Polyhedral discretizations for industrial applications

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POEMS conference at CIRM

Outline

1. Introduction
    - Context
    - Motivations to develop robust polyhedral discretizations
    - Compatible discretizations
2. Brief overview of Compatible Discrete Operators (CDO) schemes
    - The CDO framework
    - Scalar-valued diffusion problem
    - Numerical illustration
3. Groundwater flows: An example of industrial application
4. CDO schemes for the Stokes equations
5. Ongoing works & Perspectives

Context & Motivations to develop robust polyhedral discretizations

EDF Context

EDF R&D has been developping several **in-house simulation codes** for more than 30 years to study/understand/improve the safety and the life of its power plants and their efficiency.

Main simulation codes are **open-source** and developped under a quality insurance and validated for studies related to nuclear safety by the French safety authority

CODE SATURNE

- Computational fluid dynamics
- Finite Volume schemes
- Polyhedral meshes
- High Performance Computing

https://www.code-saturne.org

code_aster

- Computational structural mechanics
- Finite Element schemes
- Tetrahedral, pyramidal, hexahedral meshes
- Very broad modelling capacity

https://www.code-aster.org

Code_Saturne context

Simulate complex flows in complex geometries

Legacy discretization

- Single-phase flow solver based on co-located Finite Volume schemes
- Discretization choices close to commercial codes like Star-CD or FLUENT

↦ **V&V**: Extensive Verification & Validation process

↦ **Efficiency**: a competitive time to result on challenging problems thanks to High Performance Computing

Development of a new approach based on compatible discretizations:
Compatible Discrete Operator (CDO) schemes

↦ **Flexibility**

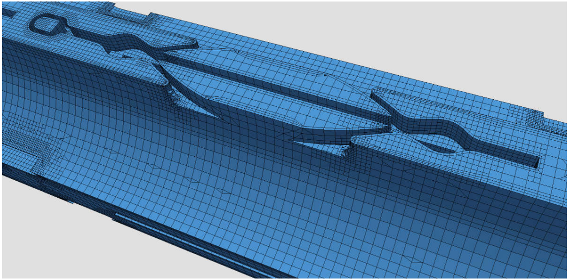
- Need a numerical scheme **less sensitive to the mesh quality**
  → Handle more efficiently polyhedral and/or poor-quality meshes

↦ **Physical fidelity**

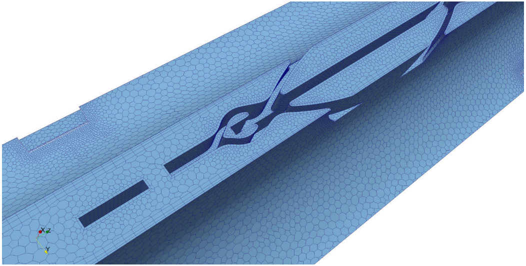
- **Preserve the structural properties** of equations/systems at the discrete level
- Build a numerical scheme relying on stronger **mathematical fundations**

Motivations to handle polyhedral meshes

Reduce time to generate meshes by use of **automatic meshing** tools



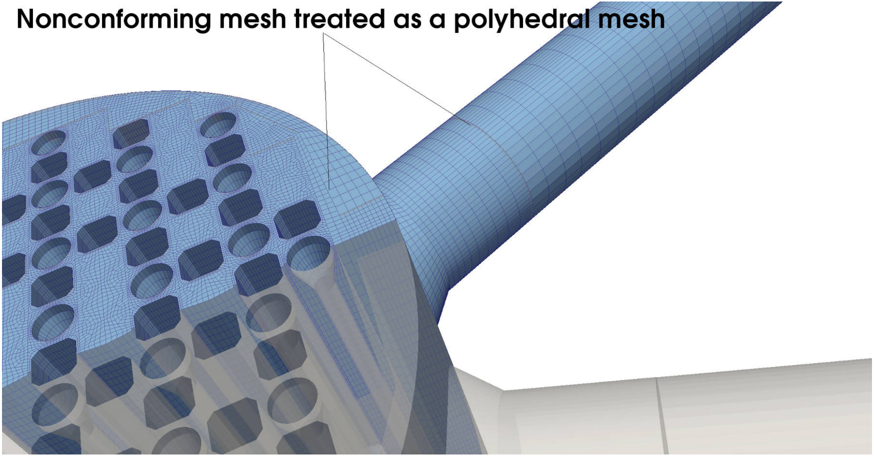
Mesh generated by a trimmer algorithm (with ANSYS)



Mesh generated by a Delaunay/Voronoï algorithm (with Star-CCM)

Motivations to handle polyhedral meshes

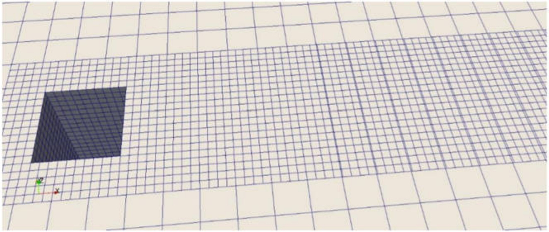
Reduce time to generate meshes by using **flexible mesh joining** process



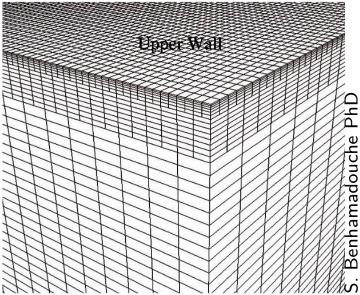
Joining process: Enable to build complex geometries from several existing meshes

Motivations to handle polyhedral meshes

Reduce time to compute the solution by using **less elements** thank to adaptative mesh refinement



Refine mesh only where it matters

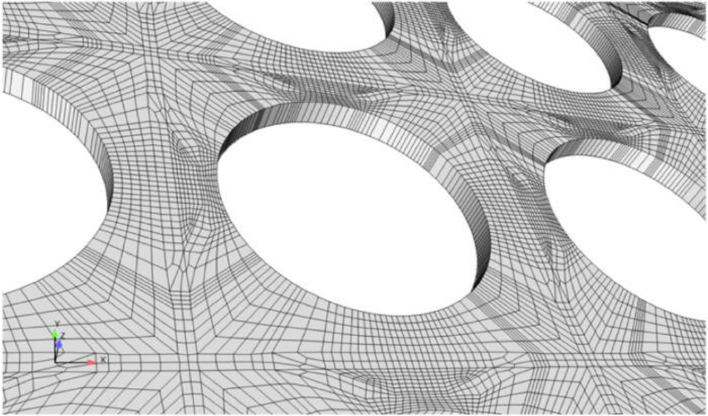


S. Benhamadouche PhD

Catch boundary layer with less element

Motivations to get robust space discetizations

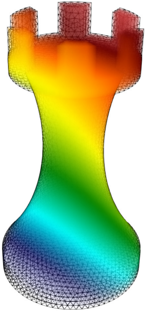
Meshing **complex geometries** can generate **distorted meshes**



Bare bundle: cut of a mesh

Compatible discretizations

Joint work with A. Ern
P. Cantin & R. Milani



Courtesy of G. Vialaneix

Compatible discretizations

Also called **structure-preserving** or **mimetic** discretizations

Aims: Preservation of the structural properties of PDEs at the discrete level

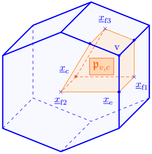
- ↦ Local discrete conservation laws
- ↦ Properties of the discrete differential operators similar to the continuous one
- ↦ Monotonicity (min/max principles) if needed
- ↦ Eliminate spurious modes

