New generation numerical methods for partial differential equations

NEMESIS

Daniele Di Pietro, 19 June 2024

UNIVERSITÉ DE MONTPELLIER
IMAG INSTITUT MONTPELLIERAIN ALEXANDER GROTHENDIECK
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- **Largest** and **most competitive** grants awarded by the ERC
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- All fields of research evaluated by a **single panel**

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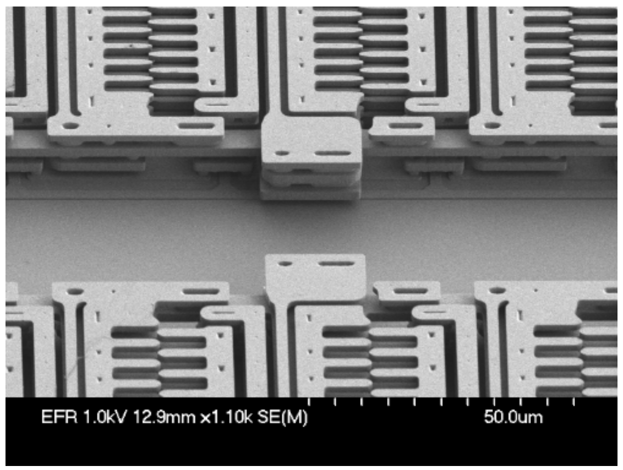
The NEMESIS project

- Principal Investigators (all researchers in Numerical Analysis!):
  - **Daniele Di Pietro**, Université de Montpellier, IMAG, corr. PI
  - **Paola Antonietti**, Politecnico di Milano, MOX
  - **Lourenço Beirão da Veiga**, Università di Milano Bicocca
  - **Jérôme Droniou**, CNRS, IMAG
- **7.8M€** (**4.4M€** at IMAG), **4** research clusters, **8** work packages
- **>70 + >15 man-year** of non-permanent + permanent researchers

From physical problems to numerical simulations

I. Physical problem



→

II. Mathematical model

$$A(u) = f$$

$$\begin{aligned} \mu H - \operatorname{curl} A &= 0 && \text{in } \Omega, \\ \operatorname{curl} H &= J && \text{in } \Omega, \\ \operatorname{div} A &= 0 && \text{in } \Omega, \\ A \times n &= 0 && \text{on } \partial\Omega \end{aligned}$$

↓

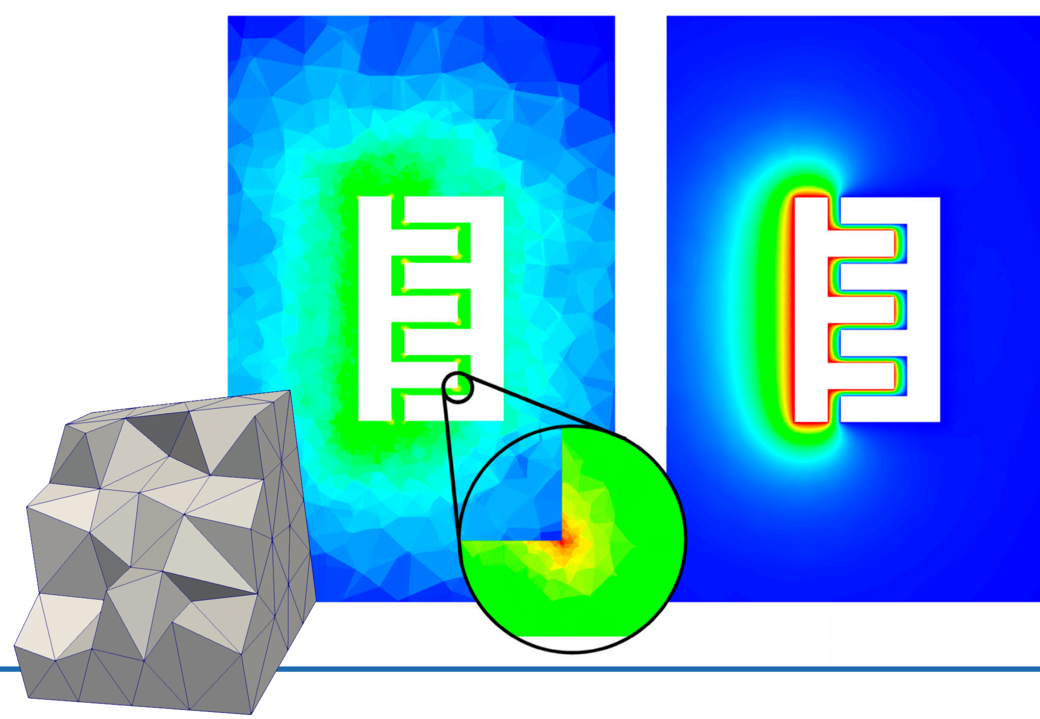
III. Numerical approximation

$$A_h(u_h) = f_h$$

→

IV. Computer simulation

$$\mathsf{A}_h \mathsf{u}_h = \mathsf{f}_h$$



NEMESIS

The challenges for next generation simulators

01.

Incomplete differential operators in Hilbert complexes

02.

Efficient solution of large, indefinite algebraic systems

03.

Nonlinear, hybrid-dimensional physics

04.

Handling all of the above at once

These challenges correspond to the **research clusters** of NEMESIS

Stability, consistency, and convergence

$$A_h(u_h) = f_h$$

- $\frac{1}{h}$ measures the **effort required to solve the discrete problem**
- Our ultimate goal is to have **convergent schemes**, for which

$$u_h \to u \text{ as } h \to 0$$

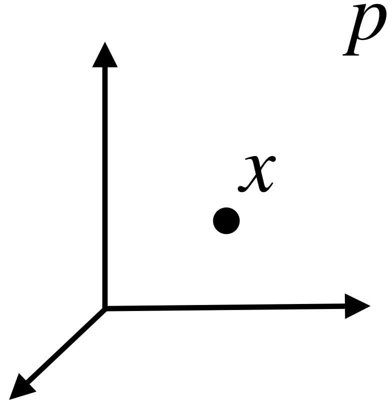
- **Stability:** Small variations of f_h induce small variations of u_h
- **Consistency:** $f_h - A_h(I_h u) \to 0$ as $h \to 0$
- For linear problems, we have the **Lax principle***:

$$\text{Stability} \implies (\text{Consistency} \iff \text{Convergence})$$

* See, e.g., [Lax & Richtmyer, 1956]

