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Discontinuous Galerkin discretization of magnetic convection

Term paper

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Abstract

The main aim of this paper is a numeric solution to magnetic convection equation in 3 dimensions. Since Discontinuous Galerkin Finite Element method leads to an unstable variational problem, upwinding technique is used. For the sake of simplicity (and ease of implementation), the upwind numerical flux is rewritten using the usual average combined with a jump penalty [BMS04]. Even though on conventional non-parallel architectures the curse of dimensionality limits the accuracy of the numerical solution, the results were sufficient for simple error analysis. In most cases, improvements in convergence rates for higher polynomial degree were observed. All numerical experiments were implemented using FEniCS finite element library; a brief motivational description of its features is also provided.

Keywords: magnetic convection, Discontinuous Galerkin, hyperbolic equations, jump-stabilization, upwind.

AMS Subject Classification: 65N12 65N22 65N30

Contents

Introduction	4
1 Preliminaries	5
1.1 Problem statement	5
1.2 Primal variational formulation	5
2 Discretization	9
2.1 Discrete variational formulation	9
2.2 Stabilization by upwinding	11
3 Implementation	13
3.1 Test problems	13
3.2 FEniCS	13
4 Results	14
4.1 Error norms	14
4.2 Plots of numerical and exact solutions	15
4.3 Test: non-linear	16
4.4 Test: zero boundary condition	17
4.5 Asymptotic error behaviour	18
4.6 Error behaviour for $p = 0$	19
5 Conclusions	21
6 Further research	21
References	22
Appendices	
A FEniCS/Python source codes	23
B Shell scripts	32
C Mathematica code	32
D Computations architecture	33

List of Figures

4.2.1 DG solution for polynomial v and A	15
4.2.2 DG solution for non-linear v and A	15
4.2.3 DG solution for zero-bc v and A	15
4.3.1 Error norm convergence for non-linear test	16
4.3.2 Convergence rates for non-linear test	16
4.4.1 Error norm convergence for zero-bc test	17
4.4.2 Convergence rates for zero-bc test	17
4.5.1 Error norm convergence for refined polynomial test	18
4.5.2 Error norm convergence for refined non-linear test	18
4.5.3 Error norm convergence for refined zero-bc test	18
4.6.1 Error norm convergence for maximally refined polynomial test	19
4.6.2 Error norm convergence for maximally refined non-linear test .	20
4.6.3 Error norm convergence for maximally refined zero-bc test . .	20

Introduction

Let M be a smooth manifold embedded into Euclidean space \mathbb{R}^d . For a smooth vector field $v \in C^\infty(M, \mathbb{R}^d)$, the *Lie derivative* w.r.t. v of a p -form $\alpha \in \Omega^k(M)$ for $0 < p < d$ is again a p -form defined as:

$$\mathcal{L}_v \alpha = d(\iota_v \alpha) + \iota_v d \alpha \quad (0.1)$$

where:

- $\iota_v : \Omega^p(M) \rightarrow \Omega^{p-1}(M)$ is the contraction w.r.t. v (an **algebraic** operation)
- $d : \Omega^p(M) \rightarrow \Omega^{p+1}(M)$ is the exterior derivative

Rigorous definitions and additional properties of contraction map and exterior derivative can be found in [Hit03].

PDEs of the form (0.1) show up in variational formulations of magnetic convection problems. In particular, interesting cases in the 3 dimensional Euclidean space occur for $p = 1$, i.e. for Lie derivatives of a 1-form.

For dimension $d = 3$, the exterior derivatives are consistent with the conventional differential operators:

$$d : \Omega^0(M) \xrightarrow{\text{grad}} \Omega^1(M) \xrightarrow{\text{curl/rot}} \Omega^2(M) \xrightarrow{\text{div}} \Omega^3(M) = \Omega^0(M) \quad (0.2)$$

Hence, for $d = 3$ and $p = 1$ identity (0.1) becomes:

$$\mathcal{L}_v \alpha \stackrel{(0.1),(0.2)}{=} d(\underbrace{\alpha \cdot v}_{\text{0-form}}) + \iota_v \underbrace{\text{curl } \alpha}_{\text{2-form}} \stackrel{(0.2)}{=} \text{grad}(\alpha \cdot v) + \text{curl } \alpha \times v \quad (0.3)$$

Here we leave the differential geometry setting aside and continue with numerical analysis of the boundary value problem associated with the differential operator in the equation (0.3).

1 Preliminaries

1.1 Problem statement

For a bounded Lipschitz domain $\Omega \in \mathbb{R}^3$ with boundary $\Gamma := \partial\Omega$, given a velocity field $v \in C^1(\overline{\Omega}, \mathbb{R}^3)$ and a function $c \in C(\Omega, \mathbb{R})$, consider a stationary PDE for a 1-form $A \in \Omega^1(\overline{\Omega})$:

$$\left. \begin{array}{l} cA + \mathcal{L}_v A = cA + \text{grad}(A \cdot v) + \text{curl } A \times v = 0 \quad \text{in } \Omega \\ A \times \eta = h \quad \text{on } \Gamma_- \\ A \cdot v = g \quad \text{on } \Gamma_- \end{array} \right\} \quad (1.1)$$

where $\Gamma_- \subset \partial\Omega$ is the *inflow boundary* defined as:

$$\Gamma_- := \{x \in \partial\Omega : \eta(x) \cdot v(x) < 0\} \subset \Gamma \quad (1.2)$$

For the completeness of notations, also define the *outflow boundary* as:

$$\Gamma_+ := \{x \in \partial\Omega : \eta(x) \cdot v(x) \geq 0\} \subset \Gamma \quad (1.3)$$

Remark: zero order term cA with a uniformly bounded sufficiently large c is required to ensure ellipticity. General CG and DG theory regarding well-posedness of continuous and discrete variational problems is available in [HS08].

Remark: notation $\Omega^1(M)$ denotes the space of 1-forms on a manifold M and is **not** related to Ω which is used to denote the domain for PDE.

1.2 Primal variational formulation

For simplicity and ease of notation, assume that Ω is a polygonal domain. Then let \mathcal{M} be the discretization of Ω into open tetrahedra. Notice, that then Γ coincides with triangulation boundary $\overline{\partial\mathcal{M}}$ (which is not always the case for arbitrary non-polygonal domains).

Fix conventional notations:

- $\mathcal{F}(\mathcal{M})$ - set of all facets of mesh \mathcal{M}
- $\mathcal{F}^o(\mathcal{M})$ - set of all interior facets of mesh \mathcal{M}
- $\mathcal{F}^\partial(\mathcal{M})$ - set of all exterior (boundary) facets of mesh \mathcal{M}

Additional notations:

- $\mathcal{F}_-^\partial(\mathcal{M})$ - set of all exterior inflow boundary facets of mesh \mathcal{M}

$$\mathcal{F}_-^\partial(\mathcal{M}) := \{f \in \mathcal{F}^\partial(\mathcal{M}) : f \subset \Gamma_- \} \quad (1.4)$$

- $\mathcal{F}_+^\partial(\mathcal{M})$ - set of all exterior outflow boundary facets of mesh \mathcal{M}

$$\mathcal{F}_+^\partial(\mathcal{M}) := \mathcal{F}^\partial(\mathcal{M}) \setminus \mathcal{F}_-^\partial(\mathcal{M}) \quad (1.5)$$

Let $K \in \mathcal{M}$. Choose the local shape functions to be polynomials of degree $p \geq 0$. Since **discontinuous** Galerkin discretization is of particular interest for this paper, the global shape functions for test space are **discontinuous** piece-wise polynomials $A'_N \in (\mathcal{P}_p(\mathcal{M}))^3$, i.e.:

$$\forall K \in \mathcal{M} \implies A'_N|_K \in (\mathcal{P}_p(K))^3 \quad (1.6)$$

Multiplying equation (1.1) by such test function A'_N and integrating over Ω gives the following variational formulation:

seek $A \in \Omega^1(\mathbb{R}^3)$ such that $\forall A'_N \in (\mathcal{P}_p(\mathcal{M}))^3$:

$$\sum_{K \in \mathcal{M}} \int_{\Omega} (cA + \operatorname{grad}(A \cdot v) + \operatorname{curl} A \times v) \cdot A'_N dx = 0 \quad (1.7)$$

Using integration by parts, every $\operatorname{grad}(A \cdot v)$ term of the summands in (1.7) can be rewritten as:

$$\int_K \operatorname{grad}(A \cdot v) \cdot A'_N dx = - \int_K (A \cdot v) \operatorname{div} A'_N dx + \int_{\partial K} (A \cdot v)(A'_N \cdot \eta) dS \quad (1.8)$$

Likewise, the $\operatorname{curl} A \times v$ term can be rewritten as:

$$\begin{aligned} \int_K (\operatorname{curl} A \times v) \cdot A'_N dx &= \int_K (v \times A'_N) \cdot \operatorname{curl} A dx = \\ &= \int_K \operatorname{curl}(v \times A'_N) \cdot A dx - \int_{\partial K} (A \times \eta) \cdot (v \times A'_N) dS \end{aligned} \quad (1.9)$$

Definition 1.2.1 (Jumps and averages). Let $K_+, K_- \in \mathcal{M}$ be adjacent, $\varphi_i : K_i \rightarrow \mathbb{R}$, $B_i : K_i \rightarrow \mathbb{R}^3$, η_i - the unit normal vector to K_i ; $i \in \{+, -\}$. Define the following maps on interface facet $f = K_+ \cap K_- \in \mathcal{F}^o(\mathcal{M})$:

(1) *Averages:*

$$\{\varphi\} := \frac{1}{2}(\varphi_+ + \varphi_-), \quad \{B\} := \frac{1}{2}(B_+ + B_-);$$

(2) Jumps:

$$[[\varphi]] := \varphi_+ - \varphi_-, \quad [[B]] := B_+ - B_-$$

(3) Jumps w.r.t. normal:

$$[[\varphi]]_\eta := \varphi_+ \eta_+ + \varphi_- \eta_-, \quad [[B]]_\eta := B_+ \cdot \eta_+ + B_- \cdot \eta_-;$$

(4) Tangential jumps w.r.t. normal:

$$[[B]]_\times := B_+ \times \eta_+ + B_- \times \eta_-;$$

On the boundary facets, the corresponding values of functions are defined as:

$$\{\varphi\} := \varphi_+, \quad \{B\} := B_+, \quad [[\varphi]]_\eta := \varphi_+ \eta_+, \quad [[B]]_\eta := B_+ \cdot \eta_+,$$

$$[[\varphi]] := \varphi_+, \quad [[B]] := B_+, \quad [[B]]_\times := B_+ \times \eta_+.$$

Note: Justification for jumps w.r.t. normal ($[[\cdot]]_\eta$ and $[[\cdot]]_\times$) is the invariance under choice of cell K : interchanging K_+ and K_- produces the same result. Reference: [DAM01].

