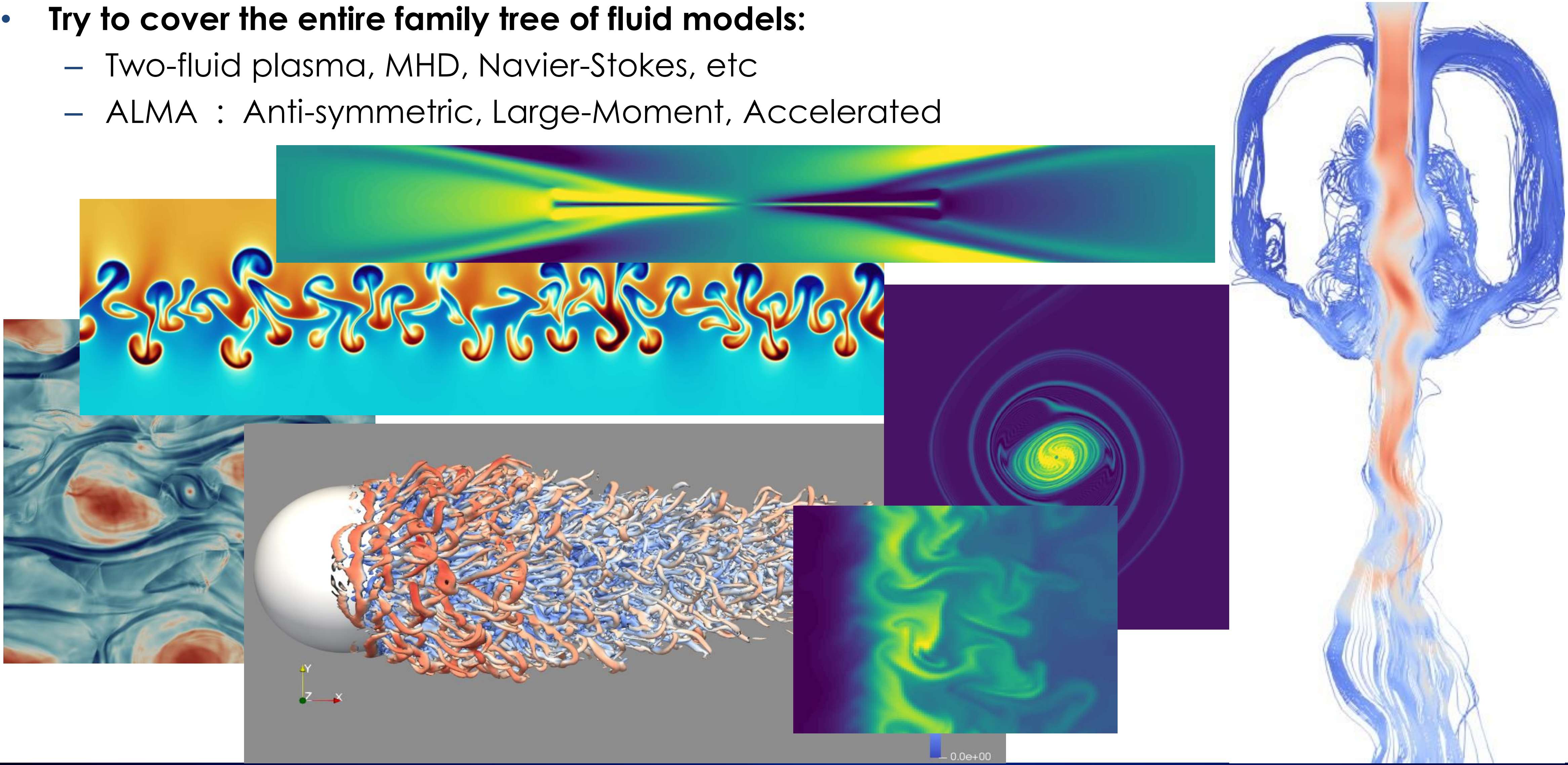
Reference: Suri et al., Materials issues in fusion reactors, J. Physics Conf. series, 2010

Computational tools for simulation and analysis of blankets

- **Commercial tools**
  - COMSOL – Multiphysics finite-element solver
  - ANSYS FLUENT
  - ANSYS CFX
  - OpenFOAM – open-source
- **Application specific**
  - HIMAG (HyPerComp Incompressible MHD solver for Arbitrary Geometry)
- **Research codes**
  - UCLA codes, DNS codes of Satake etc.

ALMA: New exascale solver for arbitrary fluid systems

- **Try to cover the entire family tree of fluid models:**
  - Two-fluid plasma, MHD, Navier-Stokes, etc
  - ALMA : Anti-symmetric, Large-Moment, Accelerated



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Formulation of the anti-symmetric equations

$$\nabla.(\psi\phi\boldsymbol{v}) = \frac{1}{2}\psi(\nabla.\boldsymbol{v} + \boldsymbol{v}.\nabla)\phi + \frac{1}{2}\phi(\nabla.\boldsymbol{v} + \boldsymbol{v}.\nabla)\psi \qquad \text{----(1)}$$

$$\nabla.\left(\psi^2\boldsymbol{v}\boldsymbol{w}\right) = \frac{1}{2}\psi(\nabla.\boldsymbol{v} + \boldsymbol{v}.\nabla)\psi\boldsymbol{w} + \frac{1}{2}\psi\boldsymbol{w}(\nabla.\boldsymbol{v} + \boldsymbol{v}.\nabla)\psi \qquad \text{----(2)}$$

Density equation formulation:

$$\nabla.(\rho\boldsymbol{v}) = \sqrt{\rho}(\nabla.\boldsymbol{v} + \boldsymbol{v}.\nabla)\sqrt{\rho}$$

$$\nabla.(\rho\boldsymbol{v}\boldsymbol{v}) = \frac{1}{2}\sqrt{\rho}(\nabla.\boldsymbol{v} + \boldsymbol{v}.\nabla)\sqrt{\rho}v + \frac{1}{2}\sqrt{\rho}\boldsymbol{v}(\nabla.\mathbf{v} + \mathbf{v}.\nabla)\sqrt{\rho}$$

$$\frac{\partial}{\partial t}(\rho\boldsymbol{v}) = \sqrt{\rho}\frac{\partial}{\partial t}(\sqrt{\rho}\boldsymbol{v}) + \sqrt{\rho}\,\boldsymbol{v}\frac{\partial}{\partial t}(\sqrt{\rho})$$

Halpern et al.(2021), Simulation of plasmas and fluids using anti-symmetric models, J. Comp. Phys., 2021

ALMA Solves the antisymmetric MHD Equations

- **Antisymmetric formulation of visco-resistive MHD equations**
  - Exposes, and tames the dynamic non-linearity by preserving square norms

Mass: $$\left[\frac{\partial}{\partial t} + (\nabla \cdot \mathbf{v} + \mathbf{v} \cdot \nabla)\right] \sqrt{\rho} = 0$$

$$J = \mu_0^{-1}(\nabla \times \boldsymbol{B})$$

Momentum: $$\left[\frac{\partial}{\partial t} + (\nabla \cdot \mathbf{v} + \mathbf{v} \cdot \nabla)\right] \sqrt{\rho}\mathbf{v}. = \boldsymbol{J} \times \frac{\boldsymbol{B}}{\sqrt{\rho}} + \left[-2\sqrt{p}\nabla\sqrt{p} + \nabla \cdot \boldsymbol{\Pi}\right]/\sqrt{\rho}$$