Physical quantities have different nature

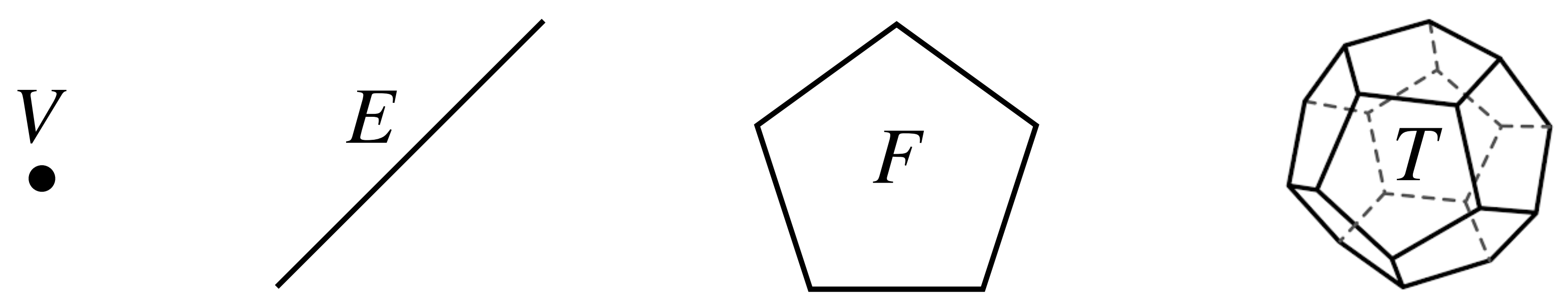
- **Scalar:** potential (pressure p) or density (energy $\mathscr{E}$)
- **Vector:** circulation (magnetic field H) or flux (heat flux Φ)
- **Tensor:** (deformation ε, etc.)



$$p(x) \qquad H(x) = \begin{pmatrix} H_1 \\ H_2 \\ H_3 \end{pmatrix} \qquad \varepsilon(x) = \begin{pmatrix} \varepsilon_{11} & \varepsilon_{12} & \varepsilon_{13} \\ \varepsilon_{12} & \varepsilon_{22} & \varepsilon_{23} \\ \varepsilon_{13} & \varepsilon_{23} & \varepsilon_{33} \end{pmatrix}$$

How can we measure these quantities?

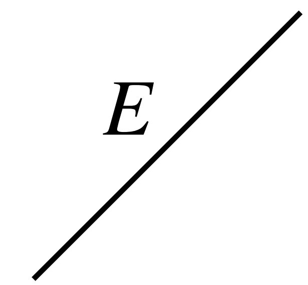
- Pressure p: evaluation at a point V
- Magnetic field H: free current in a wire E
- Heat flux Φ: normal flux through a surface F
- Energy $\mathscr{E}$: quantity in a volume T



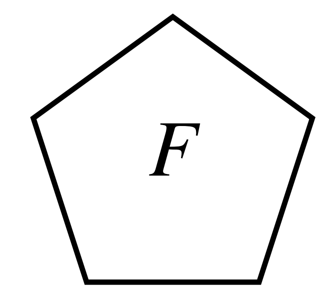
Differential forms provide a unified approach to integration over curves, surfaces, solids, etc.

Vector calculus operators

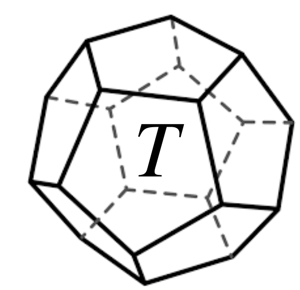
$$p(x_{V_2}) - p(x_{V_1}) = \int_E \operatorname{grad} p \cdot t_E \, d\ell \qquad \operatorname{grad} p = \begin{pmatrix} \partial_1 p \\ \partial_2 p \\ \partial_3 p \end{pmatrix}$$



$$-\oint_{\partial F} H \cdot t_{\partial F} \, d\ell = \int_F \operatorname{curl} H \cdot n_F \, dS \qquad \operatorname{curl} H = \begin{pmatrix} \partial_2 H_3 - \partial_3 H_2 \\ \partial_3 H_1 - \partial_1 H_3 \\ \partial_1 H_2 - \partial_2 H_1 \end{pmatrix}$$



$$\oint_{\partial T} \Phi \cdot n_{\partial T} \, dS = \int_T \operatorname{div} \Phi \, dV \qquad \operatorname{div} \Phi = \partial_1 \Phi_1 + \partial_2 \Phi_2 + \partial_3 \Phi_3$$



- curl and div are **incomplete differential operators**
- the notion of **exterior derivative** unifies grad, curl, and div

Betti numbers

- Let $\Omega \subset \mathbb{R}^3$ be a polyhedron with **Betti numbers** b_i
- $b_0 = 1$ (number of **connected components**) and $b_3 = 0$
- b_1 and b_2 account for the number of **tunnels** and **voids** in Ω

$(b_0, b_1, b_2, b_3) = (1,1,0,0)$ $(b_0, b_1, b_2, b_3) = (1,0,1,0)$

The de Rham cohomology

For a domain Ω of $\mathbb{R}^3$, we can form the **de Rham complex**:

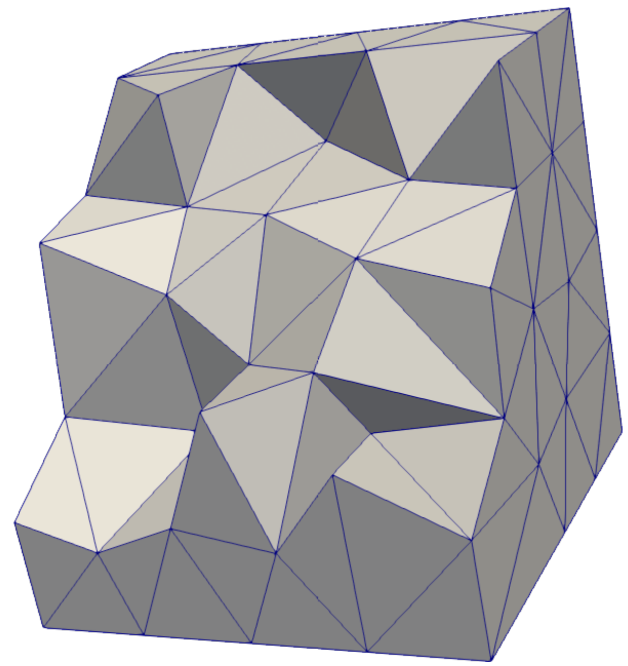
$$H^1(\Omega) \xrightarrow{\text{grad}} H(\text{curl};\Omega) \xrightarrow{\text{curl}} H(\text{div};\Omega) \xrightarrow{\text{div}} L^2(\Omega)$$

