Discrete polytopal complexes for fluid mechanics, electromagnetism and solid mechanics

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New generation methods for numerical simulations



Outline

1 Some PDE models of interest

- Stokes I
- Stokes II
- Navier–Stokes
- Magnetostatics
- 2 De Rham complex
- **3** Discrete De Rham (DDR) complex
- 4 Applications to the models of interest

Slides



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Stokes equations: standard formulation

 Ω domain, $\nu > 0$ and $f \in L^2(\Omega)$. • Strong form: Find $\boldsymbol{u}: \Omega \to \mathbb{R}^3$ and $p: \Omega \to \mathbb{R}$ s.t. $\int_{\Omega} p = 0$ and $-\nu \Delta u + \operatorname{grad} p = f$ in Ω , (momentum conservation) div $\boldsymbol{u} = 0$ in Ω , (mass conservation) u = 0 on $\partial \Omega$, (boundary condition) • Weak form: Find $(\boldsymbol{u},p) \in H^1_0(\Omega)^d \times L^2(\Omega)$ s.t. $\int_{\Omega} p = 0$ and $\nu(\operatorname{\mathbf{grad}} \boldsymbol{u}, \operatorname{\mathbf{grad}} \boldsymbol{v})_{L^2} - (p, \operatorname{div} \boldsymbol{v})_{L^2} = (\boldsymbol{f}, \boldsymbol{v})_{L^2} \quad \forall \boldsymbol{v} \in H^1_0(\Omega),$ $(\operatorname{div} \boldsymbol{u}, q)_{I^2} = 0 \qquad \forall q \in L^2(\Omega)$

Stokes equations: standard formulation

 $\begin{array}{l} \Omega \text{ domain, } \nu > 0 \text{ and } \boldsymbol{f} \in \boldsymbol{L}^2(\Omega).\\ \circ \text{ Strong form: Find } \boldsymbol{u}: \Omega \to \mathbb{R}^3 \text{ and } p: \Omega \to \mathbb{R} \text{ s.t. } \int_{\Omega} p = 0 \text{ and}\\ \quad -\nu \boldsymbol{\Delta} \boldsymbol{u} + \mathbf{grad} \, p = \boldsymbol{f} \quad \text{in } \Omega, \qquad (\text{momentum conservation})\\ \quad \text{div } \boldsymbol{u} = 0 \quad \text{in } \Omega, \qquad (\text{mass conservation})\\ \boldsymbol{u} = \boldsymbol{0} \quad \text{on } \partial\Omega, \quad (\text{boundary condition})\\ \circ \text{ Weak form: Find } (\boldsymbol{u}, p) \in H^1_0(\Omega)^d \times L^2(\Omega) \text{ s.t. } \int_{\Omega} p = 0 \text{ and}\\ \nu(\mathbf{grad} \, \boldsymbol{u}, \mathbf{grad} \, \boldsymbol{v})_{L^2} - (p, \operatorname{div} \boldsymbol{v})_{L^2} = (\boldsymbol{f}, \boldsymbol{v})_{L^2} \quad \forall \boldsymbol{v} \in H^1_0(\Omega),\\ \quad (\operatorname{div} \boldsymbol{u}, q)_{L^2} = 0 \qquad \forall q \in L^2(\Omega) \end{array}$

- \circ A priori estimates require: (¹)
 - Poincaré inequality: $\|\cdot\|_{L^2} \lesssim \|\operatorname{\mathbf{grad}} \cdot\|_{L^2}$ on $H^1_0(\Omega)$,
 - inf-sup: $\sup_{v \in H_0^1} \frac{(p, \operatorname{div} v)_{L^2}}{\|v\|_{H_0^1}} \ge C \|p\|_{L^2}$, i.e. $\operatorname{Im} \operatorname{div} = L^2(\Omega)$.

 $^{1}a \lesssim b$ means $a \leq Cb$ with C independent of a, b.

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Stokes in curl-curl formulation: weak form

• Strong form:

$$\underbrace{\nu(\operatorname{\mathbf{curl}}\operatorname{\mathbf{curl}} \boldsymbol{u} - \operatorname{\mathbf{grad}} \operatorname{div} \boldsymbol{u})}_{\nu(\operatorname{\mathbf{curl}}\operatorname{\mathbf{curl}} \boldsymbol{u} - \operatorname{\mathbf{grad}} \operatorname{div} \boldsymbol{u})} + \operatorname{\mathbf{grad}} p = \boldsymbol{f} \quad \text{in } \Omega, \quad (\text{momentum cons.}) \\ \operatorname{div} \boldsymbol{u} = 0 \quad \text{in } \Omega, \quad (\text{mass conservation}) \\ \operatorname{\mathbf{curl}} \boldsymbol{u} \times \mathbf{n} = \boldsymbol{0} \text{ and } \boldsymbol{u} \cdot \mathbf{n} = 0 \quad \text{on } \partial\Omega, \quad (\text{boundary conditions}) \\ \int_{\Omega} p = 0$$

• Weak form: Find $(\boldsymbol{u},p) \in \boldsymbol{H}(\operatorname{\mathbf{curl}};\Omega) \times H^1(\Omega)$ s.t. $\int_{\Omega} p = 0$ and

$$\begin{split} \nu(\operatorname{\mathbf{curl}} \boldsymbol{u}, \operatorname{\mathbf{curl}} \boldsymbol{v})_{L^2} + (\operatorname{\mathbf{grad}} p, \boldsymbol{v})_{L^2} &= (\boldsymbol{f}, \boldsymbol{v})_{L^2} \quad \forall \boldsymbol{v} \in \boldsymbol{H}(\operatorname{\mathbf{curl}}; \Omega), \\ -(\boldsymbol{u}, \operatorname{\mathbf{grad}} q)_{L^2} = 0 & \forall q \in H^1(\Omega), \end{split}$$

where

$$\boldsymbol{H}(\operatorname{\boldsymbol{curl}};\Omega)\coloneqq\left\{\boldsymbol{v}\in\boldsymbol{L}^2(\Omega)\,:\,\operatorname{\boldsymbol{curl}}\boldsymbol{v}\in\boldsymbol{L}^2(\Omega)\right\}.$$