Proposition 1.2.1 (Magic DG formulas). *Let \mathcal{M} be some bounded mesh in \mathbb{R}^3 , η - normal outward vector to $K \in \mathcal{M}$.*

(1) Let $A : \mathcal{M} \rightarrow \mathbb{R}^3$, $\varphi : \mathcal{M} \rightarrow \mathbb{R}$, then:

$$\sum_{K \in \mathcal{M}} \int_{\partial K} (A \cdot \eta) \varphi dS = \sum_{f \in \mathcal{F}^o(\mathcal{M})} \int_f \{A\} \cdot [[\varphi]]_\eta dS + \sum_{f \in \mathcal{F}(\mathcal{M})} \int_f [[A]]_\eta \{\varphi\} dS \quad (1.10)$$

(2) Let $A, B : \mathcal{M} \rightarrow \mathbb{R}^3$, then:

$$\sum_{K \in \mathcal{M}} \int_{\partial K} (A \times \eta) \cdot B dS = - \sum_{f \in \mathcal{F}^o(\mathcal{M})} \int_f \{A\} \cdot [[B]]_\times dS + \sum_{f \in \mathcal{F}(\mathcal{M})} \int_f [[A]]_\times \cdot \{B\} dS \quad (1.11)$$

Proof. Straightforward algebraic manipulations using identity:

$$(a \times b) \cdot c = (b \times c) \cdot a \quad (1.12)$$

(1) set $LHS := (A_1 \cdot \eta_1)\varphi_1 + (A_2 \cdot \eta_2)\varphi_2$, then:

$$\begin{aligned}
2RHS &:= (A_1 + A_2) \cdot (\varphi_1 \eta_1 + \varphi_2 \eta_2) + \\
&+ (A_1 \cdot \eta_1 + A_2 \cdot \eta_2)(\varphi_1 + \varphi_2) = \\
&= (A_1 \cdot \eta_1)\varphi_1 + (A_1 \cdot \eta_2)\varphi_2 + \\
&+ (A_2 \cdot \eta_1)\varphi_1 + (A_2 \cdot \eta_2)\varphi_2 + \\
&+ (A_1 \cdot \eta_1)\varphi_1 + \underbrace{(A_1 \cdot \eta_1)\varphi_2}_{=-(A_1 \cdot \eta_2)\varphi_2} + \\
&+ \underbrace{(A_2 \cdot \eta_2)\varphi_1}_{=-(A_2 \cdot \eta_1)\varphi_1} + (A_2 \cdot \eta_2)\varphi_2 = 2LHS;
\end{aligned}$$

(2) set $LHS := (A_1 \times \eta_1) \cdot B_1 + (A_2 \times \eta_2) \cdot B_2$, then:

$$\begin{aligned}
2RHS &:= (A_1 \times \eta_1 + A_2 \times \eta_2) \cdot (B_1 + B_2) - \\
&- (A_1 + A_2) \cdot (B_1 \times \eta_1 + B_2 \times \eta_2) = \\
&= (A_1 \times \eta_1) \cdot B_1 + (A_2 \times \eta_2) \cdot B_1 + \\
&+ (A_1 \times \eta_1) \cdot B_2 + (A_1 \times \eta_1) \cdot B_1 - \\
&- (B_1 \times \eta_1) \cdot A_1 - (B_2 \times \eta_2) \cdot A_1 - \\
&- (B_1 \times \eta_1) \cdot A_2 - (B_1 \times \eta_1) \cdot A_1 = \\
&\stackrel{((1.12))}{=} 2LHS + \\
&+ (A_1 \times \eta_1) \cdot B_2 + (A_2 \times \eta_2) \cdot B_1 - \\
&- \underbrace{(\eta_1 \times A_2) \cdot B_1}_{=A_2 \times \eta_2} - \underbrace{(\eta_2 \times A_1) \cdot B_2}_{=(A_1 \times \eta_1)} = 2LHS;
\end{aligned}$$

Finally, the desired formula for both cases is achieved by integrating and summing up the identities above over internal facets $f \in \mathcal{F}^o(\mathcal{M})$ and incorporating integrals over exterior facets $f \in \mathcal{F}^d(\mathcal{M})$. \square

Combining equations (1.8) - (1.9), applying Proposition 1.2.1 we obtain:

$$\begin{aligned}
&\sum_{K \in \mathcal{M}} \int_K cA \cdot A'_N - (A \cdot v) \operatorname{div} A'_N + \operatorname{curl}(v \times A'_N) \cdot Adx + \\
&+ \sum_{f \in \mathcal{F}(\mathcal{M})} \int_f \{A \cdot v\} [[A'_N]]_\eta dS + \sum_{f \in \mathcal{F}^o(\mathcal{M})} \int_f [[A \cdot v]]_\eta \cdot \{A'_N\} dS + \\
&+ \sum_{f \in \mathcal{F}^o(\mathcal{M})} \int_f \{A\} \cdot [[v \times A'_N]]_\times dS - \sum_{f \in \mathcal{F}(\mathcal{M})} \int_f [[A]]_\times \cdot \{v \times A'_N\} dS = 0
\end{aligned} \tag{1.13}$$

Since $A, v \in C(\Omega, \mathbb{R}^3)$ and thus $A \cdot v \in C(\Omega)$, the corresponding jumps vanish on the internal facets $f \in \mathcal{F}^o(\mathcal{M})$:

$$[[A]]_\times = 0, \quad [[A \cdot v]]_\eta = 0, \quad (1.14)$$

Hence variational formulation simplifies to:

$$\begin{aligned} & \sum_{K \in \mathcal{M}} \int_K c A \cdot A'_N - (A \cdot v) \operatorname{div} A'_N + \operatorname{curl}(v \times A'_N) \cdot A dx + \\ & \quad + \sum_{f \in \mathcal{F}(\mathcal{M})} \int_f \{A \cdot v\} [[A'_N]]_\eta dS + \\ & + \sum_{f \in \mathcal{F}^o(\mathcal{M})} \int_f \{A\} \cdot [[v \times A'_N]]_\times dS - \sum_{f \in \mathcal{F}^\partial(\mathcal{M})} \int_f [[A]]_\times \cdot \{v \times A'_N\} dS = 0 \end{aligned} \quad (1.15)$$

Remark: the idea to make use of (1.14) comes from [BMS04].

2 Discretization

2.1 Discrete variational formulation

We would like to discretize the formal variational formulation restricting A to a subspace $(\mathcal{P}_p(\mathcal{M}))^3$:

seek for $A_N \in (\mathcal{P}_p(\mathcal{M}))^3$ such that $\forall A'_N \in (\mathcal{P}_p(\mathcal{M}))^3$:

$$\begin{aligned} & \sum_{K \in \mathcal{M}} \int_K c A_N \cdot A'_N - (A_N \cdot v) \operatorname{div} A'_N + \operatorname{curl}(v \times A'_N) \cdot A_N dx + \\ & \quad + \sum_{f \in \mathcal{F}(\mathcal{M})} \int_f \{A_N \cdot v\} [[A'_N]]_\eta dS + \\ & + \sum_{f \in \mathcal{F}^o(\mathcal{M})} \int_f \{A_N\} \cdot [[v \times A'_N]]_\times dS - \sum_{f \in \mathcal{F}^\partial(\mathcal{M})} \int_f [[A_N]]_\times \cdot \{v \times A'_N\} dS = 0 \end{aligned} \quad (2.1)$$

Unfortunately, we have $\operatorname{curl}(v \times A'_N)$ in the expression which is not in general available as a finite element for arbitrary v . Applying integration by parts once again, we obtain:

$$\int_K \operatorname{curl}(v \times A'_N) \cdot A_N dx = \int_K (v \times A'_N) \cdot \operatorname{curl} A_N dx + \int_{\partial K} (A_N \times \eta) \cdot (v \times A'_N) dS \quad (2.2)$$

Applying Proposition 1.2.1 to the sum of boundary integrals in (2.2), it becomes:

$$-\sum_{f \in \mathcal{F}^o(\mathcal{M})} \int_f \{A_N\} \cdot [[v \times A'_N]]_\times dS + \sum_{f \in \mathcal{F}(\mathcal{M})} \int_f [[A_N]]_\times \cdot \{v \times A'_N\} dS \quad (2.3)$$

Notice, that when plugged into the discrete variational formulation, the following terms cancel out:

$$\sum_{f \in \mathcal{F}^o(\mathcal{M})} \int_f \{A_N\} \cdot [[v \times A'_N]]_\times dS \quad \text{and} \quad \sum_{f \in \mathcal{F}^\partial(\mathcal{M})} \int_f [[A_N]]_\times \cdot \{v \times A'_N\} dS$$

Therefore, the final expression for discrete variational formulation with already incorporated boundary conditions from (1.1) is of the following form:

$$\begin{aligned} & \sum_{K \in \mathcal{M}} \int_K c A_N \cdot A'_N - (A_N \cdot v) \operatorname{div} A'_N + (v \times A'_N) \cdot \operatorname{curl} A_N dx + \\ & + \sum_{f \in \mathcal{F}(\mathcal{M}) \setminus \mathcal{F}_-^\partial(\mathcal{M})} \int_f \{A_N \cdot v\} [[A'_N]]_\eta dS + \sum_{f \in \mathcal{F}^o(\mathcal{M})} \int_f [[A_N]]_\times \cdot \{v \times A'_N\} dS = \\ & = - \sum_{f \in \mathcal{F}_-^\partial(\mathcal{M})} \int_f g(A'_N \cdot \eta) dS \end{aligned} \quad (2.4)$$

Lemma 2.1.1. *For a vector field B and a vector η in \mathbb{R}^3 , the following holds:*

$$(\eta \times (\eta \times B)) = -(\eta \cdot \eta)B + (\eta \cdot B)\eta; \quad (2.5)$$

additionally assuming that n is a unit vector, we have the identity:

$$B = (\eta \cdot B)\eta - (\eta \times (\eta \times B)). \quad (2.6)$$

Applying Lemma 2.1.1 to A_N, A'_N, v and η as in context of formulation (2.4), we obtain the relation:

$$(v \cdot \eta)(A_N \cdot A'_N) = (v \cdot A_N)(A'_N \cdot \eta) - (A_N \times \eta)(v \times A'_N) \quad (2.7)$$

