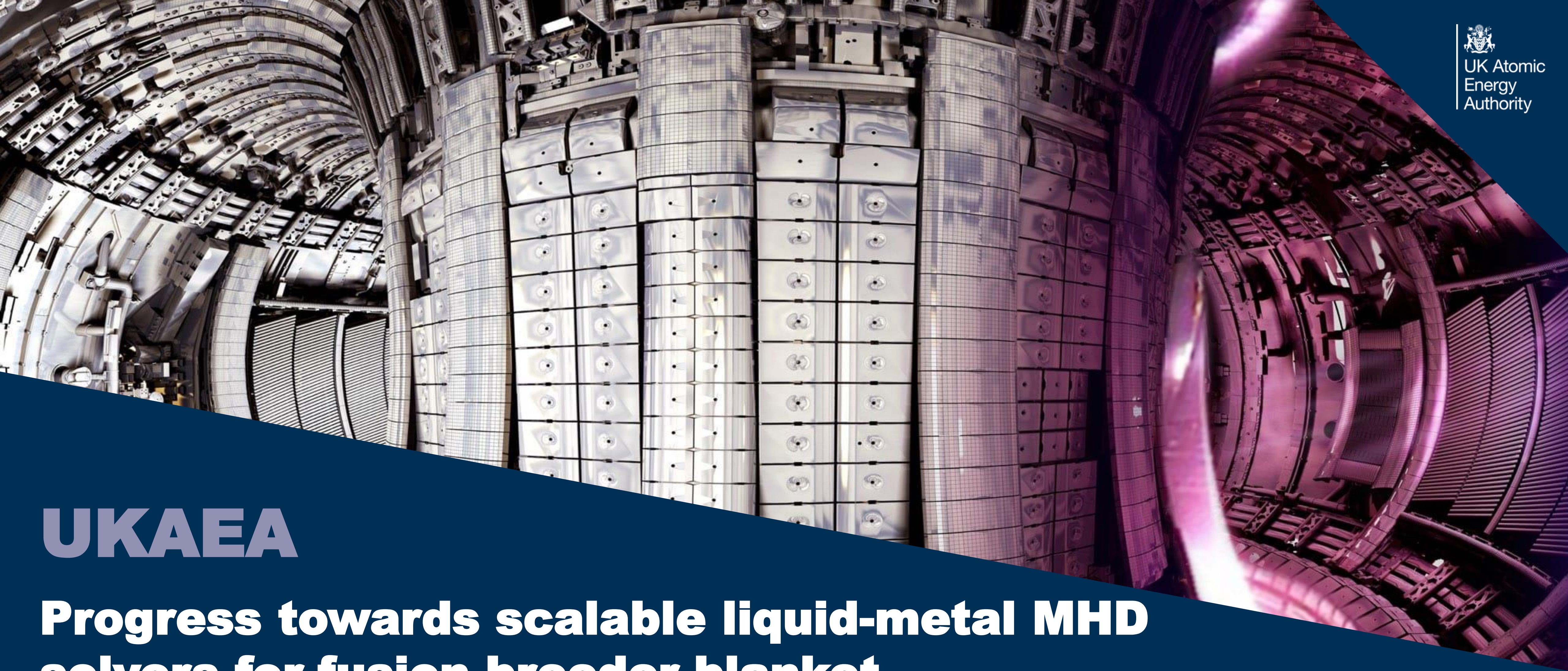

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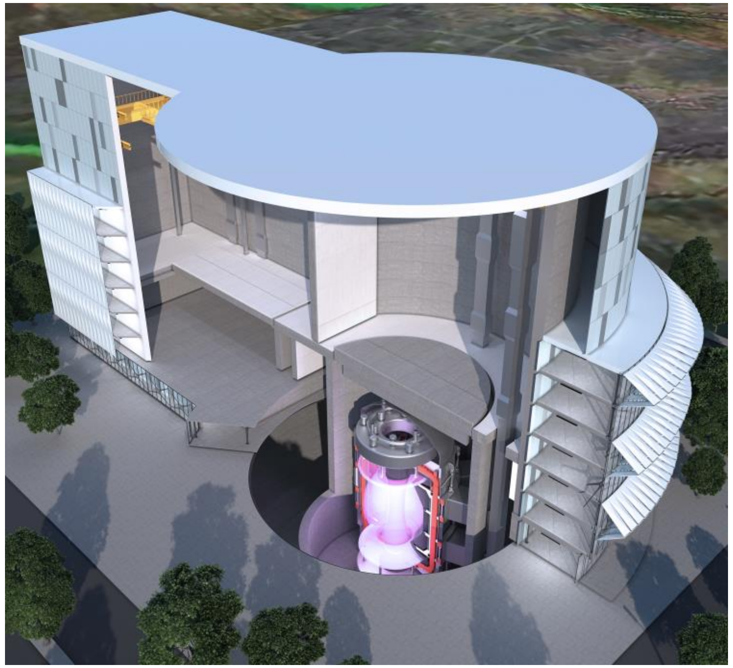
Progress towards scalable liquid-metal MHD solvers for fusion breeder blanket multiphysics applications

Rupert W Eardley, Aleksander J Dubas, Andrew Davis

Context: Digital Twins for Tokamaks

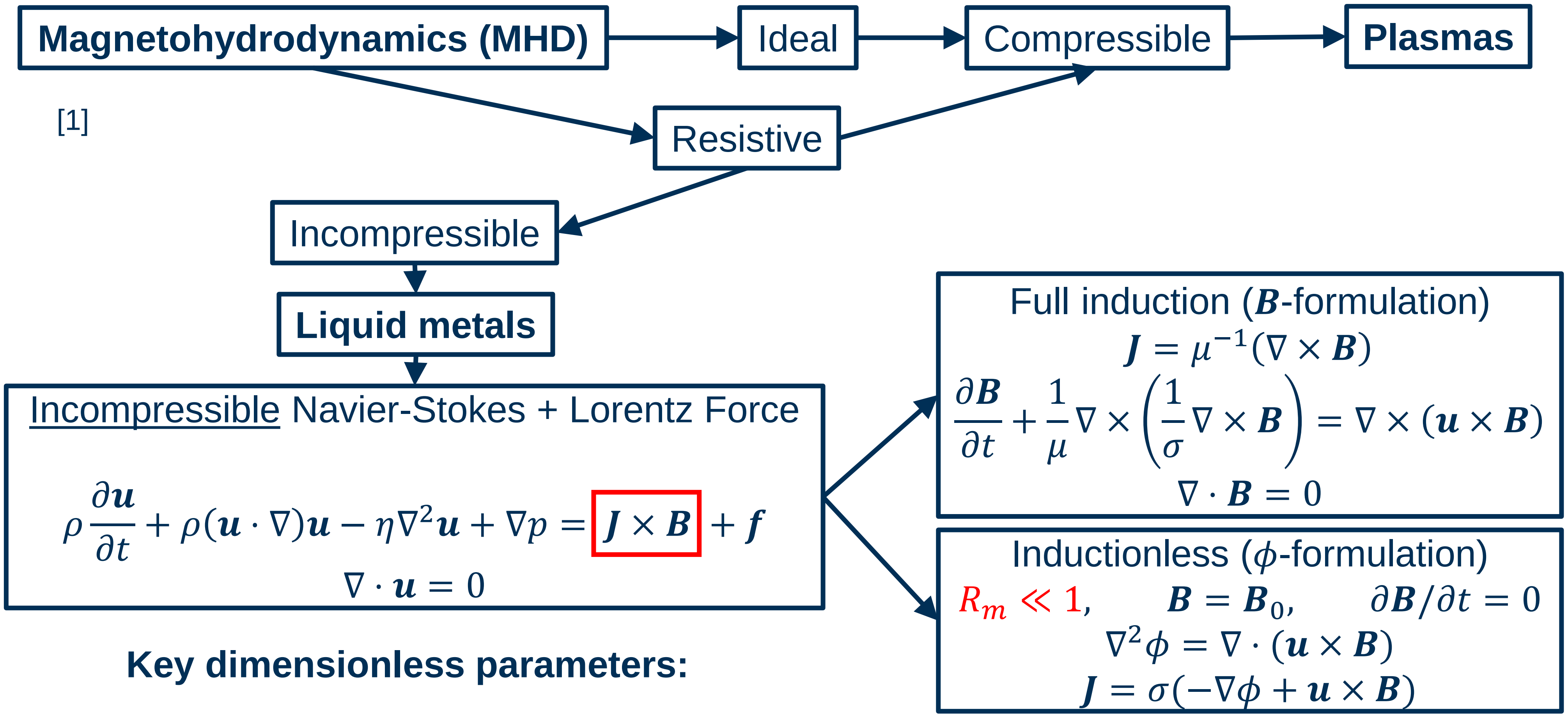
- The End Goal: Digital Twinning.
    - An exascale problem (high fidelity, multi-scale).
    - Requires validated multi-physics simulation software.
    - Must be scalable.
    - Current focus: MOOSE (Proteus).
- Why are frameworks like MOOSE a good solution?
    - Open-source: allow development of custom tools.
    - Enable developers to focus on the physics.
    - Multiphysics coupling (e.g. MOOSE multi-apps).
    - Scalable.