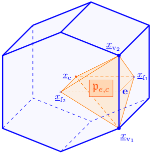
Historical viewpoint

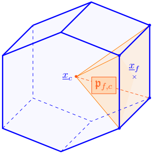
- ↦ Pioneering works
  - **Electromagnetics**: Kron *'53*, Branin *'66*, Tonti *'74* and Bossavit *'88*
  - **Mathematics**: Whitney *'57* and Dodziuk *'76*
- ↦ Seminal papers for the application (no mathematical proof): Staggered schemes on Cartesian meshes - **MAC** schemes
  - **Fluid mechanics**: Harlow & Welch *'65 "Numerical Calculation of Time-Dependent Viscous Incompressible Flow of Fluid with Free Surface"*
  - **Electromagnetics**: Yee *'66 Numerical solution of initial boundary value problems involving Maxwell's equations in isotropic media*

CDO in a nutshell

- ↦ **Low-order** method for **polyhedral meshes**
- ↦ Same building principles as in **compatible**/mimetic/structure-preserving discretizations
- ↦ **Several families** according to the location of degrees of freedom
  - Vertex- or Edge- or Face- or Cell-based schemes
- ↦ Fine-grained operators: unified analysis at the discrete/functionnal level
- ↦ Use of **sub-meshes**



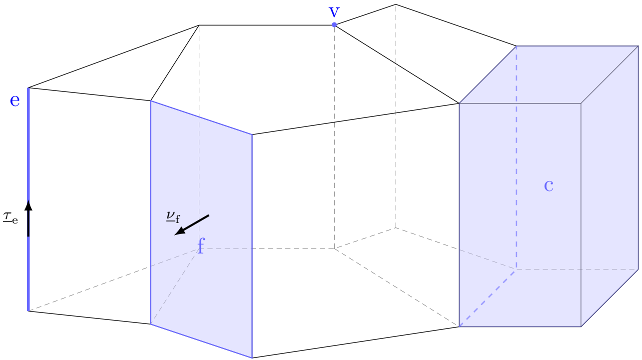




3 PhDs supervised by A. Ern

Bonelle (11-14)	• Diffusion (vertex-, face-, cell-based schemes) • Stokes in <u>curl</u> formulation (edge-/face-based schemes)
Cantin (13-16)	• Scalar-valued transport problems (vertex-based schemes) • Vector-valued transport problems (edge-based schemes)
Milani (17-)	• Navier-Stokes equations for incompressible fluids in *classical* formulation (face-based schemes)

Primal mesh



Mesh

$\mathrm{M} := \{\mathrm{V}, \mathrm{E}, \mathrm{F}, \mathrm{C}\}$

vertices $\mathrm{v} \in \mathrm{V}$
edges $\mathrm{e} \in \mathrm{E}$
faces $\mathrm{f} \in \mathrm{F}$
cells $\mathrm{c} \in \mathrm{C}$

Assign an arbitrary orientation to each edge ($\underline{\tau}_{\mathrm{e}}$) and to each face ($\underline{\nu}_{\mathrm{f}}$)

Example of subsets of entities

$$\mathrm{E}_{\mathrm{c}} := \{\mathrm{e} \in \mathrm{E} \,|\, \mathrm{e} \subset \partial \mathrm{c}\}, \qquad \mathrm{C}_{\mathrm{e}} := \{\mathrm{c} \in \mathrm{C} \,|\, \partial \mathrm{c} \subset \mathrm{e}\},$$
$$\mathrm{V}_{\mathrm{e}} := \{\mathrm{v} \in \mathrm{V} \,|\, \mathrm{v} \subset \partial \mathrm{e}\}, \qquad \mathrm{E}_{\mathrm{v}} := \{\mathrm{e} \in \mathrm{E} \,|\, \partial \mathrm{e} \subset \mathrm{v}\}.$$

Notations: X corresponds to any set in $\{\mathrm{V}, \mathrm{E}, \mathrm{F}, \mathrm{C}\}$, x to any entity in $\{\mathrm{v}, \mathrm{e}, \mathrm{f}, \mathrm{c}\}$, and $\#\mathrm{X}$ to the cardinality of X.

Degrees of freedom (DoFs)

Design principles

Potential: Evaluation **at a point** of a scalar-valued field

Circulation: Evaluation of the tangential component of a vector-valued field **along a path**

Flux: Evaluation of the normal component of a vector-valued field **across a surface**

Density: Evaluation of a scalar-valued field **inside a volume**

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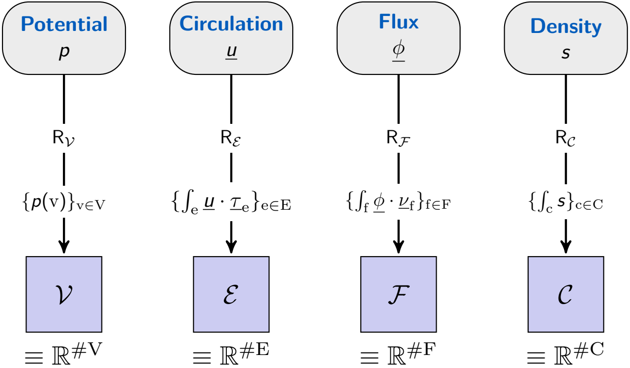
Example for the primal mesh of definitions of DoFs
=
de Rham maps



$$\begin{tikzcd}
\text{Potential } p \arrow[d, "\mathsf{R}_{\mathcal{V}}"', "\{p(\mathrm{v})\}_{\mathrm{v}\in\mathrm{V}}"] & \text{Circulation } \underline{u} \arrow[d, "\mathsf{R}_{\mathcal{E}}"', "\{\int_{\mathrm{e}} \underline{u}\cdot\underline{\tau}_{\mathrm{e}}\}_{\mathrm{e}\in\mathrm{E}}"] & \text{Flux } \underline{\phi} \arrow[d, "\mathsf{R}_{\mathcal{F}}"', "\{\int_{\mathrm{f}} \underline{\phi}\cdot\underline{\nu}_{\mathrm{f}}\}_{\mathrm{f}\in\mathrm{F}}"] & \text{Density } s \arrow[d, "\mathsf{R}_{\mathcal{C}}"', "\{\int_{\mathrm{c}} s\}_{\mathrm{c}\in\mathrm{C}}"] \\
\mathcal{V} \equiv \mathbb{R}^{\#\mathrm{V}} & \mathcal{E} \equiv \mathbb{R}^{\#\mathrm{E}} & \mathcal{F} \equiv \mathbb{R}^{\#\mathrm{F}} & \mathcal{C} \equiv \mathbb{R}^{\#\mathrm{C}}
\end{tikzcd}$$

Discrete differential operators

Building principles

Discrete gradient operator

- ↦ From a linear combination of discrete **potentials** defines a discrete **circulation**
- ↦ Key identity: Fundamental theorem of calculus

$\int_{\underline{x}_{\mathrm{v}_1}}^{\underline{x}_{\mathrm{v}_2}} \underline{\mathrm{grad}}(p) \cdot \underline{\tau}_e = p(\underline{x}_{\mathrm{v}_2}) - p(\underline{x}_{\mathrm{v}_1})$ for any path e starting at $\underline{x}_{\mathrm{v}_1}$ ending at $\underline{x}_{\mathrm{v}_2}$.

Discrete curl operator

- ↦ From a linear combination of discrete **circulations** defines a discrete **flux**
- ↦ Key identity: Kelvin–Stokes theorem

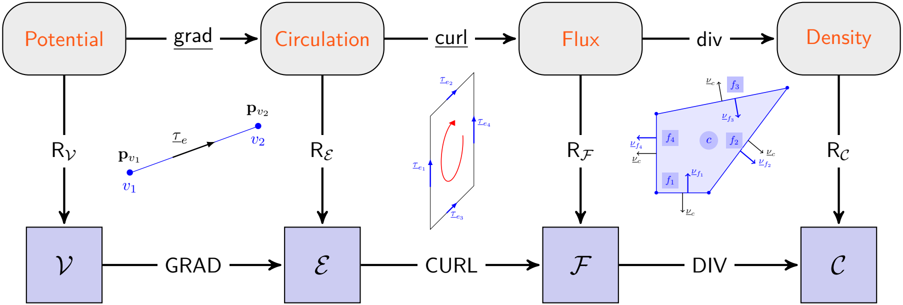
$\int_f \underline{\mathrm{curl}}(\underline{u}) \cdot \underline{\nu}_f = \int_{\partial f} \underline{u} \cdot \underline{\tau}_{\partial f}$ for a surface f with a closed contour ∂f.