Pressure: $$\left[\frac{\partial}{\partial t} + \frac{5}{6}(\nabla \cdot \mathbf{v} + \mathbf{v} \cdot \nabla)\right] \sqrt{3p} = \frac{2}{3}\left(\frac{\nabla\sqrt{3p}}{\sqrt{\rho}}\right)\sqrt{\rho}\boldsymbol{v} + \left[-\nabla \cdot \boldsymbol{q} - (\nabla \cdot (\boldsymbol{\Pi} \cdot \mathbf{v}) - \mathbf{v} \cdot (\nabla \cdot \boldsymbol{\Pi})) + \eta J^2\right]\Big/\sqrt{3p}$$

Magnetic Field: $$\left[\frac{\partial \mathbf{B}}{\partial t} + \nabla \times (\boldsymbol{B} \times \boldsymbol{v}) + \frac{\eta}{\mu_0}(\nabla \times (\nabla \times \boldsymbol{B}))\right] = 0$$

- **ALMA (Antisymmetric Large-Moment Accelerated) in-house code**
  - Solves hyperbolic transport equations on heterogeneous HPC systems
  - Originally designed to tackle complex plasma physics problems
  - Central finite-difference schemes retain the conservation properties of the continuous equations ([2]Halpern et al., 2021)

[2]Halpern et al.(2021), Simulation of plasmas and fluids using anti-symmetric models, J. Comp. Phys., 2021

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ALMA's new anti-symmetry approach results in powerful numerical integration algorithm for arbitrary hyperbolic systems

- **MHD equations using anti-symmetry formulation**

$$\begin{Bmatrix} \frac{1}{2}(\nabla\cdot v + v\cdot\nabla) & 0 & 0 & 0 \\ 0 & \frac{1}{2}(\nabla\cdot v + v\cdot\nabla) & \frac{2}{3}\frac{\left(\nabla\sqrt{3p}\right)}{\sqrt{\rho}} & \frac{B}{\sqrt{\rho}}\times\nabla\times \\ 0 & -\frac{2}{3}\frac{\left(\nabla\sqrt{3p}\right)}{\sqrt{\rho}} & \frac{5}{6}(\nabla\cdot v + v\cdot\nabla) & 0 \\ 0 & \nabla\times\frac{B}{\sqrt{\rho}}\times & 0 & 0 \end{Bmatrix} \begin{Bmatrix} \sqrt{\rho} \\ \sqrt{\rho}v \\ \sqrt{3p} \\ B \end{Bmatrix}$$

$$F = -F^T$$

- **If anti-symmetry of force operator is retained in discrete space**

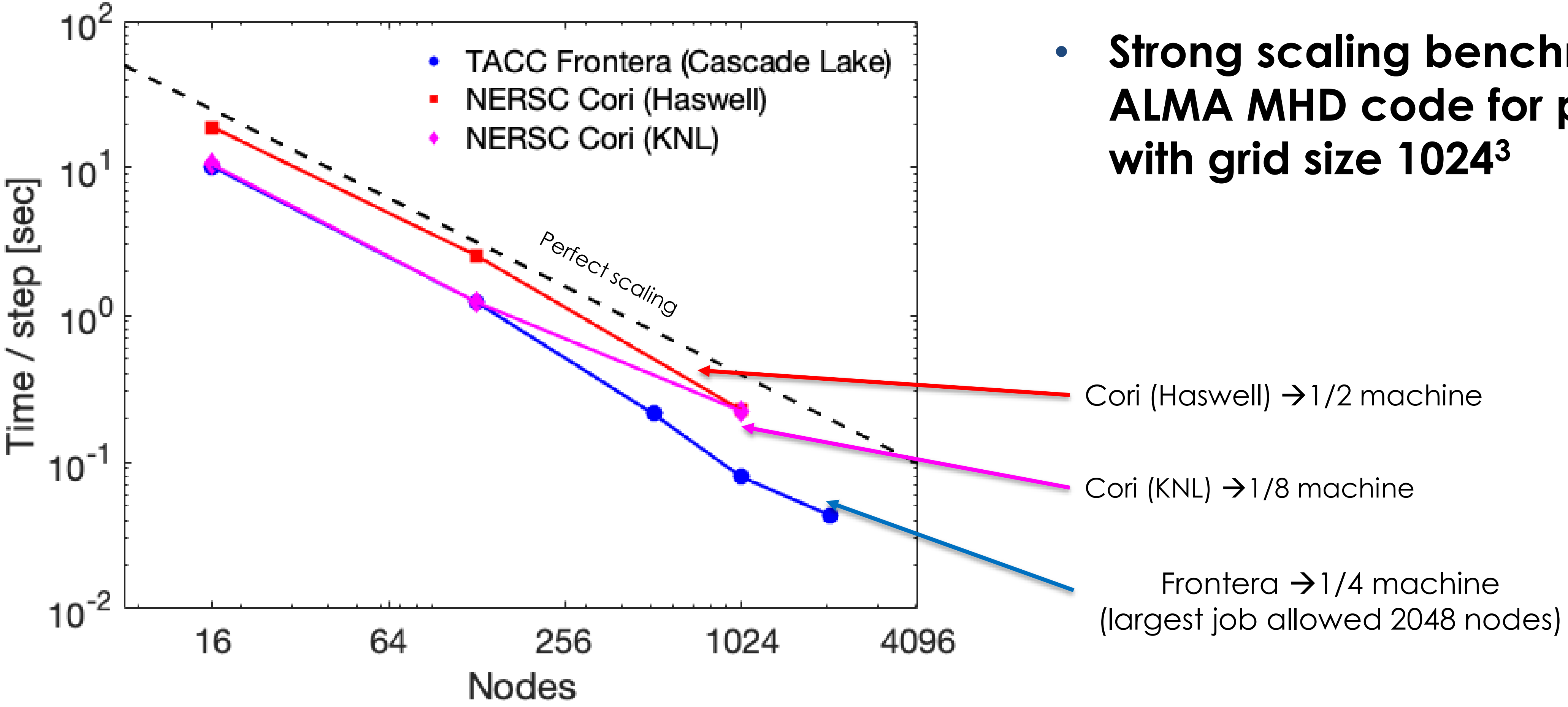
$$< \boldsymbol{\phi}|\boldsymbol{F}|\boldsymbol{\psi} > = -< \boldsymbol{\psi}|\boldsymbol{F}|\boldsymbol{\phi} >$$

  - **Conservation to numerical precision using FD methods**
  - **Multi-app structure (with native fluid-dynamics capabilities).**
  - **Modularity and scalability on heterogenous systems**

ALMA: Anti-symmetric, Large-Moment, Accelerated

- **OO Fortran2008, MPI, OpenMP (CPU), OpenACC (GPU)**
  - NVLink, async. comm., buffered, nearest neighbor communication only
  - Only dependencies: BLAS, HDF5 (output), viewable with ParaView
- **Finite difference vector calculus operators on simply connected grid**
  - 2nd, 4th, and 6th order implemented ... arbitrary order via templating
- **Explicit/Implicit RK methods for time integration**
  - add arbitrary order via Butcher tableau interface
- **Sparse 2D/3D elliptic solver based on geometric multigrid**
  - Optional 3rd party interface, e.g. Hypre
- **Compressible Navier-Stokes implementation**
  - Mach > 0.2 ; $R_e >> 1$
- **Internal boundaries conditions & obstructions via .stl file input**
  - No new meshing! automatic immersed boundary method