- Since $\text{curl}\,\text{grad} = 0$ and $\text{div}\,\text{curl} = 0$, this is a complex
- Depending on Ω, we can strengthen these relations:
  - If $b_1 = 0$, $\text{Ker}\,\text{curl} = \text{Im}\,\text{grad}$
  - If $b_2 = 0$, $\text{Im}\,\text{curl} = \text{Ker}\,\text{div}$
- When $b_1 \neq 0$ or $b_2 \neq 0$, **de Rham's cohomology** characterizes

$$\text{Ker}\,\text{curl}/\text{Im}\,\text{grad} \text{ and } \text{Ker}\,\text{div}/\text{Im}\,\text{curl}$$

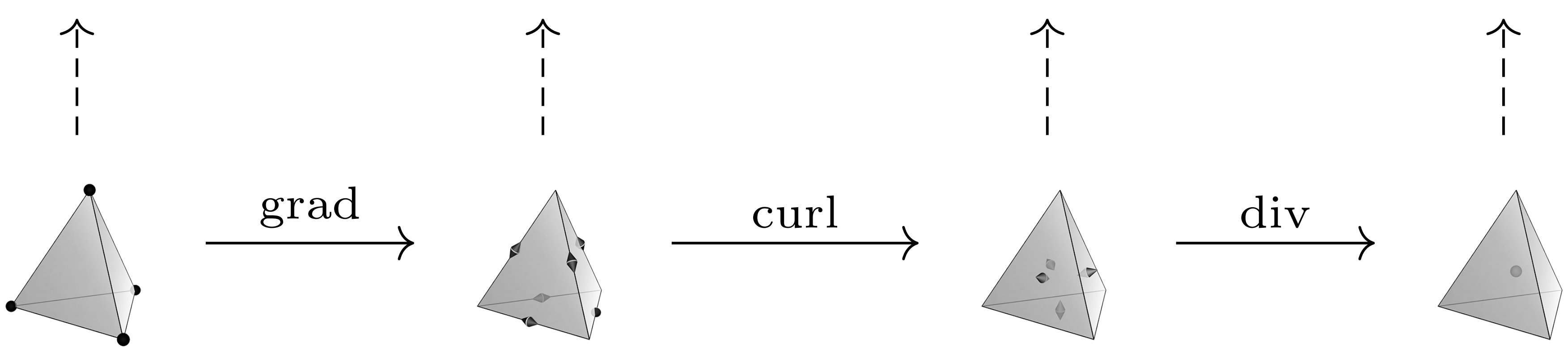
Discrete counterparts of these properties are key to **stability** when dealing with **incomplete differential operators**!

The Finite Element approach



A finite element mesh $\mathscr{T}_h$

$$
\begin{array}{ccccccc}
H^1(\Omega) & \xrightarrow{\text{grad}} & H(\text{curl};\Omega) & \xrightarrow{\text{curl}} & H(\text{div};\Omega) & \xrightarrow{\text{div}} & L^2(\Omega) \\
\uparrow & & \uparrow & & \uparrow & & \uparrow \\
\mathcal{P}^1_{\text{c}}(\mathcal{T}_h) & \xrightarrow{\text{grad}} & \mathcal{N}^1(\mathcal{T}_h) & \xrightarrow{\text{curl}} & \mathcal{RT}^1(\mathcal{T}_h) & \xrightarrow{\text{div}} & \mathcal{P}^0(\mathcal{T}_h)
\end{array}
$$



[Raviart and Thomas, 1977], [Nédélec, 1980]

Finite Element discretization

Strong formulation

Find $H : \Omega \to \mathbb{R}^3$ and $A : \Omega \to \mathbb{R}^3$ s.t.

$$\begin{aligned} \mu H - \operatorname{curl} A &= 0 && \text{in } \Omega,\\ \operatorname{curl} H &= J && \text{in } \Omega,\\ \operatorname{div} A &= 0 && \text{in } \Omega,\\ A \times n &= 0 && \text{on } \partial\Omega \end{aligned}$$

Weak formulation

Find $H \in H(\text{curl};\Omega)$ and $A \in H(\text{div};\Omega)$ s.t.

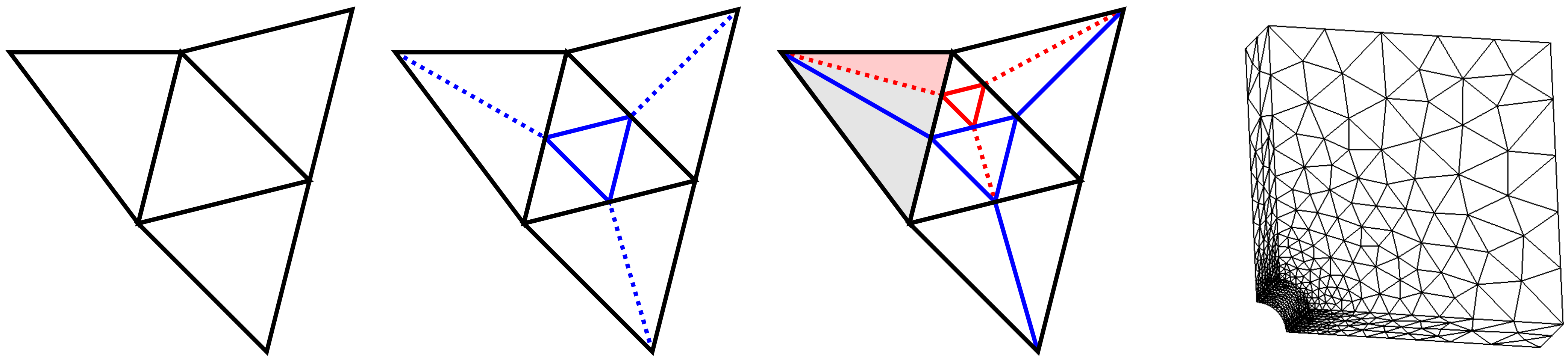
$$\begin{aligned} \int_\Omega \mu H \cdot \tau - \int_\Omega A \cdot \operatorname{curl} \tau &= 0 && \forall \tau \in H(\text{curl};\Omega),\\ \int_\Omega \operatorname{curl} H \cdot v + \int_\Omega \operatorname{div} A \ \operatorname{div} v &= \int_\Omega f \cdot v && \forall v \in H(\text{div};\Omega) \end{aligned}$$

FE scheme

Find $H_h \in \mathcal{N}^1(\mathcal{T}_h)$ and $A_h \in \mathcal{RT}^1(\mathcal{T}_h)$ s.t.