Artist's impression of STEP (image credit: UKAEA)

- Approach:
    - Break down the tokamak into critical components, e.g. breeder blankets.
    - Some breeder blanket designs rely on the flow of a liquid metal.
    - Proximity to strong magnetic fields: **liquid-metal MHD effects become dominant**.

Liquid-Metal MHD Equations



Magnetohydrodynamics (MHD)

Ideal

Compressible

Plasmas

[1]

Resistive

Incompressible

Liquid metals

Incompressible Navier-Stokes + Lorentz Force

$$\rho\frac{\partial \boldsymbol{u}}{\partial t} + \rho(\boldsymbol{u}\cdot\nabla)\boldsymbol{u} - \eta\nabla^2\boldsymbol{u} + \nabla p = \boxed{\boldsymbol{J}\times\boldsymbol{B}} + \boldsymbol{f}$$

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

Full induction ($\boldsymbol{B}$-formulation)

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

$$\frac{\partial\boldsymbol{B}}{\partial t} + \frac{1}{\mu}\nabla\times\left(\frac{1}{\sigma}\nabla\times\boldsymbol{B}\right) = \nabla\times(\boldsymbol{u}\times\boldsymbol{B})$$

$$\nabla\cdot\boldsymbol{B} = 0$$

Highly nonlinear
Strongly coupled
Feedback loop ($\boldsymbol{B}$)

Inductionless (ϕ-formulation)

$$R_m \ll 1, \qquad \boldsymbol{B} = \boldsymbol{B}_0, \qquad \partial\boldsymbol{B}/\partial t = 0$$

$$\nabla^2\phi = \nabla\cdot(\boldsymbol{u}\times\boldsymbol{B})$$

$$\boldsymbol{J} = \sigma(-\nabla\phi + \boldsymbol{u}\times\boldsymbol{B})$$

Highly nonlinear
Strongly coupled
Poisson equation

Key dimensionless parameters:

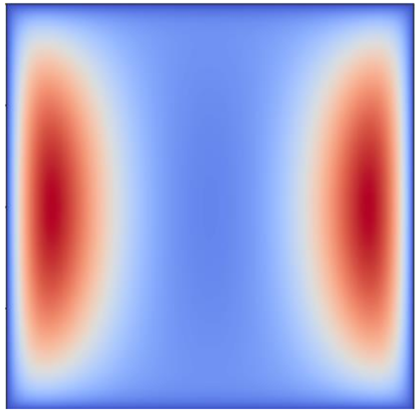
Magnetic Reynolds number: $R_m = \mu\sigma UL$

Hartmann number: $Ha = BL\sqrt{\frac{\sigma}{\eta}}$

[1] Müller U and Bühler L 2001 Magnetofluiddynamics in Channels and Containers (Berlin: Springer)

Liquid-Metal MHD in Fusion

- Liquid metals e.g. PbLi, Li, are considered as coolant and/or breeder materials due to high thermal conductivity, low viscosity and sufficient tritium breeding ratio [2].
- MHD-related issues include MHD pressure drop and flow stagnation [2].
- Recent research efforts aim to ensure LM-MHD codes are carefully validated. Smolentsev et al. 2015 [3] established 5 key validation cases:
    1. Fully-developed laminar steady MHD flow (Shercliff and Hunt flow).
    2. 3D laminar steady MHD flow (spatially varying B-field).
    3. Quasi-2D turbulent MHD flow.
    4. Turbulent MHD flow.
    5. MHD flow with heat transfer.
- Fusion breeder blankets typically expect $Ha{\sim}10^4$ [2].
- Achieving fusion-relevant Ha in codes remains a significant challenge [3].



Hunt flow

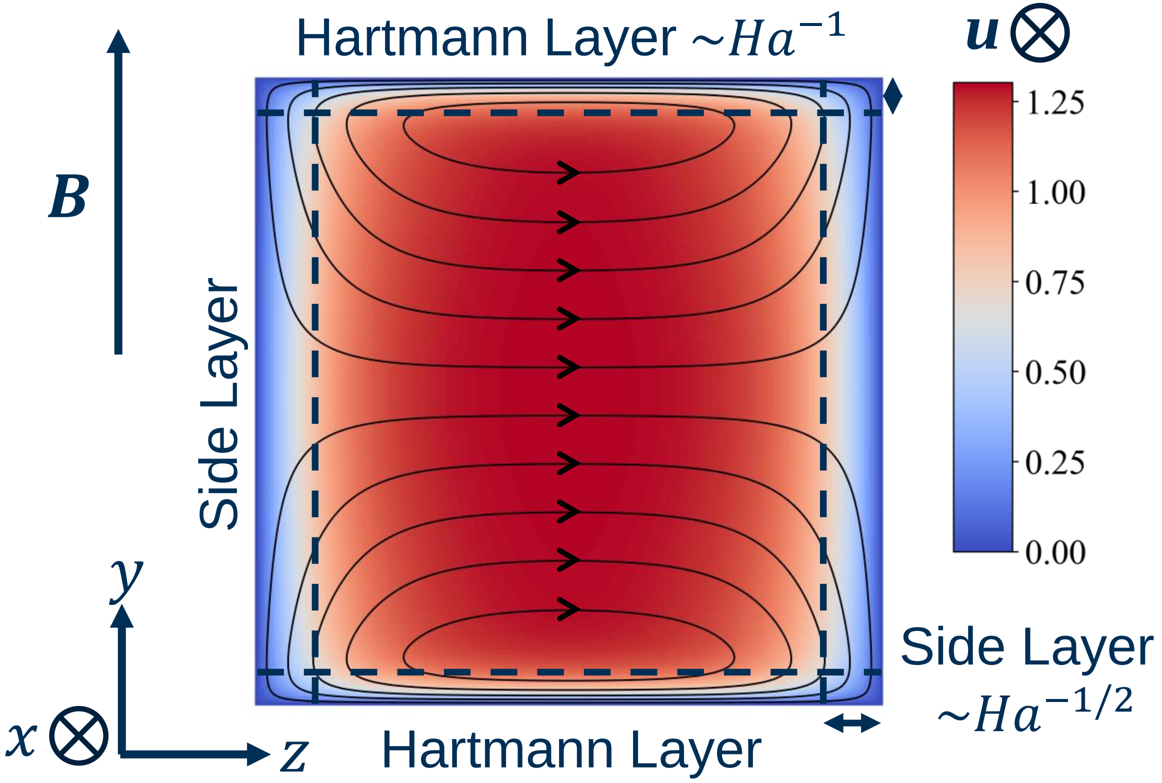
[2] Smolentsev S 2021 *Fluids* **6** (3) 110
[3] Smolentsev S et al. 2015 *Fusion Engineering and Design* **100** 65-72