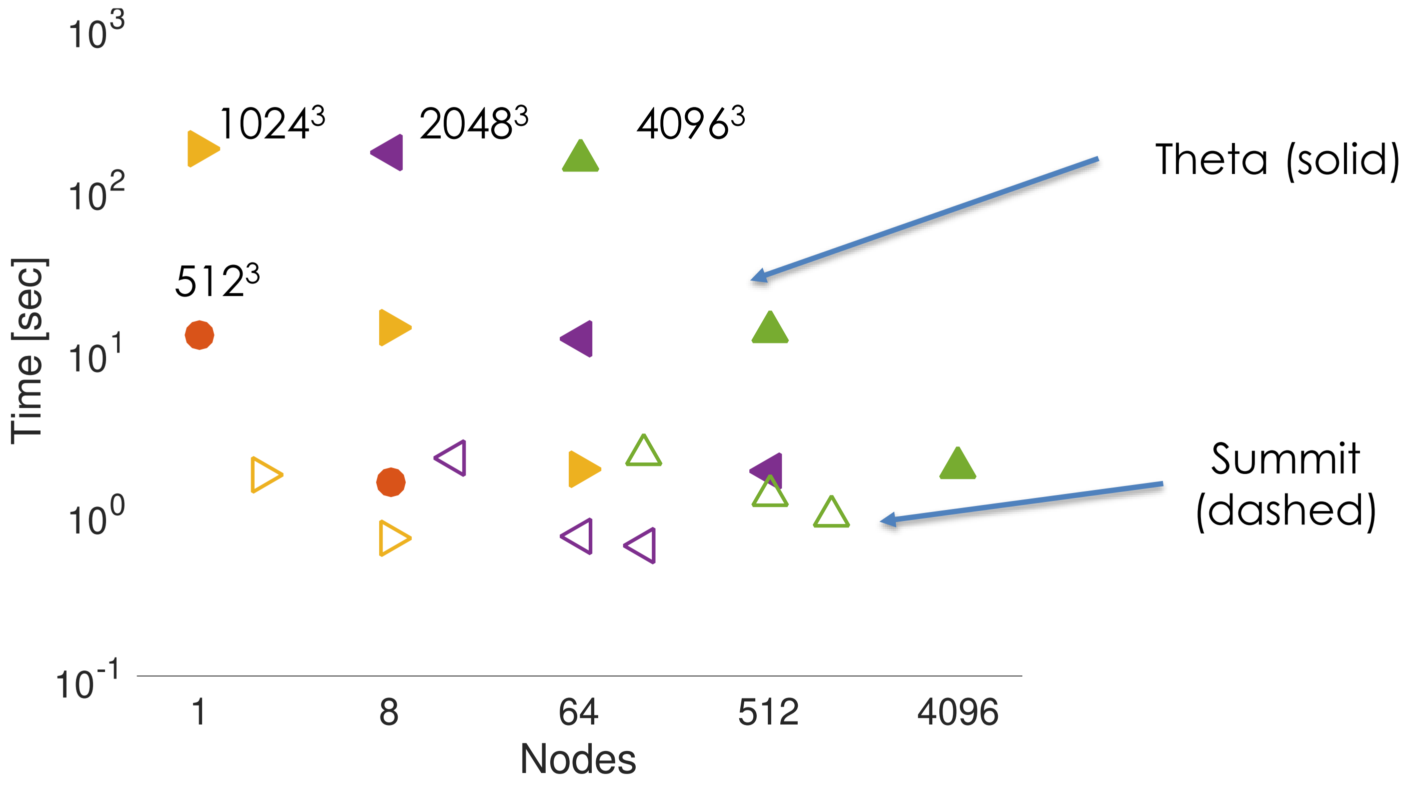
ALMA was Designed from the Ground Up to Perform on the Newest Leadership Class Systems



- **Strong scaling benchmark ALMA MHD code for problem with grid size 1024^3**

- **Benchmarks in current petascale clusters show excellent (better than ideal) strong scaling**

We Ran Some of the Largest Poisson Solves Ever on Summit Supercomputer – Up To 500 Trillion DOFs



- **Benchmark standalone MG solver at grid sizes 256^3 => 8192^3**
  - 3D linear solve of Poisson equation $\nabla^2\phi = \rho$ with sinusoidal solution
- **ALMA solutions on Summit are 20x faster than in Theta**

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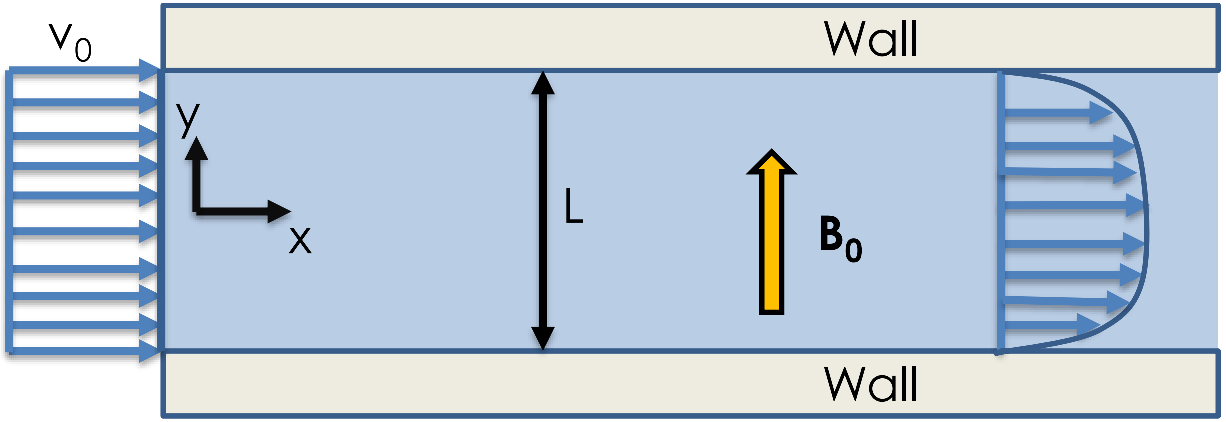
Objective : Validating liquid metal MHD benchmark cases

- Validation of Liquid metal MHD code is necessary to address the needs of the blanket design at high Hartmann number of $O(10^4)$
- Smolentsev et al. 2015[1] established key cases for verification and validation of Liquid metal MHD codes at fusion-relevant Hartmann number.
  - Fully-developed laminar steady MHD flow (Shercliff and Hunt flow)
  - 3D laminar steady MHD flow
  - Q2D turbulent MHD flow
  - 3D turbulent MHD flow
  - MHD flow with heat transfer

[1]Smolentsev, S., Badia, S., Bhattacharya, R., Buhler, L., Chen, L., Huang, Q., Jin, H.G., Krasnov, D., Lee, D.W., Valls, E.M.D.L., 2015. An approach to verification and validation of MHD codes for fusion applications. Fusion Eng. Des. 100

