Pseudospectral Simulations in Complex Geometry via Penalization

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Introduction

- The Pseudospectral Method
- The Penalty Method
- Magnetohydrodynamic Simulations
- Fluid-Structure Interactions: Insects
- `FFTW++`
- `Higher-order penalization`

The Pseudospectral Method

The incompressible Navier–Stokes equations

$$\begin{aligned} \partial_t u &= (u \cdot \nabla) u - \boldsymbol{\nabla} P + \nu \nabla^2 u \\ \nabla \cdot u &= 0 \end{aligned}$$

have Fourier transform

$$\begin{aligned} \partial_t U_k &= \mathcal{F}[(u \cdot \nabla) u] - ikP - \nu k^2 U_k \\ ik \cdot U_k &= 0. \end{aligned}$$

In Fourier space:

1. Derivatives are easy to compute.
2. Convergence is quick if the field is regular.

The Pseudospectral Method

The nonlinear term becomes a convolution in Fourier space:

$$\mathcal{F}[(u \cdot \nabla)u] = (U_k \cdot ik) * U_k.$$

Direct computation of a convolution takes $\mathcal{O}(N^2)$ operations.
It is faster to transform back to physical space:

1. Inverse FFT: $\mathcal{O}(N \log N)$ operations.
2. Multiply: $\mathcal{O}(N)$ operations.
3. Forward FFT: $\mathcal{O}(N \log N)$ operations.

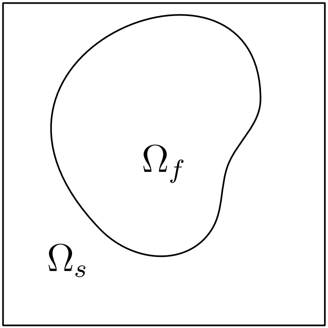
It is important to *dealias* a FFT-based convolution to recover the original nonlinear term.

The Penalty Method

The pseudospectral method uses a periodic domain.

Applications require more complicated geometries.

Let Ω_f denote the fluid domain and Ω_s the solid domain.



The Penalty Method

We *penalize* the velocity in the wall region.

$$\partial_t u = (u \cdot \nabla) u - \boldsymbol{\nabla} P + \nu \nabla^2 u - \frac{1}{\eta} \chi(x)_{\Omega_s} u$$

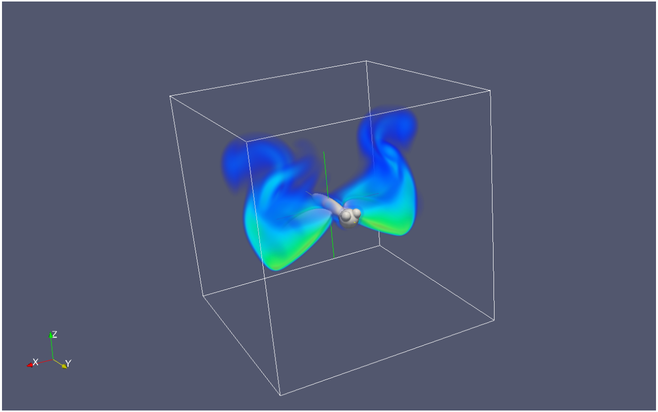
where χ_{Ω_s} is the characteristic function for the set Ω_s.

The computational domain $\Omega = \Omega_f \cup \Omega_s$ is a periodic box.

The fluid domain Ω_f can be quite general.

Application: Fluid-Structure Interaction

Thomas Engels, Kai Schneider, Dmitry Kolomenskiy.
A coupled solid-fluid system is used to simulate insect flight.

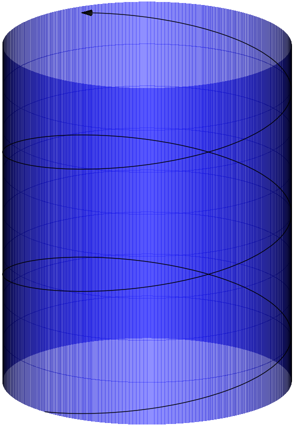


Application: Confined MHD flow

Malcolm Roberts, Matthieu Leroy, Kai Schneider

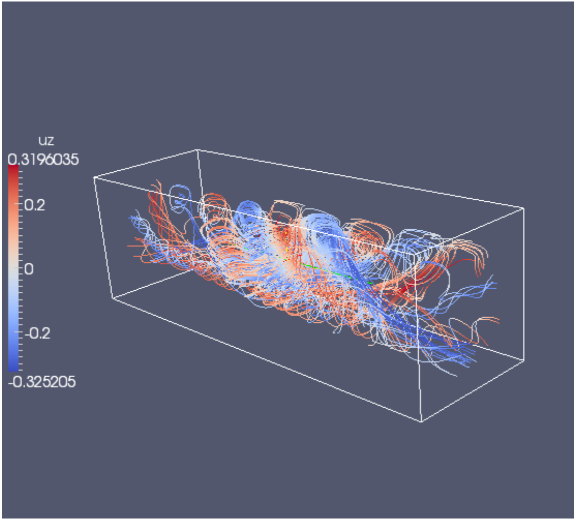
A magneto fluid is placed in a periodic cylinder.