Stokes equations in curl-curl formulation: stability

$$\begin{split} \nu(\operatorname{\mathbf{curl}} \boldsymbol{u}, \operatorname{\mathbf{curl}} \boldsymbol{v})_{L^2} + (\operatorname{\mathbf{grad}} p, \boldsymbol{v})_{L^2} & \forall \boldsymbol{v} \in \boldsymbol{H}(\operatorname{\mathbf{curl}}; \Omega), \\ -(\boldsymbol{u}, \operatorname{\mathbf{grad}} q)_{L^2} = 0 & \forall q \in H^1(\Omega) \end{split}$$

 $\label{eq:marginal} \begin{array}{l} \circ \ \mbox{Make } \boldsymbol{v} = \mathbf{grad} \, p \ \mbox{to get } \| \, \mathbf{grad} \, p \|_{L^2} \leq \| \boldsymbol{f} \|_{L^2} \ \mbox{since } \, \mathbf{curl} \, \mathbf{grad} = 0. \\ \circ \ \mbox{Make } (\boldsymbol{v}, q) = (\boldsymbol{u}, p): \end{array}$

 $\nu \|\operatorname{curl} u\|_{L^2}^2 \le \|f\|_{L^2} \|u\|_{L^2}.$

Stokes equations in curl-curl formulation: stability

$$egin{aligned} &
u(\operatorname{\mathbf{curl}}oldsymbol{u},\operatorname{\mathbf{curl}}oldsymbol{v})_{L^2}+(\operatorname{\mathbf{grad}}p,oldsymbol{v})_{L^2}&oralloldsymbol{v}\inoldsymbol{H}(\operatorname{\mathbf{curl}};\Omega),\ & -(oldsymbol{u},\operatorname{\mathbf{grad}}q)_{L^2}=oldsymbol{0}&oralloldsymbol{v}\inoldsymbol{H}^1(\Omega) \end{aligned}$$

 $\circ \text{ Make } \boldsymbol{v} = \operatorname{\mathbf{grad}} p \text{ to get } \|\operatorname{\mathbf{grad}} p\|_{L^2} \leq \|\boldsymbol{f}\|_{L^2} \text{ since } \operatorname{\mathbf{curl}} \operatorname{\mathbf{grad}} = 0. \\ \circ \text{ Make } (\boldsymbol{v}, q) = (\boldsymbol{u}, p):$

 $u \|\operatorname{curl} u\|_{L^2}^2 \le \|f\|_{L^2} \|u\|_{L^2}.$

 $\circ~$ If $\Omega~$ "is nice" ,

 $\operatorname{Im} \operatorname{\mathbf{grad}} = \operatorname{Ker} \operatorname{\mathbf{curl}}.$

The incompressibility then gives $u \in (\operatorname{Im} \operatorname{\mathbf{grad}})^{\perp} = (\operatorname{Ker} \operatorname{\mathbf{curl}})^{\perp}$ and the

Poincaré inequality: $\|\cdot\|_{L^2} \lesssim \|\operatorname{\mathbf{curl}}\cdot\|_{L^2}$ on $(\operatorname{Ker}\operatorname{\mathbf{curl}})^{\perp}$

yields

$$\|oldsymbol{u}\|_{L^2}\lesssim \|\operatorname{\mathbf{curl}}oldsymbol{u}\|_{L^2}.$$

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Navier-Stokes equations

• Additional convective term:

$$\operatorname{div}(\boldsymbol{u}\otimes\boldsymbol{u}) = (\operatorname{div}\boldsymbol{u})\boldsymbol{u} + (\operatorname{\mathbf{curl}}\boldsymbol{u}) \times \boldsymbol{u} + \frac{1}{2}\operatorname{\mathbf{grad}}|\boldsymbol{u}|^2.$$

SO

$$-\nu\Delta \boldsymbol{u} + (\boldsymbol{u}\cdot\nabla)\boldsymbol{u} + \operatorname{\mathbf{grad}} p$$

= $\nu\operatorname{\mathbf{curl}}\operatorname{\mathbf{curl}}\boldsymbol{u} + \underbrace{(\operatorname{\mathbf{curl}}\boldsymbol{u})\times\boldsymbol{u}}_{\operatorname{additional term}} + \operatorname{\mathbf{grad}}\underbrace{\left(p + \frac{1}{2}|\boldsymbol{u}|^2\right)}_{\operatorname{new pressure } p'}$

 $\circ\,$ Additional term in weak formulation

$$\int_{\Omega} \left[({f curl}\, oldsymbol{u}) imes oldsymbol{u}
ight] \cdot oldsymbol{v}.$$

It vanishes for v = u.

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Magnetostatics: weak formulation

• Strong form: For $\mu > 0$ and $J \in \operatorname{curl} H(\operatorname{curl}; \Omega)$, the magnetostatics problem reads:

Find the magnetic field $H: \Omega \to \mathbb{R}^3$ and vector potential $A: \Omega \to \mathbb{R}^3$ s.t.

| $\mu H - \operatorname{curl} A = 0$ | in Ω , | (vector potential) |
|---|----------------------|----------------------|
| $\operatorname{curl} H = J$ | in Ω , | (Ampère's law) |
| $\operatorname{div} \boldsymbol{A} = 0$ | in Ω , | (Coulomb's gauge) |
| $m{A} 	imes {f n} = m{0}$ | on $\partial \Omega$ | (boundary condition) |

• Weak form: Find $(\boldsymbol{H}, \boldsymbol{A}) \in \boldsymbol{H}(\operatorname{\mathbf{curl}}; \Omega) \times \boldsymbol{H}(\operatorname{div}; \Omega)$ s.t.

$$\int_{\Omega} \mu \boldsymbol{H} \cdot \boldsymbol{\tau} - \int_{\Omega} \boldsymbol{A} \cdot \mathbf{curl} \, \boldsymbol{\tau} = 0 \qquad \forall \boldsymbol{\tau} \in \boldsymbol{H}(\mathbf{curl}; \Omega),$$
$$\int_{\Omega} \mathbf{curl} \, \boldsymbol{H} \cdot \boldsymbol{v} + \int_{\Omega} \operatorname{div} \boldsymbol{A} \operatorname{div} \boldsymbol{v} = \int_{\Omega} \boldsymbol{J} \cdot \boldsymbol{v} \quad \forall \boldsymbol{v} \in \boldsymbol{H}(\operatorname{div}; \Omega).$$