Integrating identity (2.7) over $\mathcal{F}_-^\partial(\mathcal{M})$ and adding to variational formulation

(2.4), it becomes:

$$\begin{aligned}
& \sum_{K \in \mathcal{M}} \int_K c A_N \cdot A'_N - (A_N \cdot v) \operatorname{div} A'_N + (v \times A'_N) \cdot \operatorname{curl} A_N dx + \\
& + \sum_{f \in \mathcal{F}(\mathcal{M})} \int_f \{A_N \cdot v\} [[A'_N]]_\eta dS + \sum_{f \in \mathcal{F}^o(\mathcal{M})} \int_f [[A_N]]_\times \cdot \{v \times A'_N\} dS - \\
& - \sum_{f \in \mathcal{F}_-^\partial(\mathcal{M})} \int_f (v \cdot \eta)(A_N \cdot A'_N) dS = \tag{2.8} \\
& = - \sum_{f \in \mathcal{F}_-^\partial(\mathcal{M})} \int_f g(A'_N \cdot \eta) dS + \sum_{f \in \mathcal{F}_-^\partial(\mathcal{M})} \int_f h \cdot (v \times A'_N) dS
\end{aligned}$$

2.2 Stabilization by upwinding

The resulting numerical solution from (2.8) is only $L^2(\mathcal{M})$ -stable. To obtain the stability in a stronger norm, the "upwinding" technique is used. More precisely, $\{A_N \cdot v\}$ and $[[A_N]]_\times$ in equation (2.8) are replaced with $\{A_N\}_u \cdot v$ and $2\{A_N\}_u \times \eta$ respectively, where:

Definition 2.2.1. Setting as in the definition 1.2.1, the **upwind** value is:

$$\{\varphi\}_u := \begin{cases} \varphi_1 & \text{if } \eta_1 \cdot v > 0, \\ \varphi_2 & \text{if } \eta_1 \cdot v < 0, \\ \{\varphi\} & \text{if } \eta_1 \cdot v = 0. \end{cases}$$

The upwind value for a vector-valued function is defined analogously.

Definition 2.2.2. Weighted average is defined as:

$$\{\varphi\}_\alpha := \alpha_+ \varphi_+ + \alpha_- \varphi_-, \tag{2.9}$$

where $\alpha_+, \alpha_- \geq 0, \alpha_+ + \alpha_- = 1$.

The weighted average for a vector-valued function is defined analogously.

Notice, that (also used in [Mar06]):

$$\{\varphi\}_u = \{\varphi\}_\alpha = \{\varphi\} + \frac{[[\alpha]]}{2} [[\varphi]] \tag{2.10}$$

for $\alpha = (\operatorname{sign}(v \cdot \eta) + 1)/2$.

Remark: $\{\varphi\}_u = \varphi_+ + \frac{1}{2}\varphi_+ \neq \varphi_+$ on outflow boundary facets!

Recalling the notations from (1.5), the stabilized form of the discrete variational formulation (2.8) becomes:

$$\begin{aligned}
& \sum_{K \in \mathcal{M}} \int_K c A_N \cdot A'_N - (A_N \cdot v) \operatorname{div} A'_N + (v \times A'_N) \cdot \operatorname{curl} A_N dx + \\
& + \sum_{f \in \mathcal{F}(\mathcal{M})} \int_f (\{A_N\}_u \cdot v) [[A'_N]]_\eta dS + \sum_{f \in \mathcal{F}^o(\mathcal{M})} \int_f (2\{A_N\}_u \times \eta) \cdot \{v \times A'_N\} dS - \\
& - \sum_{f \in \mathcal{F}_-^\partial(\mathcal{M})} \int_f (v \cdot \eta) (A_N \cdot A'_N) dS = \\
& = - \sum_{f \in \mathcal{F}_-^\partial(\mathcal{M})} \int_f g (A'_N \cdot \eta) dS + \sum_{f \in \mathcal{F}_-^\partial(\mathcal{M})} \int_f h \cdot (v \times A'_N) dS
\end{aligned} \tag{2.11}$$

Alternatively, stabilization can be done by adding term

$$\sum_{f \in \mathcal{F}^o(\mathcal{M})} \int_f c_f ([[A_N]] \cdot [[A'_N]]) dS \tag{2.12}$$

to equation (2.8), where the stabilization parameter c_f related to the full up-winding was chosen to be uniformly constant on each facet (refer to [BMS04]):

$$c_f = \frac{1}{2} |v \cdot \eta| \tag{2.13}$$

and provides us with the final variational form directly used in implementation:

$$\begin{aligned}
& \sum_{K \in \mathcal{M}} \int_K c A_N \cdot A'_N - (A_N \cdot v) \operatorname{div} A'_N + (v \times A'_N) \cdot \operatorname{curl} A_N dx + \\
& + \sum_{f \in \mathcal{F}(\mathcal{M})} \int_f \{A_N \cdot v\} [[A'_N]]_\eta dS + \sum_{f \in \mathcal{F}^o(\mathcal{M})} \int_f [[A_N]]_\times \cdot \{v \times A'_N\} dS - \\
& - \sum_{f \in \mathcal{F}_-^\partial(\mathcal{M})} \int_f (v \cdot \eta) (A_N \cdot A'_N) dS + \sum_{f \in \mathcal{F}^o(\mathcal{M})} \int_f \frac{1}{2} |v \cdot \eta| ([[A_N]] \cdot [[A'_N]]) dS = \\
& = - \sum_{f \in \mathcal{F}_-^\partial(\mathcal{M})} \int_f g (A'_N \cdot \eta) dS + \sum_{f \in \mathcal{F}_-^\partial(\mathcal{M})} \int_f h \cdot (v \times A'_N) dS
\end{aligned} \tag{2.14}$$

3 Implementation

3.1 Test problems

Several test cases were available for computations. All test were conducted on the unit cube mesh \mathcal{M} in 3D (the convex hull of $\{e_1, e_2, e_3\}$). For a specific test, the velocity field v , large enough (ensuring ellipticity) factor c and the desired exact solution A were fixed. Afterwards, values for h, g on $\mathcal{F}_-^\partial(\mathcal{M})$ and right hand side f on Ω were computed using two different methods:

- numerical approximation of f using **Dolfin** from FEniCS (see 3.2)
- analytic exact expression of f using *Wolfram Mathematica* symbolic software (see Appendix C)

For detailed information on test problems refer to the source code [`tests.py`] in Appendix A.

As shortly mentioned above, test problems were implemented using FEniCS (see 3.2) finite element library. The validity of the algorithm was confirmed; additionally, various error norm convergence rates were obtained and analysed.

Linear solver used: **GMRES** (**G**eneralized **M**inimum **R**esidual) with **ILU** (**I**ncomplete **L**U-factorization) preconditioner from PETSc back-end.

3.2 FEniCS

Key features of FEniCS:

- Python and C++ interface (can be combined with SciPy and Matplotlib)
- math-like syntax for variational forms (UFL + FFC)
- custom linear algebra back-ends:
`uBLAS`, `PETSc`, `SLEPc`, `Epetra`, `MTL4`, `UMFPACK`
- additional mesh manipulation libraries: `CGAL`, `SCOTCH`
- visualization via VTK
- easy implementation of subdomains, boundary parts, variable coefficients
- MPI support

For more detailed information, refer to [AL10, Lan09].

4 Results

4.1 Error norms

Denote the error field by:

$$E := A_{\text{approx.}} - A_{\text{exact}} \quad (4.1)$$

Absolute errors were computed using two different norms:

- $(L^2(\mathcal{M}))^3$ -norm:

$$\|E\|_{(L^2(\mathcal{M}))^3} := \left(\sum_{K \in \mathcal{M}} \int_K E \cdot E dx \right)^{\frac{1}{2}} \quad (4.2)$$

- $(H(\text{curl}; \mathcal{M}))^3$ -semi-norm:

$$|E|_{(H(\text{curl}; \mathcal{M}))^3} := \left(\sum_{K \in \mathcal{M}} \int_K \text{curl } E \cdot \text{curl } E dx \right)^{\frac{1}{2}} \quad (4.3)$$

Absolute jump errors were also computed using two different norms:

- $(L^2(\mathcal{F}^o(\mathcal{M})))^3$ -norm of the jump $[[E]]$:

$$\|[[E]]\|_{(L^2(\mathcal{F}^o(\mathcal{M})))^3} := \left(\sum_{f \in \mathcal{F}^o(\mathcal{M})} \int_f [[E]] \cdot [[E]] dS \right)^{\frac{1}{2}} \quad (4.4)$$

- $(L^2(\mathcal{F}^\partial(\mathcal{M})))^3$ -norm of the jump $[[E]]$:

$$\|[[E]]\|_{(L^2(\mathcal{F}^\partial(\mathcal{M})))^3} := \left(\sum_{f \in \mathcal{F}^\partial(\mathcal{M})} \int_f [[E]] \cdot [[E]] dS \right)^{\frac{1}{2}} \quad (4.5)$$

All **error plots** are w.r.t $1/h$, i.e. **w.r.t. number of mesh cells in one space dimension**. Number of degrees of freedom in this case is of order $(1/h)^3$.