Laminar MHD Flow

2 key liquid-metal MHD analytic solutions (laminar steady flow in rectangular ducts):

- Shercliff flow [4] (all walls perfectly insulating).
- Hunt flow [5] (conducting Hartmann walls, insulating side walls).
  - Will focus on perfectly conducting/insulating case.
  - There are also solutions for arbitrary Hartmann/side wall conductivity…
  - …but BCs become more complicated (need to e.g. model wall currents).

Shercliff flow [4] ($Ha = 20$)



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[4] Shercliff J A 1953 *Mathematical Proceedings of the Cambridge Philosophical Society* **49** 136-144
[5] Hunt J C R 1965 *Journal of Fluid Mechanics* **21** (4) 577-590

Laminar MHD Flow

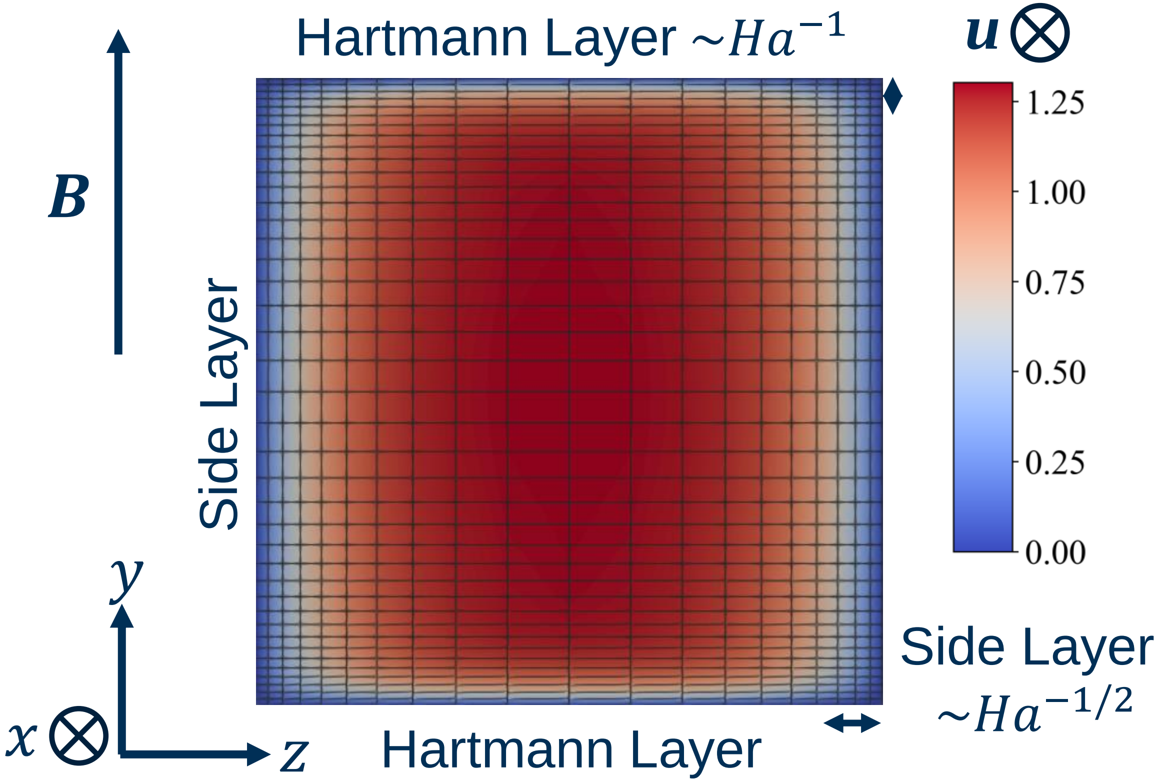
LM-MHD simulations need to resolve the Hartmann and side layers.

Increasing Ha narrows these layers [4, 5].

As Ha increases, options are:

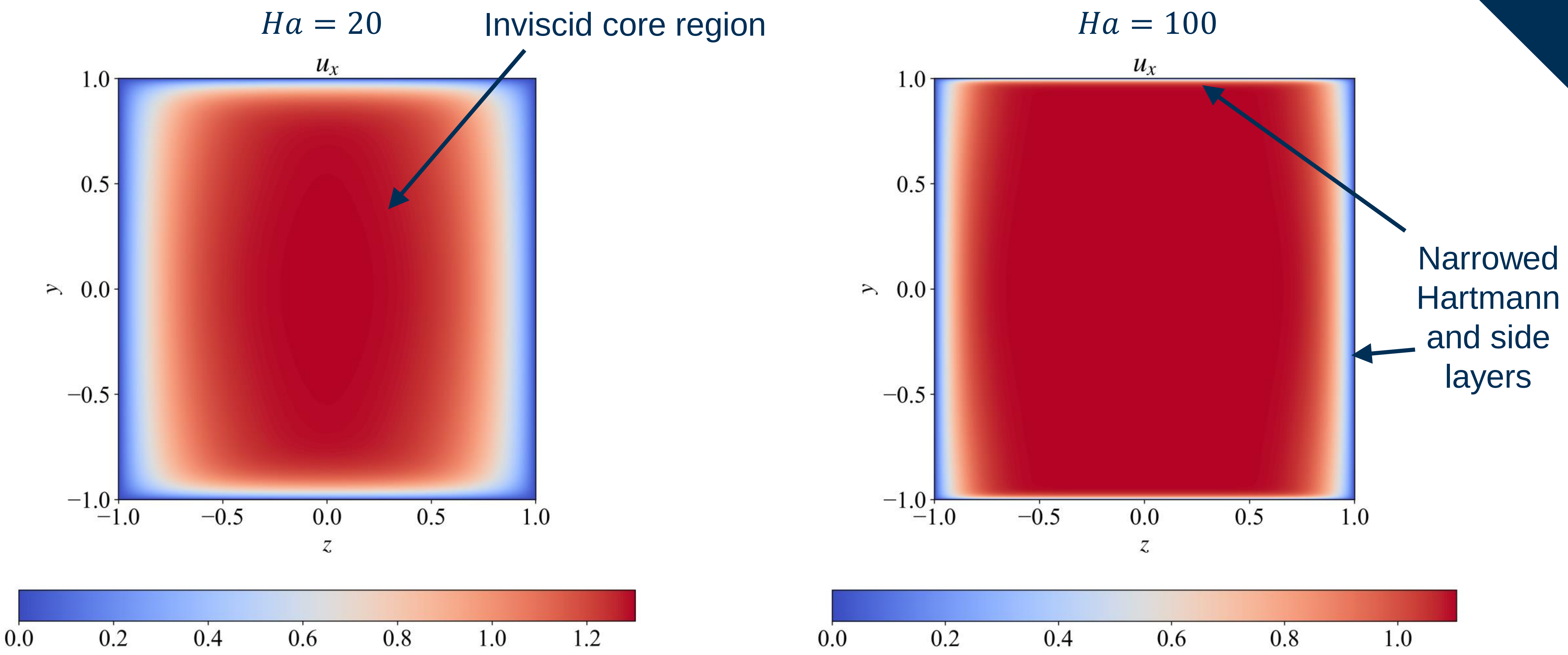
1. Sacrifice mesh uniformity to maintain low resolution.
    - Can limit ability of codes to converge.
2. Increase overall mesh element count.
    - Increases resource requirements.
    - Requires good weak scaling.