Relations images/kernels:

 $\operatorname{Im} \operatorname{\mathbf{curl}} = \operatorname{Ker} \operatorname{div},$ $\operatorname{Im} \operatorname{div} = L^2(\Omega).$

Poincaré inequalities: $\begin{aligned} \|\cdot\|_{L^2} &\leq C \|\operatorname{div} \cdot\|_{L^2} \quad \text{on } (\operatorname{Ker} \operatorname{div})^{\perp} \\ \|\cdot\|_{L^2} &\leq C \|\operatorname{\mathbf{curl}} \cdot\|_{L^2} \quad \text{on } (\operatorname{Ker} \operatorname{\mathbf{curl}})^{\perp}. \end{aligned}$

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$$H^1(\Omega) \xrightarrow{\operatorname{\mathbf{grad}}} H(\operatorname{\mathbf{curl}}; \Omega) \xrightarrow{\operatorname{\mathbf{curl}}} H(\operatorname{div}; \Omega) \xrightarrow{\operatorname{div}} L^2(\Omega) \xrightarrow{0} \{0\}$$

• Complex: image of an operator included in kernel of the next one. That is, the composition of two subsequent operators vanishes.

$$H^1(\Omega) \xrightarrow{\operatorname{\mathbf{grad}}} \boldsymbol{H}(\operatorname{\mathbf{curl}};\Omega) \xrightarrow{\operatorname{\mathbf{curl}}} \boldsymbol{H}(\operatorname{div};\Omega) \xrightarrow{\operatorname{div}} L^2(\Omega) \xrightarrow{0} \{0\}$$

Complex: image of an operator included in kernel of the next one.
Depending on the topology of Ω, some inclusions can be equalities:

no "tunnels" \implies Im grad = Ker curl (Stokes in curl-curl) no "voids" \implies Im curl = Ker div (magnetostatics) Im div = $L^2(\Omega)$ (magnetostatics, standard Stokes)

$$H^{1}(\Omega) \xrightarrow{\mathbf{grad}} \boldsymbol{H}(\mathbf{curl}; \Omega) \xrightarrow{\mathbf{curl}} \boldsymbol{H}(\mathrm{div}; \Omega) \xrightarrow{\mathrm{div}} L^{2}(\Omega) \xrightarrow{0} \{0\}$$

Complex: image of an operator included in kernel of the next one.
Depending on the topology of Ω, some inclusions can be equalities:

no "tunnels" $\implies \text{Im} \operatorname{\mathbf{grad}} = \text{Ker} \operatorname{\mathbf{curl}}$ (Stokes in curl-curl) no "voids" $\implies \text{Im} \operatorname{\mathbf{curl}} = \text{Ker} \operatorname{div}$ (magnetostatics) $\text{Im} \operatorname{div} = L^2(\Omega)$ (magnetostatics, standard Stokes)

 $\circ~$ If Ω has a non-trivial topology, the de Rham's cohomology characterizes

 $\operatorname{Ker}\operatorname{\mathbf{curl}}/\operatorname{Im}\operatorname{\mathbf{grad}}$ and $\operatorname{Ker}\operatorname{div}/\operatorname{Im}\operatorname{\mathbf{curl}}$

Reproducing these properties at the discrete level is key for stable schemes.

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The finite element approach and its limitations Global complex



 $\mathcal{T}_h = \{T\}$ conforming tetrahedral/hexahedral mesh.

• Define local polynomial spaces on each element, and glue them together to form a sub-complex of the de Rham complex:

Example: conforming *P^k*-Nédélec-Raviart-Thomas spaces [Arnold, 2018].
Gluing only works on special meshes!

The Finite Element way Shortcomings



- Approach limited to conforming meshes with standard elements
 - \implies local refinement requires to trade mesh size for mesh quality
 - ⇒ complex geometries may require a large number of elements
 - \implies the element shape cannot be adapted to the solution
- Need for (global) basis functions
 - $\implies\,$ significant increase of DOFs on hexahedral elements

Benefits of polytopal meshes I



- Local refinement (to capture geometry or solution features) is seamless, and can preserve mesh regularity.
- Agglomerated elements are also easy to handle (and useful, e.g., in multi-grid methods).
- Even on standard meshes, high-level approach can lead to leaner methods (fewer DOFs).

Benefits of polytopal meshes II

| Discrete space | k = 0 | k = 1 | k = 2 |
|--|--------------------|-----------------------------------|-----------------------------------|
| $H^1(T)$ | 4 🔷 4 | 10 \diamondsuit 10 | <mark>20</mark> \diamondsuit 20 |
| $\boldsymbol{H}(\mathbf{curl};T)$ | <mark>6</mark> | <mark>23</mark> \diamondsuit 20 | <mark>53</mark> \diamondsuit 45 |
| $\boldsymbol{H}(\operatorname{div};T)$ | 4 🔷 4 | <mark>18</mark> \diamondsuit 15 | 44 \diamondsuit 36 |
| $L^2(T)$ | $1 \diamondsuit 1$ | 4 🔷 4 | 10 \diamondsuit 10 |

Table: Tetrahedron: SDDR polytopal complex \Diamond RTN.

| Discrete space | k = 0 | k = 1 | k = 2 |
|--|--------------------|-----------------------------------|------------------------------------|
| $H^1(T)$ | 8 🔷 8 | <mark>20</mark> | <mark>32</mark> \diamondsuit 64 |
| $\boldsymbol{H}(\mathbf{curl};T)$ | 12 🔷 12 | <mark>39</mark> 🔷 54 | 77 🔷 144 |
| $\boldsymbol{H}(\operatorname{div};T)$ | <mark>6</mark> | <mark>24</mark> \diamondsuit 36 | <mark>56</mark> \diamondsuit 108 |
| $L^2(T)$ | $1 \diamondsuit 1$ | 4 🔷 8 | 10 \diamondsuit 27 |

Table: Hexahedron: SDDR polytopal complex \Diamond RTN.