4.2 Plots of numerical and exact solutions

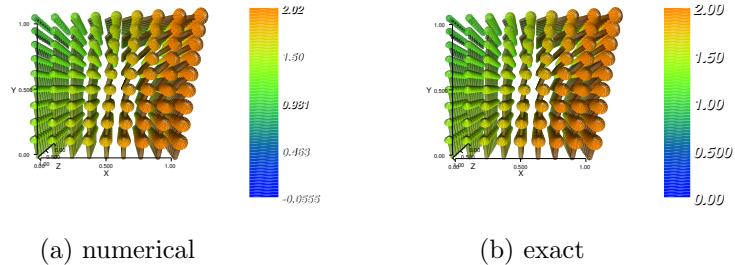


Figure 4.2.1: DG solution for polynomial v and A

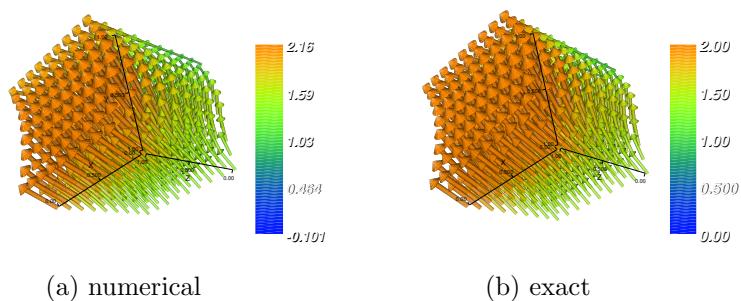


Figure 4.2.2: DG solution for non-linear v and A

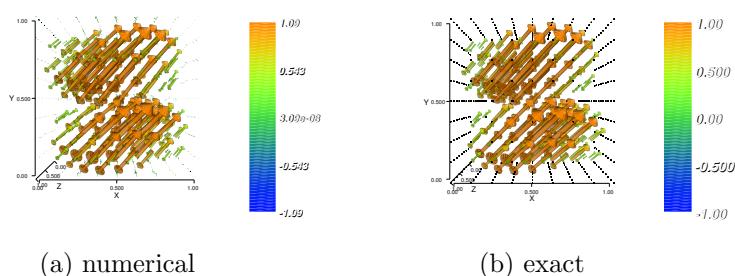


Figure 4.2.3: DG solution for zero-bc v and A

4.3 Test: non-linear

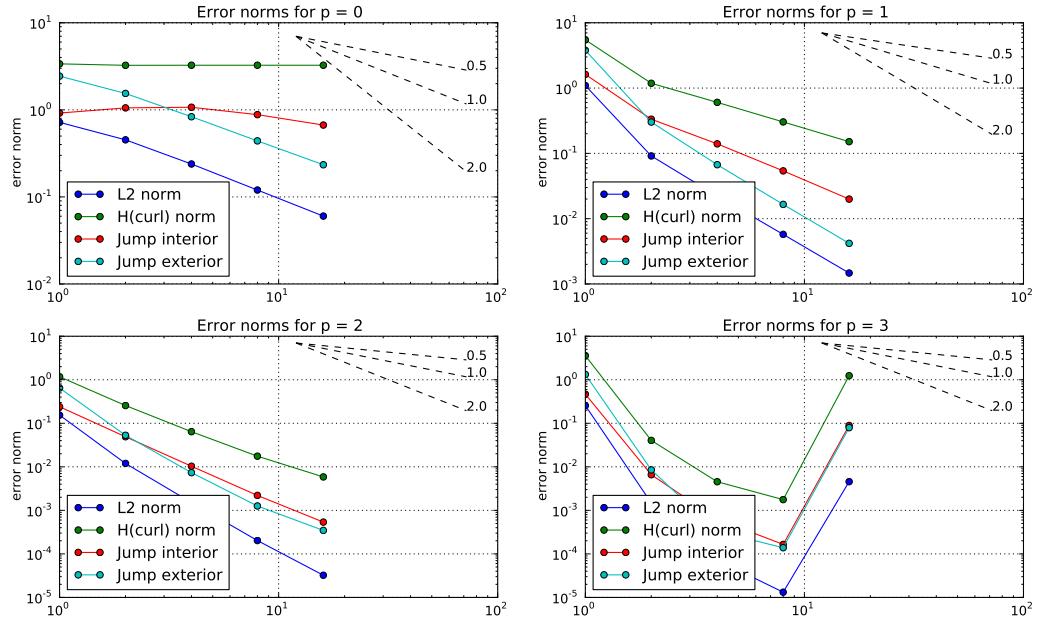


Figure 4.3.1: Error norm convergence for non-linear test

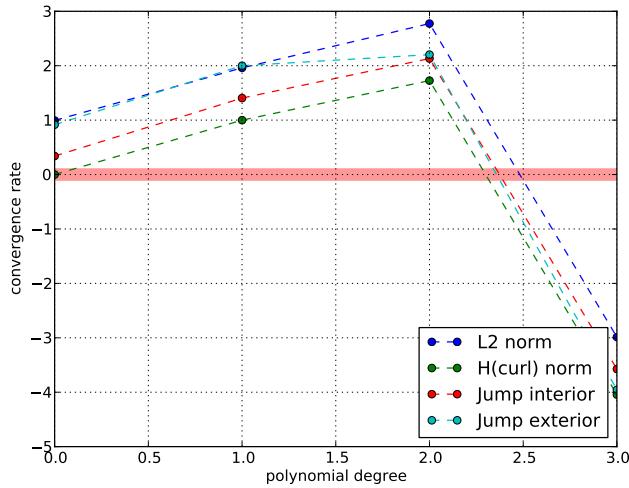


Figure 4.3.2: Convergence rates for non-linear test

4.4 Test: zero boundary condition

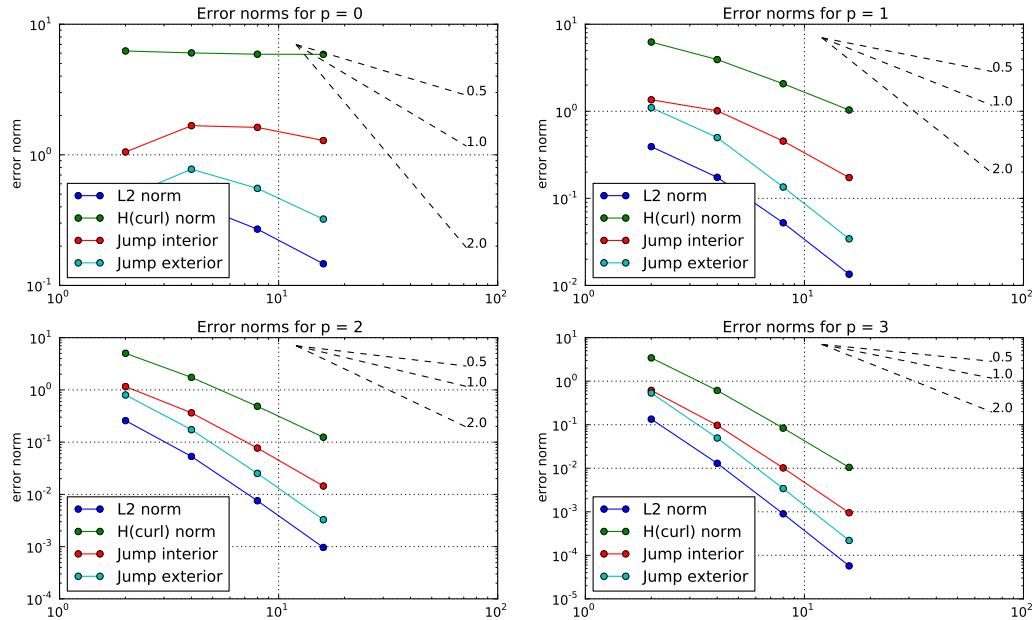


Figure 4.4.1: Error norm convergence for zero-bc test

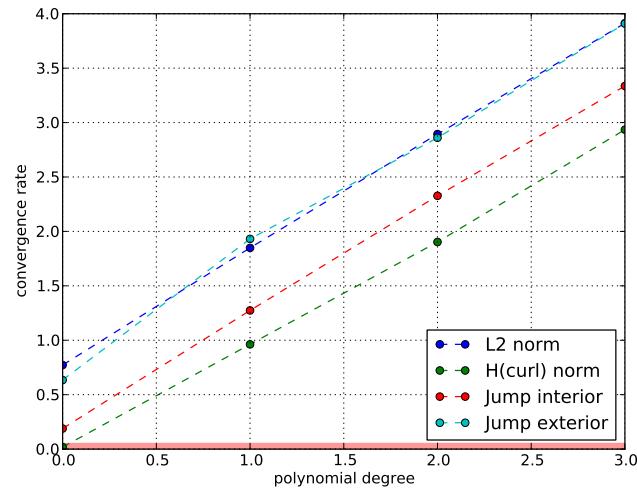


Figure 4.4.2: Convergence rates for zero-bc test

4.5 Asymptotic error behaviour

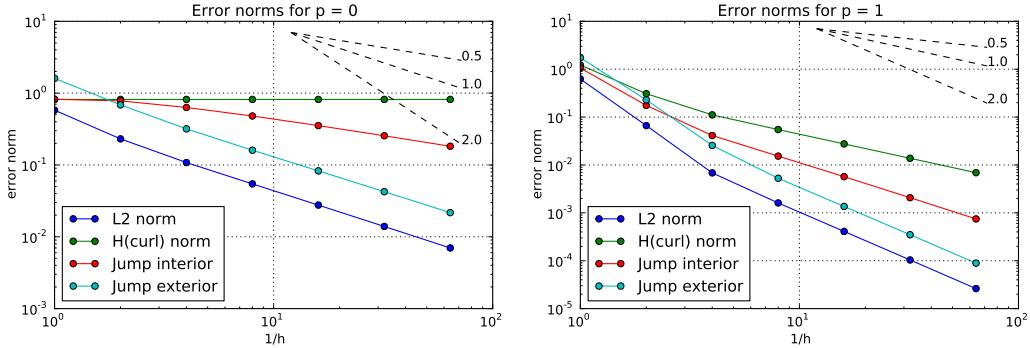


Figure 4.5.1: Error norm convergence for refined polynomial test

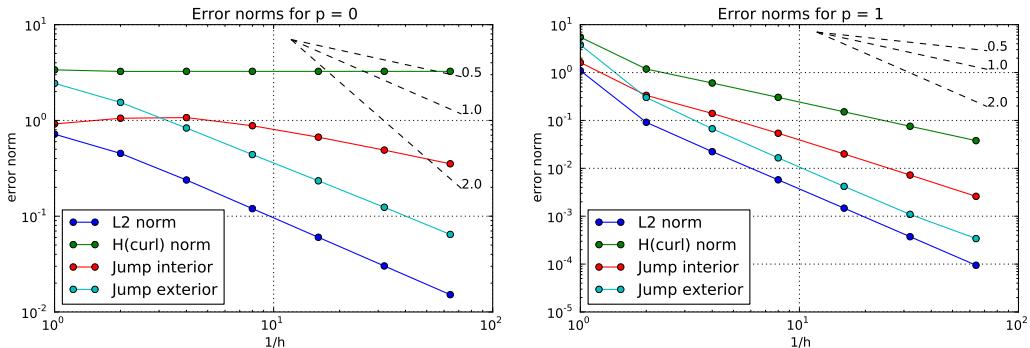


Figure 4.5.2: Error norm convergence for refined non-linear test

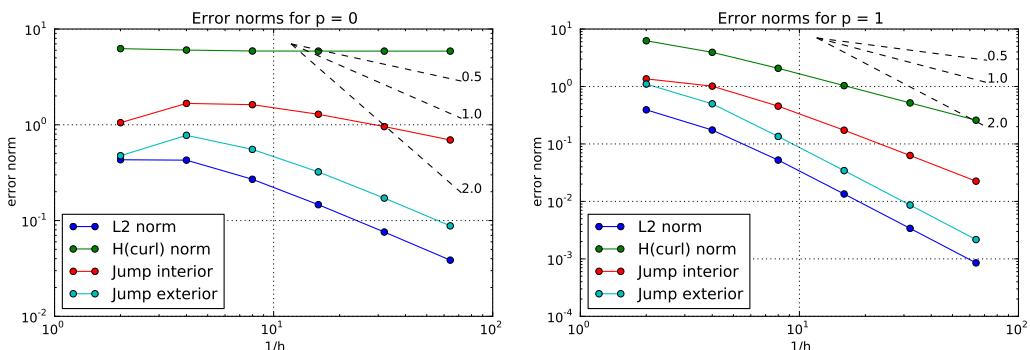


Figure 4.5.3: Error norm convergence for refined zero-bc test

4.6 Error behaviour for $p = 0$

Asymptotic convergence for higher polynomial degrees is hard to monitor due to curse of dimensionality and limited computing resources. Hence, we additionally elaborate a bit more on the case $p = 0$.

