

Tensor-product elliptic solver for liquid-metal magnetohydrodynamics

[SuperMUC-NG Status and Results Workshop, May 9 – 11, 2023](#)

Computing project: **pn68ni**

Project PI: Prof. Jörg Schumacher (TU Ilmenau)

Contributors: D. Krasnov¹, P. Vieweg¹, Yu. Kolesnikov¹, K.R. Sreenivasan², A. Pandey², O. Zikanov³, Ya. Listratov⁴, I. Belyaev⁴, Sh. Bhattacharya¹, T. Boeck¹,



Leibniz
Rechenzentrum
Garching

Research network



New York University,
NYU Abu-Dhabi⁽²⁾



University of Michigan
Dearborn⁽³⁾



MPEI, JIHT-RAS⁽⁴⁾ (Moscow)

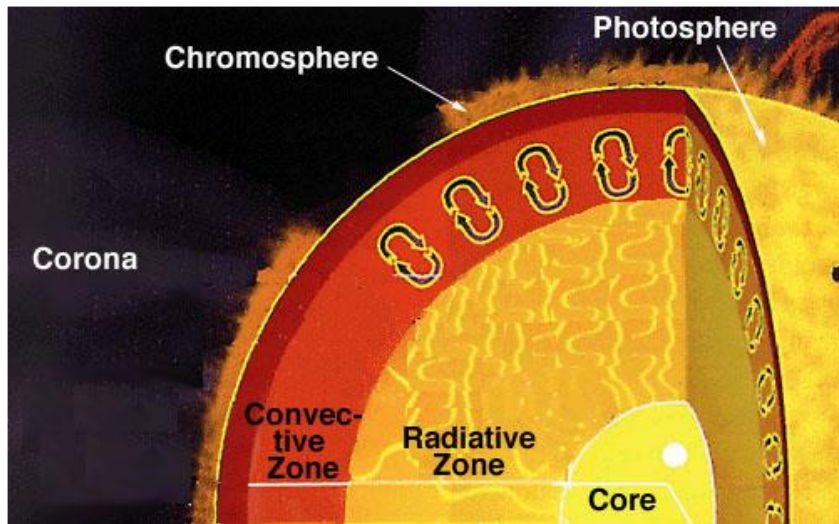


Research topics covered in 2022-2023

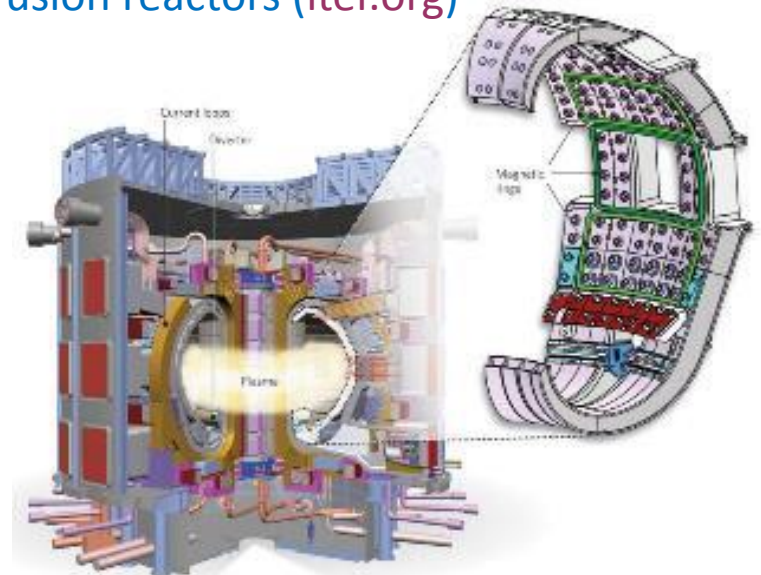
1. Turbulent convection at very low Prandtl numbers
2. Development of numerical tools for wall-bounded MHD flows
3. Evolution of MHD flows in ducts and rectangular boxes

Applications:

Solar convection with $Pr \sim 10^{-6}$



Liquid-metal cooling blankets with $Pr \sim 10^{-2}$ for fusion reactors (iter.org)



Tools applied

1. In-house flow solver for incompressible flows in rectangular geometries ([TU Ilmenau](#), [UMICH Dearborn](#))

*Key features: based on 2nd order finite-differences, conservative scheme, structured collocated grids, MPI + Open MP hybrid parallelization

2. NEK 5000 solver, open-source community driven code ([TU Ilmenau](#), [NYU](#), [NYU Abu-Dhabi](#))

*Key features: spatial discretization with spectral elements, unstructured grids, multi-domain decomposition, MPI parallelization

3. Experimental facilities with liquid mercury ([Moscow](#))

*Solenoid magnet up to 1.7T, temperature probes, electric potential sensors

Physical model:

➤ Governing equations:

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

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\nabla p + \sqrt{\frac{Pr}{Ra}} [\nabla^2 \mathbf{u} + \boxed{Ha^2 (\mathbf{j} \times \mathbf{e}_z)}] + T \mathbf{e}_z$$

$$\frac{\partial T}{\partial t} + (\mathbf{u} \cdot \nabla) T = \sqrt{\frac{1}{RaPr}} \nabla^2 T$$

$$\mathbf{j} = -\nabla \varphi + (\mathbf{u} \times \mathbf{e}_z)$$

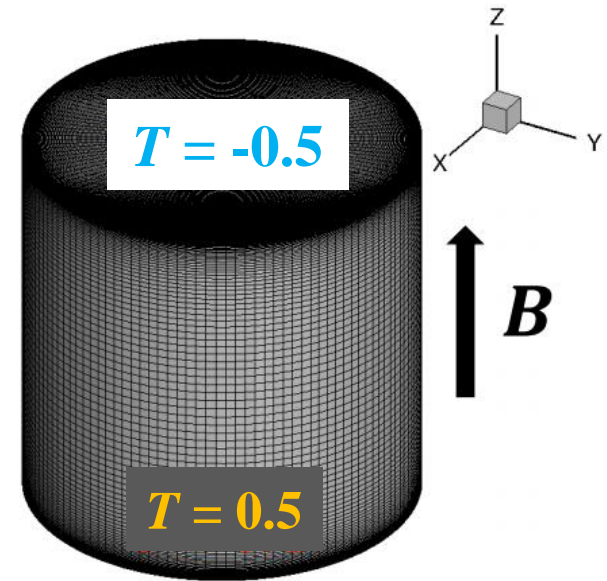
$$\boxed{\nabla^2 \varphi = \nabla \cdot (\mathbf{u} \times \mathbf{e}_z)}$$

➤ Approximations:

- The Boussinesq approximation
- The quasi-static model of electromagnetic interactions: $Re_m \ll 1$ and $Pr_m \ll 1$

➤ Non-dimensional control parameters:

$$Pr = \frac{\nu}{\kappa} \quad Ra = \frac{g\alpha\Delta TH^3}{\nu\kappa} \quad Ha = B_o H \sqrt{\frac{\sigma}{\rho\nu}} \quad \Gamma = \frac{D}{H}$$



- lateral walls are thermally insulated
- all walls are perfectly electrically insulated

Not anymore !!!