Hartmann-Poiseuille flow



$$\mu \frac{\partial^2 u}{\partial y^2} + B_0 \frac{\partial b_x}{\partial y} = \frac{\partial p}{\partial x} \quad ; \quad B_0 \frac{\partial u}{\partial y} + \eta \frac{\partial^2 b_x}{\partial y^2} = 0$$

With conducting wall BC

$$u = \frac{\eta}{B_0^2}\left\{1 - \frac{\cosh(Ha\, y)}{\cosh\left\{\frac{Ha}{2}\right\}}\right\} \quad ; \quad b_x = \frac{-1}{B_0}\left\{y - \frac{\sinh(Ha\, y)}{\mathrm{Ha}\cosh\left\{\frac{Ha}{2}\right\}}\right\}$$

u is the streamwise velocity and b_x is the induced magnetic field

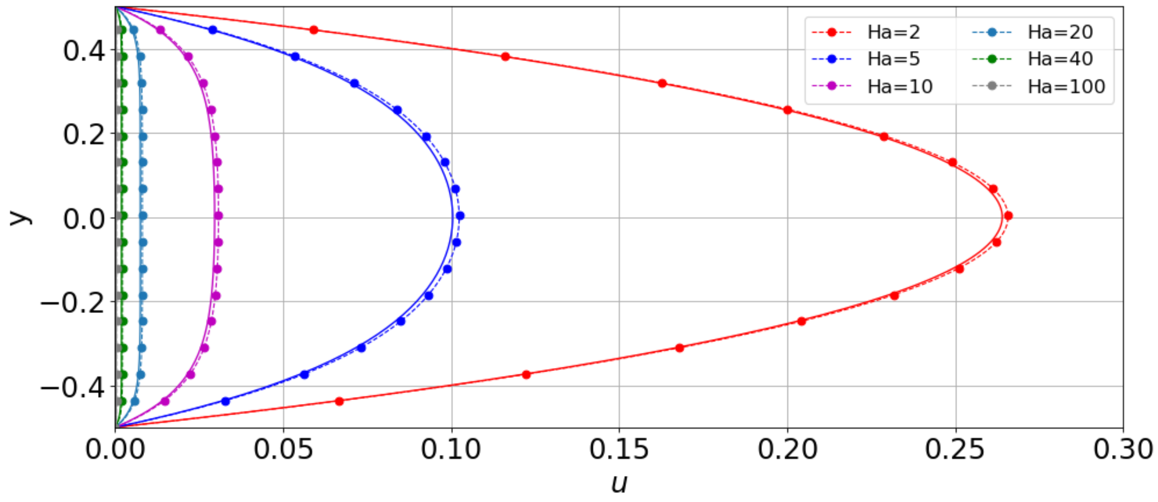
- Magnetic field B_0 is transverse to the flow direction.
- The channel width L is constant
- No-slip condition is imposed at the wall
- Constant pressure gradient
- Conducting walls : $\frac{\partial b_i}{\partial n} = 0$
- Insulating walls : $b_i = 0$

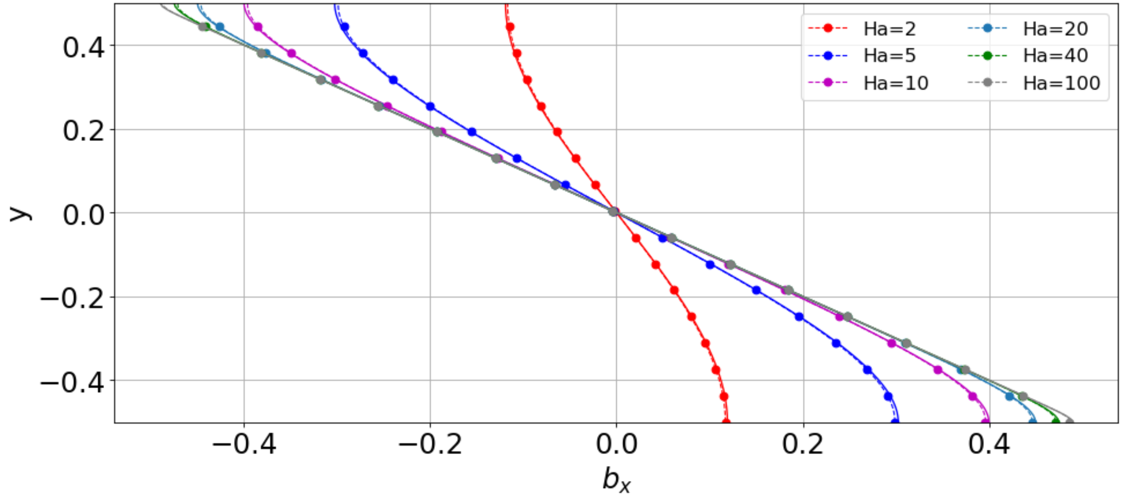
Reynolds number $Re_L = \frac{v_0 L}{\nu}$

Interaction parameter $N = \frac{L B_0^2}{\eta \rho_0 v_0}$

Hartmann number $Ha = \sqrt{N Re_L}$

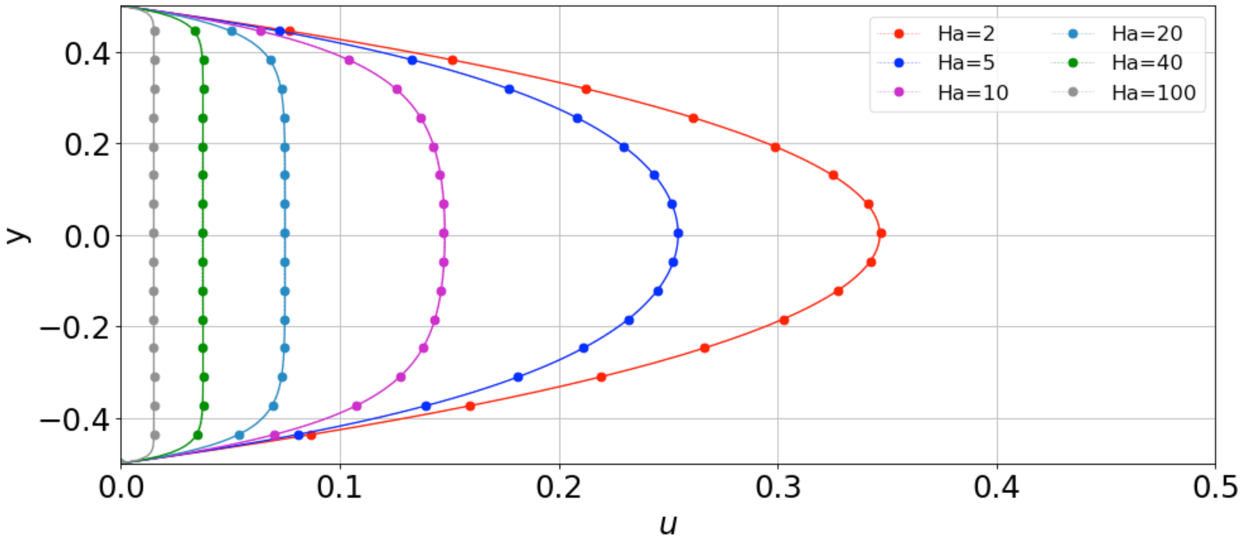
Hartmann-Poiseuille flow : Conducting walls