Shercliff flow [4] ($Ha = 20$)



[4] Shercliff J A 1953 *Mathematical Proceedings of the Cambridge Philosophical Society* **49** 136-144
[5] Hunt J C R 1965 *Journal of Fluid Mechanics* **21** (4) 577-590

Shercliff Flow



$Ha = 20$

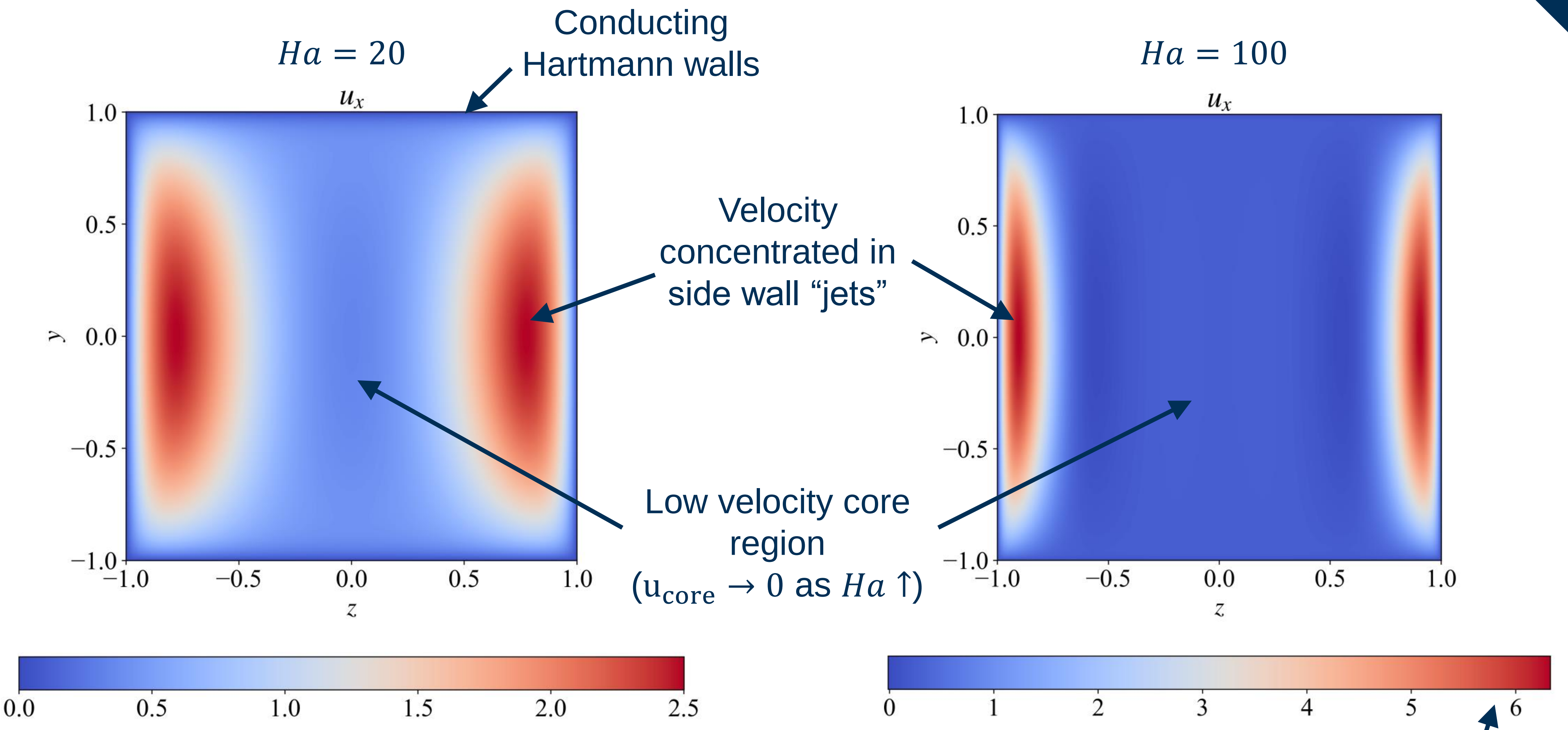
$Ha = 100$

Inviscid core region

Narrowed Hartmann and side layers

[4] Shercliff J A 1953 *Mathematical Proceedings of the Cambridge Philosophical Society* **49** 136-144

Hunt Flow



Conducting Hartmann walls

Velocity concentrated in side wall “jets”

Low velocity core region ($u_{core} \rightarrow 0$ as $Ha \uparrow$)

Increased velocity in narrower jets

[5] Hunt J C R 1965 *Journal of Fluid Mechanics* **21** (4) 577-590

OpenFOAM MHD Solvers

OpenFOAM
The OpenFOAM Foundation

Open∇FOAM®

2 prevalent versions: OpenFOAM foundation [6] version used in this work.

What is OpenFOAM [6]?

- Free open-source Finite-Volume CFD software.

There are 2 OpenFOAM MHD solver options:

- mhdFoam (native to OpenFOAM, full-induction $\boldsymbol{B}$-formulation).
- epotFoam (user-made solver [7], inductionless approximation ϕ-formulation).
- Both are transient only – no steady-state solve available.
- Relatively undeveloped compared to other OpenFOAM CFD capability.
  - Additional required features: finite wall conductivity, steady-state.

Why is OpenFOAM useful?

- Intermediate engineering applications: liquid-metal MHD without multiphysics.
- Could be coupled into MOOSE for multiphysics applications.

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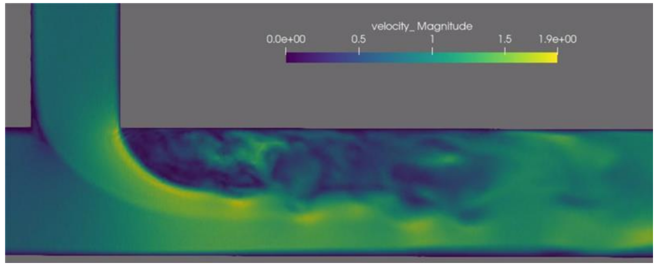
[6] The OpenFOAM Foundation Ltd: www.openfoam.org
[7] Tassone A 2016 in *Proceedings of CFD with OpenSource Software*, ed Nilsson H

Proteus

MOOSE

Proteus is a tool created using the MOOSE [8] framework, designed as an extension of the native fluid dynamics capabilities [9] in MOOSE for fusion applications.