Discrete divergence operator

- ↦ From a linear combination of discrete **fluxes** defines a discrete **density**
- ↦ Key identity: Gauss theorem

$\int_c \mathrm{div}(\underline{\phi}) = \int_{\partial c} \underline{\phi} \cdot \underline{\nu}_{\partial c}$ for a volume c with a closed surface ∂c.

Discrete differential operators on the primal mesh



$$\begin{tikzcd}
\text{Potential} \arrow[r, "\underline{\mathrm{grad}}"] \arrow[d, "\mathrm{R}_{\mathcal{V}}"] & \text{Circulation} \arrow[r, "\underline{\mathrm{curl}}"] \arrow[d, "\mathrm{R}_{\mathcal{E}}"] & \text{Flux} \arrow[r, "\mathrm{div}"] \arrow[d, "\mathrm{R}_{\mathcal{F}}"] & \text{Density} \arrow[d, "\mathrm{R}_{\mathcal{C}}"] \\
\mathcal{V} \arrow[r, "\mathsf{GRAD}"] & \mathcal{E} \arrow[r, "\mathsf{CURL}"] & \mathcal{F} \arrow[r, "\mathsf{DIV}"] & \mathcal{C}
\end{tikzcd}$$

$$\mathsf{GRAD}(\mathbf{p})|_{\mathrm{e}} = \textstyle\sum_{\mathrm{v}\in\mathrm{V}_{\mathrm{e}}} \pm 1\mathbf{p}_{\mathrm{v}}, \quad \mathsf{CURL}(\mathbf{u})|_{\mathrm{f}} = \textstyle\sum_{\mathrm{e}\in\mathrm{E}_{\mathrm{f}}} \pm 1\mathbf{u}_{\mathrm{e}}, \quad \mathsf{DIV}(\phi)|_{\mathrm{c}} = \textstyle\sum_{\mathrm{f}\in\mathrm{F}_{\mathrm{c}}} \pm 1\phi_{\mathrm{f}}$$

1. Metric-free operators: Matrix entries are exclusively 0 or ±1
2. Commuting property with De Rham's maps

   $\mathsf{GRAD}\cdot\mathrm{R}_{\mathcal{V}} = \mathrm{R}_{\mathcal{E}}\cdot\underline{\mathrm{grad}}, \qquad \mathsf{CURL}\cdot\mathrm{R}_{\mathcal{E}} = \mathrm{R}_{\mathcal{F}}\cdot\underline{\mathrm{curl}}, \qquad \mathsf{DIV}\cdot\mathrm{R}_{\mathcal{F}} = \mathrm{R}_{\mathcal{C}}\cdot\mathrm{div}$
3. Cochain complex: $\mathsf{CURL}\cdot\mathsf{GRAD}\equiv 0_{\mathcal{F}}, \qquad \mathsf{DIV}\cdot\mathsf{CURL}\equiv 0_{\mathcal{C}}$

Discretization process

Case of the diffusion problem

$$-\operatorname{div}(\underline{\underline{\kappa}}\ \underline{\operatorname{grad}}(p)) = s$$

Topological laws

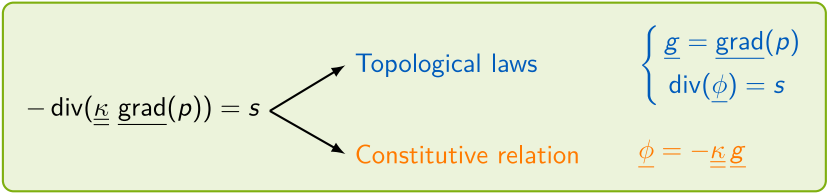
$$\begin{cases} \underline{g} = \underline{\operatorname{grad}}(p) \\ \operatorname{div}(\underline{\phi}) = s \end{cases}$$

Constitutive relation

$$\underline{\phi} = -\underline{\underline{\kappa}}\,\underline{g}$$

Discretization process

Case of the diffusion problem



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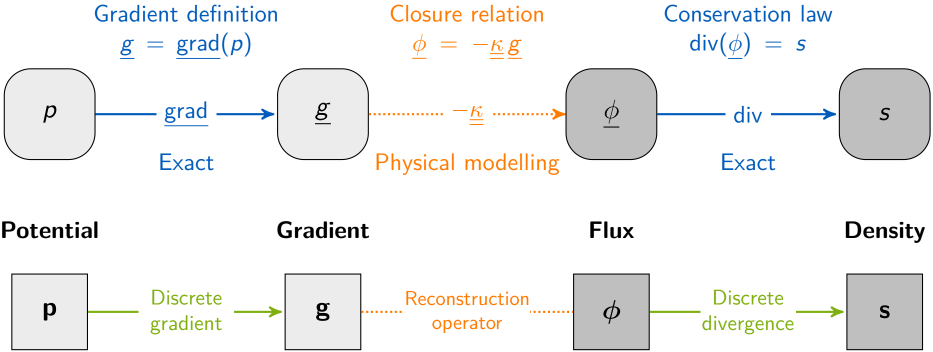


Gradient definition

$$\underline{g} = \underline{\operatorname{grad}}(p)$$

Closure relation

$$\underline{\phi} = -\underline{\underline{\kappa}}\,\underline{g}$$

Conservation law

$$\operatorname{div}(\underline{\phi}) = s$$

$$\begin{tikzcd} p \arrow[r, "\underline{\operatorname{grad}}"] & \underline{g} \arrow[r, dotted, "-\underline{\underline{\kappa}}"] & \underline{\phi} \arrow[r, "\operatorname{div}"] & s \end{tikzcd}$$

Exact

Physical modelling

Exact

Potential

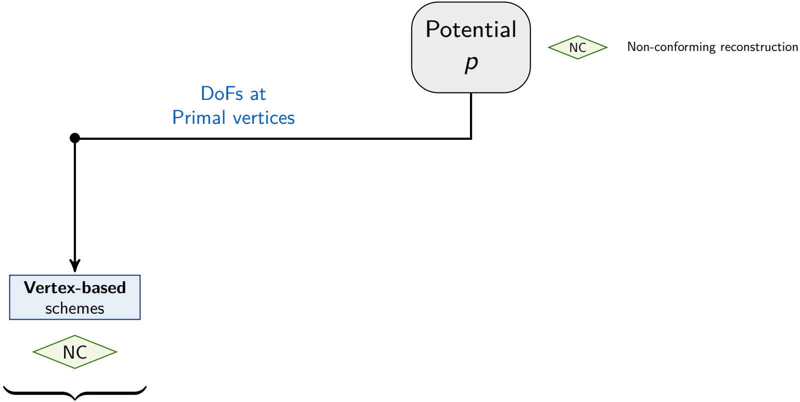
Gradient

Flux

Density

$$\begin{tikzcd} \mathbf{p} \arrow[r, "\text{Discrete gradient}"] & \mathbf{g} \arrow[r, dotted, dash, "\text{Reconstruction operator}"] & \boldsymbol{\phi} \arrow[r, "\text{Discrete divergence}"] & \mathbf{s} \end{tikzcd}$$

