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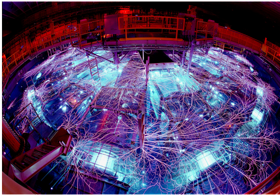

An adjoint based *a posteriori* error analysis for MHD

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Context

- Adjoint based optimization strategies explored for MHD and Grad-Shafranov[1,2]
- No adjoint based error analysis (full error decomposition) applied to MHD
- Study error contributions to inform discretizations and solver methods

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[1] Zhigang Ren et al. *Adjoint-based parameter and state estimation in 1-D magnetohydrodynamic (MHD) flow system*. Jan. 2018. URL: https://www.aimsciences.org/article/doi/10.3934/jimo.2018022.

[2] Thomas Antonsen, Elizabeth J. Paul, and Matt Landreman. *Adjoint approach to calculating shape gradients for three-dimensional magnetic confinement equilibria: Journal of Plasma Physics*. Mar. 2019. URL: https://www.cambridge.org/core/journals/journal-of-plasma-physics/article/adjoint-approach-to-calculating-shape-gradients-for-threedimensional-magnetic-confinement-equilibria/ED3C467C28CB98B2B7B036EA356120EB.

Outline

Magnetohydrodynamics (MHD)

A posteriori error analysis

Results

What is MHD?

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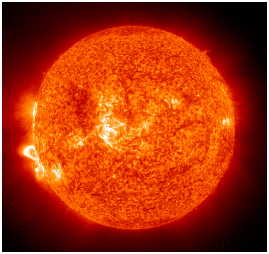

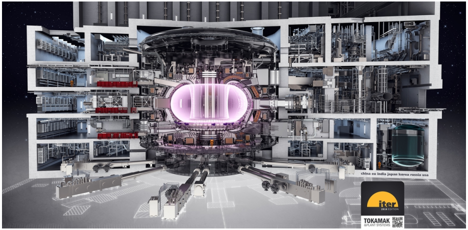

- Mathematical Model: Continuum representation of collisional plasma systems.
- Strongly coupled conducting fluid flow with reduced electromagnetics description
- Structure of simple MHD is Navier-Stokes + Lorentz force coupled with low frequency Maxwell equations.

MHD System

Stationary incompressible MHD system

$$-\frac{1}{R_f}\Delta \boldsymbol{u} + \boldsymbol{u}\cdot\nabla\boldsymbol{u} + \nabla p - \kappa(\nabla\times\boldsymbol{B})\times\boldsymbol{B} = \boldsymbol{f}$$

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

$$\frac{\kappa}{R_m}\nabla\times(\nabla\times\boldsymbol{B}) - \kappa\nabla\times(\boldsymbol{u}\times\boldsymbol{B}) = \mathbf{0},$$

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

- Unknowns: magnetic field $\mathbf{B}$, velocity $\mathbf{u}$, pressure p
- Nondimensionalized parameters: Reynold's number R_f, magnetic Reynold's number R_m, interaction parameter κ.
- Incompressibilty and solenoidal involution produce saddle point structure
- Three sources of nonlinearity + coupling between equations = complex multiphysics system

Exact Penalty Method Assumptions

- Exact penalty relies on the continuous embedding[3] of $\boldsymbol{H}(\mathrm{curl}) \cap \boldsymbol{H}(\mathrm{div}) \subset \boldsymbol{H}^1$
- Only valid for convex domains
- With this assumption, $\boldsymbol{B}$ will be in $\boldsymbol{H}^1(\Omega)$

We need to following spaces,

$$\boldsymbol{H}_0^1(\Omega) := \{\boldsymbol{w} \in \boldsymbol{H}^1(\Omega) : \boldsymbol{w}|_{\partial\Omega} \equiv \mathbf{0}\},$$
$$\boldsymbol{H}_\tau^1(\Omega) := \{\boldsymbol{w} \in \boldsymbol{H}^1(\Omega) : (\boldsymbol{w} \times \boldsymbol{n})|_{\partial\Omega} \equiv \mathbf{0}\}.$$

Then define the product spaces,

$$\mathscr{P}_{0\tau}(\Omega) := \boldsymbol{H}_0^1(\Omega) \times \boldsymbol{H}_\tau^1(\Omega),$$
$$\mathscr{P}(\Omega) := \mathscr{P}_{0\tau}(\Omega) \times L^2(\Omega).$$

[3] Martin and Monique Dauge. *Weighted regularization of Maxwell equations in polyhedral domains.* Dec. 2002. URL: `https://link.springer.com/article/10.1007/s002110100388`.