[Di Pietro and Droniou, 2023c]

Refs.: [Di Pietro et al., 2020, Di Pietro and Droniou, 2023a]

- Hierarchical constructions: from lowest-dimensional mesh entity to higher-dimensional entities.
- Enhancement:
 - □ discrete differential operator first,
 - □ potential reconstruction using the discrete differential operator.

(both polynomially consistent, both based on IBP formulas.)

• The definition of the spaces (DOFs) also guided by these IBP formulas.

Same guiding principles as the Hybrid High-Order (HHO) method [Di Pietro and Droniou, 2020].

Mesh notations

- Mesh $\mathcal{M}_h = (\mathcal{T}_h, \mathcal{F}_h, \mathcal{E}_h, \mathcal{V}_h)$ of elements/faces/edges/vertices, with intrinsic orientations (tangent, normal).
- $\circ \ \omega_{TF} \in \{+1, -1\}$ such that $\omega_{TF} \mathbf{n}_F$ outer normal to T.
- $\omega_{FE} \in \{+1, -1\}$ such that $\omega_{FE} \mathbf{t}_E$ clockwise on F.



 $\circ~\mathsf{IBP}$ is the starting point: if $q\in\mathcal{P}^{k+1}(E)$ then

$$\int_{E} q'r = -\int_{E} q \underbrace{r'}_{\in \mathcal{P}^{k-1}(E)} + q(\boldsymbol{x}_{V_2})r(\boldsymbol{x}_{V_2}) - q(\boldsymbol{x}_{V_1})r(\boldsymbol{x}_{V_1}) \qquad \forall r \in \mathcal{P}^k(E)$$

with derivatives in the direction t_E .

 $\circ~\operatorname{IBP}$ is the starting point: if $q\in \mathcal{P}^{k+1}(E)$ then

$$\int_{E} q'r = -\int_{E} \pi_{r,E}^{k-1} q \underbrace{r'}_{\in \mathcal{P}^{k-1}(E)} + q(\boldsymbol{x}_{V_{2}})r(\boldsymbol{x}_{V_{2}}) - q(\boldsymbol{x}_{V_{1}})r(\boldsymbol{x}_{V_{1}}) \qquad \forall r \in \mathcal{P}^{k}(E)$$

with $\pi_{r,E}^{k-1}$ the L^2 -projection on $\mathcal{P}^{k-1}(E)$.

 $\circ~\operatorname{IBP}$ is the starting point: if $q\in \mathcal{P}^{k+1}(E)$ then

$$\int_{E} q'r = -\int_{E} \pi_{r,E}^{k-1} q \underbrace{r'}_{\in \mathcal{P}^{k-1}(E)} + q(\boldsymbol{x}_{V_{2}})r(\boldsymbol{x}_{V_{2}}) - q(\boldsymbol{x}_{V_{1}})r(\boldsymbol{x}_{V_{1}}) \qquad \forall r \in \mathcal{P}^{k}(E)$$

 $\circ~$ Space and interpolator:

$$\underline{X}_{\mathbf{grad},E}^{k} = \left\{ \underline{q}_{E} = (q_{E}, (q_{V})_{V \in \mathcal{V}_{E}}) : q_{E} \in \mathcal{P}^{k-1}(E), \ q_{V} \in \mathbb{R} \right\},$$
$$\underline{I}_{\mathbf{grad},E}^{k} q = (\pi_{r,E}^{k-1}q, (q(\boldsymbol{x}_{V}))_{V \in \mathcal{V}_{E}}) \qquad \forall q \in C(\overline{E}).$$

 $\circ~\mbox{IBP}$ is the starting point: if $q\in \mathcal{P}^{k+1}(E)$ then

$$\int_{E} q'r = -\int_{E} \pi_{r,E}^{k-1} q \underbrace{r'}_{\in \mathcal{P}^{k-1}(E)} + q(\boldsymbol{x}_{V_{2}})r(\boldsymbol{x}_{V_{2}}) - q(\boldsymbol{x}_{V_{1}})r(\boldsymbol{x}_{V_{1}}) \qquad \forall r \in \mathcal{P}^{k}(E)$$

- Space: $\underline{X}_{\mathbf{grad},E}^{k} = \Big\{ \underline{q}_{\underline{E}} = (\underline{q}_{\underline{E}}, (q_{V})_{V \in \mathcal{V}_{E}}) : q_{E} \in \mathcal{P}^{k-1}(E), q_{V} \in \mathbb{R} \Big\}.$
- $\circ \text{ Edge gradient } G^k_E: \underline{X}^k_{\mathbf{grad},E} \to \mathcal{P}^k(E) \text{ s.t.}$

$$\int_E (G_E^k \underline{q}_E) r = -\int_E q_E r' + q_{V_2} r(\boldsymbol{x}_{V_2}) - q_{V_1} r(\boldsymbol{x}_{V_1}) \qquad \forall r \in \mathcal{P}^k(E).$$

 $\circ~\mbox{IBP}$ is the starting point: if $q\in \mathcal{P}^{k+1}(E)$ then

$$\int_{E} q'r = -\int_{E} \pi_{r,E}^{k-1} q \underbrace{r'}_{\in \mathcal{P}^{k-1}(E)} + q(\boldsymbol{x}_{V_{2}})r(\boldsymbol{x}_{V_{2}}) - q(\boldsymbol{x}_{V_{1}})r(\boldsymbol{x}_{V_{1}}) \qquad \forall r \in \mathcal{P}^{k}(E)$$

• Space: $\underline{X}_{\mathbf{grad},E}^{k} = \left\{ \underline{q}_{E} = (q_{E}, (q_{V})_{V \in \mathcal{V}_{E}}) : q_{E} \in \mathcal{P}^{k-1}(E), q_{V} \in \mathbb{R} \right\}.$ • Edge gradient $G_{E}^{k} : \underline{X}_{\mathbf{grad}}^{k} \to \mathcal{P}^{k}(E)$ s.t.

$$\int_{E} (G_{E}^{k} \underline{q}_{E}) r = -\int_{E} q_{E} r' + q_{V_{2}} r(\boldsymbol{x}_{V_{2}}) - q_{V_{1}} r(\boldsymbol{x}_{V_{1}}) \qquad \forall r \in \mathcal{P}^{k}(E).$$