#1: Turbulent convection at low Prandtl numbers

Parameters of simulations with FD in-house solver

rectangular box with aspect ratio $L/H = 25/1$ (width/height)

$Ra = 10^5 \dots 10^7$ and $Pr = 0.021, 0.005, 0.001$

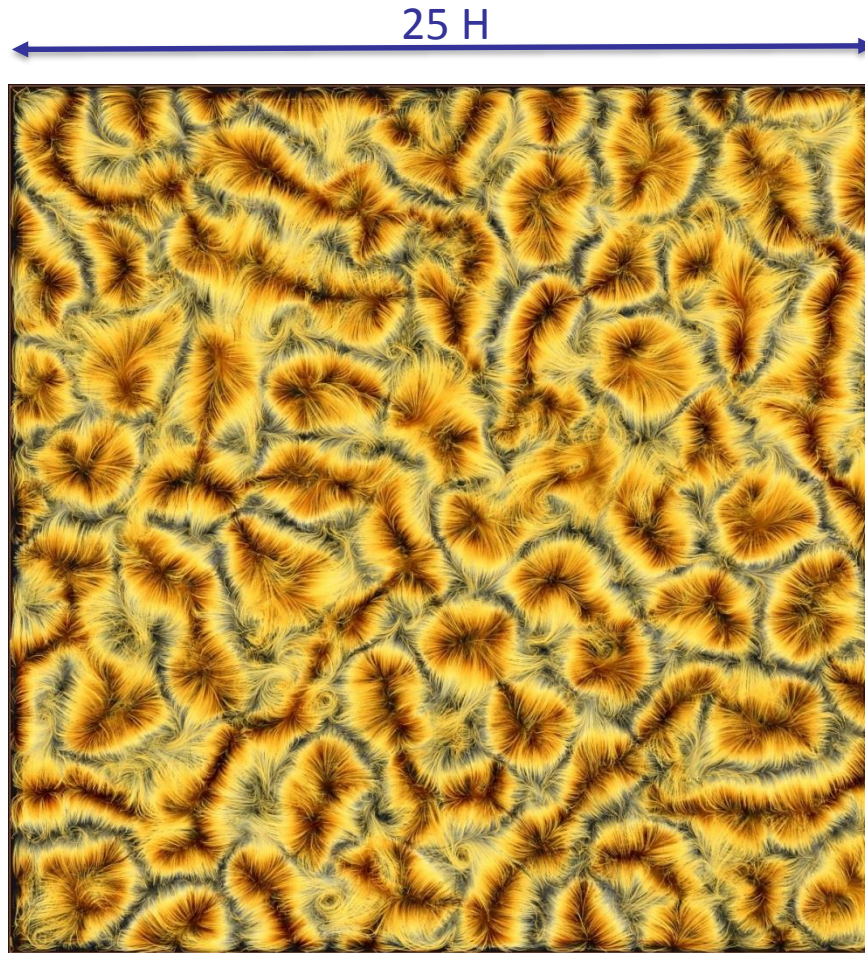
Simulation	Resolution	Computing information	Nu	Re
$Ra = 1e6, Pr = 0.021$	$8192^2 \times 512$	34 Bill. points, @ 24576 cores	4.74282523	3155
$Ra = 1e6, Pr = 0.005$	$8192^2 \times 512$	34 Bill. points, @ 24576 cores	3.48979662	7638
$Ra = 1e6, Pr = 0.001$	$12800^2 \times 800$	131 Bill. points, @ 38400 cores	2.47784979	19901
$Ra = 1e5, Pr = 0.001$	$9600^2 \times 640$	60 Bill. points, @ 28800 cores	1.21289961	4776
$Ra = 1e7, Pr = 0.001$	$20480^2 \times 1280$	0.54 Trill. points, @ 144000 cores	4.60336402	56103

Information about the largest simulation at $Ra = 10^7$ and $Pr = 10^{-3}$

- (*) consumed compute time totals 35 Mill. core-hours (one run at 144000 cores)
- (*) highest resolution maxed out at $22400^2 \times 1400 = 0.7$ Trill. points
- (*) one snapshot with 3D flow field exceeds 17 TB
- (*) total data to be post-processed more than 190 TB

#1: Turbulent convection at low Prandtl numbers

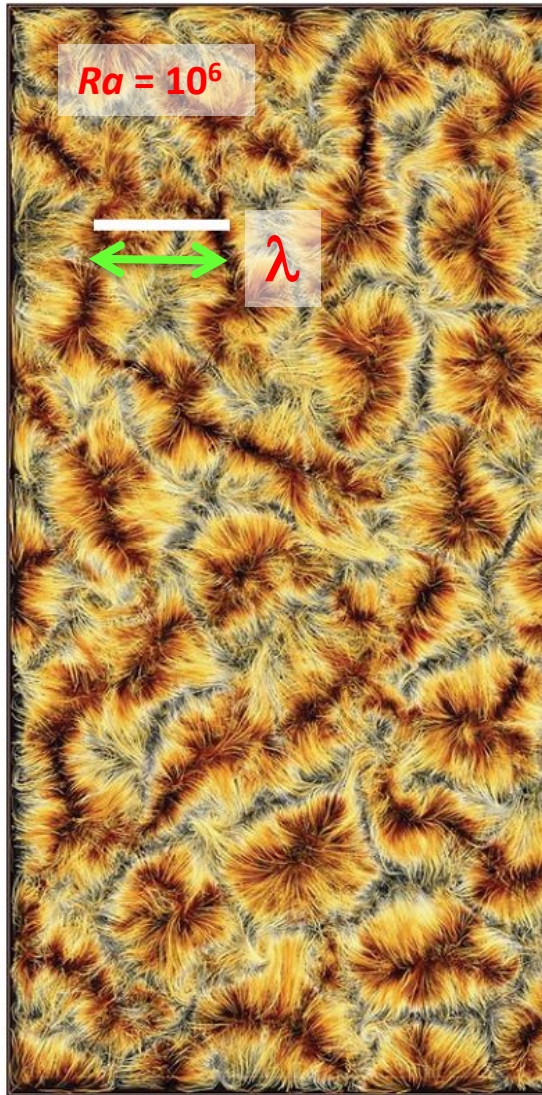
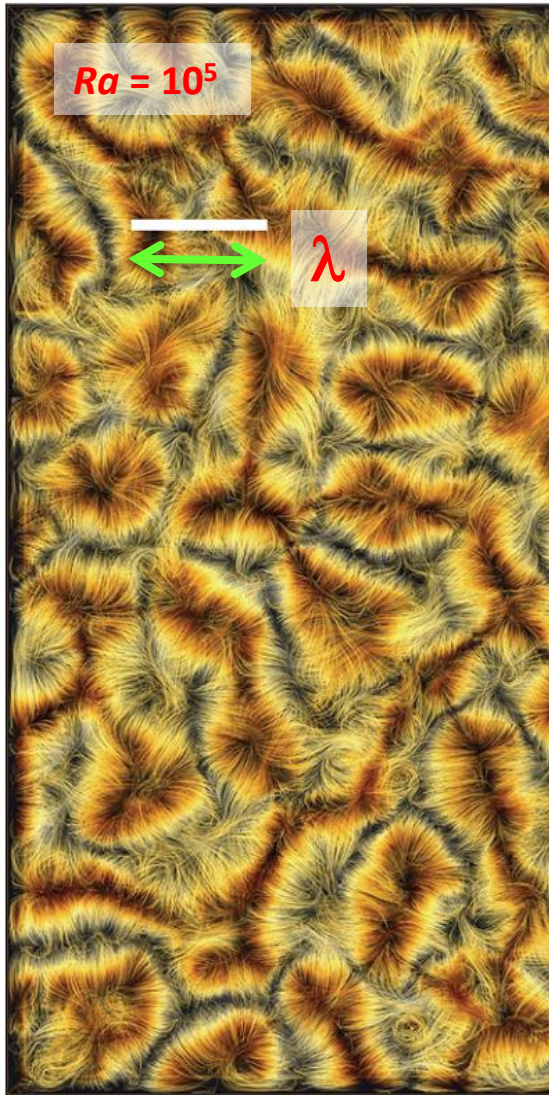
Flow field at $Ra = 10^5$ and $Pr = 0.001$ and $\Gamma = 25$ (L/H)