CDO discretizations



Potential
p

NC Non-conforming reconstruction

DoFs at
Primal vertices

Vertex-based
schemes

NC

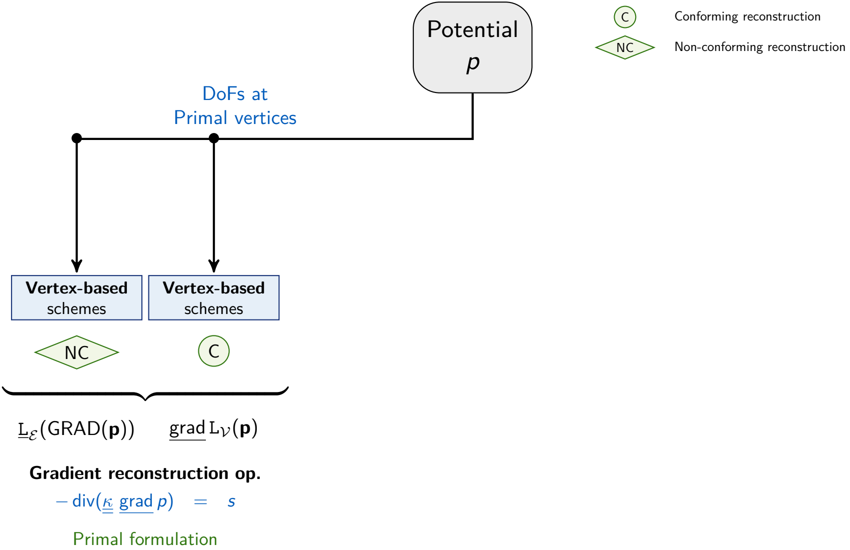
$\underline{\mathrm{L}}_{\mathcal{E}}(\mathrm{GRAD}(\mathbf{p}))$

Gradient reconstruction op.

$$-\mathrm{div}(\underline{\underline{\kappa}}\,\underline{\mathrm{grad}}\,p) = s$$

Primal formulation

CDO discretizations



Potential
p

C Conforming reconstruction

NC Non-conforming reconstruction

DoFs at
Primal vertices

Vertex-based schemes

NC

Vertex-based schemes

C

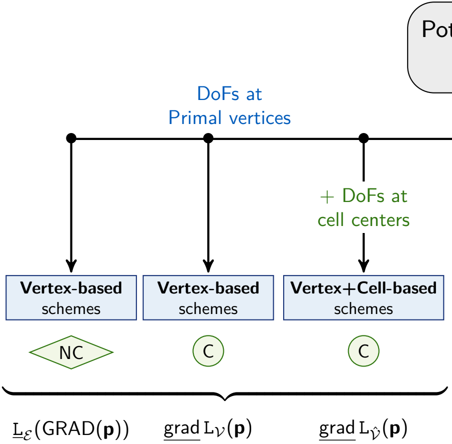
$\underline{\mathrm{L}}_{\mathcal{E}}(\mathrm{GRAD}(\mathbf{p}))$ $\underline{\mathrm{grad}}\,\mathrm{L}_{\mathcal{V}}(\mathbf{p})$

Gradient reconstruction op.

$$-\,\mathrm{div}(\underline{\underline{\kappa}}\,\underline{\mathrm{grad}}\,p) \quad = \quad s$$

Primal formulation

CDO discretizations



Potential
p

DoFs at
Primal vertices

$+$ DoFs at
cell centers

Vertex-based schemes

Vertex-based schemes

Vertex+Cell-based schemes

NC

C

C

$\underline{\mathrm{L}}_{\mathcal{E}}(\mathrm{GRAD}(\mathbf{p}))$

$\underline{\mathrm{grad}}\,\mathrm{L}_{\mathcal{V}}(\mathbf{p})$

$\underline{\mathrm{grad}}\,\mathrm{L}_{\hat{\mathcal{V}}}(\mathbf{p})$

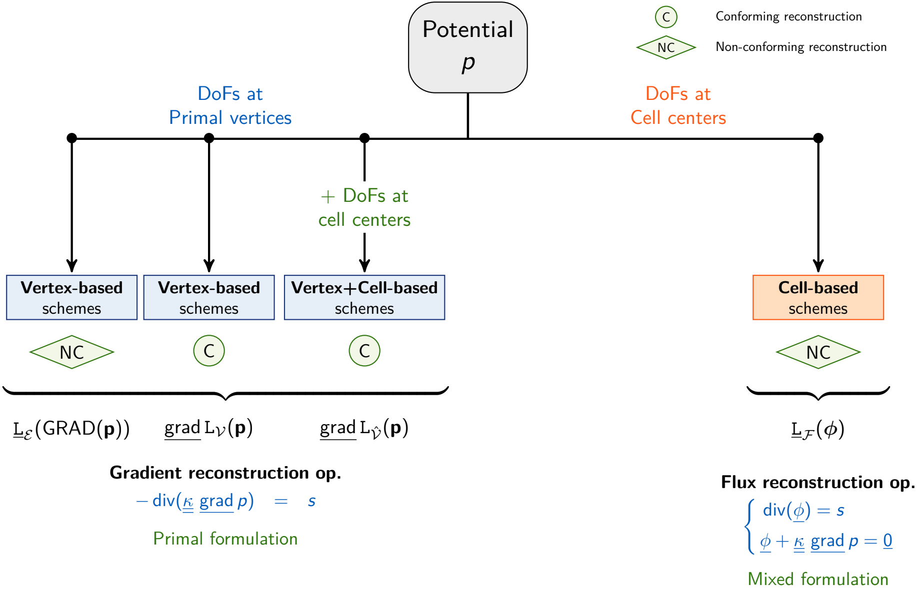
C	Conforming reconstruction
NC	Non-conforming reconstruction

Gradient reconstruction op.

$$-\,\mathrm{div}(\underline{\underline{\kappa}}\ \underline{\mathrm{grad}}\,p) \quad = \quad s$$

Primal formulation

CDO discretizations



C Conforming reconstruction

NC Non-conforming reconstruction

Potential
p

DoFs at
Primal vertices

DoFs at
Cell centers

+ DoFs at
cell centers

Vertex-based schemes — NC

Vertex-based schemes — C

Vertex+Cell-based schemes — C

Cell-based schemes — NC

$\underline{\mathrm{L}}_{\mathcal{E}}(\mathrm{GRAD}(\mathbf{p}))$ $\quad\underline{\mathrm{grad}}\,\mathrm{L}_{\mathcal{V}}(\mathbf{p})$ $\quad\underline{\mathrm{grad}}\,\mathrm{L}_{\hat{\mathcal{V}}}(\mathbf{p})$

$\underline{\mathrm{L}}_{\mathcal{F}}(\phi)$

Gradient reconstruction op.

$$-\mathrm{div}(\underline{\underline{\kappa}}\,\underline{\mathrm{grad}}\,p) \quad = \quad s$$

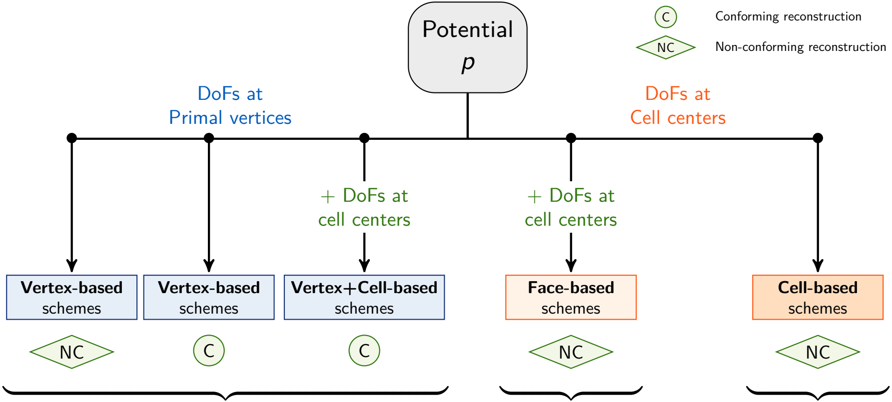
Primal formulation

Flux reconstruction op.

$$\begin{cases} \mathrm{div}(\underline{\phi}) = s \\ \underline{\phi} + \underline{\underline{\kappa}}\,\underline{\mathrm{grad}}\,p = \underline{0} \end{cases}$$