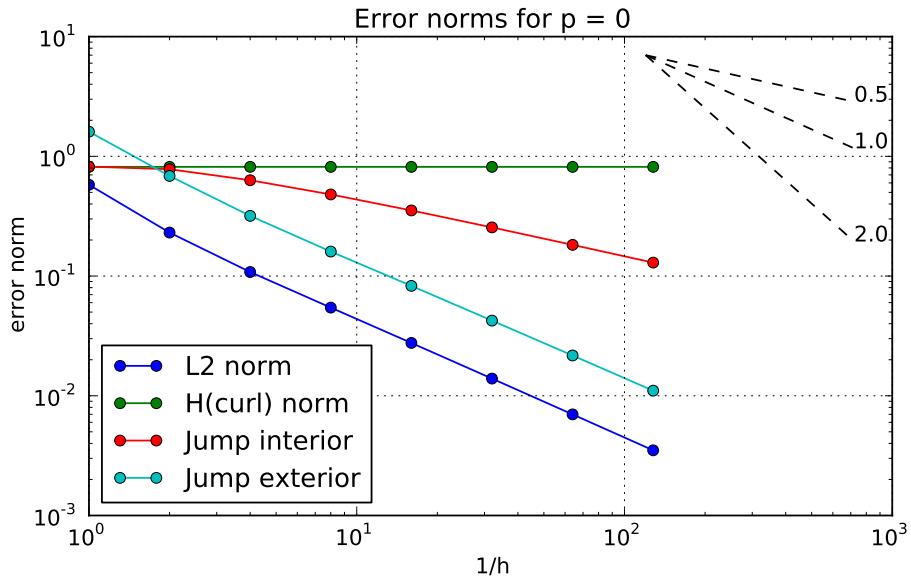


Figure 4.6.1: Error norm convergence for maximally refined polynomial test

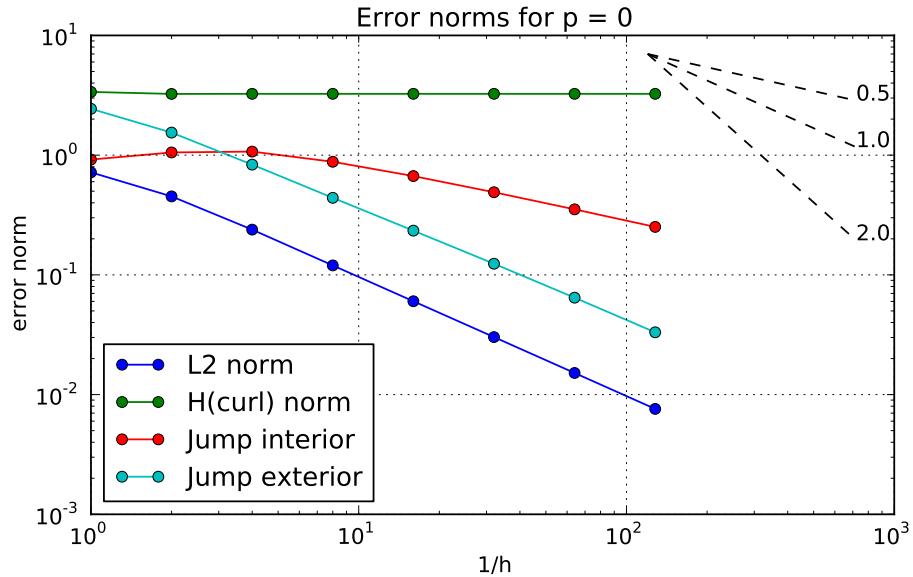


Figure 4.6.2: Error norm convergence for maximally refined non-linear test

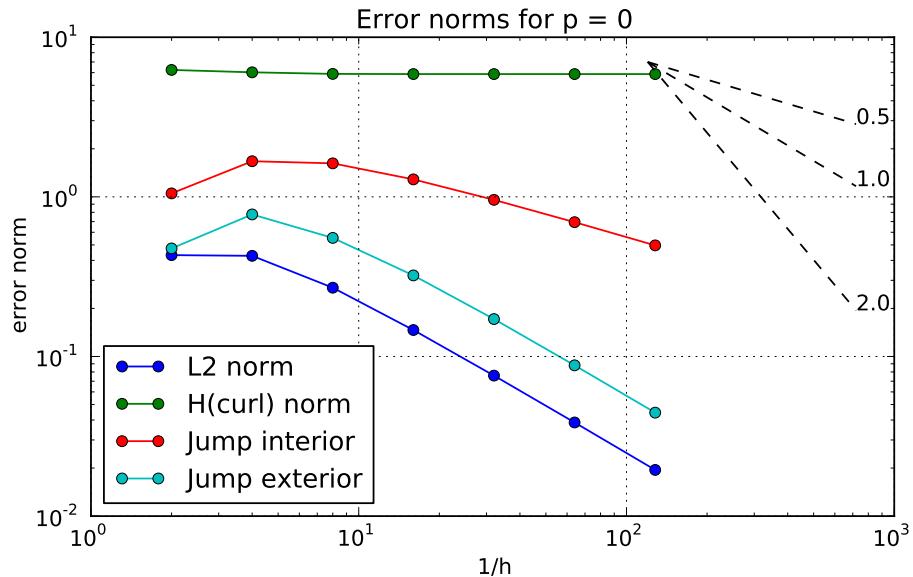


Figure 4.6.3: Error norm convergence for maximally refined zero-bc test

5 Conclusions

Order of convergence increases with polynomial degree p and empirical relation for every error norm is:

$(L^2(\mathcal{M}))^3$ -norm	$2p$
$(H(\text{curl}; \mathcal{M}))^3$ -semi-norm	p
$(L^2(\mathcal{F}^o(\mathcal{M})))^3$ -norm	$p + 1/2$
$(L^2(\mathcal{F}^\partial(\mathcal{M})))^3$ -norm	$2p$

Remark: The convergence rates above are w.r.t $1/h$, i.e. **w.r.t. number of mesh cells in one space dimension**. Dividing them by 3 gives convergence rates w.r.t. number of degrees of freedom.

6 Further research

- Scalability of the code. Most of the CPU time is spent on:
 - assembling matrices: finite elements can be easily distributed over nodes
 - solving linear system: configure PETSc solver as a back-end and enable its parallel capabilities
- Zero order term. Getting rid of the cA term in PDE (1.1).
- Diffusion term. Introducing additional $\epsilon \text{curl curl } A$ term in PDE (1.1).
- Consistency. Come up with a test having load vector $f = 0$ (not so easy for non-linear velocity fields v) and monitor error behaviour, since $f = 0$ shows up in magnetic convection equations.

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Appendices

A FEniCS/Python source codes

Source code is available for download at:

www.sukys.lt/search/label/publications

Listing 1: [config.py] main configuration:

```

1 # === MAIN CONFIGURATION ===
2
3 # === PARAMETERS [ feel free to play around ] ===
4
5 test      = 'polynomial'      # default test to use: polynomial, non-linear, zero-bc
6 P         = 1                 # polynomial degree to be used
7 levels    = 3                 # number of refinement levels
8
9 pylab_on = True              # plots errors and convergence rates (using pylab)
10 show_fig = True              # shows all pylab plots in xsession
11 save_fig = False             # saves all pylab plots into files
12
13 viper_on = False             # plots the exact and approximated fields
14 save_viper = False            # saves all viper plots into files | set to 'False' to
15 prevent HUGE files in 'viper' directory
16
17 errors_skip = 0              # number of first error norms to ignore when plotting
18 errors_slopes = [0.5, 1.0, 2.0] # slopes to be added to plots as a referece for
19 convergence rates
20
21 rates_wrt   = 'hmax'          # compute convergence rates w.r.t.: 'hmax' OR 'ndofs'
22 rates_method = 'average'       # compute convergence rates from: 'last' 2 errors OR
23 average, of all errors
24
25 rates_skip = 0               # number of first error norms to ignore when computing
26 AVERAGE convergence rates for plots
27
28 compute_all = True            # computes solution for polynomial degress p = 0, 1, 2,
29 ..., P and plots the order of convergence for every error
30 debug_on    = False             # includes debugging branches ( plots inflow boundary
31 parts, etc. )
32
33 level_offset = 0              # first refinement level
34 stability    = 1               # stability parameter
35
36 # === CONSTANTS [ no need to modify in general ] ===
37
38 FE_TYPE     = 'DG'              # finite elements to use: 'DG' – Discontinuous Galerkin;
39 'CG' – Continuous Galerkin
40 RHS_BACKEND = 'Mathematica'     # compute load vector for the right hand side using: '
41 Dolfin' OR 'Mathematica'
42
43 QUAD_FACTOR = 1                # parameters for quadrature order (for error norm
44 computation)
45 QUAD_OFFSET = 2                # parameters for quadrature order (for error norm
46 computation)
47
48 FIGURE_FORMAT = 'pdf'           # default format for saving figures to files
49 ERRORS_FORMAT = '%1.0e'          # format string for errors
50 RATES_FORMAT = '%+1.2f'          # format string for convergence rates
51 SUFFIX_FORMAT = '_test=%s_P=%d_levels=%d' # output file suffix format | usage:
52 SUFFIX_FORMAT % (test, P, levels)
53
54 VIPER_PATH   = 'viper/'          # default path for saving viper VTK files
55 PYLAB_PATH   = 'pylab/'          # default path for saving pylab plots
56 TEXT_PATH    = 'text/'           # default path for saving text output
57 DUMP_PATH    = 'dump/'           # default path for saving dumped objects
58
59 # === CONSISTENCY CHECKS [ do NOT modify ] ===
60
61 if FETYPE == 'CG':
62     SUFFIX_FORMAT += '_CG'        # to avoid conflicts with 'DG' FETYPE
63     MIN_P      = 1
64 else:
65     MIN_P      = 0               # minimal polynomial degree for FE space