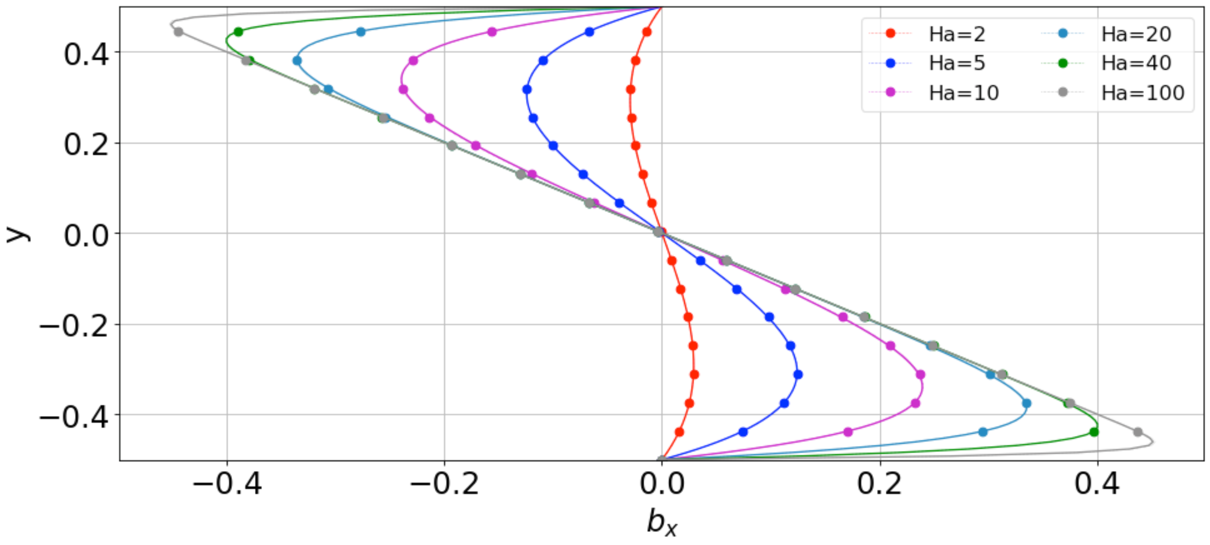




Solid lines represent the analytical solution.
Dotted line with symbols represent the solution from ALMA

Hartmann-Poiseuille flow : Insulating walls





Flow in a 3D periodic square duct

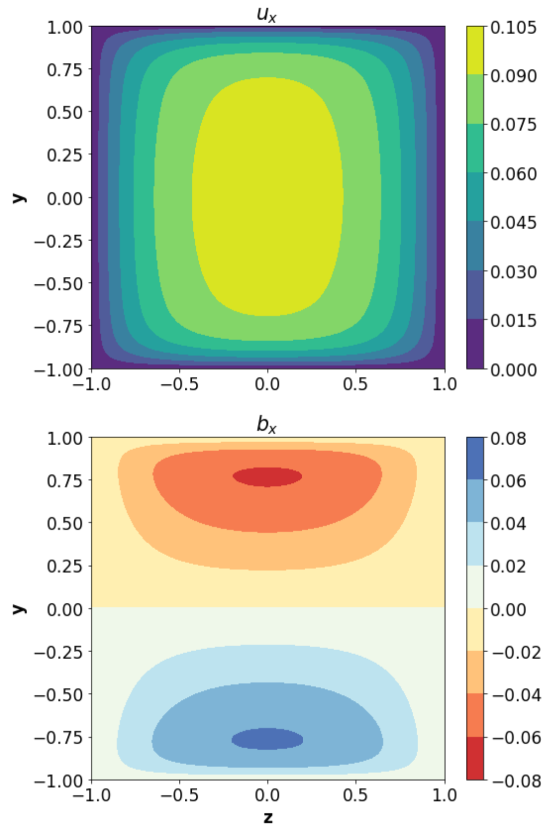
Boundary conditions :

1. Conducting walls $(c_w = \infty)$
2. Insulating walls $(c_w = 0)$

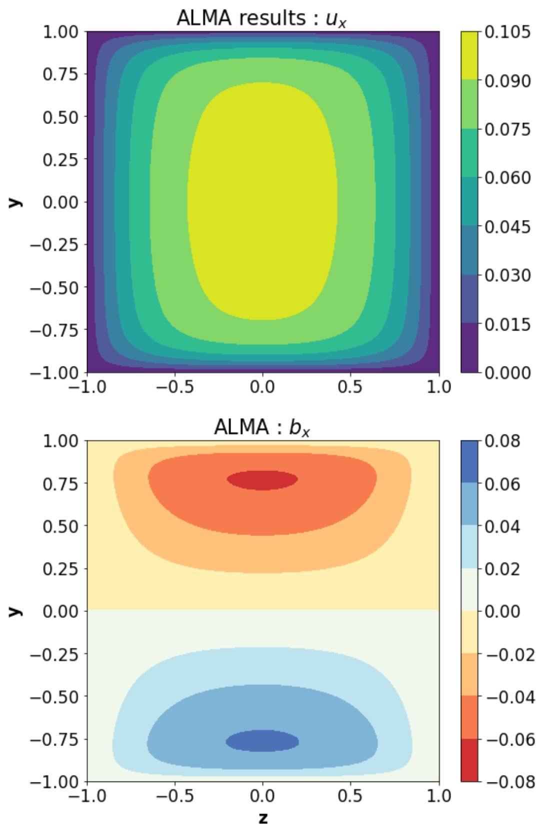
$$c_w \frac{\partial b_i}{\partial z} + b_i = 0\ at\ z = \pm L;$$

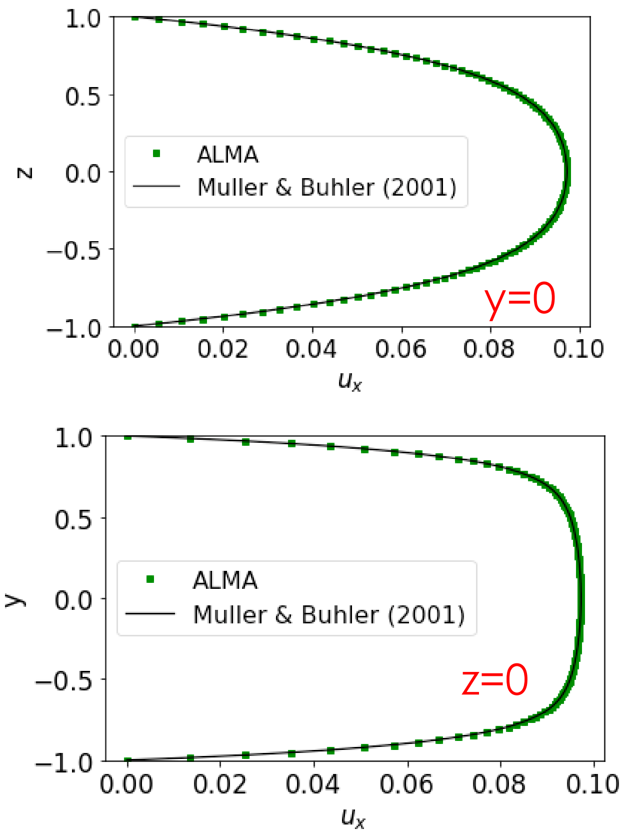
$$c_w \frac{\partial b_i}{\partial y} + b_i = 0 \text{ at y} = \pm L$$