Mixed formulation

CDO discretizations



C Conforming reconstruction

NC Non-conforming reconstruction

Potential p

DoFs at Primal vertices

DoFs at Cell centers

+ DoFs at cell centers

+ DoFs at cell centers

Vertex-based schemes — NC

Vertex-based schemes — C

Vertex+Cell-based schemes — C

Face-based schemes — NC

Cell-based schemes — NC

$\underline{\mathrm{L}}_{\mathcal{E}}(\mathrm{GRAD}(\mathbf{p}))$ $\underline{\mathrm{grad}}\,\mathrm{L}_{\mathcal{V}}(\mathbf{p})$ $\underline{\mathrm{grad}}\,\mathrm{L}_{\hat{\mathcal{V}}}(\mathbf{p})$

$\mathrm{L}_{\widetilde{\mathcal{E}}_c}(\hat{\mathrm{G}}_c(\mathbf{p}))$

$\underline{\mathrm{L}}_{\mathcal{F}}(\phi)$

Gradient reconstruction op.

$$-\mathrm{div}(\underline{\underline{\kappa}}\,\underline{\mathrm{grad}}\,p) \quad = \quad s$$

Primal formulation

Gradient reconstruction op.

$$\begin{cases} -\mathrm{div}(\underline{\underline{\kappa}}\,\underline{\mathrm{grad}}\,p)|_{\mathrm{c}} = s|_{\mathrm{c}} \\ \underline{\underline{\kappa}}\,\underline{\mathrm{grad}}\,p|_{\mathrm{f},\mathrm{c}_1} + \underline{\underline{\kappa}}\,\underline{\mathrm{grad}}\,p|_{\mathrm{f},\mathrm{c}_2} = \underline{0} \end{cases}$$

Hybrid formulation

Flux reconstruction op.

$$\begin{cases} \mathrm{div}(\underline{\phi}) = s \\ \underline{\phi} + \underline{\underline{\kappa}}\,\underline{\mathrm{grad}}\,p = \underline{0} \end{cases}$$

Mixed formulation

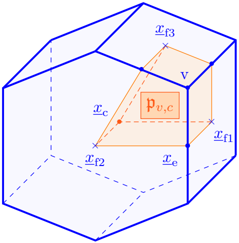
Non-conforming CDO vertex-based schemes

- ↦ Potentials **p** located at **primal vertices** and its DoF space is denoted $\mathcal{V}$
- ↦ Gradient $\mathbf{g} = \mathrm{GRAD}(\mathbf{p}) \in \mathcal{E}$ located at primal edges

Find $\mathbf{p} \in \mathcal{V}$ s.t.

$$\sum_{c\in C}\int_c \underline{\mathrm{L}}_{\mathcal{E}_c}(\mathrm{GRAD}(\mathbf{p}))\cdot\underline{\underline{\kappa}}\cdot\underline{\mathrm{L}}_{\mathcal{E}_c}(\mathrm{GRAD}(\mathbf{q})) = \sum_{c\in C}\int_c s\,\mathrm{L}^0_{\mathcal{V}_c}(\mathbf{q}),\quad \forall\mathbf{q}\in\mathcal{V}$$

Key operator: Gradient reconstruction



↦ Vertex-based partition

$\mathfrak{P}_{\mathrm{V,c}} := \{\mathfrak{p}_{v,c}\}_{v\in V_c}$

$\mathrm{L}^0_{\mathcal{V}_c}(\mathbf{p})|_{\mathfrak{p}_{v,c}} := \mathbf{p}_v$

Non-conforming CDO vertex-based schemes

- ↦ Potentials **p** located at **primal vertices** and its DoF space is denoted $\mathcal{V}$
- ↦ Gradient $\mathbf{g} = \mathrm{GRAD}(\mathbf{p}) \in \mathcal{E}$ located at primal edges

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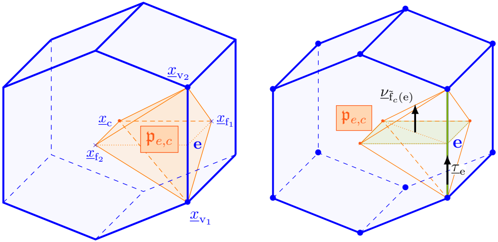
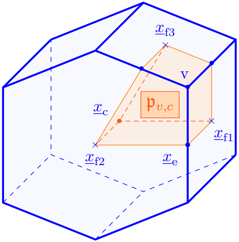
Key operator: Gradient reconstruction



↦ Edge-based partition $\mathfrak{P}_{E,c} := \{\mathfrak{p}_{e,c}\}_{e\in E_c}$

$$\underline{\mathrm{L}}_{\mathcal{E}_c}(\mathbf{g})|_{\mathfrak{p}_{e,c}} := \underline{\mathrm{C}}_{\mathcal{E}_c}(\mathbf{g}) + \beta\frac{\underline{\tilde{\mathrm{f}}}_c(e)}{|\mathfrak{p}_{e,c}|}\left(\mathbf{g}_e - \underline{e}\cdot\underline{\mathrm{C}}_{\mathcal{E}_c}(\mathbf{g})\right) \in \mathbb{P}^3_0$$

where $\underline{\mathrm{C}}_{\mathcal{E}_c}(\mathbf{g}) := \frac{1}{|c|}\sum_{e\in E_c}\mathbf{g}_e\underline{\tilde{\mathrm{f}}}_c(e)$ (constant in c)



↦ Vertex-based partition

$\mathfrak{P}_{V,c} := \{\mathfrak{p}_{v,c}\}_{v\in V_c}$

$\mathrm{L}^0_{\mathcal{V}_c}(\mathbf{p})|_{\mathfrak{p}_{v,c}} := \mathbf{p}_v$

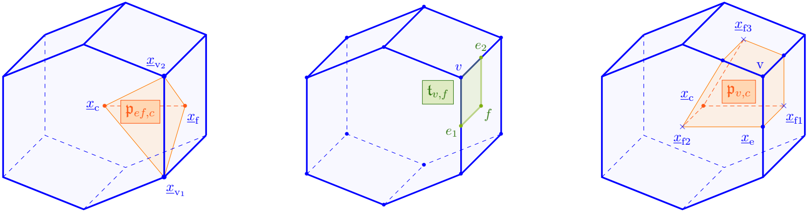
Conforming CDO Vertex-based schemes

↦ Potentials **p** located at **primal vertices** and its DoF space is denoted $\mathcal{V}$

∼ **FE for polyhedral meshes**

Find $\mathbf{p} \in \mathcal{V}$ s.t.

$$\sum_{c \in C} \int_c \underline{\mathrm{grad}}\, \mathrm{L}_{\mathcal{V}_c}(\mathbf{p}) \cdot \underline{\underline{\kappa}} \cdot \underline{\mathrm{grad}}\, \mathrm{L}_{\mathcal{V}_c}(\mathbf{q}) = \sum_{c \in C} \int_c \mathrm{L}_{\mathcal{V}_c} \mathrm{R}_{\mathcal{V}_c}(s)\, \mathrm{L}_{\mathcal{V}_c}(\mathbf{q}), \qquad \forall \mathbf{q} \in \mathcal{V}$$



↦ Based on an **implicit tetrahedral partition**: $\mathfrak{P}_{\mathrm{EF,c}} := \{\mathfrak{p}_{ef,c}\}_{e \in E_f, f \in F_c}$

↦ In $\mathfrak{p}_{ef,c}$ consider the $\mathbb{P}_1$-Lagrange FE with basis functions: $\theta_{v1}, \theta_{v2}, \theta_f$ and θ_c

- Need a linear interpolation at face center: $\mathbf{p}_f := \frac{1}{|f|} \sum_{v \in V_f} |\mathfrak{t}_{v,f}| \mathbf{p}_v$
- Need a linear interpolation at cell center: $\mathbf{p}_c := \frac{1}{|c|} \sum_{v \in V_c} |\mathfrak{p}_{v,c}| \mathbf{p}_v$