- Open-source (LGPLv2): https://github.com/aurora-multiphysics/proteus
- Advantages of MOOSE:
  - Multiphysics coupling (multi-app structure), modularity, scalablility.
- Target scope includes liquid-metal MHD:
  - Starting with inductionless ($R_m \ll 1$) incompressible MHD.
  - ϕ-formulation (like epotFoam).
  - Finite Element Method, automatic differentiation [10] for Jacobians.
  - Fully coupled – monolithic Navier-Stokes + electromagnetic solve.
  - Using PSPG + SUPG stabilisation to enable equal (1st) order velocity and pressure.



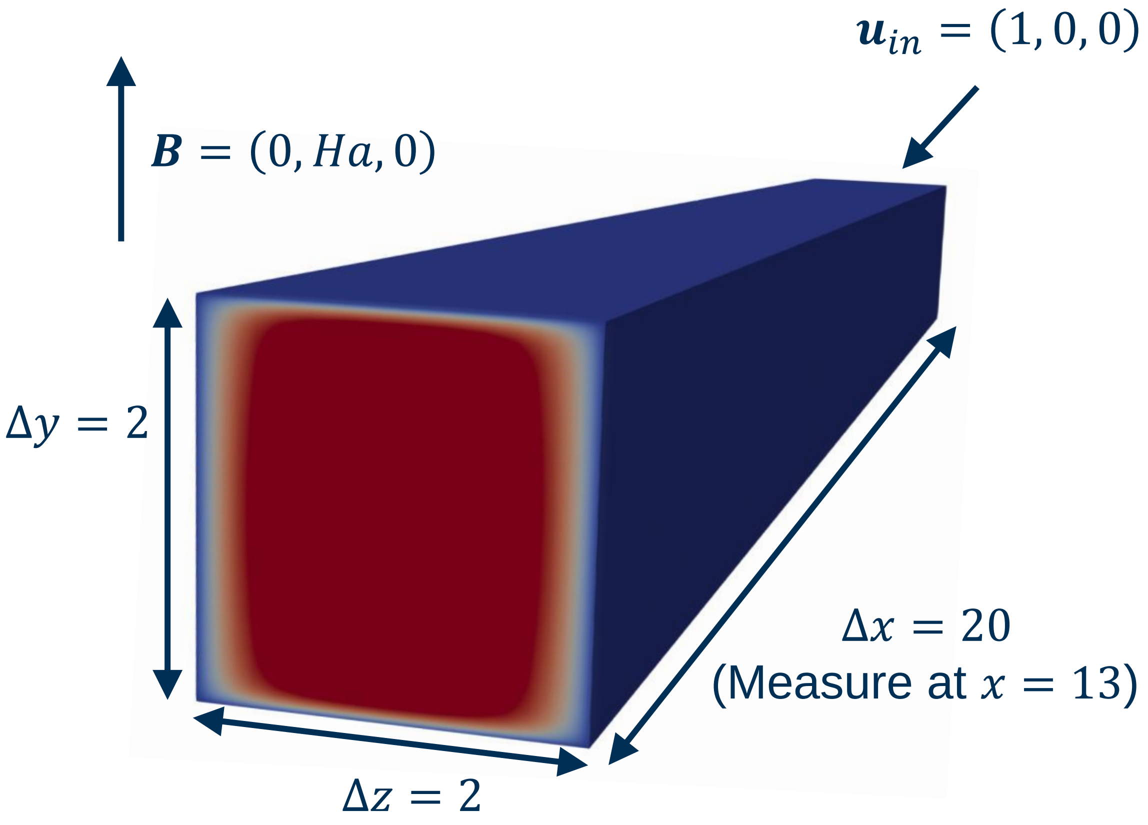
[8] Lindsay A D et al. 2022 *SoftwareX* **20** 101202
[9] Peterson J W, Lindsay A D and Kong F 2018 *Advances in Engineering Software* **119** 68-92
[10] Lindsay A D et al. 2021 *Nuclear Technology* **207** 905-922

OpenFOAM Scaling

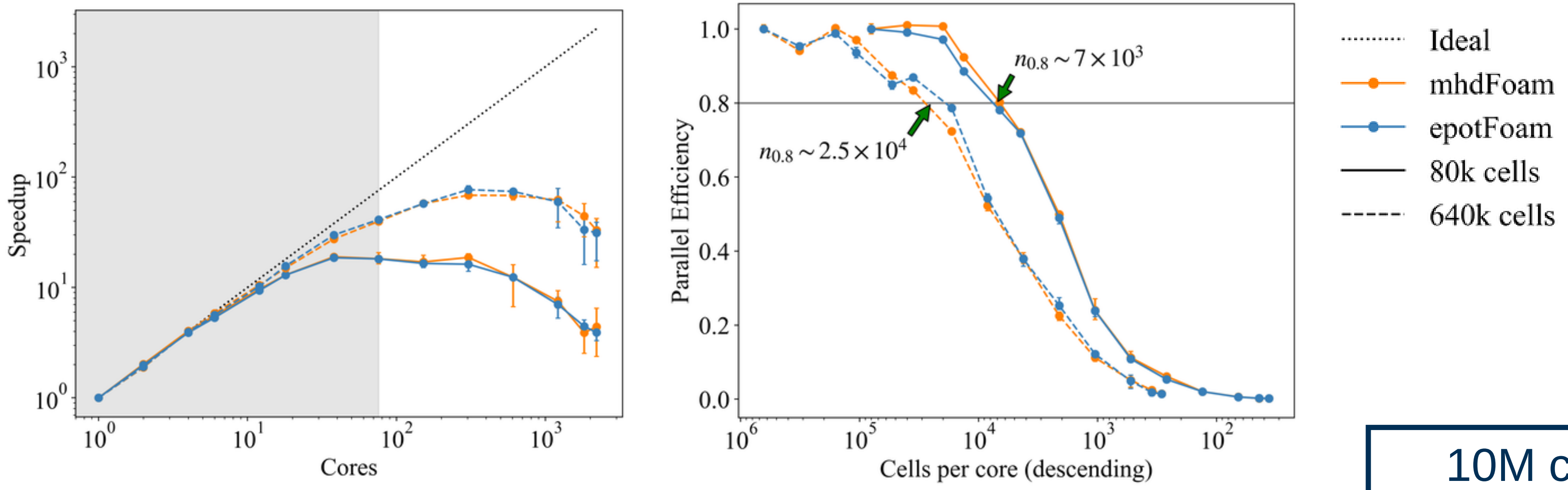
Reference case:

- $Ha = 20$ Shercliff flow (insulating walls).
- 3D simulation (solution is 2D) – more cells.
- Scaling tests used CSD3.
- Studied strong scaling for 80k, 640k and 10M cells.
  - Mesh grading used for 80k and 640k cell cases.
- Studied weak scaling up to 2206 cores.
  - 10k cells per core.
  - Timestep reduced for stability (CFL condition).
- Measuring time per timestep.