Analytical solution (c_w=0)

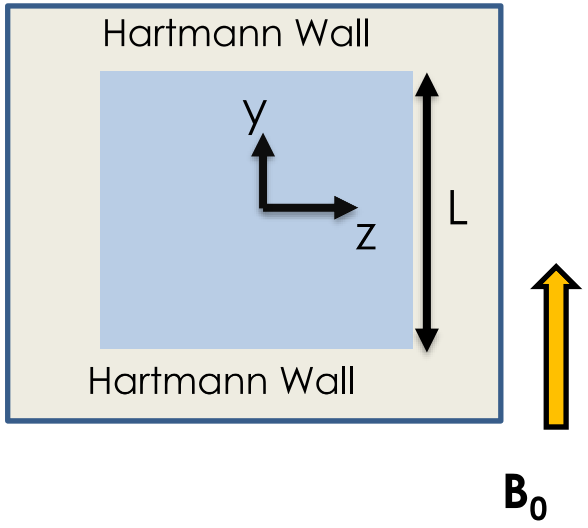


Numerical solution : ALMA





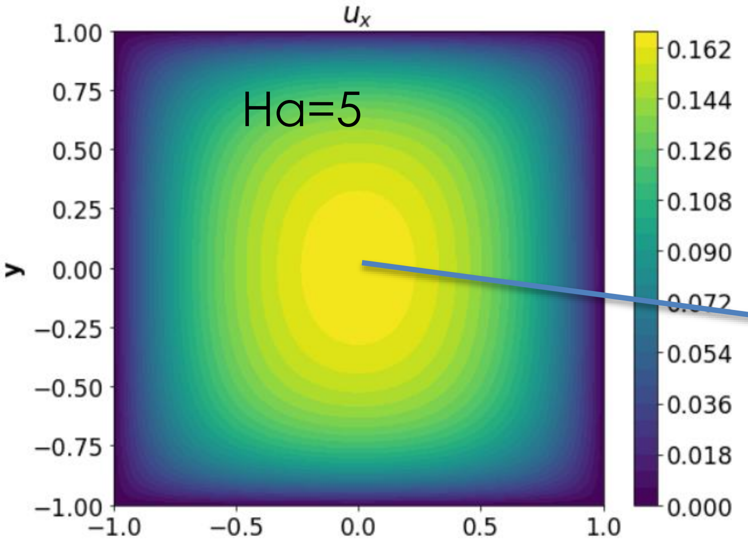
Flow into the plane



Hartmann number
Ha = 10

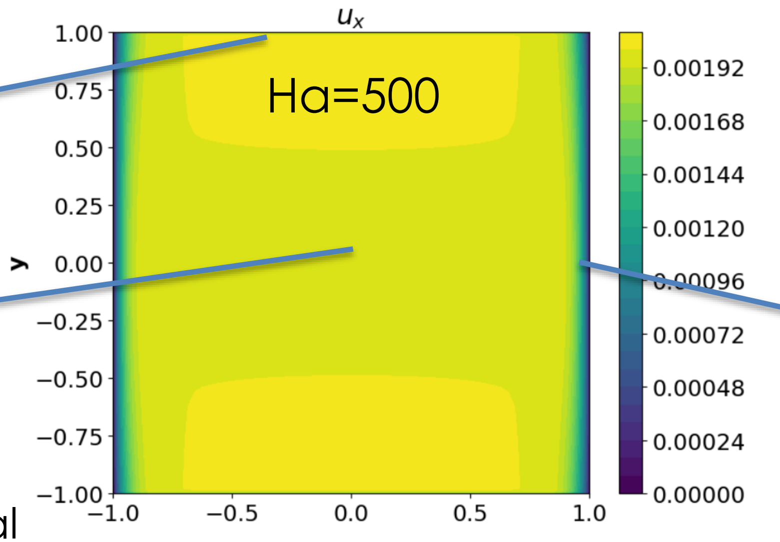
Hartmann layer ~ Ha^{-1}

Shercliff's[3] case : Insulating side and Hartmann walls



Hartmann layers ~ Ha^{-1}

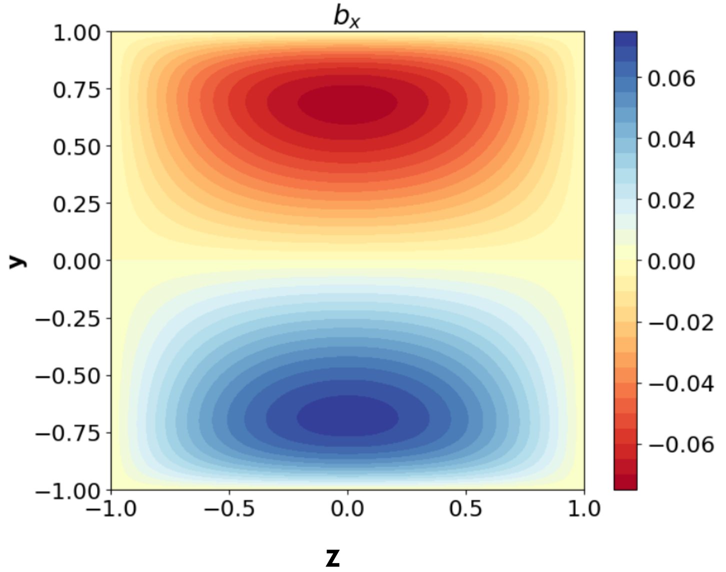
Inviscid core

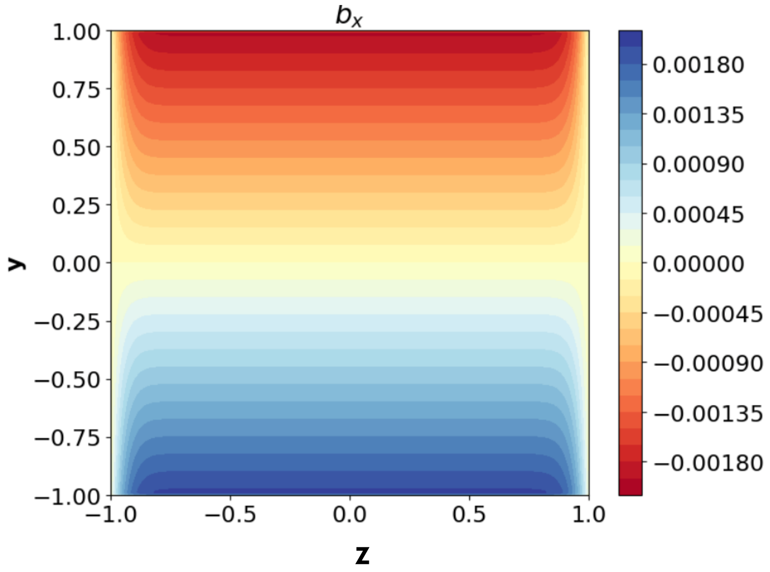


Resolution nz=144, ny=150

Side layers scaling ~ $Ha^{-1/2}$

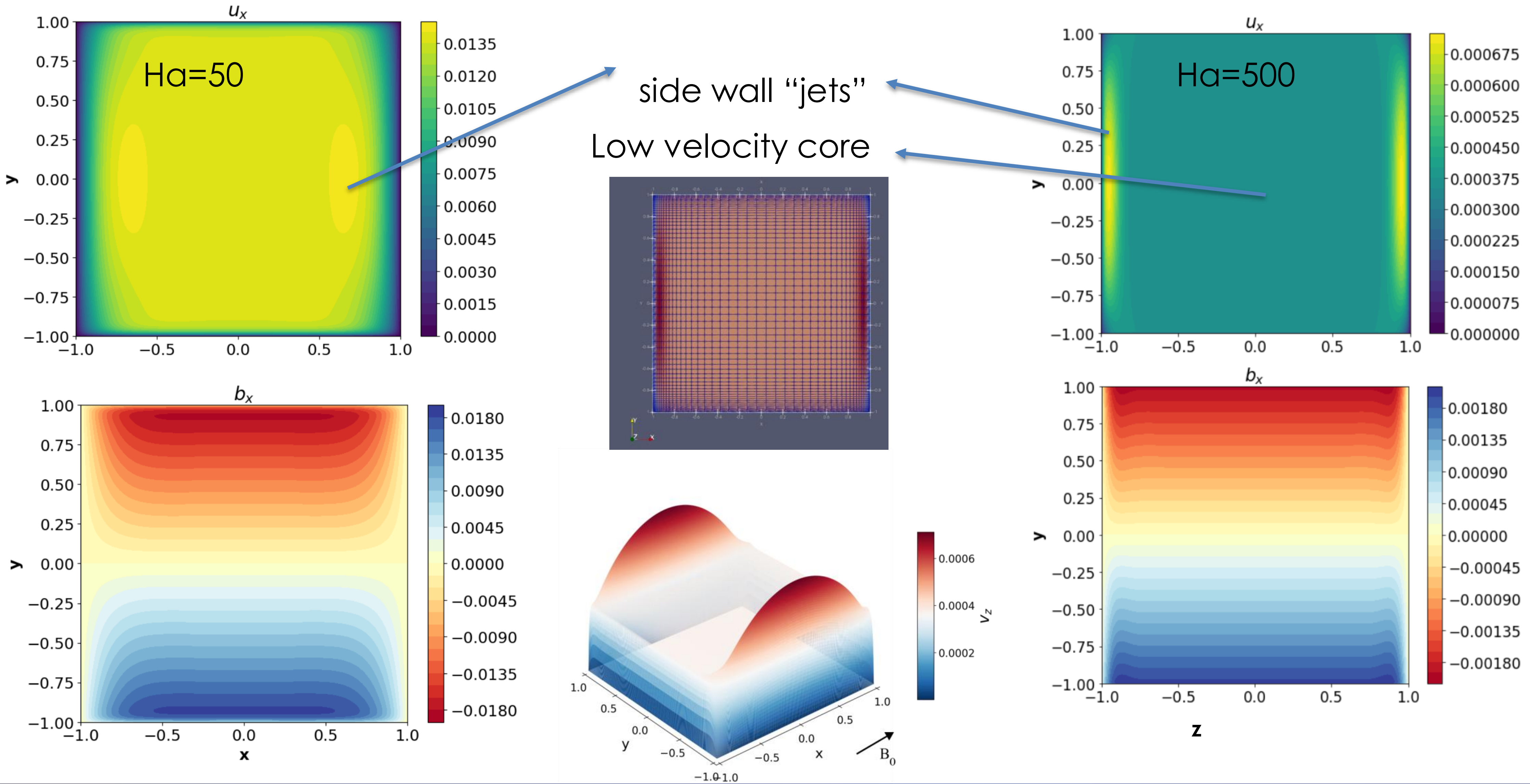
Near wall grid density presents a computational challenge





[3] Shercliff, 1953, Steady motion of conducting fluids in pipes under transverse magnetic fields

Hunt's case[4] : Insulating side walls and conducting (c_w=0.01) Hartmann walls



[4]Hunt, 1965, Magnetohydrodynamic flow in rectangular ducts, JFM