Conforming potential reconstruction

$$\mathrm{L}_{\mathcal{V}_c}(\mathbf{p})(\underline{x})|_{\mathfrak{p}_{ef,c}} := \mathbf{p}_{\mathrm{v}_1}\theta_{\mathrm{v}_1} + \mathbf{p}_{\mathrm{v}_2}\theta_{\mathrm{v}_2} + \left(\frac{1}{|\mathrm{f}|} \sum_{\mathrm{v} \in \mathrm{V}_\mathrm{f}} |\mathfrak{t}_{\mathrm{v},\mathrm{f}}| \mathbf{p}_\mathrm{v} \right) \theta_\mathrm{f} + \left(\frac{1}{|c|} \sum_{\mathrm{v} \in V_c} |\mathfrak{p}_{v,c}| \mathbf{p}_v \right) \theta_\mathrm{c}$$

Conforming CDO Vertex+Cell-based schemes

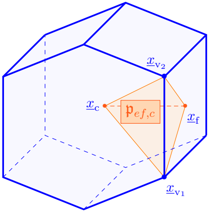
↦ **Hybrid** set of DoFs: Potentials $\mathbf{p} \in \widehat{\mathcal{V}}$ located at **primal vertices** and **cell centers**

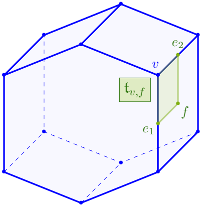
↦ **Static condensation** for cell unknows: Linear system reduce to $\#\mathrm{V}$

∼ **FE for polyhedral meshes**

Find $\mathbf{p} \in \widehat{\mathcal{V}}$ s.t.

$$\sum_{c \in C} \int_c \underline{\mathrm{grad}}\, \mathrm{L}_{\widehat{\mathcal{V}}_c}(\mathbf{p}) \cdot \underline{\underline{\kappa}} \cdot \underline{\mathrm{grad}}\, \mathrm{L}_{\widehat{\mathcal{V}}_c}(\mathbf{q}) = \sum_{c \in C} \int_c \mathrm{L}_{\widehat{\mathcal{V}}_c} \mathrm{R}_{\widehat{\mathcal{V}}_c}(s)\, \mathrm{L}_{\widehat{\mathcal{V}}_c}(\mathbf{q}), \qquad \forall \mathbf{q} \in \widehat{\mathcal{V}}$$





↦ Based on an **implicit tetrahedral partition**: $\mathfrak{P}_{\mathrm{EF,c}} := \{\mathfrak{p}_{ef,c}\}_{e \in E_f, f \in F_c}$

↦ In $\mathfrak{p}_{ef,c}$ consider the $\mathbb{P}_1$-Lagrange FE with basis functions: $\theta_{v1}, \theta_{v2}, \theta_f$ and θ_c

- Need a linear interpolation at face center: $\mathbf{p}_f := \frac{1}{|f|} \sum_{v \in V_f} |\mathfrak{t}_{v,f}| \mathbf{p}_v$

Conforming potential reconstruction

$$\mathrm{L}_{\widehat{\mathcal{V}}_c}(\mathbf{p})(\underline{x})|_{\mathfrak{p}_{ef,c}} := \mathbf{p}_{\mathrm{v}_1}\theta_{\mathrm{v}_1} + \mathbf{p}_{\mathrm{v}_2}\theta_{\mathrm{v}_2} + \left(\frac{1}{|\mathrm{f}|} \sum_{\mathrm{v} \in \mathrm{V_f}} |\mathfrak{t}_{\mathrm{v,f}}| \mathbf{p}_{\mathrm{v}} \theta_{\mathrm{f}} \right) + \mathbf{p}_c \theta_{\mathrm{c}}$$

Non-conforming CDO cell-based schemes

- ↦ Potentials $\mathbf{p} \in \widetilde{\mathcal{V}}$ located at **cell centers** and fluxes $\phi \in \mathcal{F}$ located at **(primal) faces**
- ↦ Divergence op.: $\mathsf{DIV}(\phi) \in \mathcal{C}$ *i.e.* constant inside each cell
- ↦ **Saddle-point** system
- ↦ Simple potential reconstruction in each cell: $\mathrm{L}^0_{\widetilde{\mathcal{V}}}(\mathbf{p})|_c := \mathbf{p}_c$

Find $(\mathbf{p}, \phi) \in \widetilde{\mathcal{V}} \times \mathcal{F}$ s.t.

$$\begin{cases} \displaystyle\sum_{c \in C} \left(\int_c \underline{\mathrm{L}}_{\mathcal{F}_c}(\phi) \cdot \underline{\underline{\kappa}}^{-1} \cdot \underline{\mathrm{L}}_{\mathcal{F}_c}(\mathbf{\Psi}) - \int_c \mathsf{DIV}(\mathbf{\Psi}) \cdot \mathrm{L}^0_{\widetilde{\mathcal{V}}}(\mathbf{p}) \right) = 0, & \forall \mathbf{\Psi} \in \mathcal{F} \\ \displaystyle -\sum_{c \in C} \int_c \mathsf{DIV}(\phi) \cdot \mathrm{L}^0_{\widetilde{\mathcal{V}}}(\mathbf{q}) = \sum_{c \in C} \int_c s \cdot \mathrm{L}^0_{\widetilde{\mathcal{V}}}(\mathbf{q}), & \forall \mathbf{q} \in \widetilde{\mathcal{V}} \end{cases}$$

Key operator: Flux reconstruction

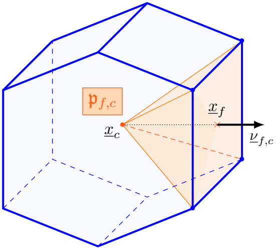
Non-conforming CDO cell-based schemes

- ↦ Potentials $\mathbf{p} \in \widetilde{\mathcal{V}}$ located at **cell centers** and fluxes $\phi \in \mathcal{F}$ located at **(primal) faces**
- ↦ Divergence op.: $\mathsf{DIV}(\phi) \in \mathcal{C}$ *i.e.* constant inside each cell
- ↦ **Saddle-point** system
- ↦ Simple potential reconstruction in each cell: $\mathrm{L}^0_{\widetilde{\mathcal{V}}}(\mathbf{p})|_c := \mathbf{p}_c$

Find $(\mathbf{p}, \phi) \in \widetilde{\mathcal{V}} \times \mathcal{F}$ s.t.

$$\begin{cases} \displaystyle\sum_{c\in C}\left(\int_c \underline{\mathrm{L}}_{\mathcal{F}_c}(\phi)\cdot \underline{\underline{\kappa}}^{-1}\cdot \underline{\mathrm{L}}_{\mathcal{F}_c}(\boldsymbol{\Psi}) - \int_c \mathsf{DIV}(\boldsymbol{\Psi})\cdot \mathrm{L}^0_{\widetilde{\mathcal{V}}}(\mathbf{p})\right) = 0, & \forall \boldsymbol{\Psi}\in\mathcal{F} \\ \displaystyle -\sum_{c\in C}\int_c \mathsf{DIV}(\phi)\cdot\mathrm{L}^0_{\widetilde{\mathcal{V}}}(\mathbf{q}) = \sum_{c\in C}\int_c s\cdot \mathrm{L}^0_{\widetilde{\mathcal{V}}}(\mathbf{q}), & \forall \mathbf{q}\in\widetilde{\mathcal{V}} \end{cases}$$