Superstructures shown by **streamlines**, seeded with 15000 lines

#1: Turbulent convection at low Prandtl numbers

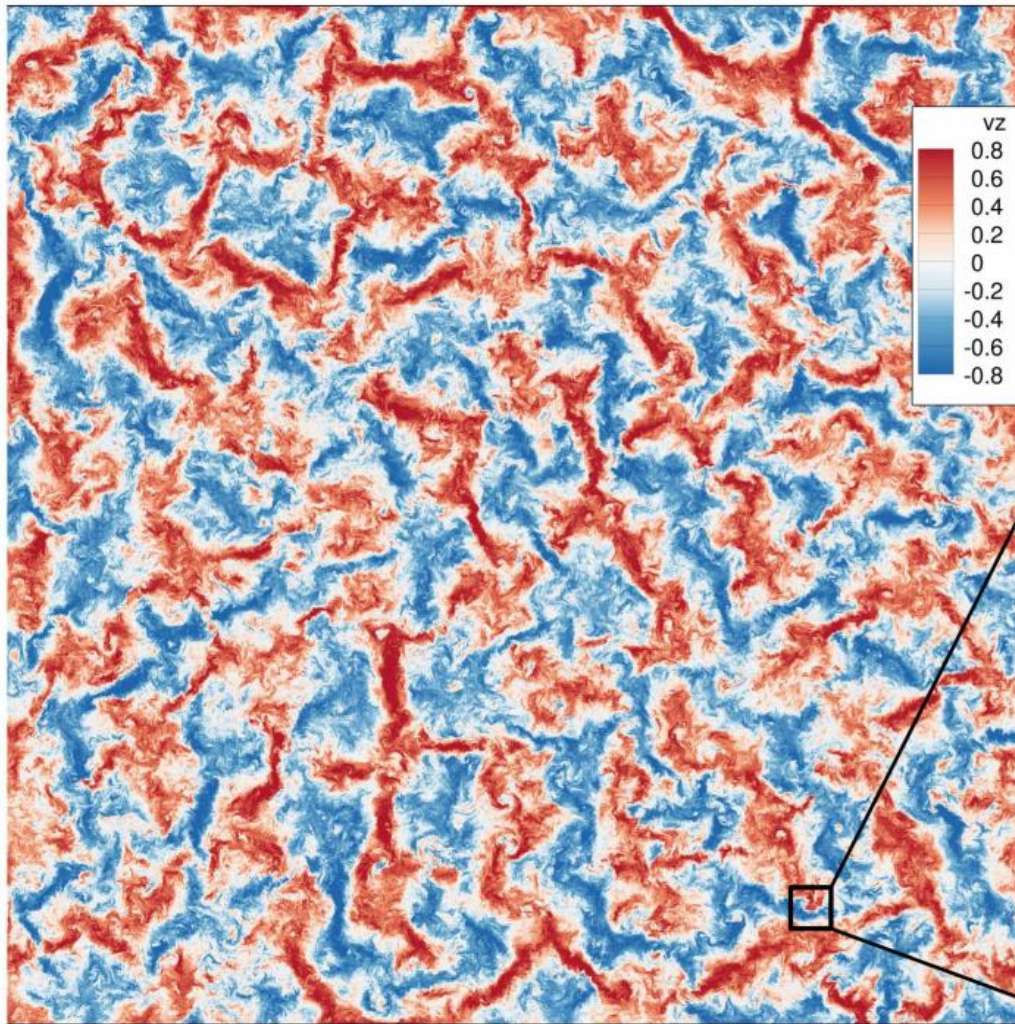
Flow fields at $Pr = 0.001$



λ – characteristic length of superstructures as typical distance between two up- or down-welling regions, about $\sim 3H$

#1: Turbulent convection at low Prandtl numbers

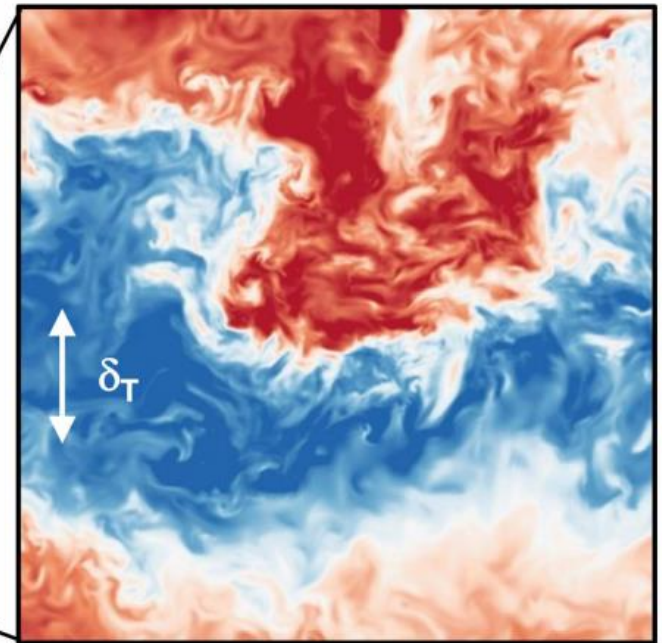
Vertical velocity V_z in the mid-plane at $Ra = 10^6$ and $Pr = 0.001$



On the left – entire domain, visualized at full resolution of 12800×12800 pixels (i.e. one pixel = one grid point)

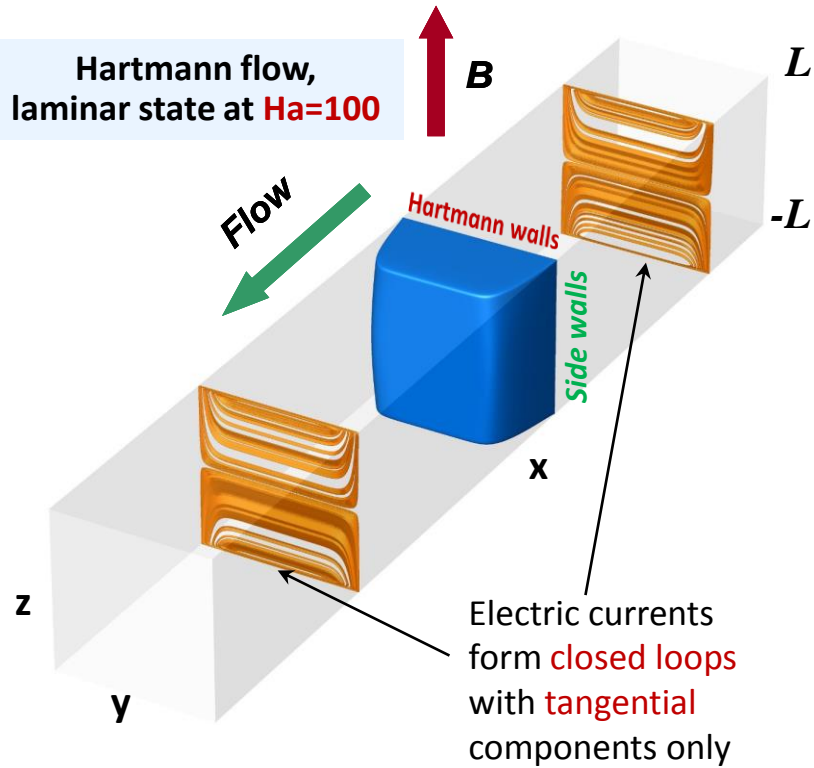
Zoom into a 1/1 region, displaying highly inertial small-scale turbulence