```

Listing 2: [initialization.py]: initialization routines:

```

2 # === INITIALIZATION ROUTINES ===
from config import *
from auxiliary import initializeList, getRefinements
from errors import TYPE_SIZE
import sys
7
try:
    test      = sys.argv[1]                      # test to use
    P         = int(sys.argv[2])                  # polynomial degree
    levels   = int(sys.argv[3])                  # number of refinements
12 except:
    print '\n'== SETTING PARAMETERS FROM: [config.py] ==\n' + \
          'Alternative usage: main.py [test-name] [pol-degree] [number-of-refinements] [env]\n'
17
try:
    env = sys.argv[4]                         # environment: 'cluster' OR 'xsession'
except:
    env = 'xsession'
22
if env == 'cluster':
    print '\n'== CLUSTER ENVIRONMENT: DISABLING VIPER & PYLAB ==\n'
    pylab_on     = False
    viper_on     = False
27
if RHS_BACKEND == 'Dolfin':
    print '==> LOAD VECTOR BACKEND: DOLFIN (FEniCS) ==\n'
else: # RHS_BACKEND == 'Mathematica'
    print '==> LOAD VECTOR BACKEND: Mathematica (Wolfram) ==\n'
SUFFIX      = SUFFIX_FORMAT % (test, P, levels)
32
# initializing lists
errors      = initializeList(P+1, TYPE_SIZE)
rates       = initializeList(P+1, TYPE_SIZE)
ndofs      = initializeList(P+1, 0)
37 hmax      = initializeList(P+1, 0)
cpu_time   = initializeList(P+1, 0)
refinements = getRefinements(level_offset, levels)

```

Listing 3: [main.py] main source code:

```

"""
For the detailed explanation refer to paper:
"Discontinuous Galerkin discretization of magnetic convection"
available at: [pdf] http://sukys.lt/search/label/publications
[doi] !!! add link here !!!
"""

__author__   = "Jonas Sukys (sukys.jonas@gmail.com)"
__date__     = "2010-02-19 -- 2010-08-01"
10 __copyright__ = "Copyright (C) 2010 Jonas Sukys, D-MATH, ETH Zurich"
__license__  = "GNU LGPL Version 2.1"

# === IMPORTS ===
from dolfin import *
15 import sys
import time

# === LOCAL IMPORTS ===
from config import *
from tests import *
from errors import *
from debug import *
from auxiliary import *
from dumpload import *
20
# === INITIALIZATION ===
from initialization import *

# === BEGIN ITERATION over polynomial degrees
30 for p in range(MIN_P, P+1):

    # timer for CPU effort consumption
    cpu_time_start = time.clock()

35    # compute only for the polynomial degree p = P
    if not compute_all: p = P

```

```

# quadrature accuracy order
quad_degree = QUAD.FACTOR * p + QUAD.OFFSET
40
# === BEGIN ITERATION over refinement levels
for M in refinements:
    # === PROBLEM DATA ===
45
    # mesh and function space
    mesh = UnitCube(M, M, M)
    hmax[p].append(mesh.hmax())
    V = VectorFunctionSpace(mesh, FE_TYPE, p)
    ndofs[p].append(V.dim())
    # velocity field
    v = getVelocity(test, quad_degree)
    # ellipticity fix
    c = getZeroOrderTerm(test)
    # exterior normal
    n = FacetNormal(mesh)

    # inflow boundary
    class Boundary_Inflow(SubDomain):
        def __init__(self, normal, velocity):
            self.n = normal
            self.v = velocity
            SubDomain.__init__(self)

        def inside(self, x, on_boundary):
            return on_boundary and dot3D(normal3D(x), self.v(x)) < DOLFIN_EPS
    70
    # === PROBLEM PARAMETERS ===
    # vector field on inflow boundary
    A_0 = getSolution(test, quad_degree)

    # marking boundary parts
    boundary_parts = MeshFunction('uint', mesh, mesh.topology().dim() - 1)
    boundary_parts.set_all(1)
    inflow = Boundary_Inflow(n, v)
    inflow.mark(boundary_parts, 0)

    # === VARIATIONAL FORMULATION ===
    A_- = TestFunction(V)
    A = TrialFunction(V)

    def upwind(u, v, n):
        return avg(u) + jump((sgn(dot(v, n)) + 1)/2)/2 * jump(u)

    def jump_cross(u, n):
        return cross(u('+'), n('+')) + cross(u(')'), n(')')
    90
    c_f = stability * 0.5 * abs(dot(v('+'), n('+')))

    a = c*dot(A, A_0)*dx - dot(A, v)*div(A_-)*dx + dot(cross(v, A_-), curl(A))*dx \
        + avg(dot(A, v))*jump(A_0, n)*dS + dot(A, v)*dot(A_0, n)*ds(0) + dot(A, v)*dot(A_0, n)*ds
    95
        (1) \
        + dot(jump_cross(A, n), avg(cross(v, A_-)) )*dS \
        - dot(v, n)*dot(A, A_-)*ds(0) \
        + c_f*dot(jump(A), jump(A_-))*dS
    100
    # boundary conditions
    g = dot(A_0, v)
    h = cross(A_0, n)

    # source term
    if RHS.BACKEND == 'Dolfin':
        f = getRHS.Dolfin(A_0, A_-, v)
    else: # RHS.BACKEND == 'Mathematica'
        f = dot(getRHS.Mathematica(test, quad_degree), A_-)
    105
    L = c*dot(A_0, A_-)*dx + f*dx - g*dot(A_0, n)*ds(0) + dot(h, cross(v, A_-))*ds(0)
    problem = VariationalProblem(a, L, exterior_facet_domains=boundary_parts)

    # configuring solver for the linear system
    problem.parameters['linear_solver'] = 'iterative',
    itsolver = problem.parameters['krylov_solver']
    itsolver['absolute_tolerance'] = 1e-15 # default: 1e-15
    115

```

```

120     itsolver['relative_tolerance'] = 1e-6 # default: 1e-6
121     itsolver['divergence_limit'] = 10000.0 # default: 10000.0
122     itsolver['gmres_restart'] = 30 # default: 30
123     itsolver['monitor_convergence'] = True # default: False
124     itsolver['report'] = True # default: True

125     # compute solution
126     A_discrete = problem.solve()

127     # === A POSTERIORI ERROR ANALYSIS ===

128     computeErrors(errors, p, A_discrete, A_0, mesh, quad_degree, FE_TYPE)

129     # END ITERATION over refinement levels

130     # computing convergence rates w.r.t. mesh size h
131     computeConvergenceRates(rates, errors, p, hmax, rates_wrt)

132     # compute CPU effort
133     cpu_time[p] = time.clock() - cpu_time_start

134     if not compute_all: break

135     # END ITERATION over polynomial degrees

136     # === TEXT OUTPUT to stdout and fout ===

137     output('ERRORS', errors, compute_all, cpu_time, TEXT_PATH, SUFFIX, ERRORS_FORMAT)
138     output('RATES', rates, compute_all, cpu_time, TEXT_PATH, SUFFIX, RATES_FORMAT)

139     # === DUMPING RESULTS to files ===

140     dump(errors, DUMP_PATH + 'ERRORS' + SUFFIX)
141     dump(rates, DUMP_PATH + 'RATES' + SUFFIX)

142     # === PYLAB PLOTTING & SAVING ===

143     if pylab_on:

144         plotErrors(refinements, errors, compute_all, errors_skip, errors_slopes, 'Error norms',
145                     , show_fig, save_fig, PYLAB_PATH, SUFFIX, FIGURE_FORMAT)
146         if compute_all:
147             plotConvergenceRates(rates, rates_method, rates_skip, '', show_fig, save_fig,
148                                   PYLAB_PATH, SUFFIX, FIGURE_FORMAT)

149     # === VIPER PLOTTING ===

150     if viper_on:

151         plot(v, title='Velocity field', mesh=mesh, axes=True)
152         if debug_on: plotInflowSurface(n, v, mesh)
153         plot(A_0, title='Exact solution', mesh=mesh, axes=True)
154         try:
155             plot(A_discrete, title='Discrete solution', axes=True)
156         except:
157             print '\nERROR :: Discrete solution was not computed!\n'
158             interactive()

159     # === VIPER SAVING ===

160     if save_viper:

161         file = File(VIPER_PATH + 'velocity' + SUFFIX + '.pvd')
162         file << interpolate(v, V)

163         file = File(VIPER_PATH + 'exact' + SUFFIX + '.pvd')
164         file << interpolate(A_0, V)

165         file = File(VIPER_PATH + 'discrete' + SUFFIX + '.pvd')
166         file << A_discrete

```

Listing 4: [auxiliary.py]: auxiliary routines:

```

# === AUXILIARY ROUTINES ===

def dot3D(u,v):
4   return u[0]*v[0] + u[1]*v[1] + u[2]*v[2]

# for unit cube only!
def normal3D(x):

9   from dolfin import DOLFIN_EPS

```

```

14     n = x
15     for i in range(0, 2):
16         if abs(x[0]) < DOLFIN_EPS:
17             return (-1,0,0)
18         elif abs(x[1]) < DOLFIN_EPS:
19             return (0,-1,0)
20         elif abs(x[2]) < DOLFIN_EPS:
21             return (0,0,-1)
22         elif abs(x[0] - 1) < DOLFIN_EPS:
23             return (1,0,0)
24         elif abs(x[1] - 1) < DOLFIN_EPS:
25             return (0,1,0)
26         elif abs(x[2] - 1) < DOLFIN_EPS:
27             return (0,0,1)

28     def sgn(x):
29         return 0 if x == 0 else x/abs(x)

30     # returns list of numbers of the form: 2** (offset + level)
31     def getRefinements(offset, levels):
32         M_all = range(offset, offset + levels)

33         for i in range(len(M_all)):
34             M_all[i] = 1 << M_all[i]

35         return M_all

36     def initializeList(CASE_SIZE, TYPE_SIZE):
37         err = []
38         for i in range(CASE_SIZE):
39             err.append([])
40             for j in range(TYPE_SIZE):
41                 err[i].append([])

42     return err