Key operator: Flux reconstruction



↦ Face-based partition $\mathfrak{P}_{\mathrm{F,c}} := \{\mathfrak{p}_{f,c}\}_{f\in\mathrm{F}_c}$

$$\underline{\mathrm{L}}_{\mathcal{F}_c}(\phi)|_{\mathfrak{p}_{f,c}} := \underline{\mathrm{C}}_{\mathcal{F}_c}(\phi) + \beta\frac{\underline{\tilde{\mathrm{e}}}_c(f)}{|\mathfrak{p}_{f,c}|}\left(\phi_f - \underline{\mathrm{f}}\cdot\underline{\mathrm{C}}_{\mathcal{F}_c}(\phi)\right) \in \mathbb{P}^3_0$$

where $\underline{\mathrm{C}}_{\mathcal{F}_c}(\phi) := \dfrac{1}{|\mathrm{c}|}\displaystyle\sum_{f\in\mathrm{F}_c}\phi_f\underline{\tilde{\mathrm{e}}}_c(f)$ (constant in c)

- $\underline{\tilde{\mathrm{e}}}_c(f) := \underline{x}_f - \underline{x}_c$
- $\underline{\mathrm{f}} := |\mathrm{f}|\underline{\nu}_{f,c}$

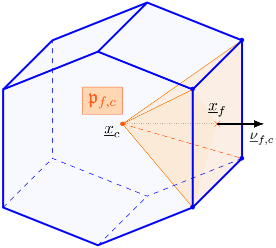
Non-conforming CDO face-based schemes

- ↦ **Hybrid** set of DoFs: Potentials $\mathbf{p} \in \widehat{\mathcal{U}}$ located at **face centers** and at **cell centers**
- ↦ Gradient on dual edges $\tilde{\mathrm{e}}_c(f)$ (segment $[\underline{x}_f, \underline{x}_c]$): $\mathbf{g}_{\tilde{\mathrm{e}}_c(f)} := \widehat{\mathsf{G}}(\mathbf{p})|_{\tilde{\mathrm{e}}_c(f)} := \mathbf{p}_f - \mathbf{p}_c \in \widetilde{\mathcal{E}}_c$
- ↦ **Static condensation** for cell unknows: Linear system reduced to $\#\mathrm{F}$
- ↦ Simple potential reconstruction in each cell: $\mathrm{L}^0_{\widehat{\mathcal{U}}}(\mathbf{p})|_c := \mathbf{p}_c$

Find $\mathbf{p} \in \widehat{\mathcal{U}}$ s.t.

$$\sum_{c \in C} \int_c \underline{\mathrm{L}}_{\widetilde{\mathcal{E}}_c}(\widehat{\mathsf{G}}(\mathbf{p})) \cdot \underline{\underline{\kappa}} \cdot \underline{\mathrm{L}}_{\widetilde{\mathcal{E}}_c}(\widehat{\mathsf{G}}(\mathbf{q})) = \sum_{c \in C} \int_c s \cdot \mathrm{L}_{\widehat{\mathcal{U}}}(\mathbf{q}), \qquad \forall \mathbf{q} \in \widehat{\mathcal{U}}$$

Key operator: Gradient reconstruction



↦ Face-based partition $\mathfrak{P}_{\mathrm{F,c}} := \{\mathfrak{p}_{f,c}\}_{f \in \mathrm{F}_c}$

$$\underline{\mathrm{L}}_{\widetilde{\mathcal{E}}_\mathrm{c}}(\mathbf{g})|_{\mathfrak{p}_{f,c}} := \underline{\mathrm{C}}_{\widetilde{\mathcal{E}}_c}(\mathbf{g}) + \beta \frac{\underline{\mathrm{f}}}{|\mathfrak{p}_{f,c}|}\left(\mathbf{g}_{\tilde{\mathrm{e}}_c(f)} - \underline{\tilde{\mathrm{e}}}_c(f) \cdot \underline{\mathrm{C}}_{\widetilde{\mathcal{E}}_c}(\mathbf{g})\right) \in \mathbb{P}^3_0$$

where $\underline{\mathrm{C}}_{\mathcal{F}_\mathrm{c}}(\mathbf{g}) := \dfrac{1}{|\mathrm{c}|} \displaystyle\sum_{f \in \mathrm{F}_c} \mathbf{g}_{\tilde{\mathrm{e}}_c(f)} \underline{\mathrm{f}}$ (constant in c)

- $\underline{\tilde{\mathrm{e}}}_c(f) := \underline{x}_f - \underline{x}_c$
- $\underline{\mathrm{f}} := |\mathrm{f}| \underline{\nu}_{f,c}$

A unified analysis

Mesh regularity: shape-regularity of a simplicial submesh with a bounded number of entities

Vertex-,Face-,Cell-based schemes

↦ Stability and well-posedness relying on the stability of the reconstruction and discrete Poincaré inequalities

↦ Error estimates (for smooth enough solutions)
- First-order CV rate in energy norm for the gradient (or flux)
- Second-order CV rate in L^2-norm for the potential (under elliptic regularity)

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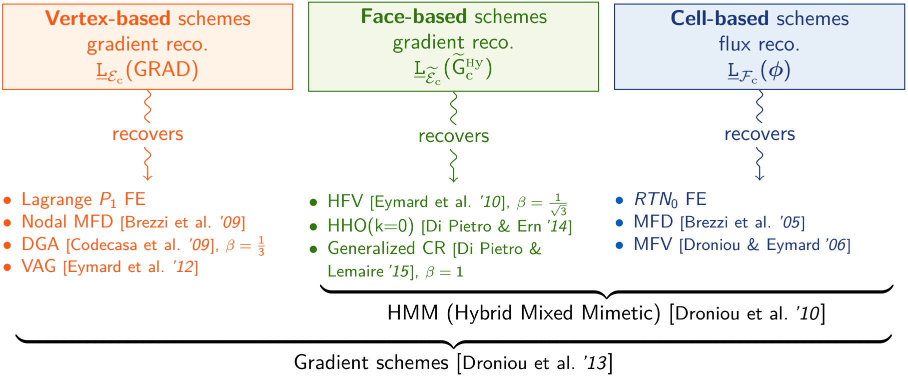


Vertex-based schemes
gradient reco.
$\underline{\mathrm{L}}_{\mathcal{E}_c}(\mathrm{GRAD})$

recovers

- Lagrange P_1 FE
- Nodal MFD [Brezzi et al. *'09*]
- DGA [Codecasa et al. *'09*], $\beta = \frac{1}{3}$
- VAG [Eymard et al. *'12*]

Face-based schemes
gradient reco.
$\underline{\mathrm{L}}_{\widetilde{\mathcal{E}}_c}(\widetilde{\mathrm{G}}_c^{\mathrm{Hy}})$

recovers

- HFV [Eymard et al. *'10*], $\beta = \frac{1}{\sqrt{3}}$
- HHO(k=0) [Di Pietro & Ern *'14*]
- Generalized CR [Di Pietro & Lemaire *'15*], $\beta = 1$

Cell-based schemes
flux reco.
$\underline{\mathrm{L}}_{\mathcal{F}_c}(\phi)$

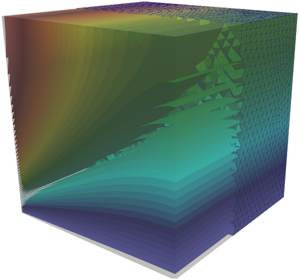
recovers

- *RTN*$_0$ FE
- MFD [Brezzi et al. *'05*]
- MFV [Droniou & Eymard *'06*]

HMM (Hybrid Mixed Mimetic) [Droniou et al. *'10*]

Gradient schemes [Droniou et al. *'13*]