δ_T indicates thickness of the thermal boundary layer

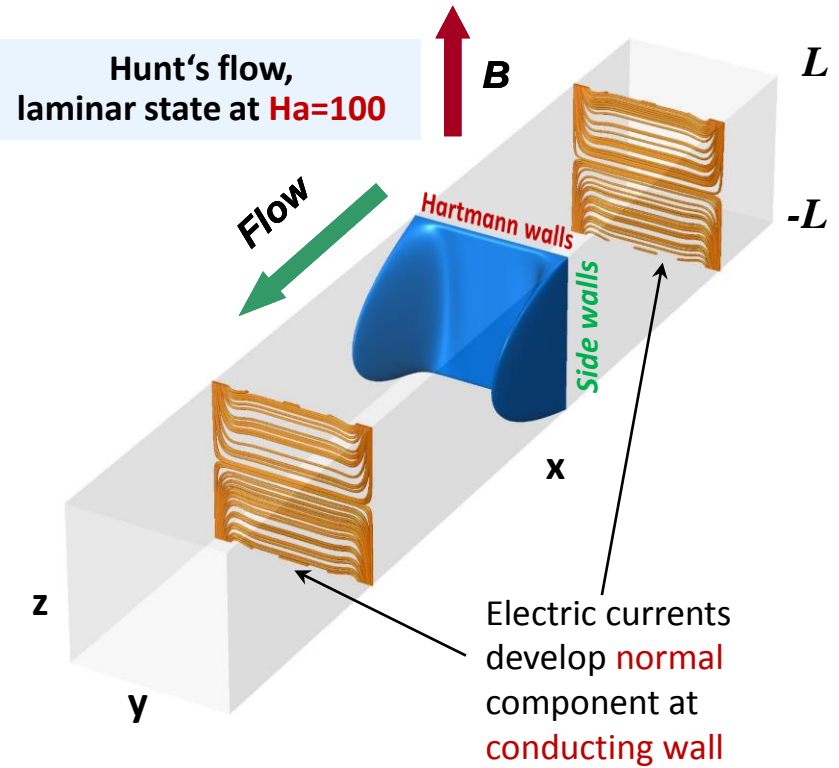


Important finding: Turbulence in the bulk is Kolmogorov-like with $E(k) \sim k^{-5/3}$

Archetypal system: MHD flow in square duct



Hartmann case: all 4 walls are insulating



Hunt's case: conducting Hartmann walls, insulating sidewalls (Shercliff walls)

- Boundary condition for electric potential, idealized cases

Side wall	$\partial\phi/\partial n = 0$	$\partial\phi/\partial n = 0$
Hartmann wall	$\partial\phi/\partial n = 0$	$\phi = const$

perfectly insulating

perfectly conducting

Finite-wall conductivity (realistic scenario)

Wall conductance ratio

$$C_w = \frac{\sigma_w \tau_w}{\sigma L}$$

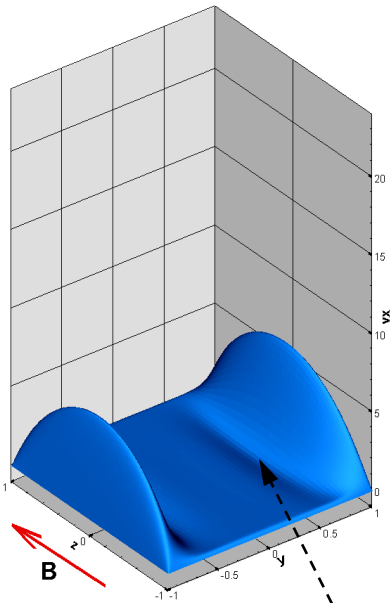
σ_w and τ_w – conductivity and thickness of the wall

σ and L – conductivity and thickness of the fluid layer

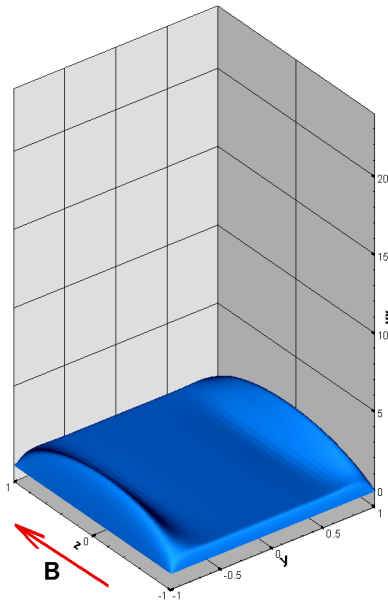
Case 1: $Ha = 100$



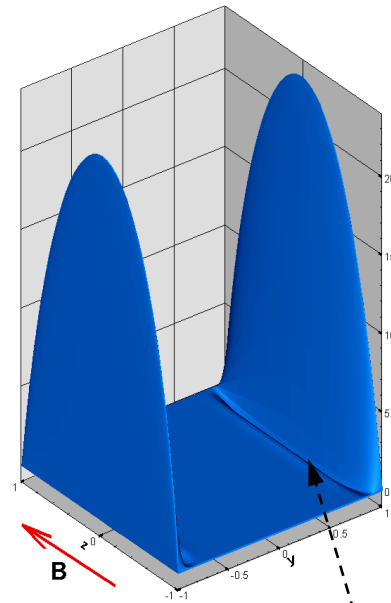
Case 2: $Ha = 1000$



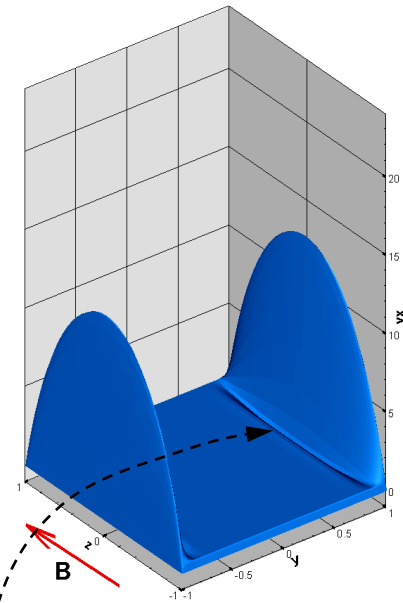
Ideally conducting Hartmann walls



Finite conductance ratio $C_w = 0.1$



Ideally conducting Hartmann walls

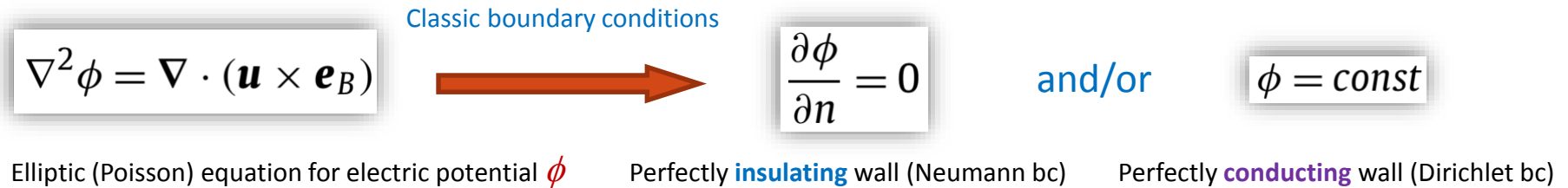


Finite conductance ratio $C_w = 0.1$

Importance: at high Ha the basic velocity profile develops **inflection points** in the region of side-jets – the flow, therefore, may (and do!) become **unstable** even at very **low- Re**

#2: Development of numerical tools for wall-bounded MHD flows

Tensor-product Elliptic solver for finite-wall conductivity



Realistic boundary condition for thin-walls with finite conductivity

$$\left. \frac{\partial \phi}{\partial n} \right|_{\text{wall}} = C_w \nabla_{\perp}^2 \phi \Big|_{\text{wall}}$$

Wall-normal derivative

Tangential 2D Laplace operator at the wall

$$C_w = \frac{\sigma_w \tau_w}{\sigma L}$$

Wall conductance ratio C_w

First proposed: J.S. Walker, J. Méc. (1981)

Main issue: solution depends on boundary conditions, whereas boundary conditions depend on solution – **chicken and egg** problem



Efficient and simple **direct** solution:

Tensor-product approach, based on identifying the eigenmodes expansion for tridiagonal matrices of **discrete** Laplace operator, modified by **embedded** thin-wall conditions

The approach can be applied on structured grids with **arbitrary clustering/stretching**

#2: Development of numerical tools for wall-bounded MHD flows

What is tensor-product approach for elliptic equations?