ρ	ν	μ	σ
1	1	1	1

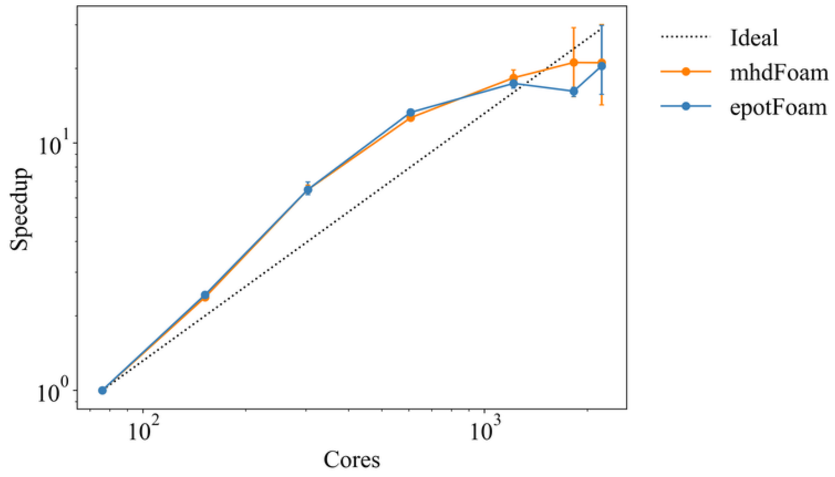


OpenFOAM Strong Scaling

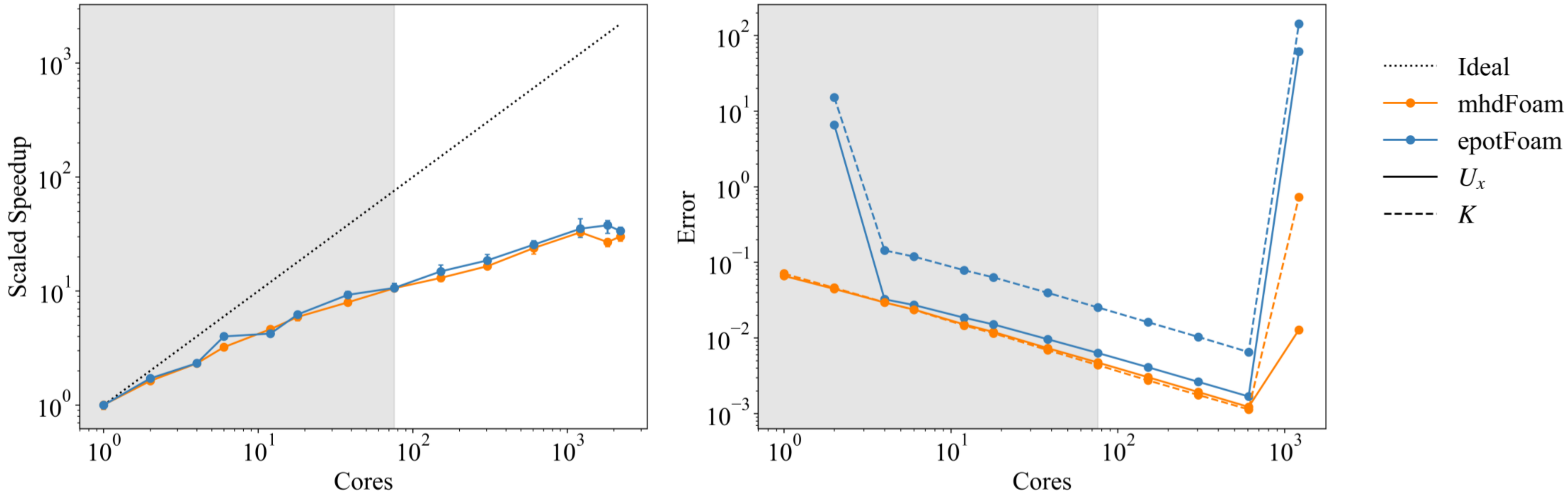


- Target $n = \frac{cells}{core} \geq n_{0.8}$
- $n_{0.8} =$ value of n below which efficiency drops below 80%
- Find that $n_{0.8}$ increases as resolution increases.

10M cells: super-linear scaling



OpenFOAM Weak Scaling



Weak scaling is not ideal, but reasonable.

Iterations per field per timestep increases with resolution (sparse matrix problem).

Careful choice of preconditioners may improve weak scaling.

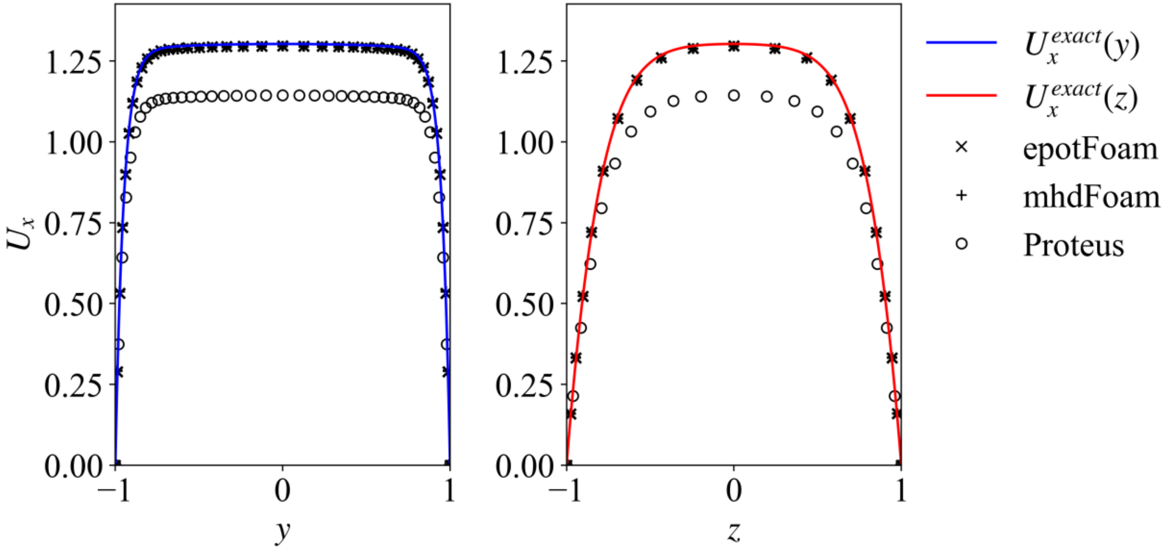
epotFoam struggles when under-resolved.

High pressure drop error for epotFoam.

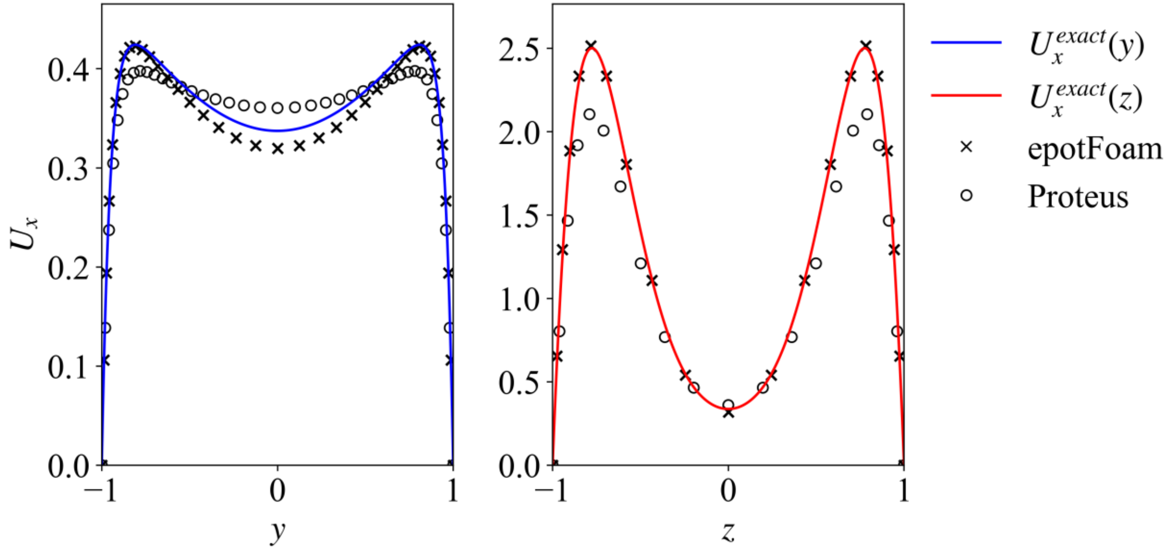
Both solvers failed above 12M cells; potentially required smaller timestep.