```

Listing 5: [tests.py]: tests for the solver:

```

from dolfin import *
quad_degree = 4

5 def getVelocity(test, quad_degree):
    if test == 'linear' : return Expression( ('1.2','1.4','0.7'), degree=quad_degree )
    if test == 'polynomial' : return Expression( ('0.66*(1 - pow(x[1], 2))', '0.2 + x[2]*x[0]', '0.8 - pow(x[0], 2)'), degree=quad_degree )
    if test == 'non-linear' : return Expression( ('0.66*(1 - pow(x[1], 2))', '0.2 + sin(pi*x[0])', '0.8 - pow(x[0], 2)'), degree=quad_degree )
    if test == 'zero-bc' : return Expression( ('1.2','1.4','0.7'), degree=quad_degree )

10 def getZeroOrderTerm(test):
    if test == 'linear' : return 1.0
    if test == 'polynomial' : return 10.0
    if test == 'non-linear' : return 10.0
    if test == 'zero-bc' : return 1.0

15 def getSolution(test, quad_degree):
    if test == 'linear' : return Expression( ('2*x[0] - 1.5*x[1] + 0.6*x[2]', '1.2*x[0] + 2.4*x[1] - 0.6*x[2]', '1.4*x[0] + 0.3*x[1] - 2.5*x[2]'), degree=quad_degree )
    if test == 'polynomial' : return Expression( ('x[0]*x[1]', '1 - pow(x[1], 2)', '1 + x[2]*x[0]'), degree=quad_degree )
20    if test == 'non-linear' : return Expression( ('sin(pi*x[1])', '1 - pow(x[1], 2)', '1 + pow(x[2], 2)'), degree=quad_degree )
    if test == 'zero-bc' :
        sol = 'sin(pi*x[0])*sin(2*pi*x[1])*sin(3*pi*x[2])'
        return Expression( (sol, sol, sol), degree=quad_degree )

25 def getRHS_Mathematica(test, quad_degree):

    if test == 'linear' : return Expression( ('0.72', '4.38', '0.35'), degree=
        quad_degree )

    if test == 'polynomial':
        rhs1 = '0.2*x[0] + 0.66*x[1]*(1 - pow(x[1], 2)) - 0.8*x[2] + 2*pow(x[0], 2)*x[2] +
        (0.8 - pow(x[0], 2))*x[2] + (1 - pow(x[1], 2))*x[2] - 2*x[0]*(1 + x[0]*x[2])',
        rhs2 = '-0.66*x[0] - 0.66*x[0]*pow(x[1], 2) + 0.66*x[0]*(1 - pow(x[1], 2)) - 2*x[1]*(0.2 + x[0]*x[2])',
        rhs3 = 'x[0]*(0.8 - pow(x[0], 2)) + x[0]*(1 - pow(x[1], 2)) + 0.66*x[2] - 0.66*pow(x[1], 2)*x[2]',
        return Expression( (rhs1, rhs2, rhs3), degree=quad_degree )

```

```

35   if test == 'non-linear':
36     rhs1 = '-2*x[0]*(1 + pow(x[2], 2)) + 0.6283185307179586*cos(pi*x[1]) + pi*cos(pi*x
37       [1])*sin(pi*x[0])',
38     rhs2 = '-2.0734511513692637*cos(pi*x[1]) + 2.0734511513692637*pow(x[1], 2)*cos(pi*x
39       [1]) + 2.0734511513692637*(1 - pow(x[1], 2))*cos(pi*x[1]) - 1.32*x[1]*sin(pi*x
40       [1]) - 2*x[1]*(0.2 + sin(\pi*x[0]))',
41     rhs3 = '2*(0.8 - pow(x[0], 2))*x[2]',
42     return Expression( (rhs1, rhs2, rhs3), degree=quad_degree )
43
44   if test == 'zero-bc':
45     rhs1 = '6.597344572538565*cos(3*pi*x[2])*sin(pi*x[0])*sin(2*pi*x[1]) +
46       8.79645943005142*cos(2*pi*x[1])*sin(pi*x[0])*sin(3*pi*x[2]) +
47       3.7699111843077517*cos(pi*x[0])*sin(2*pi*x[1])*sin(3*pi*x[2]),
48     rhs2 = '6.597344572538565*cos(3*pi*x[2])*sin(pi*x[0])*sin(2*pi*x[1]) +
49       8.79645943005142*cos(2*pi*x[1])*sin(pi*x[0])*sin(3*pi*x[2]) +
50       3.7699111843077517*cos(pi*x[0])*sin(2*pi*x[1])*sin(3*pi*x[2]),
51     rhs3 = '6.597344572538564*cos(3*pi*x[2])*sin(pi*x[0])*sin(2*pi*x[1]) +
52       8.79645943005142*cos(2*pi*x[1])*sin(pi*x[0])*sin(3*pi*x[2]) +
53       3.7699111843077517*cos(pi*x[0])*sin(2*pi*x[1])*sin(3*pi*x[2]),
54     return Expression( (rhs1, rhs2, rhs3), degree=quad_degree )
55
56 def getRHS_Dolfin(A_0, A_, v):
57   return dot(cross(curl(A_0), v), A_) + graddot(A_, A_0, v)
58
59 def graddot(A_, A_0, v):
60   return (A_[0]*v[0].dx(0)*A_0[0] + A_[0]*v[1].dx(0)*A_0[1] + A_[0]*v[2].dx(0)*A_0[2] + \
61     A_[1]*v[0].dx(1)*A_0[0] + A_[1]*v[1].dx(1)*A_0[1] + A_[1]*v[2].dx(1)*A_0[2] + \
62     A_[2]*v[0].dx(2)*A_0[0] + A_[2]*v[1].dx(2)*A_0[1] + A_[2]*v[2].dx(2)*A_0[2] + \
63     A_[0]*A_0[0].dx(0)*v[0] + A_[0]*A_0[1].dx(0)*v[1] + A_[0]*A_0[2].dx(0)*v[2] + \
64     A_[1]*A_0[0].dx(1)*v[0] + A_[1]*A_0[1].dx(1)*v[1] + A_[1]*A_0[2].dx(1)*v[2] + \
65     A_[2]*A_0[0].dx(2)*v[0] + A_[2]*A_0[1].dx(2)*v[1] + A_[2]*A_0[2].dx(2)*v[2])

```

Listing 6: [errors.py]: error computation and plotting:

```

# ===== ROUTINES FOR ERROR COMPUTATION, PRINTING AND PLOTTING =====
from config import FE_TYPE
4
# initializing error types
if FE_TYPE == 'DG':
  L2, CURL, JUMP, JUMP_EXT, TYPE_SIZE = range(5)
  TYPE_NAMES = ['L2 norm', 'H(curl) norm', 'Jump interior', 'Jump exterior']
9 else: # FE_TYPE == 'CG':
  L2, CURL, TYPE_SIZE = range(3)
  TYPE_NAMES = ['L2 norm', 'H(curl) norm']

def computeErrors(errors, case, A, A_0, mesh, quad_degree, FE_TYPE):
14
  from dolfin import VectorFunctionSpace, interpolate, Function, sqrt, assemble, dot,
    curl, jump, dx, dS, ds
  # interpolation in higher degree space for better error approximation
  VE = VectorFunctionSpace(mesh, FE_TYPE, quad_degree)
  A_0_VE = interpolate(A_0, VE)
  A_VE = interpolate(A, VE)

  # computing error field
  E = Function(VE)
  E.vector()[:] = A_VE.vector()[:] - A_0_VE.vector()[:]

  # computing error field norms
  # L2:
29  try:
    errors[case][L2].append(sqrt(assemble(dot(E,E)*dx, mesh = mesh)))
  except: print 'Skipping L2 error...'

  # CURL:
34  try:
    errors[case][CURL].append(sqrt(assemble(dot(curl(E),curl(E))*dx, mesh = mesh)))
  except: print 'Skipping CURL error...'

  # JUMP:
39  try:
    errors[case][JUMP].append(sqrt(assemble(dot(jump(E),jump(E))*dS, mesh = mesh)))
  except: print 'Skipping JUMP error...'

  # JUMP_EXT:
44  try:
    errors[case][JUMP_EXT].append(sqrt(assemble(dot(E,E)*ds, mesh = mesh)))
  except: print 'Skipping JUMP_EXT error...'

```

```

49 def plotErrors(refinements, err, compute_all, skip, slopes, title_text, show_fig,
    save_fig, PYLAB_PATH, SUFFIX, FIGURE_FORMAT):
50     from pylab import figure, gcf, gca, subplot, loglog, grid, legend, xlabel, ylabel,
    title, show
51
52     if compute_all:
53         if len(err) == 1:
54             cols = 1
55         else:
56             cols = 2
57
58         rows = (len(err) - 1) / cols + 1
59         figure(figsize=(cols*8, rows*4.62))
60
61         for p in range(len(err)):
62             subplot(rows, cols, p + 1)
63
64             for err_type in range(TYPE_SIZE):
65                 loglog(refinements[skip:], err[p][err_type][skip:], '-o')
66
67             for slope in slopes:
68                 plotSlope(slope, gca())
69
70             grid()
71             legend(TYPE_NAMES, loc='lower left')
72
73             ylabel('error norm')
74             xlabel('1/h')
75             title(title_text + ' for p = ' + str(p))
76
77     else:
78
79         figure(figsize=(8, 4.62))
80
81         p = len(err) - 1
82         for err_type in range(TYPE_SIZE):
83             loglog(refinements[skip:], err[p][err_type][skip:], '-o')
84
85             for slope in slopes:
86                 plotSlope(slope, gca())
87
88             grid()
89             legend(TYPE_NAMES, loc='lower left')
90
91             ylabel('error norm')
92             xlabel('1/h')
93             title(title_text + ' for p = ' + str(p))
94
95             if save_fig: savefig(gcf(), PYLAB_PATH + 'ERRORS' + SUFFIX + '.' + FIGURE_FORMAT,
96                                 FIGURE_FORMAT)
97             if show_fig: show()
98
99 # returns the list of convergence rates
100 def computeConvergenceRates(rates, errors, p, ref, wrt):
101
102     from math import log as ln # (log is a dolfin name too)
103
104     for err_type in range(TYPE_SIZE):
105         for i in range(1, len(errors[p][err_type])):
106             try:
107                 if wrt == 'hmax':
108                     rates[p][err_type].append(ln(float(errors[p][err_type][i-1])/float(errors[p][err_type][i]))/ln(float(ref[p][i-1])/float(ref[p][i])))
109                 elif wrt == 'ndofs':
110                     rates[p][err_type].append(ln(float(errors[p][err_type][i-1])/float(errors[p][err_type][i]))/ln(float(ref[p][i])/float(ref[p][i-1])))
111                 else:
112                     print 'wrt must be either \'meshsize\' or \'ndofs\''
113                     return
114             except:
115                 rates[p][err_type].append(0.0)
116
117 def plotConvergenceRates(rates, method, skip, title_text, show_fig, save_fig, PYLAB_PATH,
118                           SUFFIX, FIGURE_FORMAT):
119
120     from pylab import axhline, gcf, plot, grid, legend, xlabel, ylabel, title, show
121
122     # line splitting converge and divergence regions