Tensor-product approach can be seen as the most **generalized form** of Fourier expansion, i.e. expansion into **eigenmodes**

$$\frac{\delta^2 \phi}{\delta x^2} + \frac{\delta^2 \phi}{\delta y^2} + \frac{\delta^2 \phi}{\delta z^2} = r$$

Discrete 3D Poisson equation for ϕ



Each of these operators $\frac{\delta^2 \phi}{\delta x^2}, \frac{\delta^2 \phi}{\delta y^2}, \frac{\delta^2 \phi}{\delta z^2}$ can be represented as tridiagonal matrix for the 3-point stencils of 2nd derivative

$$\frac{\delta^2}{\delta x^2} = \frac{1}{h^2} \begin{bmatrix} -2 & \dots & \dots \\ 1 & -2 & 1 \\ \dots & \dots & -2 \end{bmatrix}$$

Tridiag. matrix T_x for x-uniform grid

(1) Core idea – find eigenvalues λ , **eigenvectors** and **inverse** eigenvectors for tridiagonal matrices T_x and T_y corresponding to horizontal operators in **x**- and **y**-directions:

$T_x \rightarrow A$ (direct), λ_x and A^{-1} (inverse) and $T_y \rightarrow B$ (direct), λ_y and B^{-1} (inverse)

(2) 3D elliptic problem can be converted to the **eigenmodes space** as series of 1D problems amenable to fast Thomas tridiagonal solver in the remaining **z**-direction

$$\left(\lambda_{x,i} + \lambda_{y,j} + \frac{\delta^2}{\delta z^2} \right) \hat{\phi}_{i,j}(z) = \hat{r}_{i,j}(z), \quad i = 1, \dots, N_x, \quad j = 1, \dots, N_y$$

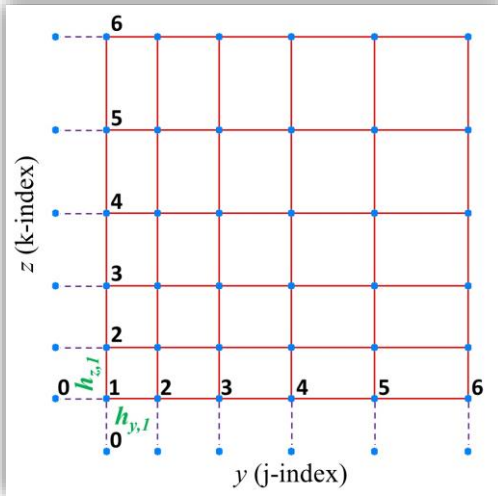
For **uniform grids** this approach retains full compatibility with **fast transforms** (FFT, cosFT, sinFT)!!!

The eigenvectors A, B converge to  **Fourier** modes for periodic conditions
Cosine modes for Neumann conditions
Sine modes for Dirichlet conditions

The eigenvalues λ_x and λ_y become $-k_x^2$ and $-k_y^2$, i.e. negatives of the square of the wave-numbers

#2: Development of numerical tools for wall-bounded MHD flows

Embedding thin-wall b.c. into eigenmode expansion



Example of rectangular grid in (y,z)

$$\frac{\phi_2 - \phi_0}{2h_1} = C_w \left(\frac{\delta^2 \phi}{\delta x^2} + \frac{\delta^2 \phi}{\delta y^2} \right)_{z_1}$$

Discrete thin-wall boundary condition



$$\frac{\delta^2 \phi}{\delta x^2} + \frac{\delta^2 \phi}{\delta y^2} + \frac{\delta^2 \phi}{\delta z^2} = r$$

Discrete 3D Poisson equation

$$\frac{2\phi_2}{h_1^2} - \frac{2\phi_1}{h_1^2} + \left(1 - \frac{2C_w}{h_1} \right) \left(\frac{\delta^2 \phi}{\delta x^2} + \frac{\delta^2 \phi}{\delta y^2} \right)_{z_1} = r_1$$

This form of thin-wall condition can be implemented with **eigenmodes** expansion

Two methods are possible, both amount to modification of the tridiagonal matrices

Method 1. Solving problem in **transformed** (eigenmodes) space, corner elements of the tridiag. matrix for **Thomas solver** are modified

$$\frac{2\hat{\phi}_2}{h_1^2} - \frac{2\hat{\phi}_1}{h_1^2} + \left(1 - \frac{2C_w}{h_1} \right) (\lambda_{x,i} + \lambda_{y,j}) \hat{\phi}_1 = \hat{r}_1 \quad \Rightarrow \quad [a_1, b_1, c_1] = \left[\times, -\frac{2}{h_1^2} + \left(1 - \frac{2C_w}{h_1} \right) (\lambda_{x,i} + \lambda_{y,j}), \frac{2}{h_1^2} \right]$$

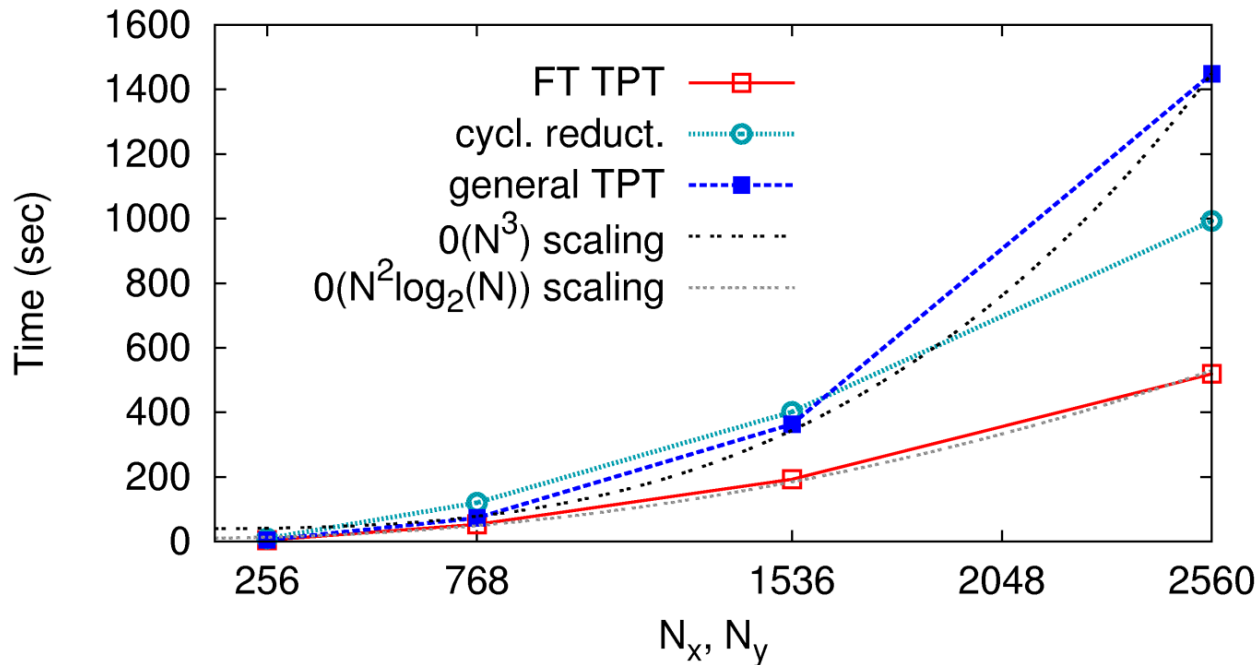
Method 2. Modify tridiag. matrix in **real** space, then use this matrix to identify **modified** eigenmodes, then transform and solve

$$\frac{2\phi_2}{h_1^2} \frac{h_1}{h_1 - 2C_w} - \frac{2\phi_1}{h_1^2} \frac{h_1}{h_1 - 2C_w} + \left(\frac{\delta^2 \phi}{\delta x^2} + \frac{\delta^2 \phi}{\delta y^2} \right)_{z_1} = r_1 \frac{h_1}{h_1 - 2C_w} \quad \Rightarrow \quad [a_1, b_1, c_1] = \left[\times, -\frac{2}{h_1^2} \frac{h_1}{h_1 - 2C_w}, \frac{2}{h_1^2} \frac{h_1}{h_1 - 2C_w} \right]$$