Validation Results: Ha=20

- 100x40x20 cells/elements, mesh grading factor 10 (ratio between smallest/largest cell width).
  - Grading factor 5 in Proteus – struggles to converge when higher.
- Proteus implementation miscalculates the velocity magnitude: RMSE(U_x) $\sim 10\%$.
  - Continuing to investigate this.
- Steady-state solve used for Proteus.



Shercliff flow



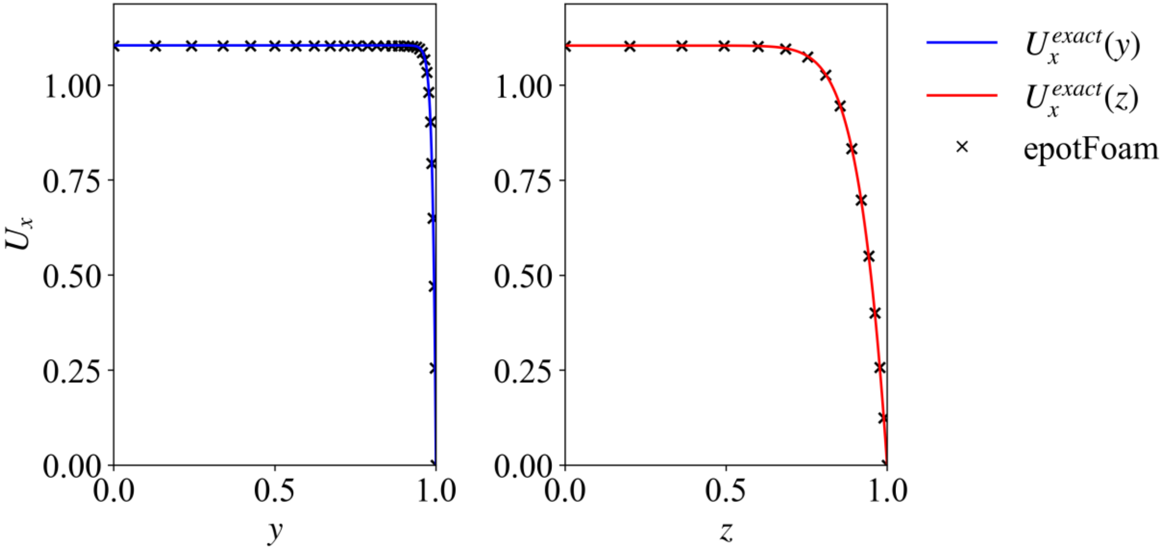
Hunt flow

Validation Results: Ha=100

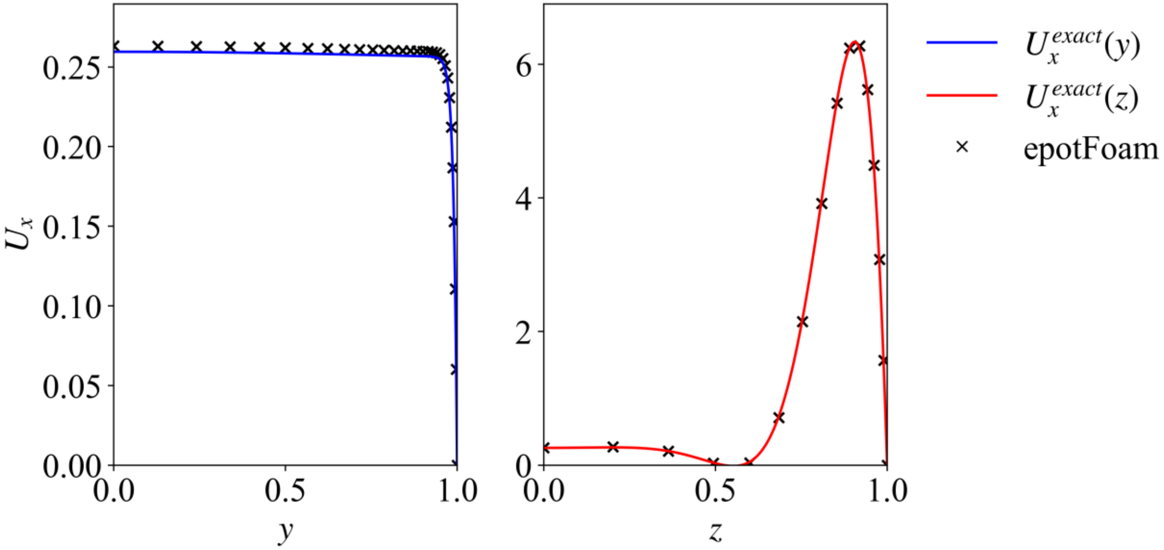
- 100x60x30 cells/elements:
    - Mesh grading factor 50 along y.
    - Mesh grading factor 20 along z.
- No Proteus results yet – fails to converge with mesh grading > 8.
- Timestep scaled with magnetic damping time to maintain stability:

$$\tau = \frac{\rho}{\sigma|\boldsymbol{B}|^2} \propto \frac{1}{Ha^2}$$

- RMSE(U_x) $\lesssim 3\%$, pressure drop error $\sim 1\%$.