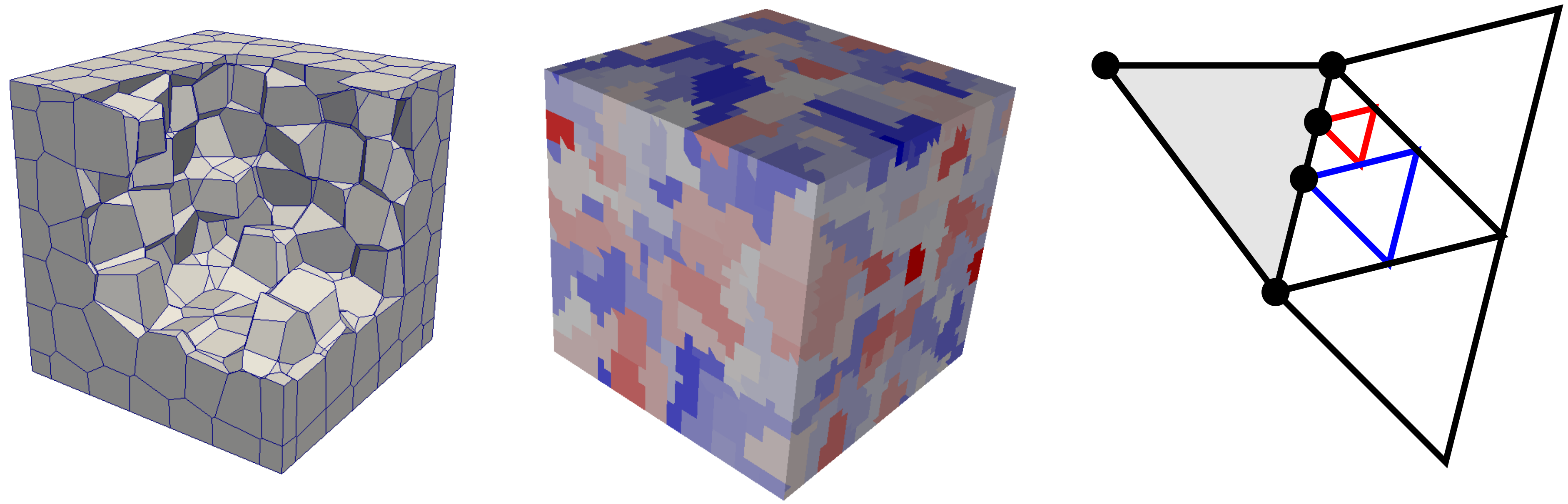
$$\begin{aligned} \int_\Omega \mu H_h \cdot \tau_h - \int_\Omega A_h \cdot \operatorname{curl} \tau_h &= 0 && \forall \tau_h \in \mathcal{N}^1(\mathcal{T}_h),\\ \int_\Omega \operatorname{curl} H_h \cdot v_h + \int_\Omega \operatorname{div} A_h \ \operatorname{div} v_h &= \int_\Omega f \cdot v_h && \forall v \in \mathcal{RT}^1(\mathcal{T}_h) \end{aligned}$$

Limitations of Finite Elements



- Approach limited to conforming meshes with standard elements:
  - Local refinement requires to trade mesh quality for size
  - Complex geometries may require a large number of elements
  - The element shape cannot be adapted to the solution
- The extension to more advanced cases is not straightforward
- Solution of algebraic systems cannot benefit from agglomeration

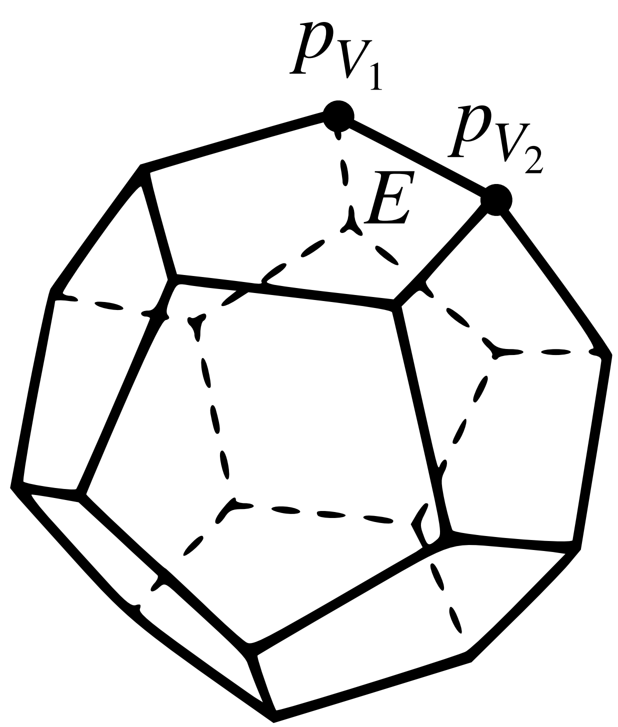
The fully discrete polyhedral approach

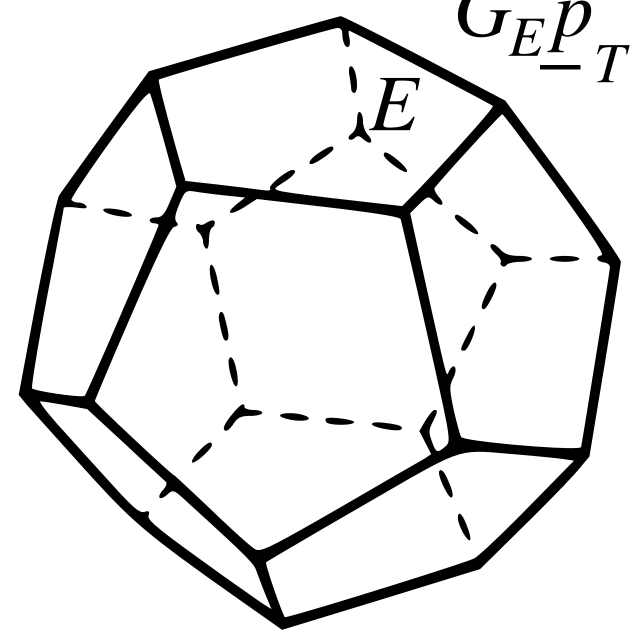


- **Key idea:** use discrete spaces *and* operators
- Support of general polyhedral meshes and high-order
- Several strategies to reduce the size of algebraic systems
- Agglomeration-based multi-grid solvers for algebraic systems