#2: Development of numerical tools for wall-bounded MHD flows

Benchmarks of tensor-product vs. other methods (performed on SuperMUC-NG)

Rayleigh-Bénard convection in a rectangular box computed on grids with various $N_x = N_y = N$ and $N_z = 256$
 Clock time required to compute 100 time steps on 256 cores is shown as a function of N
 Matrix multiplications in **general TPT** are performed with **MKL multi-thread** routines



General TPT = Tensor-Product-Thomas solver, i.e. MatMul in x,y and Thomas method in z
 Cycl. Reduct. = Cosine-FT in x and 2D Cyclic reduction method (Fishpack) in y,z
 FT TPT = Fast Transform Tensor-Product-Thomas, i.e. Cosine-FT in x,y and Thomas method in z



Only **TPT** allows for arbitrary grid-clustering in x,y,z

#2: Tensor-product elliptic solver, list of pros and cons

(in part inspired by car reviews 😊 from Mat Watson/carwow youtube)

Prerequisite – elliptic problem should be **separable**, thus decomposition into eigenmodes can be applied (basically that implies constant coefficients and structured grids)

Good points

- Direct solver – no iterations, no convergence **issues**
- Arbitrary **grid-clustering** in all 3 directions
- MKL matmul routines scale up **almost linearly** vs. number of threads
- Can be extended to curvilinear grid if separable (e.g. **cylinder** coords.)
- No **speed-penalty** vs. classic Neumann and Dirichet conditions
- Each wall can be assigned its **own** conductance ratio C_w
- Can be applied for finite **thermal conductivity**, even for unsteady form

Annoying points

- Transform matrices grow in size as n^2 – potential issue at hi-res
- Matrix multiplication scales as $O(n^3)$, vs. $O(n^2 \log_2(n))$ for FFT/CosFT/SinFT

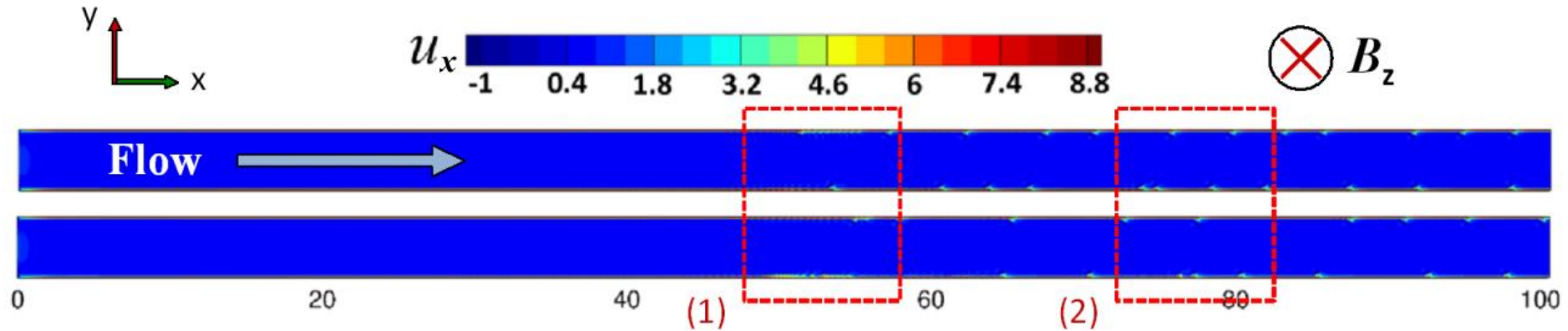
- Five good points about the car
- Five annoying points about the car



Copyright carwow.co.uk and Mat Watson

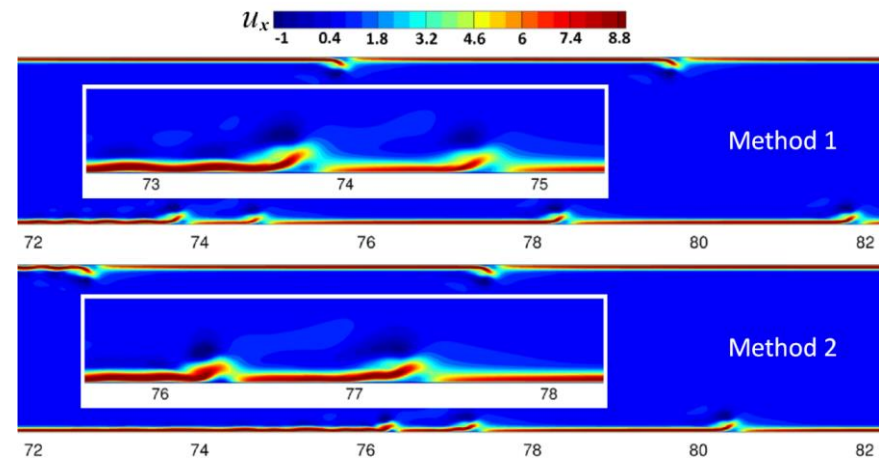
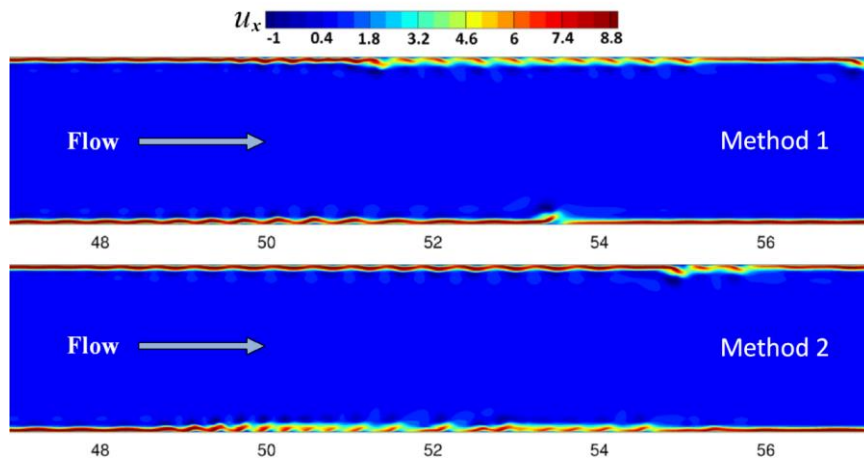
#3: Evolution of MHD flows in ducts and rectangular boxes (examples)

MHD flows in **ducts** with conducting walls – typical configuration for liquid-metal **fusion blankets**
 Spatial evolution of Hunt's flow at $Re = 2000$, $Ha = 2000$ and $C_w = 0.03$