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Comparison of flow rates

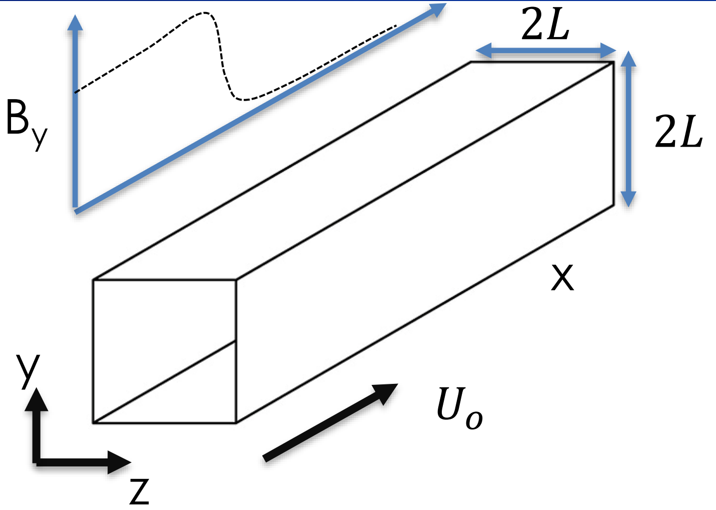
Shercliff's case : Insulating side and Hartmann walls

Ha	Q	$Q_{analytical}$	Error (%)
500	7.68000E-04	7.68000E-04	0
5000	7.90180E-04	7.90200E-04	0.00253
10000	3.965000E-04	3.96500E-04	0

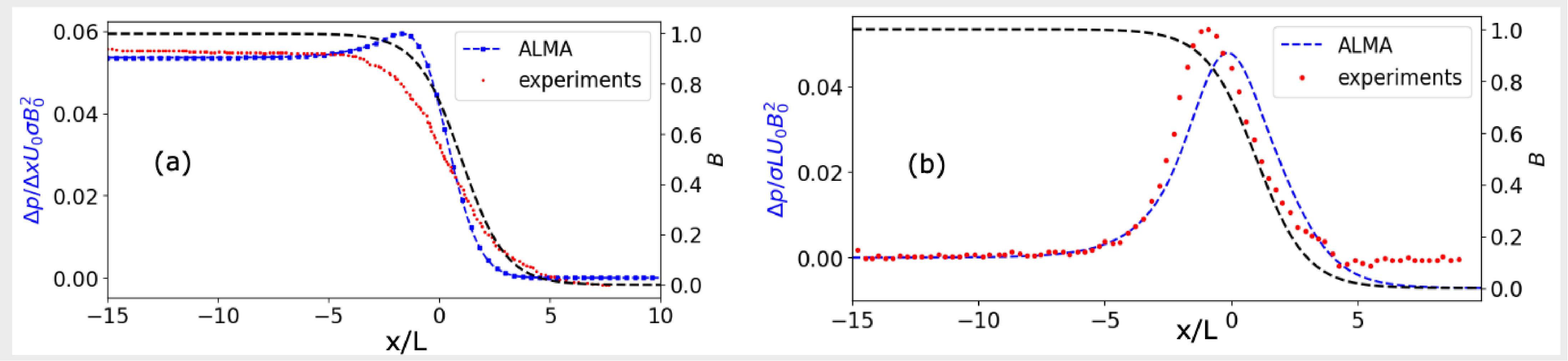
Hunt's case : Conducting Hartmann walls (c_w=0.01) and Insulating side walls

Ha	Q	$Q_{analytical}$	Error (%)
500	1.88000E-03	1.86500E-03	1.06
5000	2.0E-05	1.90700E-05	4.9
10000	5.98E-6	5.16900E-06	13.7

3D laminar flow with spatially varying magnetic field



- Domain : 2L x 2L x 25L , where L =1m
- [5] Ha = 2900 , N = 540, c_w = 0.07
- **Background magnetic field** : $B_y = 0.5B_0(1 - \tanh(0.5(z - z_c)))$ (represented using **black dashed line** below)
- No slip walls
- Results compared against **experiments** of Reed at al. ALEX results.