 $\circ \ \, \text{Potential reconstruction} \ \, \gamma^{k+1}_E:\underline{X}^k_{\mathbf{grad},E}\to \mathcal{P}^{k+1}(E) \ \, \text{s.t.}$

$$\int_{E} (\gamma_{E}^{k+1} \underline{q}_{E}) z' = -\int_{E} (G_{E}^{k} \underline{q}_{E}) z + q_{V_{2}} z(\boldsymbol{x}_{V_{2}}) - q_{V_{1}} z(\boldsymbol{x}_{V_{1}}) \qquad \forall z \in \mathcal{P}^{k+2}(E).$$

(Works because $\frac{d}{dx}: \mathcal{P}^{k+2}(E)/\mathbb{R} \to \mathcal{P}^{k+2}(E)$ is an isomorphism.)

 $\circ~ {\rm IBP}$ is the starting point: if $q\in {\cal P}^{k+1}(F)$,

$$\int_{F} (\operatorname{\mathbf{grad}}_{F} q) \cdot \boldsymbol{v} = -\int_{F} q \operatorname{\underline{div}}_{F} \boldsymbol{v}_{F} + \sum_{E \in \mathcal{E}_{F}} \omega_{FE} \int_{E} q \boldsymbol{v} \cdot \mathbf{n}_{FE} \quad \forall \boldsymbol{v} \in \mathcal{P}^{k}(F)^{2}.$$

 $\circ~ {\rm IBP}$ is the starting point: if $q\in {\cal P}^{k+1}(F)$,

$$\int_{F} (\operatorname{\mathbf{grad}}_{F} q) \cdot \boldsymbol{v} = -\int_{F} \pi_{r,F}^{k-1} q \underbrace{\operatorname{div}_{F} \boldsymbol{v}}_{\in \mathcal{P}^{k-1}(F)} + \sum_{E \in \mathcal{E}_{F}} \omega_{FE} \int_{E} q \boldsymbol{v} \cdot \mathbf{n}_{FE} \quad \forall \boldsymbol{v} \in \mathcal{P}^{k}(F)^{2}.$$

 $\circ~\operatorname{IBP}$ is the starting point: if $q\in \mathcal{P}^{k+1}(F)$,

$$\int_{F} (\operatorname{\mathbf{grad}}_{F} q) \cdot \boldsymbol{v} = -\int_{F} \pi_{r,F}^{k-1} q \underbrace{\operatorname{div}_{F} \boldsymbol{v}}_{\in \mathcal{P}^{k-1}(F)} + \sum_{E \in \mathcal{E}_{F}} \omega_{FE} \int_{E} q \boldsymbol{v} \cdot \mathbf{n}_{FE} \quad \forall \boldsymbol{v} \in \mathcal{P}^{k}(F)^{2}.$$

 $\circ~$ Space and interpolator:

$$\underline{X}_{\mathbf{grad},F}^{k} = \left\{ \underline{q}_{F} = (q_{F}, (q_{E})_{E \in \mathcal{E}_{F}}, (q_{V})_{V \in \mathcal{V}_{F}}) : \\ q_{F} \in \mathcal{P}^{k-1}(F), \ q_{E} \in \mathcal{P}^{k-1}(E), \ q_{V} \in \mathbb{R} \right\},$$
$$\underline{I}_{\mathbf{grad},F}^{k}q = (\pi_{r,F}^{k-1}q, (\pi_{r,E}^{k-1}q_{|E})_{E \in \mathcal{E}_{F}}, (q(\boldsymbol{x}_{V}))_{V \in \mathcal{V}_{F}}) \quad \forall q \in C(\overline{F}).$$

 $\circ~ {\rm IBP}$ is the starting point: if $q\in {\cal P}^{k+1}(F)$,

$$\int_{F} (\operatorname{\mathbf{grad}}_{F} q) \cdot \boldsymbol{v} = -\int_{F} \pi_{r,F}^{k-1} q \operatorname{div}_{F} \boldsymbol{v}_{F} + \sum_{E \in \mathcal{E}_{F}} \omega_{FE} \int_{E} q \boldsymbol{v} \cdot \mathbf{n}_{FE} \quad \forall \boldsymbol{v} \in \mathcal{P}^{k}(F)^{2}.$$

 $\circ~\mbox{Space}$:

$$\underline{X}_{\mathbf{grad},F}^{k} = \left\{ \underline{q}_{F} = (q_{F}, (q_{E})_{E \in \mathcal{E}_{F}}, (q_{V})_{V \in \mathcal{V}_{F}}) : q_{F} \in \mathcal{P}^{k-1}(F), \ q_{E} \in \mathcal{P}^{k-1}(E), \ q_{V} \in \mathbb{R} \right\},$$

 $\circ \text{ Face gradient } \mathbf{G}_F^k: \underline{X}_{\mathbf{grad},F}^k \to \mathcal{P}^k(F)^2 \text{ s.t.}$

$$\int_{F} (\mathbf{G}_{F}^{k} \underline{q}_{F}) \cdot \boldsymbol{v} = -\int_{F} q_{F} \operatorname{div}_{F} \boldsymbol{v} + \sum_{E \in \mathcal{E}_{F}} \omega_{FE} \int_{E} (\gamma_{E}^{k+1} \underline{q}_{E}) \boldsymbol{v} \cdot \mathbf{n}_{FE} \quad \forall \boldsymbol{v} \in \mathcal{P}^{k}(F)^{2}.$$

• Space :

$$\underline{X}_{\mathbf{grad},F}^{k} = \left\{ \underline{q}_{F} = (q_{F}, (q_{E})_{E \in \mathcal{E}_{F}}, (q_{V})_{V \in \mathcal{V}_{F}}) : q_{F} \in \mathcal{P}^{k-1}(F), \ q_{E} \in \mathcal{P}^{k-1}(E), \ q_{V} \in \mathbb{R} \right\}$$