The magnetic field is forced helically at the boundaries.

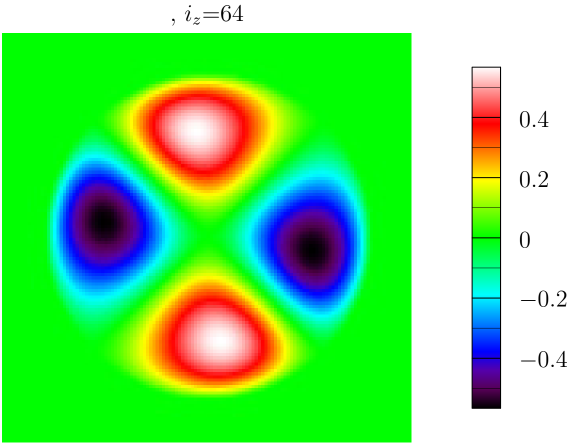


Confined MHD flow: Circular Geometry

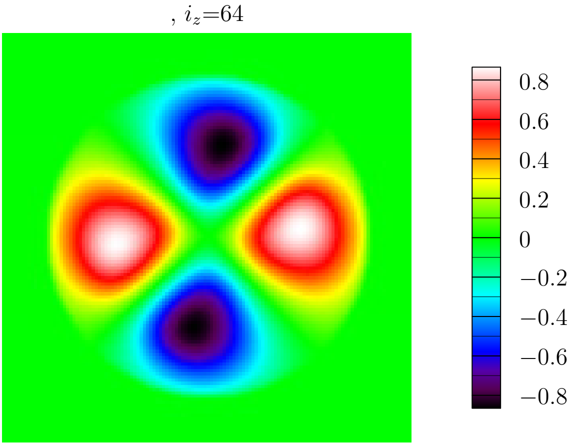
For large forcing parameters, helical vortices emerge.