Reed at al, [5]ALEX RESULTS-A COMPARISON OF MEASUREMENTS FROM A ROUND AND A RECTANGULAR DUCT WITH 3-D CODE PREDICTIONS

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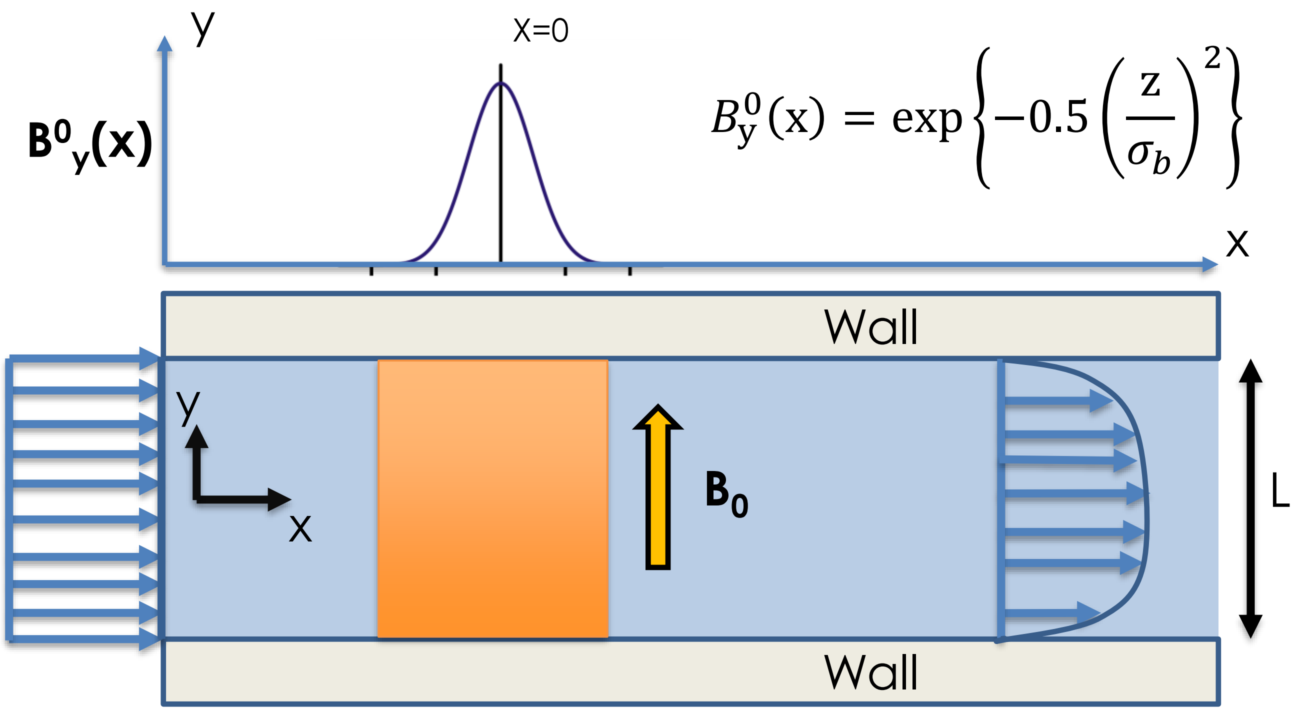
Ongoing work

3D MHD turbulence: Test parameters adopted from Andreev et al[6]

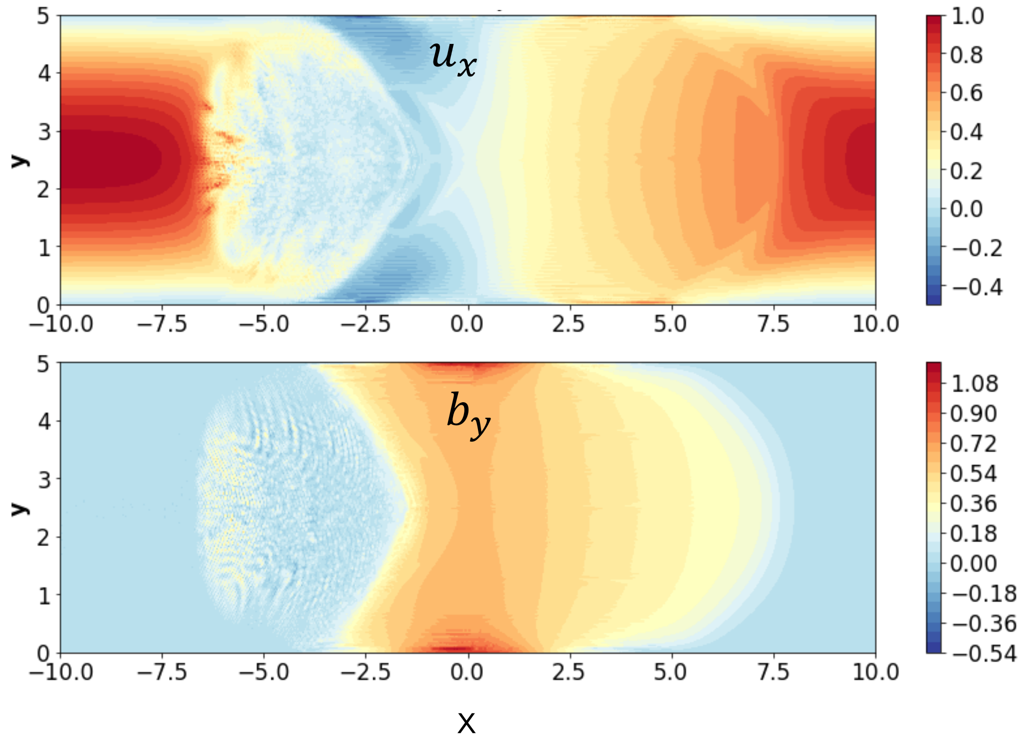
Re = 4000
Ha = 400
N = 40

[6]Experimental study of liquid metal channel flow under the influence of a nonuniform magnetic field, Andreev et al, POF, 2006



$$B_y^0(x) = \exp\left\{-0.5\left(\frac{z}{\sigma_b}\right)^2\right\}$$

Preliminary results



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Summary and Future Work

- The antisymmetric form of the MHD equations are solved using the ALMA framework
- The method was successfully applied in a laminar MHD flow in 2D channels and 3D ducts, subject to uniform and spatially varying magnetic field.
- Future work includes:
  - Validating the solver for MHD flows that lie in the turbulent regime – Q2D and 3D turbulence
  - Simulation of liquid metal flows and plasmas in the presence of time-varying background magnetic field.

Acknowledgement

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Thank you!

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