Exact Penalty Weak Form

Find $U := ((\boldsymbol{u}, \boldsymbol{B}), p) \in \mathscr{P}(\Omega)$ such that

$$\mathcal{N}_{EP}(U, V) = (F, V), \quad \forall\, V \in \mathscr{P}(\Omega),$$

where

$$\mathcal{N}_{EP}(U, V) = \frac{1}{R_f}(\nabla \boldsymbol{u}, \nabla \boldsymbol{v}) + (\boldsymbol{u} \cdot \nabla \boldsymbol{u}, \boldsymbol{v}) - (p, \nabla \cdot \boldsymbol{v}) + (q, \nabla \cdot \boldsymbol{u})$$
$$+ \kappa((\nabla \times \boldsymbol{B}) \times \boldsymbol{B}, \boldsymbol{v}) + \kappa(\nabla \times (\boldsymbol{u} \times \boldsymbol{B}), \boldsymbol{C}) + \frac{\kappa}{R_m}(\nabla \times \boldsymbol{B}, \nabla \times \boldsymbol{C})$$
$$+ \frac{\kappa}{R_m}(\nabla \cdot \boldsymbol{B}, \nabla \cdot \boldsymbol{C}).$$

and

$$F = ((\boldsymbol{f}, \mathbf{0}), 0).$$

Well posedness of the exact penalty weak form already shown[4]

[4] Max D. Gunzburger, Amnon J. Meir, and Janet S. Peterson. "On the existence, uniqueness, and finite element approximation of solutions of the equations of stationary, incompressible magnetohydrodynamics". In: *Mathematics of Computation* 56.194 (1991), pp. 523–523. DOI: 10.1090/s0025-5718-1991-1066834-0.

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Galerkin Discretization for linear problems

Abstract variational problem: find $u \in V$ such that

$$a(u, v) = (f, v), \forall v \in V,$$

for some data $f \in V$. Consider a finite dimensional subspace $V_h \subset V$ and solution of the approximate problem: find $u_h \in V_h$ such that

$$a(u_h, v) = (f, v), \forall v \in V_h.$$

Denote the error $e_h = u - u_h$.

Error representation

The adjoint form a^* can be defined by the relation (modulo boundary conditions)[5]

$$a^*(v, u) = a(u, v), \ \forall u, v \in V.$$

If ϕ solves the dual problem: find $\phi \in V$ such that

$$a^*(\phi, v) = (\psi, v), \ \forall v \in V,$$

the we have the following error representation,

Theorem

The error in a (linear) QoI represented by QoI $= (\psi, u)$ is computable as $(\psi, e) = (f, \phi) - a(u_h, \phi)$.

[5] Roland Becker and Rolf Rannacher. *An optimal control approach to a posteriori error estimation in finite element methods: Acta Numerica*. Jan. 2003. DOI: `https://doi.org/10.1017/S0962492901000010`.

Adjoint for nonlinear maps

- Let $N \in C^1(V, V)$. For u, u_h fixed, define[6]

$$\bar{N}_{u,u_h}(w) = \int_0^1 N'(su + (1-s)u_h)\,ds\,w,$$

where N' is the derivative of N. By the integral mean value theorem,

$$\bar{N}_{u,u_h}(u - u_h) = N(u) - N(u_h),$$

- Suppose $\mathcal{N}(u, v) = (N(u), v)$, and define $\overline{\mathcal{N}}^*(u, v) = (\bar{N}^*_{u,u_h}(u), v)$
- Solve the (linear) problem

$$\overline{\mathcal{N}}^*(\phi, v) = (\psi, v), \quad \forall v \in V,$$

we have the error representation,

$$\begin{aligned}(\psi, e) = \overline{\mathcal{N}}^*(\phi, e) &= (\bar{N}^*_{u,u_h}(\phi), e) = (\phi, \bar{N}_{u,u_h}(e)) \\ &= (\phi, \bar{N}_{u,u_h}(u - u_h)) = (\phi, N(u) - N(u_h)).\end{aligned}$$

[6] Donald Estep. *A Short Course on Duality, Adjoint Operators, Green's Functions, and A Posteriori Error Analysis*. URL: `https://pdfs.semanticscholar.org/a7f9/59110a2442e55b696d0b89c2d5cef5dcee51.pdf`.