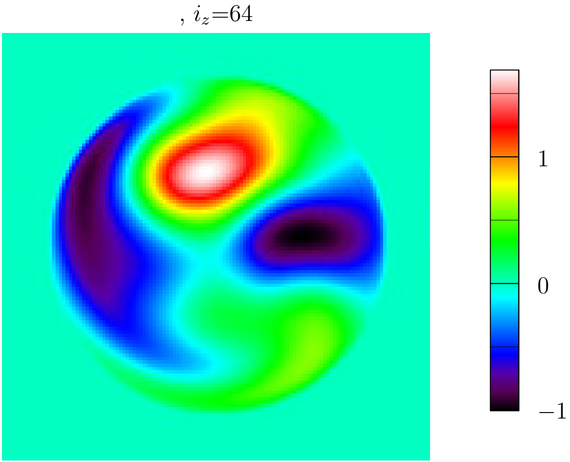
Confined MHD flow: Circular Geometry



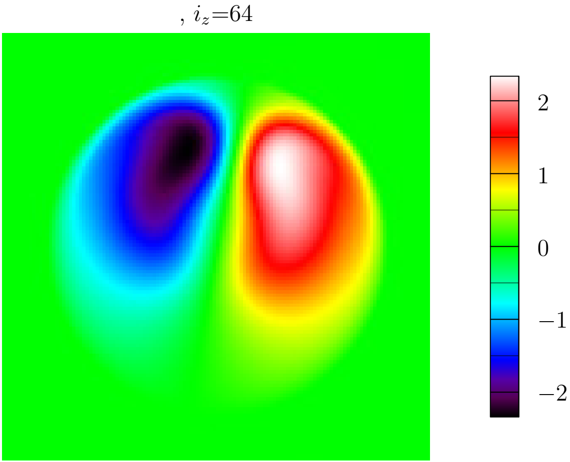
Confined MHD flow: Circular Geometry



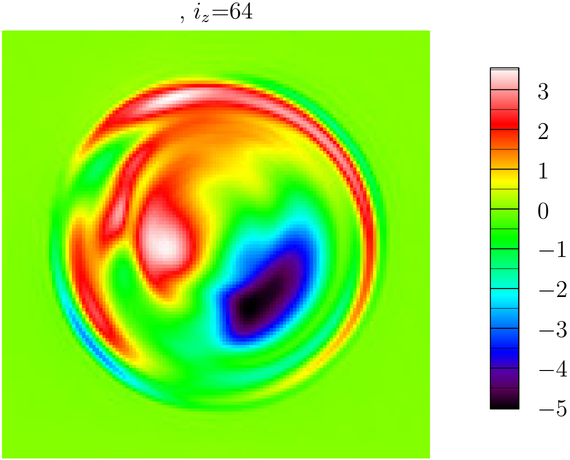
Confined MHD flow: Circular Geometry



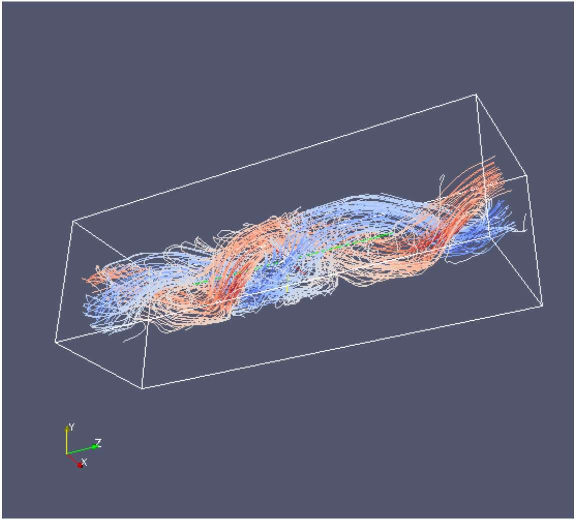
Confined MHD flow: Circular Geometry



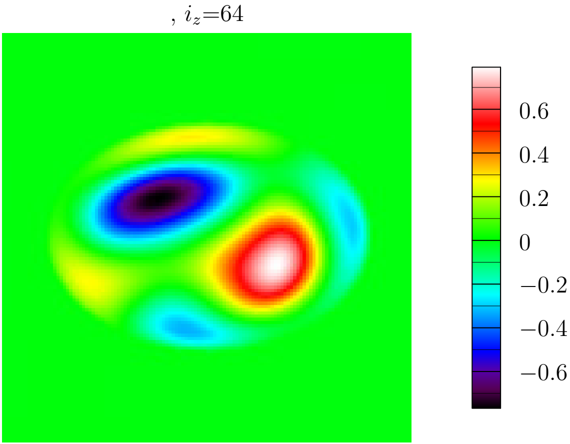
Confined MHD flow: Circular Geometry



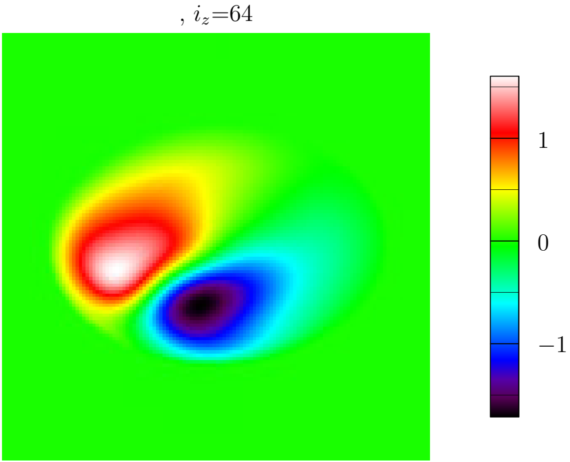
MHD flow: Elliptical Geometry



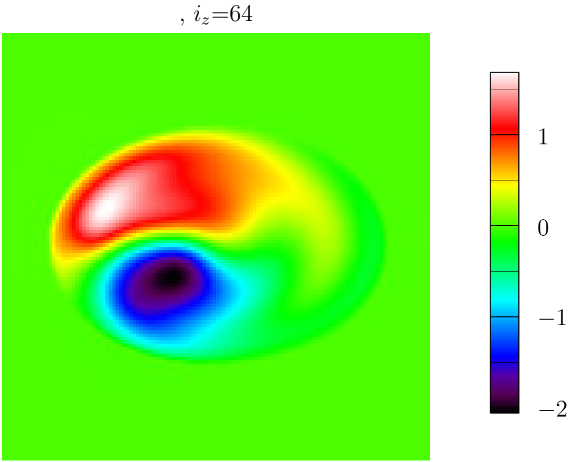
MHD flow: Elliptical Geometry



MHD flow: Elliptical Geometry



MHD flow: Elliptical Geometry



FFTW++

FFTW++ wraps FFTW for C++. John C Bowman (University of Alberta) and Malcolm Roberts Hybrid MPI/OpenMP, $2D$ decomposition. Features *implicitly dealiased convolutions*.

1. Convolutions on d-dimensional data use $(1/2)^{d-1}$ or $(2/3)^{d-1}$ less memory.
2. Single-core convolutions $\approx 2\times$ as fast as the explicit method.
3. Multi-threaded convolutions $\approx 4\times$ as fast.
4. Multi-process convolutions $\approx 6\times$ as fast.

Current work: implementation and use in and MPI pseudospectral code.

Penalty method

The accuracy of the penalty method is

$$\mathcal{O}(\sqrt{\eta} \times dx)$$

Improving regularity of the penalty field may improve convergence. The time-step is restricted by

$$dt < \eta.$$

It may be possible to remove this condition.

Conclusion

Code is open-source and online:

- github.com/pseudospectators/FLUSI
- fftwpp.sf.net

Thank you for your attention!