 $\circ \ \ {\rm Face \ gradient} \ \ {\rm G}^k_F: \underline{X}^k_{{\rm grad},F} \to {\mathcal P}^k(F)^2 \ {\rm s.t.}$

$$\int_{F} (\mathbf{G}_{F}^{k} \underline{q}_{F}) \cdot \boldsymbol{v} = -\int_{F} q_{F} \operatorname{div}_{F} \boldsymbol{v} + \sum_{E \in \mathcal{E}_{F}} \omega_{FE} \int_{E} (\gamma_{E}^{k+1} \underline{q}_{E}) \boldsymbol{v} \cdot \mathbf{n}_{FE} \quad \forall \boldsymbol{v} \in \mathcal{P}^{k}(F)^{2}.$$

• Potential reconstruction $\gamma_F^{k+1} : \underline{X}_{\mathbf{grad},F}^k \to \mathcal{P}^{k+1}(F)$ s.t.

$$\int_{F} (\gamma_{F}^{k+1} \underline{q}_{F}) \operatorname{div}_{F} \boldsymbol{z} = -\int_{F} \mathbf{G}_{F}^{k} \underline{q}_{F} \cdot \boldsymbol{z} + \sum_{E \in \mathcal{E}_{F}} \omega_{FE} \int_{F} (\gamma_{E}^{k+1} \underline{q}_{E}) \boldsymbol{z} \cdot \mathbf{n}_{FE}$$
$$\forall \boldsymbol{z} \in \boldsymbol{\mathcal{R}}^{c,k+2}(F) := (\boldsymbol{x} - \boldsymbol{x}_{F}) \mathcal{P}^{k+1}(F).$$

 $(\operatorname{div}_F : \mathcal{R}^{c,k+2}(F) \to \mathcal{P}^{k+1}(F) \text{ is an isomorphism.})$

Same principle! Based on IBP we determine:

- An additional unknown $(q_T \in \mathcal{P}^{k-1}(T))$ to get the space $\underline{X}_{\mathbf{grad},T}^k$, and its meaning (polynomial moment on T) to get the interpolator $\underline{I}_{\mathbf{grad},T}^k$.
- $\circ \text{ A formula for the element gradient } \mathbf{G}^k_T:\underline{X}^k_{\mathbf{grad},T} \to \mathcal{P}^k(T)^3.$
- $\circ \text{ A potential reconstruction } P^{k+1}_{\mathbf{grad},T}: \underline{X}^k_{\mathbf{grad},T} \to \mathcal{P}^{k+1}(T).$

The Discrete de Rham method I

- Contrary to FE, do not seek explicit (or any!) basis functions.
- Fully discrete spaces made of vectors of polynomials, representing polynomial moments when interpreted through the interpolator.
- Polynomials attached to geometric entities to emulate expected continuity properties of each space,
- Create discrete operators (differential, potential reconstruction) between the spaces.



DDR complex:

$$\mathbb{R} \xrightarrow{\underline{I}^{k}_{\operatorname{\mathbf{grad}},h}} \underline{X}^{k}_{\operatorname{\mathbf{grad}},h} \xrightarrow{\underline{G}^{k}_{h}} \underline{X}^{k}_{\operatorname{\mathbf{curl}},h} \xrightarrow{\underline{C}^{k}_{h}} \underline{X}^{k}_{\operatorname{div},h} \xrightarrow{D^{k}_{h}} \mathcal{P}^{k}(\mathcal{T}_{h}) \xrightarrow{0} \{0\}.$$

• Reproduces key properties of the continuous de Rham complex:

- Same cohomology [Di Pietro et al., 2023] (exact complex if trivial topology.)
 Uniform Poincaré inequalities [Di Pietro and Droniou, 2021a,
 - Di Pietro and Droniou, 2023a, Di Pietro and Hanot, 2024b].
- Analytical properties [Di Pietro et al., 2023]:
 - Primal consistency: approximation properties of potential reconstructions, discrete operators and inner products
 - □ Adjoint consistency: estimate the error in discrete integration-by-parts involving the discrete operators.

 L^2 -like inner products: for $\bullet \in \{ \mathbf{grad}, \mathbf{curl}, \mathrm{div} \}$, on $\underline{X}_{\bullet,h}^k$,

$$\begin{split} (\underline{\boldsymbol{v}}_h,\underline{\boldsymbol{w}}_h)_{\bullet,h} &:= \sum_{T\in\mathcal{T}_h} (\underline{\boldsymbol{v}}_h,\underline{\boldsymbol{w}}_h)_{\bullet,T} \\ \text{with } (\underline{\boldsymbol{v}}_h,\underline{\boldsymbol{w}}_h)_{\bullet,T} &= \int_T \boldsymbol{P}_{\bullet,h}^k \underline{\boldsymbol{v}}_h \cdot \boldsymbol{P}_{\bullet,h}^k \underline{\boldsymbol{w}}_h + \mathbf{s}_{\bullet,T} (\underline{\boldsymbol{v}}_h,\underline{\boldsymbol{w}}_h), \end{split}$$

where $s_{\bullet,T}$ penalises differences on the boundary between element and face/edge potentials on T.

DDR scheme: replace continuous spaces/operators/ L^2 -products with discrete space/operators/ L^2 -like inner products.

Open-source C++ *implementation available in* HArDCore (https://github.com/jdroniou/HArDCore).

Outline

1 Some PDE models of interest

- Stokes I
- Stokes II
- Navier–Stokes
- Magnetostatics
- 2 De Rham complex
- 3 Discrete De Rham (DDR) complex
- 4 Applications to the models of interest

Slides



Theorem (Error estimates [Beirão da Veiga et al., 2022])

With the discrete $oldsymbol{H}(\mathbf{curl})$ -like and H^1 -like norms

$$\begin{split} \|\underline{\boldsymbol{v}}_{h}\|_{\mathbf{curl},1,h}^{2} &= \|\underline{\boldsymbol{v}}_{h}\|_{\mathbf{curl},h}^{2} + \|\underline{\boldsymbol{C}}_{h}^{k}\underline{\boldsymbol{v}}_{h}\|_{\mathrm{div},h}^{2}, \\ \|\underline{\boldsymbol{q}}_{h}\|_{\mathbf{grad},1,h}^{2} &= \|\underline{\boldsymbol{q}}_{h}\|_{\mathbf{grad},h}^{2} + \|\underline{\boldsymbol{G}}_{h}^{k}\underline{\boldsymbol{q}}_{h}\|_{\mathbf{curl},h}, \end{split}$$

we have the pressure robust estimates

$$\|\underline{\boldsymbol{u}}_h - \underline{\boldsymbol{I}}_{ ext{curl},h}^k \boldsymbol{u}\|_{ ext{curl},1,h} + \|\underline{p}_h - \underline{\boldsymbol{I}}_{ ext{grad},h}^k p\|_{ ext{grad},1,h} \lesssim C_1(\boldsymbol{u}) h^{k+1}$$

with $C_1(u)$ depending u and some of its derivatives, but not p.