Exact penalty framework

- Let $V = \prod_{i=1}^{n} V_i$ be a product space of vector valued Hilbert spaces $V_i = V_i(\Omega)$, with $\Omega \subset \mathbb{R}^d$ (e.g. $\boldsymbol{H}_0^1(\Omega) \times \boldsymbol{H}_\tau^1(\Omega)$). Suppose we have the following nonlinear problem: find $u \in V$ such that

$$\mathcal{N}(u, v) = (f, v), \forall v \in V,$$

- $\mathcal{N} : V \times V \to \mathbb{R}$ is now more generally given by

$$\mathcal{N}(u, v) = \sum_{i=1}^{m} (N_i(u), v_{\ell_i}) + a(u, v),$$

- $a(u, v)$ is a billinear form and $\ell_i \in \{1, \ldots, n\}$, for each i.
- define the vector operator

$$N(u) = \left[N_1(u), \quad \ldots \quad , N_m(u)\right]^T.$$

Necessary constructions

- For fixed solution/approxmiate pair u/u_h, define the averaged Jacobian matrix $\overline{\mathcal{J}}(N)$, by

$$\overline{\mathcal{J}}_{ij} = \int_0^1 \frac{\partial N_i}{\partial u_j}(su + (1-s)u_h)\, ds,$$

- $\frac{\partial N_i}{\partial u_j}(\cdot)$ denotes the derivative of N_i w.r.t. the argument u_j. The linearized operator $\bar{N}_i$ is next defined for $w \in V$, by

$$\begin{aligned}\bar{N}_i(w) &= \int_0^1 \frac{\partial N_i}{\partial u}(su + (1-s)u_h)\, ds\, w \\ &= \sum_{j=1}^{n} \int_0^1 \frac{\partial N_i}{\partial u_j}(su + (1-s)u_h)\, ds\, w_j = \sum_{j=1}^{n} \overline{\mathcal{J}}_{ij} w_j.\end{aligned}$$

- Next define

$$\overline{\nu}_i(u,v) = (\bar{N}_i(u), v_{\ell_i}) = \left(\sum_{j=1}^{n} \overline{\mathcal{J}}_{ij} u_j, v_{\ell_i} \right) = \sum_{j=1}^{n} \left(\overline{\mathcal{J}}_{ij} u_j, v_{\ell_i} \right).$$

with $a(u,v) = \nu_i(u,v)$. The full linearized adjoint operator is thus,

$$N^*(u,v) = \sum_{i=1}^{m} \overline{\nu}_i^*(u,v) + a^*(u,v).$$

Nonlinear error representation

Then if ϕ solves the dual problem,

$$\overline{\mathcal{N}}^*(\phi, v) = (\psi, v), \ \forall v \in V,$$

we have the following theorem

Theorem

The error in a QoI represented by $Q(u) = (\psi, u)$ is computable as $(\psi, e) = (f, v) - \mathcal{N}(u_h, \phi)$.

Takeaway: we just need to adjoints to the linear operators $\overline{\mathcal{J}}_{ij}$.

MHD Specific Cases

We consider the three nonlinear terms,

$$\begin{aligned}
(N_1(\boldsymbol{u}, \boldsymbol{B}), \boldsymbol{C}) &= (\nabla \times (\boldsymbol{u} \times \boldsymbol{B}), \boldsymbol{C}), \\
(N_2(\boldsymbol{B}), \boldsymbol{v}) &= ((\nabla \times \boldsymbol{B}) \times \boldsymbol{B}, \boldsymbol{v}) \\
(N_3(\boldsymbol{u}), \boldsymbol{v}) &= (\boldsymbol{u} \cdot \nabla \boldsymbol{u}, \boldsymbol{v}).
\end{aligned}$$