See [Bassi et al., 2012] and [Antonietti et al., 2013] for mesh agglomeration

Discrete vector calculus operators





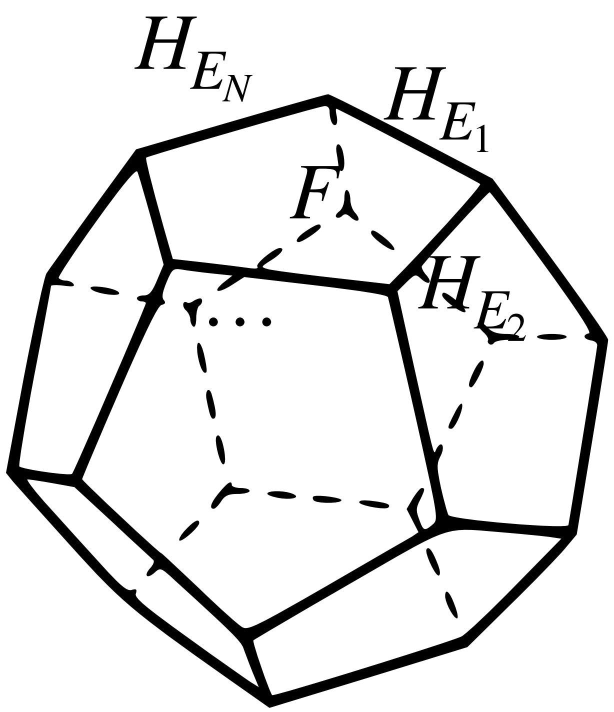
$$G_E \underline{p}_T = \frac{p_{V_2} - p_{V_1}}{|E|}$$

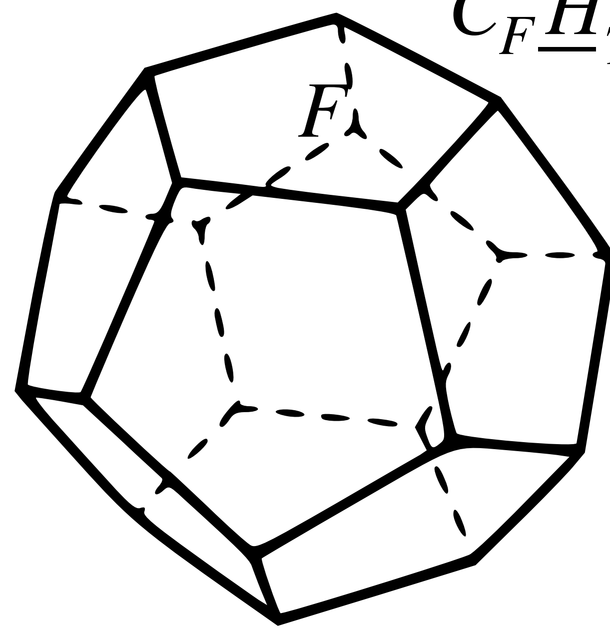
$$\underline{p}_T := (p_V)_{V \in \mathcal{V}_T} \in \mathbb{R}^{\mathcal{V}_T} \qquad \underline{G}_T \underline{p}_T := (G_E \underline{p}_T)_{E \in \mathcal{E}_T} \in \mathbb{R}^{\mathcal{E}_T}$$

$$\underline{X}_{\mathrm{grad},T} := \mathbb{R}^{\mathcal{V}_T} \xrightarrow{\underline{G}_T} \underline{X}_{\mathrm{curl},T} := \mathbb{R}^{\mathcal{E}_T}$$

See [Beirão da Veiga et al., 2014], [Bonelle and Ern, 2014]

Discrete vector calculus operators





$$C_F \underline{H}_T = -\frac{1}{|F|} \sum_{E \subset \partial F} \omega_{FE} \int_E H_E$$

$$\underline{H}_T := (H_E)_{E \in \mathscr{E}_T} \in \mathbb{R}^{\mathscr{E}_T}$$

$$\underline{C}_T := (C_F \underline{H}_T)_{F \in \mathscr{F}_T} \in \mathbb{R}^{\mathscr{F}_T}$$

$$\underline{X}_{\mathrm{grad},T} \xrightarrow{\underline{G}_T} \underline{X}_{\mathrm{curl},T} \xrightarrow{\underline{C}_T} \underline{X}_{\mathrm{div},T} := \mathbb{R}^{\mathcal{F}_T}$$

A lowest-order polyhedral scheme

$$\underline{X}_{\mathrm{grad},h} \xrightarrow{\underline{G}_h} \underline{X}_{\mathrm{curl},h} \xrightarrow{\underline{C}_h} \underline{X}_{\mathrm{div},h} \xrightarrow{D_h} \mathbb{R}^{\mathcal{T}_h}$$

Weak formulation

Find $H \in H(\mathrm{curl};\Omega)$ and $A \in H(\mathrm{div};\Omega)$ s.t.

$$\int_\Omega \mu H \cdot \tau - \int_\Omega A \cdot \mathrm{curl}\,\tau = 0 \qquad \forall \tau \in H(\mathrm{curl};\Omega),$$

$$\int_\Omega \mathrm{curl}\,H \cdot v + \int_\Omega \mathrm{div}\,A\ \mathrm{div}\,v = \int_\Omega f \cdot v \qquad \forall v \in H(\mathrm{div};\Omega)$$

Polyhedral scheme

Find $\underline{H}_h \in \underline{X}_{\mathrm{curl},h}$ and $\underline{A}_h \in \underline{X}_{\mathrm{div},h}$ s.t.

$$\mu(\underline{H}_h, \underline{\tau}_h)_{\mathrm{curl},h} - (\underline{A}_h, \underline{C}_h \underline{\tau}_h)_{\mathrm{div},h} = 0 \qquad \forall \underline{\tau}_h \in \underline{X}_{\mathrm{curl},h},$$

$$(\underline{C}_h \underline{H}_h, \underline{v}_h)_{\mathrm{div},h} + \int_\Omega D_h \underline{A}_h\, D_h \underline{v}_h = \int_\Omega f \cdot P_{\mathrm{div},h} \underline{v}_h \qquad \forall \underline{v}_h \in \underline{X}_{\mathrm{div},h}$$