Robustness comes from:

Commutation property
$$\underline{G}_{h}^{k}(\underline{I}_{\mathbf{grad},h}^{k}p) = \underline{I}_{\mathbf{curl},h}^{k}(\mathbf{grad}\,p).$$

Stokes equations in curl-curl formulation: tests I

 $\circ \ \Omega = (0,1)^3.$

• Voronoi mesh families (similar results on tetrahedral meshes):



(a) Voronoi mesh

 $\circ~$ Exact solution: for some $\lambda\geq 0$,

$$p(x, y, z) = \lambda \sin(2\pi x) \sin(2\pi y) \sin(2\pi z),$$
$$u(x, y, z) = \begin{bmatrix} \frac{1}{2} \sin(2\pi x) \cos(2\pi y) \cos(2\pi z) \\ \frac{1}{2} \cos(2\pi x) \sin(2\pi y) \cos(2\pi z) \\ -\cos(2\pi x) \cos(2\pi y) \sin(2\pi z) \end{bmatrix}$$

- Measured errors:
 - \square E^{d} in discrete norms between the approximate solutions and the *interpolates* of the exact solution (as in the theorems).
 - \square *E*^c in continuous norms between reconstructed potentials of the approximate solutions and the exact solution.

Stokes equations in curl-curl formulation: tests III

$$\begin{array}{c} \bullet & E^{c}, \ k = 0; \ \bullet & E^{c}, \ k = 1; \ \bullet & E^{c}, \ k = 2\\ \bullet & \bullet & E^{d}, \ k = 0; \ \bullet & E^{d}, \ k = 1; \ \bullet & E^{d}, \ k = 2 \end{array}$$



Stokes equations in curl-curl formulation: tests IV

$$\begin{array}{c} \bullet & E^{c}, \ k = 0; \ \bullet & E^{c}, \ k = 1; \ \bullet & E^{c}, \ k = 2\\ \bullet & \bullet & E^{d}, \ k = 0; \ \bullet & E^{d}, \ k = 1; \ \bullet & E^{d}, \ k = 2 \end{array}$$



Navier-Stokes in curl-curl formulation: theorem

Theorem (Error estimates [Di Pietro et al., 2024])

Define the discrete L^4 -Sobolev constant by

$$C_{\mathrm{S},h} \coloneqq \max\left\{\frac{\|\boldsymbol{P}_{\mathrm{curl},h}^{k} \underline{\boldsymbol{\upsilon}}_{h}\|_{\boldsymbol{L}^{4}(\Omega)}}{\|\underline{\boldsymbol{C}}_{h}^{k} \underline{\boldsymbol{\upsilon}}_{h}\|_{\mathrm{div},h}} : \underline{\boldsymbol{\upsilon}}_{h} \in (\mathrm{Im}\,\underline{\boldsymbol{G}}_{h}^{k})^{\perp} \backslash \{\mathbf{0}\}\right\}$$

With \mathbf{R}_u solenoidal part of forcing term f (depends only on u), if

 $C_{\mathrm{S},h}^2 \| \underline{I}_{\mathrm{curl},h}^k(\mathbf{R}_u) \|_{\mathrm{curl},h}$ is small enough,

then

$$\| \underline{u}_h - \underline{I}_{ ext{curl},h}^k u \|_{ ext{curl},h} + \| \underline{C}_h^k (\underline{u}_h - \underline{I}_{ ext{curl},h}^k u) \|_{ ext{div},h} \lesssim C(u) h^{k+1}$$

- Robust estimate with respect to the pressure.
- Boundedness of $C_{S,h}$ w.r.t. h still an open question (expected for convex domains).

Navier-Stokes in curl-curl formulation: convergence tests I

$$\begin{array}{c} \bullet & E^{c}, \ k = 0; \ \bullet & E^{c}, \ k = 1; \ \bullet & E^{c}, \ k = 2 \\ \bullet & \star^{-} E^{d}, \ k = 0; \ \bullet & - E^{d}, \ k = 1; \ \bullet & - E^{d}, \ k = 2 \end{array}$$



Navier-Stokes in curl-curl formulation: convergence tests II

$$\begin{array}{c} \bullet & E^{c}, \ k = 0; \ \bullet & E^{c}, \ k = 1; \ \bullet & E^{c}, \ k = 2 \\ \bullet & \star^{-} E^{d}, \ k = 0; \ \bullet & E^{d}, \ k = 1; \ \bullet & E^{d}, \ k = 2 \end{array}$$



In the unit cube $\Omega = (0,1)^3$:

• Essential BCs (pressure and tangential velocity):

p(x, y, z) = -z and $u \times n = 0$

on the bottom corner $\{0\} \times (0, 0.25) \times (0, 0.25)$ of the face x = 0.

• Natural BCs (tangential vorticity and flux):

 $\operatorname{curl} \boldsymbol{u} \times \mathbf{n} = \mathbf{0}$ and $\boldsymbol{u} \cdot \mathbf{n} = 1$

on the bottom corner $\{1\} \times (0, 0.25) \times (0, 0.25)$ of the face x = 1,

• Homogeneous natural BCs elsewhere.