Region (1): Onset of sidewall **jet instabilities**

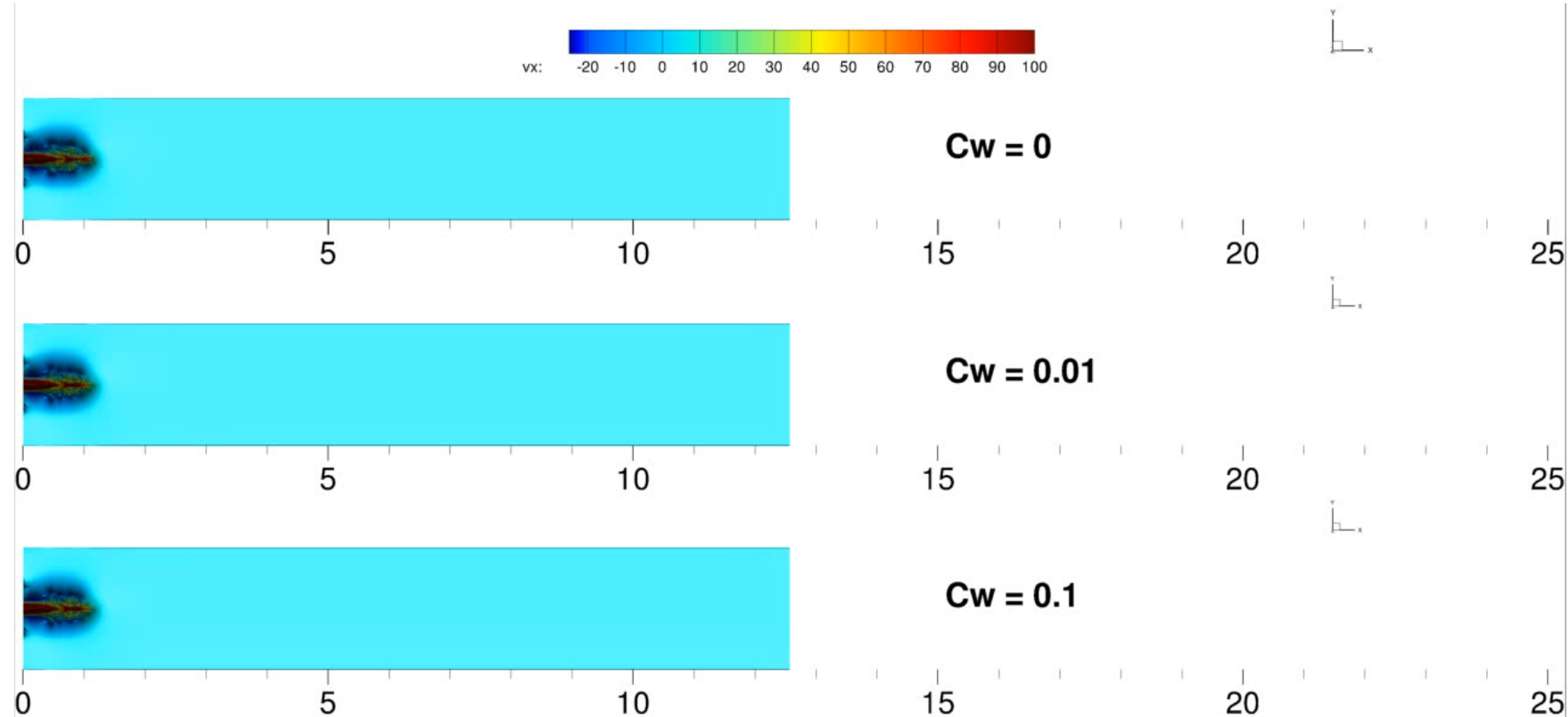
Region (2): Fully developed **jet detachments**



- Krasnov et.al. *J. Comp. Phys.* (2023)

#3: Evolution of MHD flows in ducts and rectangular boxes (examples)

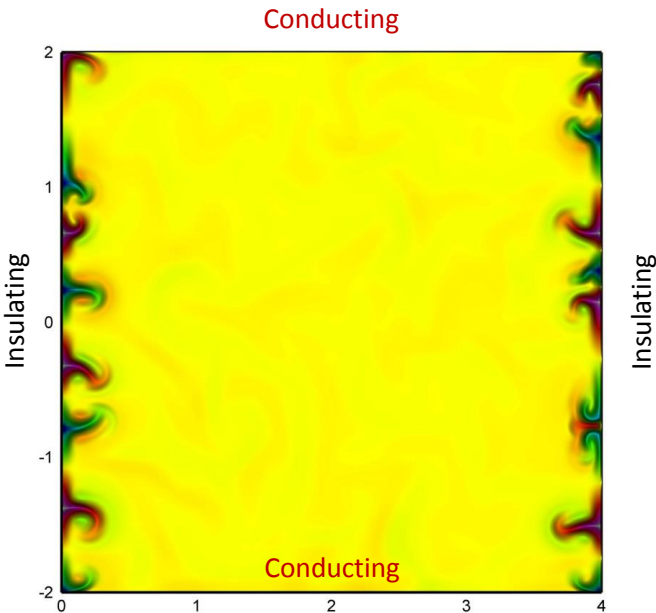
Effect of wall conductivity on instability of a submerged round jet, entering square duct
Uniform vertical magnetic field B_z at $Ha=500$, flow at $Re=1000$



#3: Evolution of MHD flows in ducts and rectangular boxes (examples)

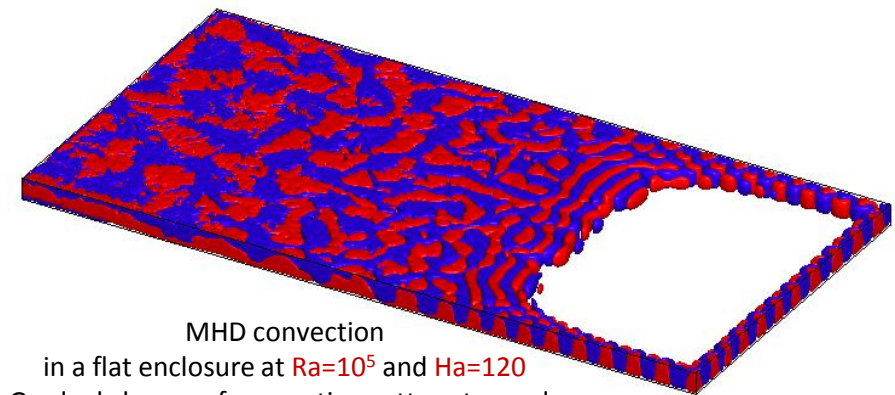
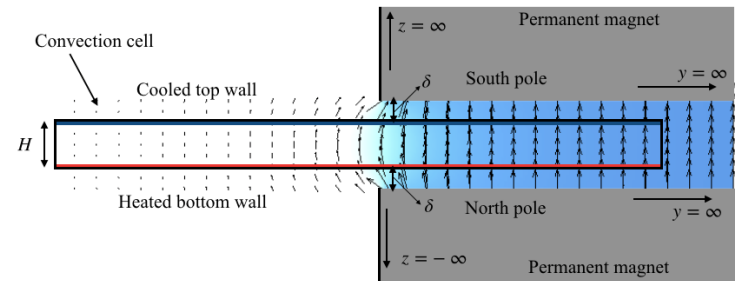
Magneto-thermal convection flows around and above the Chandrasekhar stability limit
 At these conditions convective motion is expected to be fully **suppressed** by strong magnetic field
 However, residual motion at the sidewalls – **wall-modes** – can exist far above even if the rest has “died”

Fundamental: effect of wall conductivity
 on the wall-modes at uniform magnetic field



MHD convection in a rectangular box at $Ra=10^7$ and $Ha=1000$
 Wall-modes are killed at conducting side-walls $C_w=0.1$

Fusion relevant:
 wall-modes at fringing magnetic field



MHD convection
 in a flat enclosure at $Ra=10^5$ and $Ha=120$
 Gradual change of convective pattern towards
 anisotropic structures and wall-modes

- Bhattacharya et.al., *J. Fluid Mech.* (2023)