Increasing the approximation order

- With the previous construction, one can hope for the error

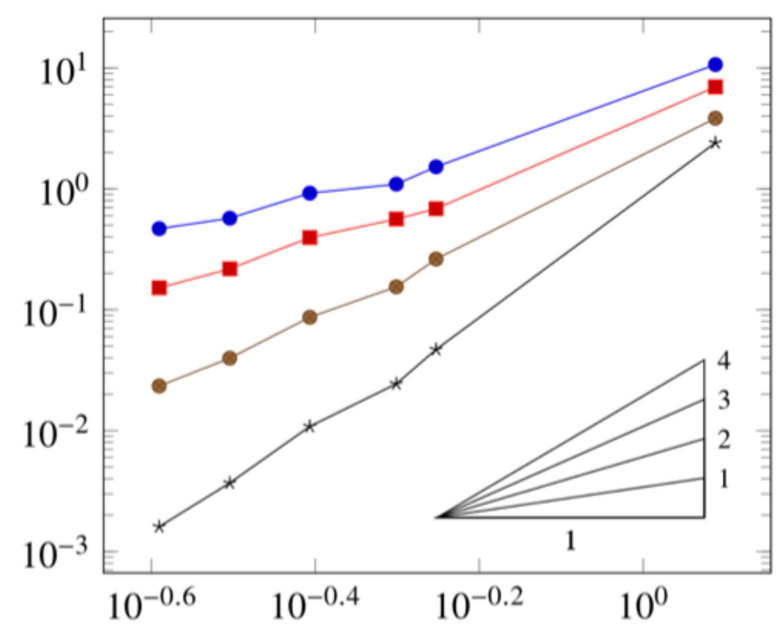
$$\|u - I_h u\|_h \lesssim h$$

- However, for u smooth, it would be desirable to have instead

$$\|u - I_h u\|_h \lesssim h^k \text{ with } k \geq 1$$

- This requires **high-order discrete de Rham complexes**

$\|u_h - I_h u\|_h$



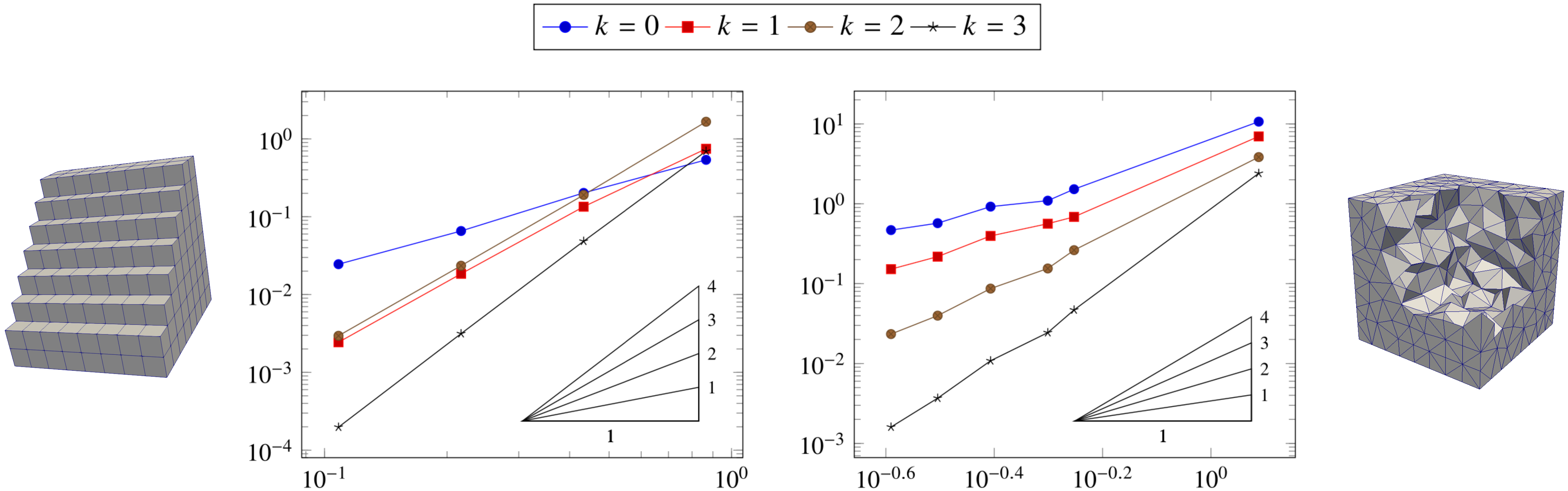
h

Arbitrary order discrete de Rham complexes

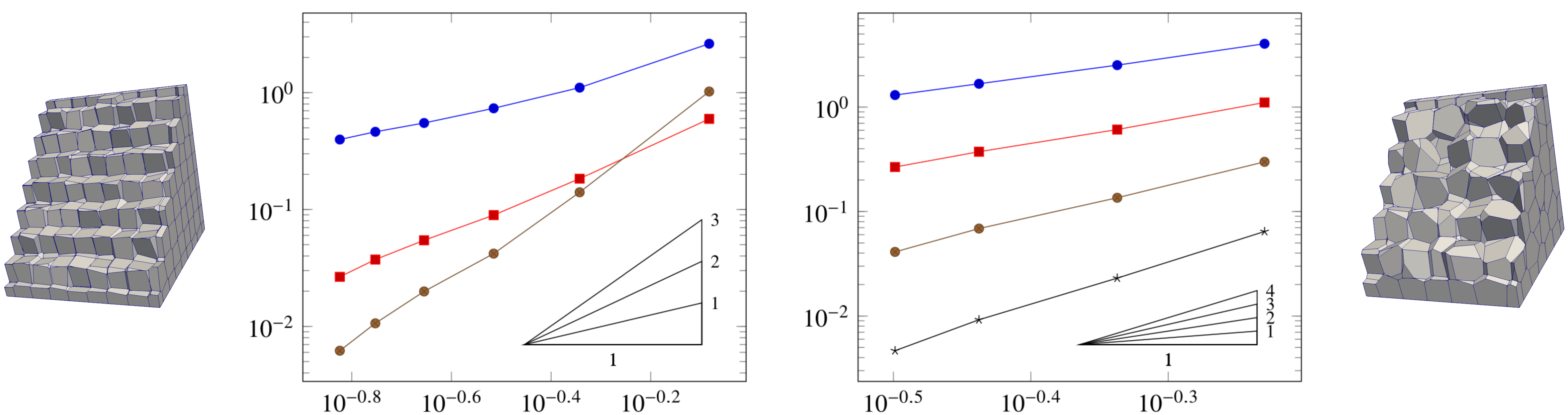
$$\underline{X}^k_{\mathrm{grad},h} \xrightarrow{\underline{G}^k_h} \underline{X}^k_{\mathrm{curl},h} \xrightarrow{\underline{C}^k_h} \underline{X}^k_{\mathrm{div},h} \xrightarrow{D^k_h} \mathcal{P}^k(\mathcal{T}_h)$$

- First ideas based on FE [Beirão da Veiga et al., 2016—18]
- First DDR complex [DP, Droniou, and Rapetti, 2020]
- First complete set of analytical properties [DP and Droniou, 2023]
- Extension to differential forms [Bonaldi, DP, Droniou, Hu, 2023]
- **Key preliminary developments for the NEMESIS project!**

Convergence for the magnetostatics problem



(a) "Cubic-Cells" mesh (b) "Tetgen-Cube-0" mesh



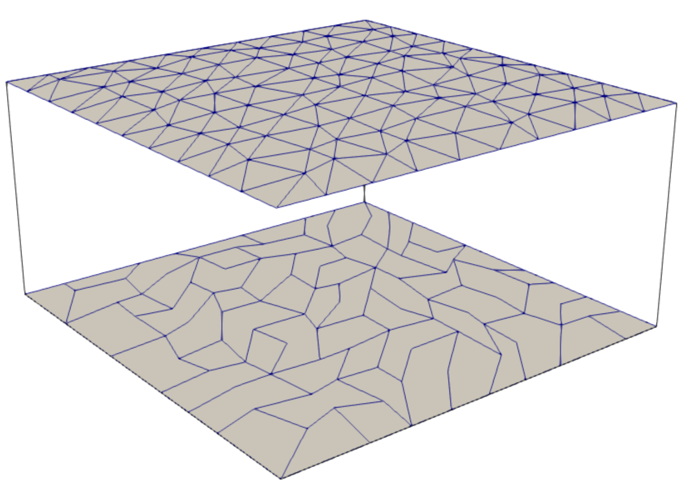
(c) "Voro-small-0" mesh (d) "Voro-small-1" mesh