The linearized forms $\overline{\mathcal{J}}_{ij}$ as described before are are

$$\begin{aligned}
&\overline{\mathcal{J}}^*_{11}(v_1) = \tfrac{1}{2}(\boldsymbol{B} + \boldsymbol{B}_h) \times (\nabla \times \boldsymbol{C}), \\
&\overline{\mathcal{J}}^*_{12}(v_2) = \tfrac{1}{2}(\boldsymbol{u} + \boldsymbol{u}_h) \times (\nabla \times \boldsymbol{v}), \\
&\overline{\mathcal{J}}^*_{21}(v_1) = \tfrac{1}{2}(-(\nabla \times (\boldsymbol{B} + \boldsymbol{B}_h) \times \boldsymbol{v}) + \nabla \times ((\boldsymbol{B} + \boldsymbol{B}_h) \times \boldsymbol{v}), \\
&\overline{\mathcal{J}}^*_{31}(v_1) = \tfrac{1}{2}\left[\boldsymbol{v} \cdot \left((\nabla \boldsymbol{u} + \nabla \boldsymbol{u}_h)^T\right) - ((\boldsymbol{u} + \boldsymbol{u}_h) \cdot \nabla \boldsymbol{v}) - ((\nabla \cdot (\boldsymbol{u} + \boldsymbol{u}_h)\boldsymbol{v})\right]
\end{aligned}$$

Error representation for MHD

Theorem (Error representation for MHD)

For a given QoI represented by $\Psi = ((\boldsymbol{\psi}_{\boldsymbol{u}}, \boldsymbol{\psi}_{\boldsymbol{B}}), \psi_p)^T$, the numerical error satisfies

$$
\begin{aligned}
(\Psi, E) &= \overline{\mathcal{N}}^*_{EP}(\Phi, E) = \mathcal{N}_{EP}(U, \Phi) - \mathcal{N}_{EP}(U_h, \Phi) \\
&= (F, \Phi) - \mathcal{N}_{EP}(U_h, \Phi) \\
&= (F, \Phi) - \Bigg[\frac{1}{R_f}(\nabla \boldsymbol{u}_h, \nabla \boldsymbol{\phi}) + (\boldsymbol{u}_h \cdot \nabla \boldsymbol{u}_h, \boldsymbol{\phi}) \\
&- (p_h, \nabla \cdot \boldsymbol{\phi}) - \kappa((\nabla \times \boldsymbol{B}_h) \times \boldsymbol{B}_h, \boldsymbol{\phi}) + (\nabla \cdot \boldsymbol{u}_h, \pi) \\
&- \frac{\kappa}{R_m}(\nabla \times \boldsymbol{B}_h, \nabla \times \boldsymbol{\beta}) - \kappa(\nabla \times (\boldsymbol{u}_h \times \boldsymbol{B}_h), \boldsymbol{\beta}) \\
&+ \frac{\kappa}{R_m}(\nabla \cdot \boldsymbol{B}_h, \nabla \cdot \boldsymbol{\beta}) \Bigg].
\end{aligned}
$$

Error components

1. The discretization error in the momemtum equation is

$$D_{mom} = \frac{1}{R_f}(\nabla \boldsymbol{u}_h, \nabla \boldsymbol{\phi}) + (\boldsymbol{u}_h \cdot \nabla \boldsymbol{u}_h, \boldsymbol{\phi}) - (p_h, \nabla \cdot \boldsymbol{\phi})$$
$$- \kappa((\nabla \times \boldsymbol{B}_h) \times \boldsymbol{B}_h, \boldsymbol{\phi}).$$

2. The discretization error in the continuity equations is

$$D_{con} = (\nabla \cdot \boldsymbol{u}_h, \pi).$$

3. the "magnetic" discretization error is

$$D_M = -\frac{\kappa}{R_m}(\nabla \times \boldsymbol{B}_h, \nabla \times \boldsymbol{\beta}) - \kappa(\nabla \times (\boldsymbol{u}_h \times \boldsymbol{B}_h), \boldsymbol{\beta})$$
$$+ \frac{\kappa}{R_m}(\nabla \cdot \boldsymbol{B}_h, \nabla \cdot \boldsymbol{\beta}).$$

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Hartmann Problem

- Consider the flow of a conducting fluid in a channel $\Omega = [-1/2, 1/2]^2$, with an external magnetic field $\boldsymbol{B}_{ext} = (0, 1)$ prescribed on $\partial\Omega$.
- Analytic solution[7], $\boldsymbol{u} = (u_x, 0)$, $\boldsymbol{B} = (B_x, 1)$