Shercliff flow

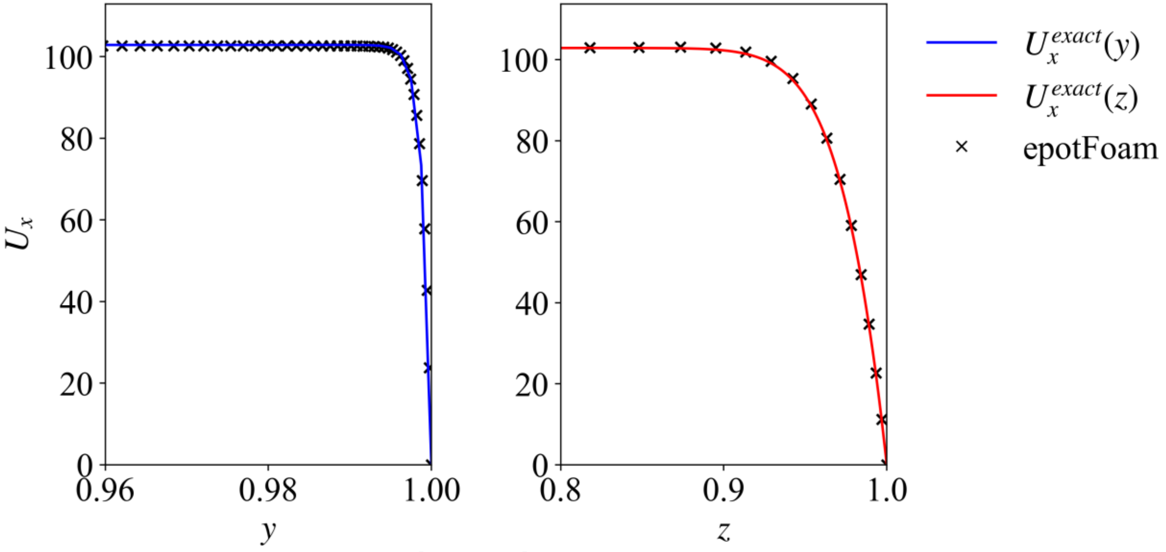


Hunt flow

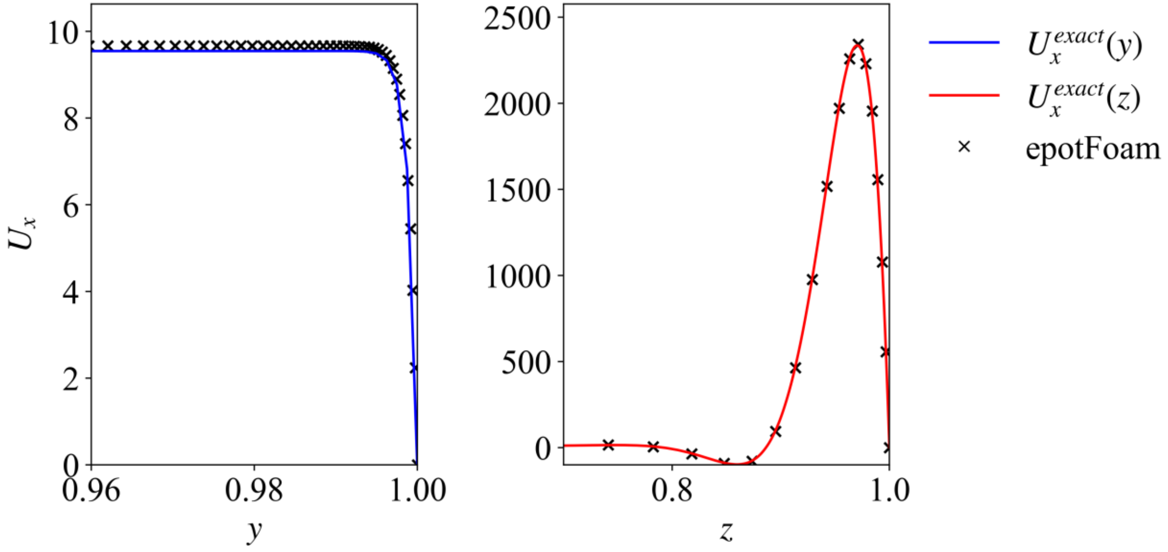
Validation Results: Ha=1000

- 300x200x50 cells/elements:
    - Mesh grading factor 200 along y.
    - Mesh grading factor 50 along z.
- Increased velocity to speed up computation (still laminar flow, $Re \sim 200$).

- Shercliff: 3 hrs on 76 cores.
    - Error $\sim 1\%$ for both RMSE(U_x) and pressure drop.
- Hunt: 1.5 hrs on 76 cores.
    - Pressure drop error ~1%
    - RMSE(U_x) $\sim 30\%$ (high where velocity crosses 0).



Shercliff flow

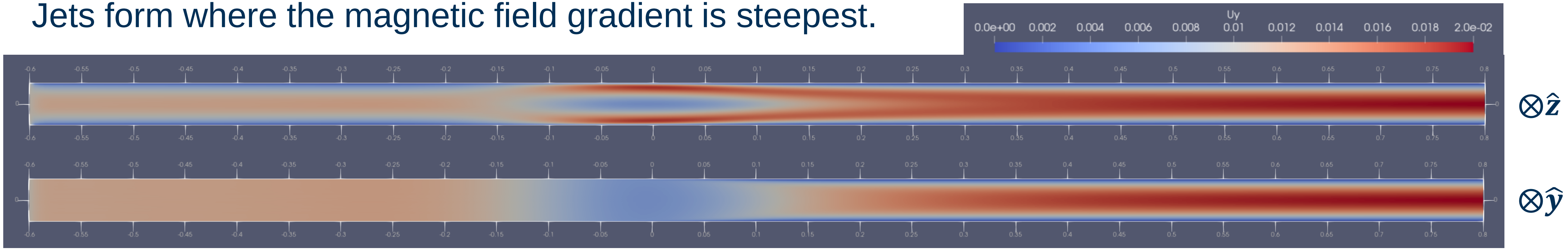


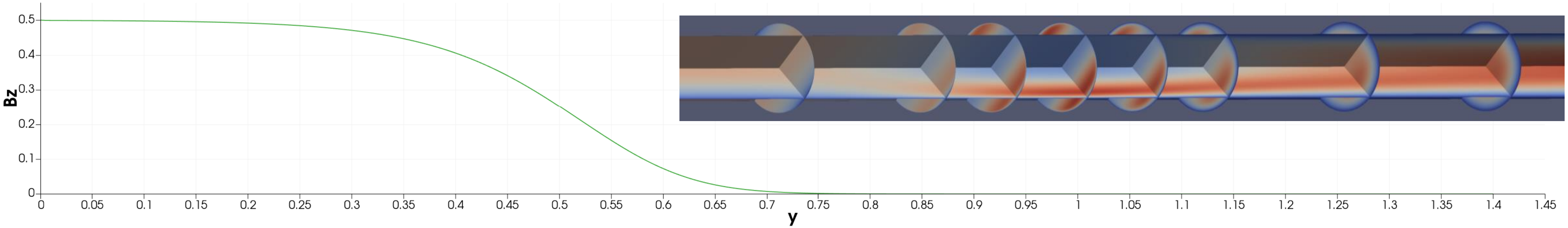
Hunt flow

Nonuniform Magnetic Field

Testing epotFoam in a more complex case – axially varying B-field.

- Based on [11] – but perfectly insulating rather than using arbitrary wall conductivity.
- Required modifying epotFoam to enable nonuniform magnetic field: https://github.com/rweardley/epotFoam/tree/epotFoamNonuniform
- Jets form where the magnetic field gradient is steepest.





[11] Reed C B, Picologlou B F, Hua T Q and Walker J S 1987 ALEX results: A comparison of measurements from a round and a rectangular duct with 3-D code predictions (CONF-871007--90) (United States)

Conclusions

- Results from OpenFOAM
  - Limitations – further work to implement more general BCs, coupling to other solvers etc, currently only transient.
  - But results are currently promising.
  - epotFoam RMSE(U_x) and pressure drop error consistently $< 3\%$ (except Hunt at $Ha = 1000$).
- Results from Proteus
  - Inaccuracy in flow profile magnitude.
  - Limitations with convergence for nonuniform meshes – prevents increasing to higher Ha.
  - Identifying the best preconditioners may help.
  - But an early start – new to MOOSE, only in early stages of development; will be continuing to investigate and develop the implementation.

Thank you

Any questions/suggestions?

Please feel free to contact me:

- Rupert Eardley (UKAEA)
- rupert.eardley@ukaea.uk

References:

[1] Müller U and Bühler L 2001 Magnetofluiddynamics in Channels and Containers (Berlin: Springer)

[2] Smolentsev S 2021 *Fluids* **6** (3) 110

[3] Smolentsev S et al. 2015 *Fusion Engineering and Design* **100** 65-72

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Acknowledgements

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