Navier-Stokes: flow in cavity with mixed BCs II





Reissner-Mindlin

Model:

$$\boldsymbol{\gamma} + \operatorname{div}(\boldsymbol{C}\operatorname{\mathbf{grad}}_s\boldsymbol{\theta}) = \boldsymbol{0} \qquad \qquad \text{in } \Omega,$$

$$-\operatorname{div}\boldsymbol{\gamma} = f \qquad \qquad \text{in } \Omega,$$

$$\gamma = \frac{\kappa}{t^2} (\operatorname{grad} u - \theta) \quad \text{in } \Omega,$$
$$\theta = 0, \quad u = 0 \quad \text{on } \partial\Omega$$

$$oldsymbol{ heta} = oldsymbol{0}, \quad u = 0 \qquad \qquad ext{on } \partial \Omega.$$

- Ω polygonal domain (2D), t: plate thickness.
- $\circ \gamma$: shear strain; θ : fibers rotations; u: transverse displacement.
- f: transverse load; C: linear elasticity tensor; κ : shear modulus.

Reissner-Mindlin

Model:

$$\boldsymbol{\gamma} + \operatorname{div}(\boldsymbol{C}\operatorname{\mathbf{grad}}_s\boldsymbol{\theta}) = \boldsymbol{0} \qquad \qquad \text{in } \Omega,$$

$$-\operatorname{div}\boldsymbol{\gamma} = f \qquad \qquad \text{in } \Omega,$$

$$\gamma = \frac{\kappa}{t^2} (\operatorname{grad} u - \theta) \quad \text{in } \Omega,$$
$$\theta = 0 \quad u = 0 \quad \text{on } \partial \Omega$$

$$\boldsymbol{\theta} = \mathbf{0}, \quad u = 0 \qquad \qquad \text{on } \partial \Omega.$$

- Ω polygonal domain (2D), t: plate thickness.
- γ : shear strain; θ : fibers rotations; u: transverse displacement.
- \circ f: transverse load; C: linear elasticity tensor; κ : shear modulus.

Scheme: [Di Pietro and Droniou, 2021b].

- Approximation space for $u: \underline{X}_{\mathbf{grad},h}^k$.
- Approximation space for θ : $\underline{X}_{curl,h}^{k}$ enriched with full vector-valued polynomials on the edges (not just tangential components).

Theorem (Error estimate for arbitrary k)

If the solution (η, u) satisfies $u \in C^1(\overline{\Omega}) \cap H^{k+2}(\Omega)$ and $\theta \in H^1(\Omega)^2 \cap H^{k+2}(\Omega)^2$, then

$$\|(\underline{\boldsymbol{\theta}}_h - \underline{I}_{\boldsymbol{\Theta},h} \boldsymbol{\theta}, \underline{u}_h - \underline{I}_{\mathbf{grad},h} u)\|_{L^2} \lesssim h^{k+1} \left(|\boldsymbol{\theta}|_{H^{k+2}} + |\boldsymbol{\gamma}|_{H^{k+1}}\right).$$

- Optimal rate of convergence, but not robust w.r.t. $t \to 0$ (even for k = 0).
- \circ Lack of robustness for $k \geq 1$ observed on solutions s.t. $|\gamma|_{H^{k+1}} \sim t^{-k-\frac{1}{2}}$.

Theorem (Locking-free error estimate for k = 0)

Under the previous assumptions and k = 0, it holds

$$\begin{split} \|(\underline{\boldsymbol{\theta}}_h - \underline{I}_{\mathbf{\Theta},h} \boldsymbol{\theta}, \underline{u}_h - \underline{I}_{\mathbf{grad},h} u)\|_{L^2} \\ \lesssim h\left(|\boldsymbol{\theta}|_{H^2} + t|\boldsymbol{\gamma}|_{H^1} + \|\boldsymbol{\gamma}\|_{L^2} + \|f\|_{L^2}\right). \end{split}$$

• Fully robust w.r.t. t: $|\boldsymbol{\theta}|_{H^2} + t|\boldsymbol{\gamma}|_{H^1} + \|\boldsymbol{\gamma}\|_{L^2} + \|f\|_{L^2} \lesssim 1$. \rightsquigarrow Observed in numerical tests.

- Proof relies on:

 - □ Conforming lifting of U_h , and a piecewise-constant lifting on Θ_h based on a local discrete Hodge decomposition.

Both challenging because of the polygonal mesh...

Reissner-Mindlin: test



- Discrete version of the de Rham complex, of arbitrary degree of accuracy and applicable to polytopal meshes.
 Other discrete polytopal complex based on VEM [Beirão da Veiga et al., 2018], see connexions in [Beirão da Veiga et al., 2022].
- Full theory:
 - □ Algebraic properties: same cohomology as the continuous de Rham complex on any domain, commutation properties between interpolants and discrete operators, etc.
 - Analytic properties: Poincaré inequalities, primal and adjoint consistency, etc.
- Polytopal exterior calculus version: complex written in the framework of differential forms (see Finite Element Exterior Calculus for FE methods). [Bonaldi et al., 2024].
- DDR on manifolds, with application to Maxwell [Droniou et al., 2024].

- Other polytopal complexes based on DDR approach (see Marwa Salah's presentation to follow): plate complexes, divdiv complexes (2D and 3D), Stokes complex...
- Applications:
 - □ Magnetostatics. [Di Pietro and Droniou, 2021a]
 - □ Stokes equations in standard form. [Hanot, 2023]
 - □ Kirchoff plate. [Di Pietro and Droniou, 2023b]
 - □ Quad-rot problem. [Di Pietro, 2024]
 - □ Biharmonic problems. [Di Pietro and Hanot, 2024a]

 $\circ\,$ Notes and series of introductory lectures to DDR:

https://math.unice.fr/~massonr/Cours-DDR/Cours-DDR.html



COURSE OF JEROME DRONIOU FROM MONASH UNIVERSITY, INVITED PROFESSOR AT UCA

Introduction to Discrete De Rham complexes

- Short description (in french)
- Summary of notations and formulas
- Part 1, first course: the de Rham complex and its usefulness in PDEs, 22/09/22 (video)
- Part 1, second course: Low order case, 29/09/22 (video)
- Part 1, third course: Design of the DDR complex in 2D, 07/10/22 (video)
- Part 1, fourth course: Exactness of the DDR complex in 2D, 10/10/22 (video)
- Part 2, fifth course: DDR in 3D, analysis tools, 17/11/22 (video)



NEMESIS

New generation methods for numerical simulations

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Thank you for your attention!

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