$$u_x = \frac{G\, R_f(\cosh(H/2) - \cosh(Hy))}{2H \sinh(H/2)}$$

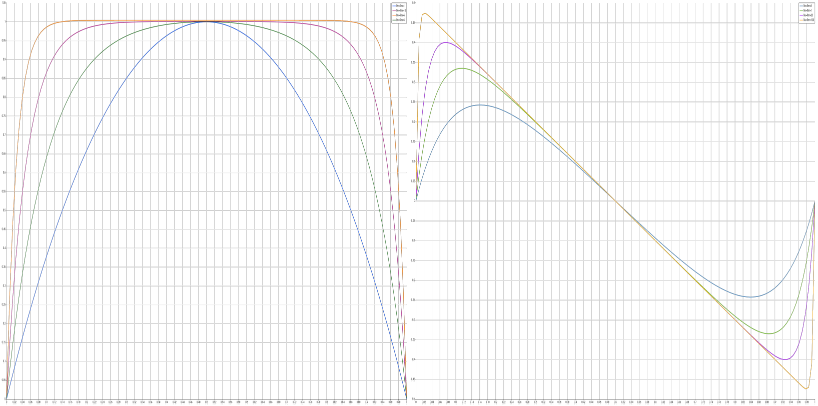
$$B_x = \frac{G(\sinh(Hy) - 2\sinh(H/2)y)}{2\kappa \sinh(H/2)}$$

$$p = -Gx - \kappa B_x^2/2,$$

- $G = -\frac{dp}{dx}$ is an arbitrary pressure drop
- so-called Hartmann number $H = \sqrt{R_f R_m \kappa}$

[7] Edward G. Phillips et al. "A Block Preconditioner for an Exact Penalty Formulation for Stationary MHD". In: *SIAM Journal on Scientific Computing* 36.6 (2014). DOI: 10.1137/140955082.

Hartmann profiles with increasing H



(a) Velocity (b) B field

Hartmann adjoint results

$$\text{Eff.} = \text{Effectivity} = \frac{\text{true error}}{\text{error estimate}}$$

2D Elem.	Computed QoI	True Error	Eff.	D_{mom}	D_{con}	D_M
1024	3.56e-01	-6.07e-03	0.994	-2.74e-07	1.98e-06	6.03e-03
4096	3.51e-01	-1.53e-03	0.998	-6.28e-09	6.29e-08	1.52e-03
16384	3.50e-01	-3.82e-04	1.000	1.00e-08	1.34e-09	3.82e-04
65536	3.50e-01	-9.57e-05	1.000	7.51e-08	2.32e-11	9.56e-05

Table: Results using $((\mathbb{P}^2, \mathbb{P}^1), \mathbb{P}^1)$ elements for $((\boldsymbol{u}, \boldsymbol{B}), p)$.

2D Elem.	Computed QoI	Error	Eff.	D_{mom}	D_{con}	D_M
1024	3.50e-01	-1.11e-06	0.900	-3.86e-05	1.51e-06	3.81e-05
4096	3.50e-01	-4.90e-08	0.931	-2.47e-06	6.03e-08	2.45e-06
16384	3.50e-01	-6.93e-09	0.989	-1.49e-07	1.37e-09	1.54e-07
65536	3.50e-01	1.94e-07	1.000	-2.04e-07	2.57e-11	9.67e-09

Table: Results using $((\mathbb{P}^2, \mathbb{P}^2), \mathbb{P}^1)$ elements for $((\boldsymbol{u}, \boldsymbol{B}), p)$.

Magnetic lid driven cavity

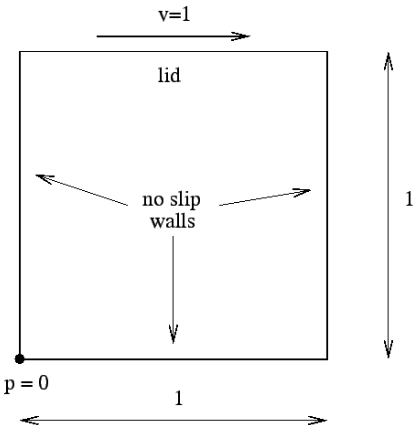


Figure: Boundary condtions for u_x

Augmented with constant $B_y = -1$ on top and bottom to retard flow

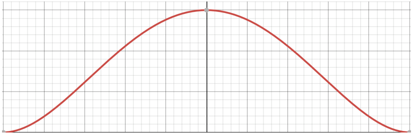
Regularization of the lid velocity

- Use a polynomial regularization of the lid velocity[8] to get expected orders of convergence

$$u_{top}(x) = C\left(x - \tfrac{1}{2}\right)^2 \left(x + \tfrac{1}{2}\right)^2,$$