```

```

124     axhline(y=0, linewidth=10, color='r', alpha=0.4, label='_nolegend_')
125
126     for err_type in range(TYPE_SIZE):
127         avg_rate = []
128         for case in range(len(rates)):
129             if method == 'average':
130                 if len(rates[case][err_type]) > skip:
131                     avg_rate.append( sum(rates[case][err_type][skip:]) / ( len(rates[case][err_type]) - skip ) )
132                 else:
133                     avg_rate.append( sum(rates[case][err_type]) / len(rates[case][err_type]) )
134             elif method == 'last':
135                 avg_rate.append( rates[case][err_type][-1] )
136             else:
137                 print 'method must be either \'average\' or \'last\''
138
139     plot(range(len(rates)), avg_rate, '--o', label=TYPE_NAMES[err_type])
140
141     grid()
142     legend(loc='lower right')
143     xlabel('polynomial degree')
144     ylabel('convergence rate')
145     title(title_text)
146
147     if save_fig: savefig(gcf(), PYLAB_PATH + 'RATES' + SUFFIX + '.' + FIGURE_FORMAT,
148                           FIGURE_FORMAT)
149     if show_fig: show()
150
151     # text output to stdout and fout
152     def output(title, data, compute_all, cpu_time, OUTPUT_PATH, SUFFIX, format_string):
153
154         from datetime import timedelta
155
156         # makes array into a compactly formatted string
157         def format(array, format_string):
158             line = ''
159             for idx in range(len(array)):
160                 line += format_string % array[idx] + '\t'
161             return line.rstrip()
162
163         # writes @param line into stdout & fout
164         def record(fout, line):
165             print line
166             fout.write(line + '\n')
167
168         fout = open(OUTPUT_PATH + title + SUFFIX, 'w')
169
170         for p in range(len(data)):
171
172             # compute only for the value p = P
173             if not compute_all: p = len(data) - 1
174
175             record(fout, '\n====| ' + title + ' for p = ' + str(p) + ' |===' [CPU time: ' + str(
176                 timedelta(seconds=round(cpu_time[p]))) + ']\n')
177             for err_type in range(TYPE_SIZE):
178                 record(fout, str(TYPE_NAMES[err_type]) + ':')
179                 record(fout, format(data[p][err_type], format_string))
180                 record(fout, '') # adds an additional line between err-type's
181
182             # compute only for the value p = P
183             if not compute_all: break
184
185         fout.close()
186
187         # writes pylab figure to file
188         def savefig(fig, path, FIGURE_FORMAT):
189             fig.savefig(path, dpi=None, facecolor='w', edgecolor='w', orientation='portrait',
190                         papertype=None, format=FIGURE_FORMAT, transparent=False)
191
192         # plots slopes
193         def plotSlope(slope, plt):
194
195             from pylab import xlim, ylim, loglog
196             from math import pow, log as ln # (log is a dolfin name too)
197
198             xmin, xmax = xlim()
199             ymin, ymax = ylim()
200
201             xmin = xmax / 10 * 1.2
202             xmax = 6 * xmin
203
204             ymax = ymax * 0.7
205             ymin = pow( 10, ln(ymax, 10) - slope * (ln(xmax, 10) - ln(xmin, 10)) )

```

```
204 plt.plot([xmin, xmax], [ymax, ymin], '--k', label='_nolegend_')
plt.annotate(str(slope), xy=(xmax, ymin), xycoords='data')
```

Listing 7: [debug.py]: debugging routines:

```
# === DEBUGGING ROUTINES ===

from dolfin import *
from auxiliary import *

5 def plotInflowSurface(n, v, mesh):
    # inflow surface
    class Surface_Inflow(SubDomain):
        def __init__(self, normal, velocity):
10        self.n = normal
            self.v = velocity
        SubDomain.__init__(self)

15    def inside(self, x, on_boundary):
        return dot3D(normal3D(x), self.v(x)) < 0

    # plotting inflow surface
    surface_mesh = BoundaryMesh(mesh)
    surface_parts = MeshFunction('uint', surface_mesh, surface_mesh.topology().dim())
20    surface_parts.set_all(1)
    inflow = Surface_Inflow(n, v)
    inflow.mark(surface_parts, 0)
    plot(surface_parts, title='Inflow surface (in red)', axes=True)
```

Listing 8: [dumupload.py]: file I/O for objects:

```
# dumps obj to file
2 def dump(obj, path):
    import cPickle
    cPickle.dump(obj, open(path, 'wb'))

# loads obj from file
7 def load(path):
    import cPickle
    return cPickle.load(open(path, 'rb'))
```

Listing 9: [loadplot.py]: routines for dumped files:

```
1 # LOADS FROM FILES AND PLOTS DUMPED ERRORS AND CONVERGENCE RATES
#( Dolfin isn'tallation is NOT needed, MatPlotLib is sufficient )

from config import *
from auxiliary import *
6 from dumupload import *
from errors import *

import sys

11 # === QUICK CONFIG [ overrides config.py ] ===

errors_skip = 0    # number of first error norms to ignore when plotting
rates_skip = 2     # number of first error norms to ignore when computing average
                    convergence rates

16 # ===

try:
    test      = sys.argv[1] # test to use
    P         = int(sys.argv[2]) # polynomial degree
21    levels   = int(sys.argv[3]) # number of refinements
except:
    test      = 'polynomial'
    P         = 1
    levels   = 7
26 try:
    show_fig = sys.argv[4]
    save_fig = sys.argv[5]
except:
31    show_fig = True
    save_fig = False
```

```

36 if test == 'zero-bc':
    errors_skip = 1
    rates_skip = 2
SUFFIX = SUFFIX_FORMAT % (test, P, levels)
41 errors = load (DUMP_PATH + 'ERRORS' + SUFFIX)
rates = load (DUMP_PATH + 'RATES' + SUFFIX)
plotErrors(getRefinements(level_offset, levels), errors, compute_all, errors_skip,
           errors_slopes, 'Error norms', show_fig, save_fig, PYLAB_PATH, SUFFIX, FIGUREFORMAT)
if compute_all: plotConvergenceRates(rates, 'average', rates_skip, '', show_fig,
                                     save_fig, PYLAB_PATH, SUFFIX, FIGUREFORMAT)

```

B Shell scripts

Listing 10: [batch_job.sh]: executes multiple configurations:

```

1 #!/bin/bash
# executes computations for multiple configurations
#
# P          : 0 1 2 3 4
# max LEVELS : 8 7 6 5 4
6 # cpu_time   : 2 2 2 2 2 // in hours per one test
#
ENV='cluster'
DEGREES='0 1 2 3'
11 TESTS='polynomial non-linear zero-bc'
MAX='8'
16 for P in $DEGREES
do
    LEVELS=$((MAX-$P))
    for TEST in $TESTS
    do
21        python main.py $TEST $P $LEVELS $ENV;
    done
done

```

Listing 11: [save_figs.sh]: saves multiple pylab figures:

```

#!/bin/bash cd '/media/data/Dropbox/ETH Zurich/Lectures/Term Paper/fenics/sukysj-dgdmc'
2 # saves pylab figures for multiple configurations
#
DEGREES='0 1 2 3'
TESTS='polynomial non-linear zero-bc'
7 MAX='8'
SHOWFIG='False'
SAVEFIG='True'
12 for P in $DEGREES
do
    LEVELS=$((MAX-$P))
    for TEST in $TESTS
    do
17        python loadplot.py $TEST $P $LEVELS $SHOWFIG $SAVEFIG;
    done
done

```

C Mathematica code

Listing 12: [rhs.nb]: computes f on Ω :

```
<< VectorAnalysis`
```

```

SetCoordinates[Cartesian[x, y, z]];

5 Linear test :
a1 = 2 x - 1.5 y + 0.6 z;
a2 = 1.2 x + 2.4 y - 0.6 z;
a3 = 1.4 x + 0.3 y - 2.5 z;
A = {a1, a2, a3};

10 v1 = 1.2;
v2 = 1.4;
v3 = 0.7;
v = {v1, v2, v3};

15 CForm[Grad[A.v] + Cross[Curl[A], v]]

Polynomial test :

20 a1 = x y;
a2 = (1 - y^2);
a3 = (1 + z x);
A = {a1, a2, a3};

25 v1 = 0.66*(1 - y^2);
v2 = 0.2 + z x;
v3 = 0.8 - x^2;
v = {v1, v2, v3};

30 CForm[Grad[A.v] + Cross[Curl[A], v]]

Non-linear test :

35 a1 = Sin[\[Pi] y];
a2 = (1 - y^2);
a3 = (1 + z^2);
A = {a1, a2, a3};

40 v1 = 0.66*(1 - y^2);
v2 = 0.2 + Sin[\[Pi] x];
v3 = 0.8 - x^2;
v = {v1, v2, v3};

CForm[Grad[A.v] + Cross[Curl[A], v]]

45 Zero - bc test :

a1 = Sin[\[Pi] x]*Sin[2 \[Pi] y]*Sin[3 \[Pi] z];
a2 = Sin[\[Pi] x]*Sin[2 \[Pi] y]*Sin[3 \[Pi] z];
a3 = Sin[\[Pi] x]*Sin[2 \[Pi] y]*Sin[3 \[Pi] z];
A = {a1, a2, a3};

50 v1 = 1.2;
v2 = 1.4;
v3 = 0.7;
v = {v1, v2, v3};

55 CForm[Grad[A.v] + Cross[Curl[A], v]]

```

D Computations architecture

Arch x86-64

Kernel 2.6.30.9-90

CPU 16 x Quad-Core 2.3Ghz

Memory 64 GB

OpenMP not enabled

MPI not enabled

Usage per test for `levels = 8 - degree`:

CPU: ~ 2 hours

Memory: ~ 40 GB

Location: cmath-7 node in SAM, D-MATH, ETH Zurich