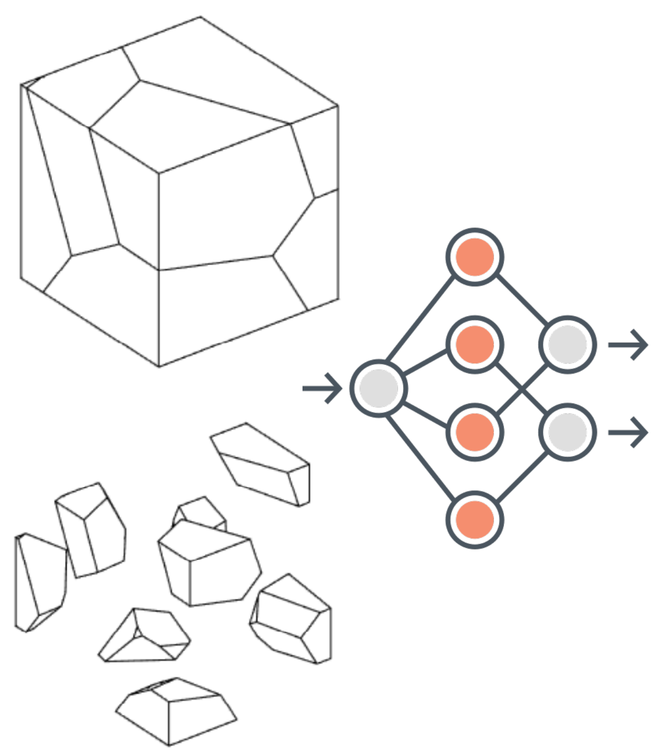
$\|(H_h - I^k_{\mathrm{curl},h}H, A_h - I^k_{\mathrm{div},h}A)\|_h$ vs. h for $k \in \{0,1,2,3\}$, [DP and Droniou, 2021]

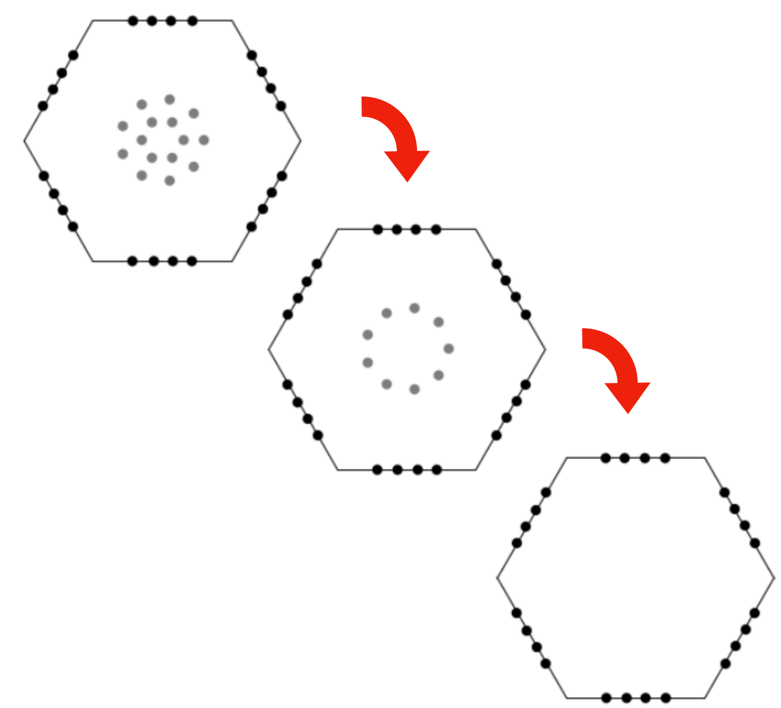
Efficiency boost

$$A_h u_h = f_h$$

- Agglomeration-based **multigrid solvers**
- AI-driven **mesh adaptation**
- Serendipity and static condensation to **reduce system size**

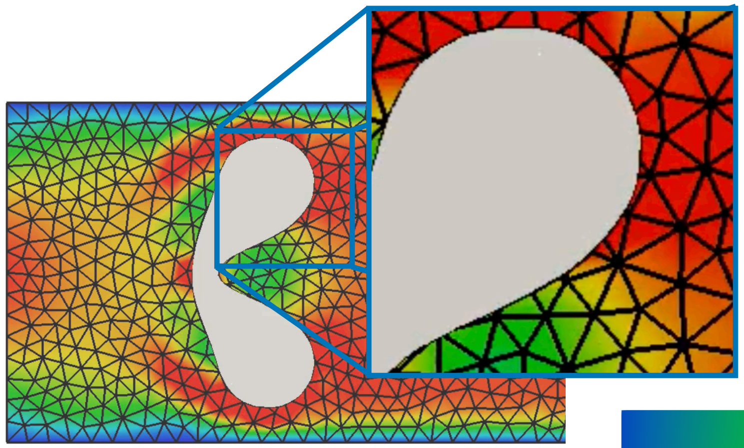






Hybrid-dimensional, coupled, nonlinear physics

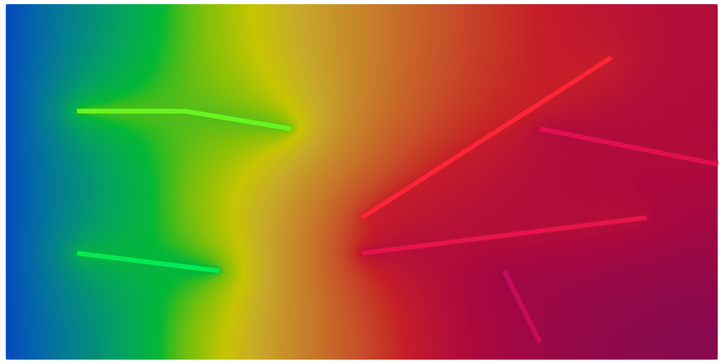
- Rigorous mathematical tools for **highly non linear problems**
- Development of methods for **problems set on surfaces**
- Polyhedral meshes for **moving interface problems**



Discrete Rellich—Kondrachov on domains and manifolds:

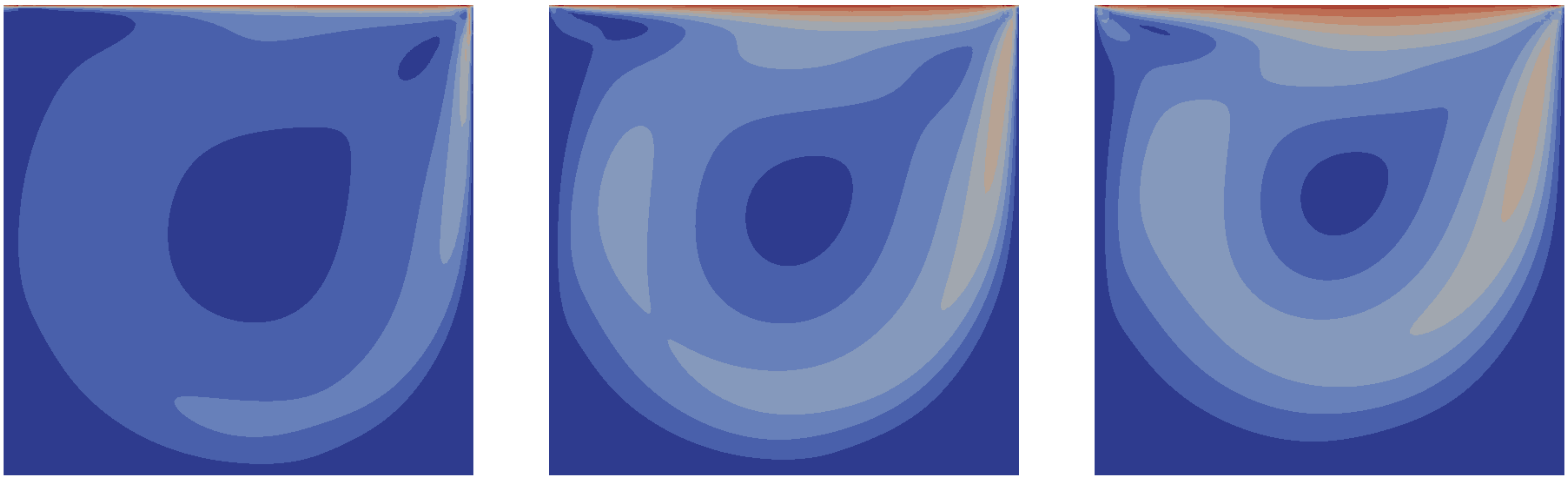
$(D_h u_h)_{h\in\mathscr{H}}$ bounded $\Longrightarrow$ $(u_h)_{h\in\mathscr{H}}$ compact

with D_h discrete $\mathbf{curl}, \mathrm{div}, \mathbf{grad}_s, \ldots$



An example of highly nonlinear problem

The non-Newtonian Navier—Stokes equations



$p = 1.5$ $p = 2$ $p = 2.5$

$$\partial_t u - \nabla \cdot \sigma(u) + (u \cdot \nabla)u + \nabla p = f$$
$$\nabla \cdot u = 0$$

with $\sigma(u) = \nu \, |\, \varepsilon(u) \,|^{p-2} \varepsilon(u)$

[Castanon Quiroz, DP, Harnist, 2023]

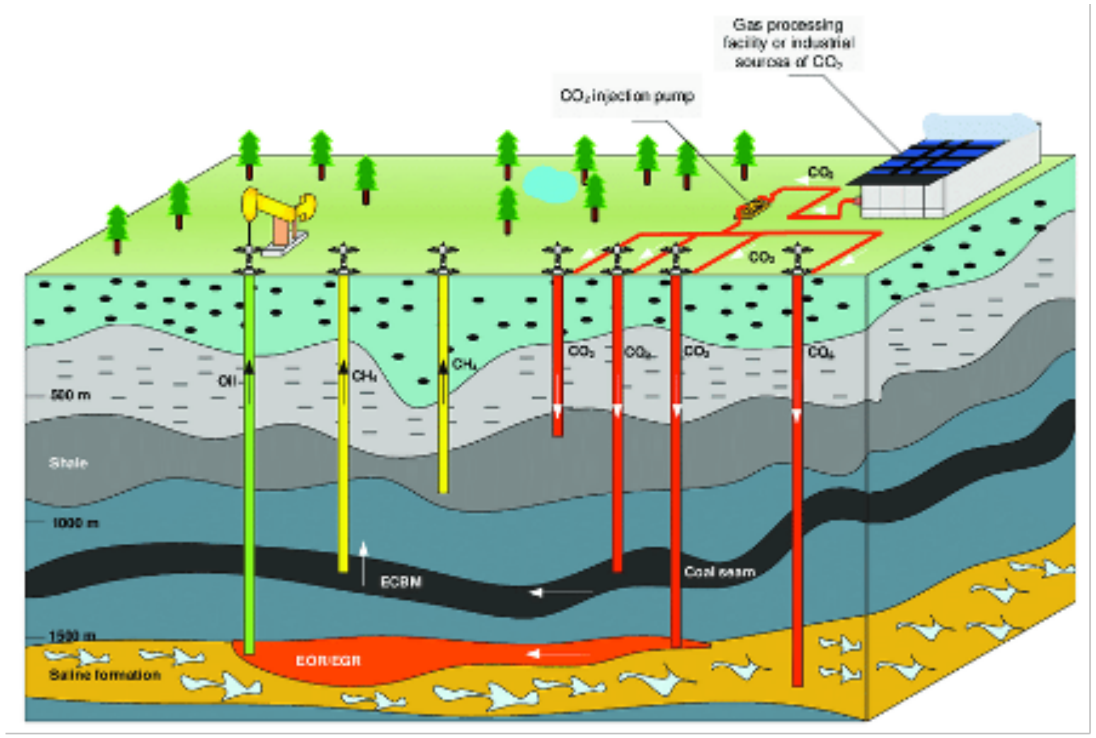
Example of mathematical challenges

- Development of **discrete elasticity complexes**
- Corresponding **discrete Poincaré and Sobolev inequalities**
- **Compactness results**
- …

$$H^1(\Omega) \xrightarrow{\nabla_{\rm sym}} H_{\mathbb{S}}(\mathrm{Rot\,Rot}^\top;\Omega) \xrightarrow{\mathrm{Rot\,Rot}^\top} H_{\mathbb{S}}(\mathrm{Div};\Omega) \xrightarrow{\mathrm{Div}_{\mathbb{S}}} L^2(\Omega)$$

Proof-of-concept applications

Magnetohydrodynamics



Geological flows

These applications require to combine all the advances of the NEMESIS project!

NEMESIS

New generation methods
for numerical simulations

Funded by
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Thank you for your attention!