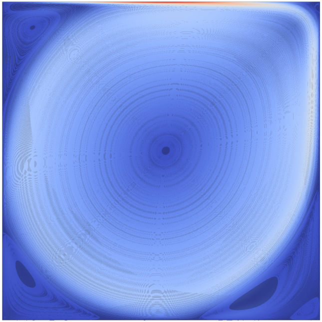
- C chosen so that

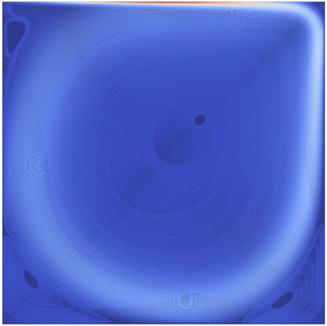
$$\int_{-1/2}^{1/2} u_{top}(x)\,dx = 1$$

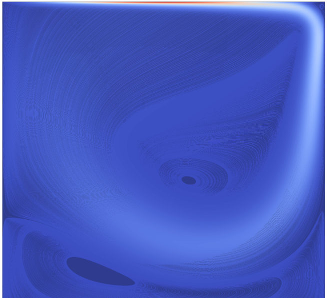


[8] Michael W. Lee, Earl H. Dowell, and Maciej J. Balajewicz. *A study of the regularized lid-driven cavity's progression to chaos*. Nov. 2018. DOI: https://doi.org/10.1016/j.cnsns.2018.11.010.

Regularized plots for varying Rm







Discontinuous plots

Results for discontinuous magnetic lid velocity[9]

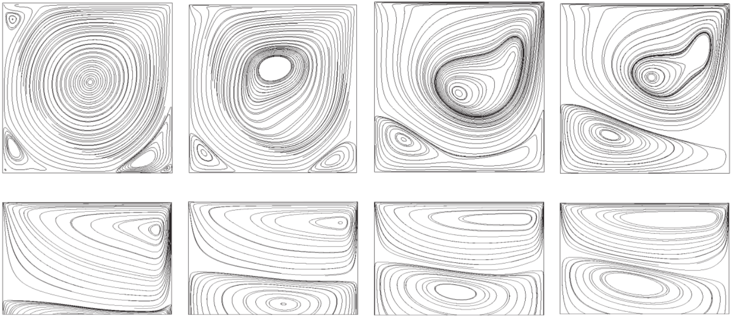


FIG. 1. *Streamlines for the MHD lid driven cavity problem with* $R = 5000$ *and* $R_m = 0, 0.1, 0.3, 0.4, 5, 10, 20, 30$. *The four latter cases are zoomed in to* $[0, 1] \times [0.8, 1]$.

[9] Edward G. Phillips et al. "A Block Preconditioner for an Exact Penalty Formulation for Stationary MHD". In: *SIAM Journal on Scientific Computing* 36.6 (2014). DOI: 10.1137/140955082.

Lid driven cavity adjoint results

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$$\text{Eff.} = \text{Effectivity} = \frac{\text{true error}}{\text{error estimate}}$$

2D Elem.	Computed QoI	Error	Eff.	D_{mom}	D_{con}	D_M
1600	-2.09e-02	-6.64e-04	1.080	-2.83e-04	-4.27e-04	-6.81e-06
3600	-2.04e-02	-2.00e-04	0.949	-4.34e-05	-1.37e-04	-9.07e-06
6400	-2.03e-02	-6.99e-05	0.948	-1.49e-05	-4.37e-05	-7.71e-06

Table: Results using $((\mathbb{P}^2, \mathbb{P}^1), \mathbb{P}^1)$ elements for $((\boldsymbol{u}, \boldsymbol{B}), p)$.

2D Elem.	Computed QoI	Error	Eff.	D_{mom}	D_{con}	D_M
1600	-2.03e-02	6.08e-05	0.702	-1.42e-05	-2.88e-05	2.31e-07
3600	-2.03e-02	2.13e-05	0.876	-2.24e-06	-4.40e-06	-1.21e-05
6400	-2.03e-02	1.06e-05	0.954	-5.00e-07	-1.08e-06	-8.50e-06

Table: Results using $((\mathbb{P}^3, \mathbb{P}^2), \mathbb{P}^1)$ elements for $((\boldsymbol{u}, \boldsymbol{B}), p)$.

- χ_L=-0.25, χ_R=0.25, χ_B=-0.5, χ_T=0.0.
- The overkill solution is compted on a 400x400 mesh, Re=2000, Rm=0.4, $\kappa = 1$.