References

- A. Pandey, D. Krasnov, K. R. Sreenivasan and J. Schumacher, *Convective mesoscale turbulence at very low Prandtl numbers*, *J. Fluid Mech.* vol. 948, A23, 2022
- A. Pandey, D. Krasnov, J. Schumacher, R. Samtaney, K. R. Sreenivasan, *Similarities between characteristics of convective turbulence in confined and extended domains*, *Physica D.* 422, 2022
- *High Performance Computing in Science and Engineering*, **LRZ Garching/Munich 2022**
- I.A. Belyaev, I.S. Mironov, N.A. Luchinkin, Ya.I. Listratov, Yu. Kolesnikov, D. Krasnov, O. Zikanov and S. Molokov, *Experimental study of submerged liquid metal jet in a rectangular duct in a transverse magnetic field*, *J. Fluid Mech.*, 2023 (in press)
- D. Krasnov, A. Akhtari, O. Zikanov, J. Schumacher, Tensor-product-Thomas elliptic solver for liquid-metal magnetohydrodynamics, *J. Comp. Phys.* Vol. 474, 2023
- S. Bhattacharya, T. Boeck, D. Krasnov and J. Schumacher, *Effects of strong fringing magnetic fields on turbulent thermal convection*, *J. Fluid Mech.* 2023 (just accepted)

P. Bastian • D. Kranzlmüller • H. Brühle • G. Mathias
EDITORS

High Performance Computing

in Science and Engineering
Garching/Munich 2022



KONWIHR
Leibniz Supercomputing Centre
of the Bavarian Academy of Sciences and Humanities

GCS

J. Fluid Mech. (2022), vol. 948, A23, doi:10.1017/jfm.2022.694

JFM PAPERS

Convective mesoscale turbulence at very low Prandtl numbers

Amrish Pandey^{1,†}, Dmitry Krasnov², Katepalli R. Sreenivasan^{1,3,4} and Jörg Schumacher^{2,1,†}

¹Center for Space Science, New York University Abu Dhabi, PO Box 129188, Abu Dhabi, UAE
²Institut für Thermo- und Fluidodynamik, Technische Universität Ilmenau, PO Box 100565, D-98684 Ilmenau, Germany
³Tandon School of Engineering, New York University, New York, NY 11201, USA
⁴Department of Physics and Courant Institute of Mathematical Sciences, New York University, New York, NY 11201, USA

(Received 18 February 2022; revised 17 June 2022; accepted 5 August 2022)

Horizontally extended turbulent convection, termed mesoscale convection in natural systems, remains a challenge to investigate in both experiments and simulations. This is particularly so for very low molecular Prandtl numbers, such as occur in stellar convection and in the Earth's outer core. The present study reports three-dimensional direct numerical simulations of turbulent Rayleigh-Bénard convection in square boxes of side length L and height H with the aspect ratio $\Gamma = L/H$ of 25, for Prandtl numbers that span almost 4 orders of magnitude, $10^{-3} \leq Pr \leq 7$, and Rayleigh numbers $10^5 \leq Ra \leq 10^7$, obtained by massively parallel computations on grids of up to 5.36×10^6 points. The low end of this Pr -range cannot be accessed in controlled laboratory measurements. We report the essential properties of the flow and their trends with the Rayleigh and Prandtl numbers, in particular, the global transport of momentum and heat – the latter decomposed into convective and diffusive contributions – across the convection layer, mean vertical profiles of the temperature and temperature fluctuations and the kinetic energy and thermal dissipation rates. We also explore the degree to which the turbulence in the bulk of the convection layer resembles classical homogeneous and isotropic turbulence in terms of spectra, increment moments and dissipative anomaly, and find close similarities. Finally, we show that a characteristic scale of the order of the mesoscale scale to saturate to a wavelength of $\lambda \approx 3H$ for $Pr \leq 0.005$. We briefly discuss possible implications of these results for the development of subgrid-scale parameterization of turbulent convection.

† Email addresses for correspondence: amrish.pandey@nyu.edu, joerg.schumacher@tu-ilmenau.de

© The Author(s), 2022. Published by Cambridge University Press. This is an Open Access article, distributed under the terms of the Creative Commons Attribution licence (<http://creativecommons.org/licenses/by/4.0/>), which permits unrestricted re-use, distribution and reproduction, provided the original article is properly cited.

948 A23-1

Journal of Computational Physics 474 (2022) 11784

Contents lists available at ScienceDirect
Journal of Computational Physics
journal homepage: www.elsevier.com/locate/jcp

ELSEVIER

Tensor-product-Thomas elliptic solver for liquid-metal magnetohydrodynamics

Dmitry Krasnov^{1,*}, Ali Akhtari², Oleg Zikanov³, Jörg Schumacher⁴

¹ Institut für Thermo und Fluidodynamik, Technische Universität Ilmenau, D-98684 Ilmenau, Germany
² Department of Mechanical Engineering, University of Michigan - Dearborn, 4901 Evergreen Road, Dearborn, MI 48126, MI, USA

ARTICLE INFO

Article history:
Received 12 March 2022
Received in revised form 23 September 2022
Accepted 12 November 2022
Available online 24 November 2022

ABSTRACT

A new approach to numerical simulation of magnetohydrodynamic flows of liquid metals is presented. It combines the conservative finite-difference discretization with a tensor-product-Thomas solution of the elliptic problems for pressure, electric potential, velocity, and temperature. The method is realizable on an arbitrarily clustered structured grid. The main novelty of the approach is the efficient solution of the practically important and computationally challenging elliptic problems for electric potential in flow domains with thin electrically conducting walls. The method is verified via solution of benchmark problems for streamwise-uniform and nonuniform, steady and unsteady magnetohydrodynamic flows in ducts, and for thermal convection in boxes of various aspect ratios. Computational efficiency of the method in comparison to the existing ones is demonstrated.

© 2022 Elsevier Inc. All rights reserved.

Keywords:
Elliptic solvers
Magnetohydrodynamic flows
Flow instability
Wall conductivity
Thermal convection

1. Introduction

Magnetohydrodynamic (MHD) flows of liquid metals and other strongly electrically conducting fluids are found in traditional and emerging technologies, such as casting and remelting of steel and aluminum [1], growth of semiconductor crystals [2], or liquid-metal blankets and divertors conceptualized for future nuclear fusion reactors [3]. A steady magnetic field is either purposely imposed to control the flow, as e.g., in casting of metals and growth of crystals, or required by technological needs unrelated to the flow, as in fusion reactors. In practically all such systems, perturbations of the magnetic field caused by motion of the fluid are weak in comparison to the imposed magnetic field. The problem can be simplified by neglecting the perturbations in the expressions of the Ohm's law and Lorentz force. Derivation and discussion of applicability of this quasi-static (inductionless) approximation can be found, e.g., in [4]. Another commonly valid approximation is that of modeling the liquid metal as an incompressible (or Boussinesq in systems with thermal convection) constant-property fluid.

Despite being simpler than the full MHD model, the quasi-static approximation presents significant and yet not fully answered challenges to computational analysis. The main reason is the profound transformation of the flow caused by the magnetic field. Mechanisms of the transformation and its types are discussed in literature (see, e.g., the recent reviews [5–8]). Here we only list the main features: suppression of turbulent velocity fluctuations, development of thin MHD boundary and internal shear layers, and transformation of a flow into an anisotropic state, in which gradients of flow variables along the magnetic field lines are reduced. If the effect of the magnetic field is strong, i.e., the Hartmann and Stuart N numbers

* Corresponding author.
E-mail address: dmitry.krasnov@tu-ilmenau.de (D. Krasnov).

<https://doi.org/10.1016/j.jcp.2022.11784>
0021-9991/© 2022 Elsevier Inc. All rights reserved.

Outlook & Possible next steps

- Convection at low Pr : exploring broader parameter space and longer statistics (time-evolution)
- Extension of the tensor-product approach to solve problems with finite *thermal* wall-conductivity → *conjugate* heat transport “made easy”
- It would be interesting to explore application of practical algorithms of fast matrix multiplication possibly utilizing the symmetry properties of the transform matrices to achieve scaling better than $O(n^3)$

Thanks a lot for your attention!

Project support/Acknowledgements



National Science
Foundation