Numerical results for diffusion problem

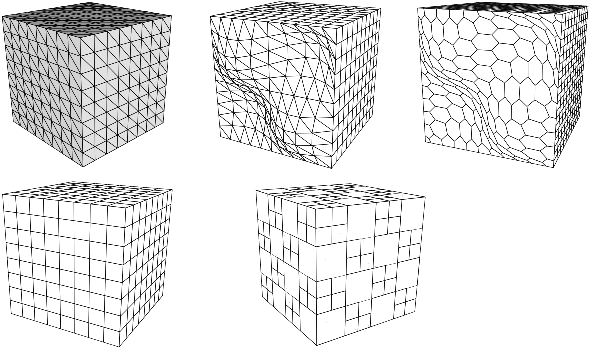


FVCA6 benchmark: Test case 1

Anisotropic diffusion problem: $-\mathrm{div}(\underline{\underline{\kappa}}\,\underline{\mathrm{grad}}(p)) = s$ **+ Dirichlet BCs**

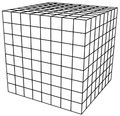
$$p(x,y,z) := 1 + \sin(\pi x)\sin\left(\pi\left(y+\frac{1}{2}\right)\right)\sin\left(\pi\left(z+\frac{1}{3}\right)\right), \quad \underline{\underline{\kappa}} := \begin{bmatrix} 1 & 0.5 & 0 \\ 0.5 & 1 & 0.5 \\ 0 & 0.5 & 1 \end{bmatrix}$$

Mesh sequences:

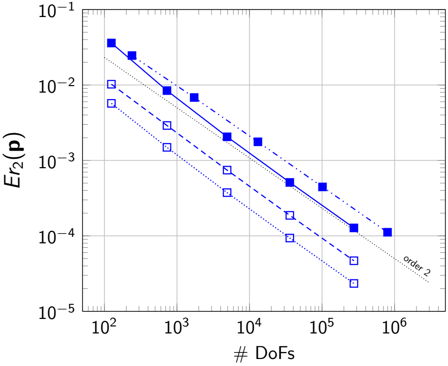


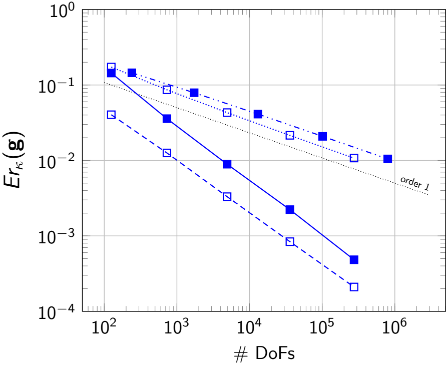
Comparative study of CDO schemes

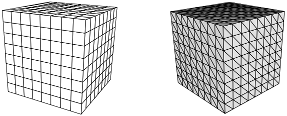
- $Er_2(\mathbf{p})$: Error on the potential in L^2 norm
- $Er_\kappa(\mathbf{g})$: Error on the gradient or flux in energy norm



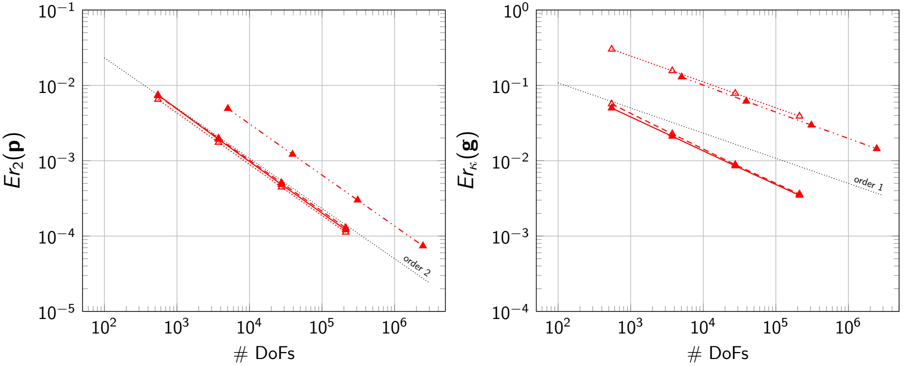
Vb-DGA	—■—	**p** : $1.3e-4$ **g** : $4.8e-4$
Vb-Conf	- -□- -	**p** : $4.7e-5$ **g** : $2.1e-4$
VCb	···□···	**p** : $2.3e-5$ **g** : $1.1e-2$
Fb-SUSHI	-·■-·	**p** : $1.1e-4$ **g** : $1.0e-2$

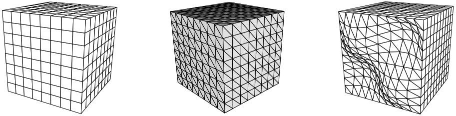




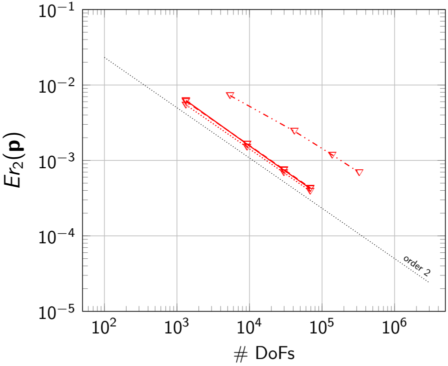


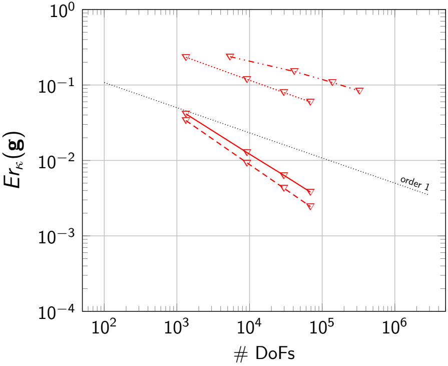
`Vb-DGA`	■	$\mathbf{p}: 1.3e-4$ $\mathbf{g}: 4.8e-4$	▲	$\mathbf{p}: 1.2e-4$ $\mathbf{g}: 3.5e-3$
`Vb-Conf`	□	$\mathbf{p}: 4.7e-5$ $\mathbf{g}: 2.1e-4$	△	$\mathbf{p}: 1.3e-4$ $\mathbf{g}: 3.6e-3$
`VCb`	□	$\mathbf{p}: 2.3e-5$ $\mathbf{g}: 1.1e-2$	△	$\mathbf{p}: 1.1e-4$ $\mathbf{g}: 3.9e-2$
`Fb-SUSHI`	■	$\mathbf{p}: 1.1e-4$ $\mathbf{g}: 1.0e-2$	▲	$\mathbf{p}: 7.4e-5$ $\mathbf{g}: 1.4e-2$

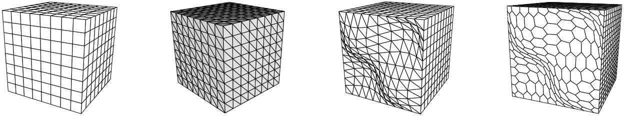




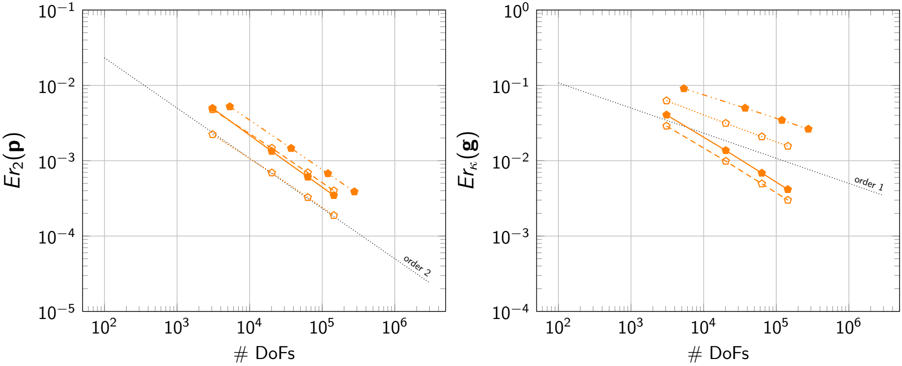
`Vb-DGA`	■ **p** : $1.3e-4$ **g** : $4.8e-4$	▲ **p** : $1.2e-4$ **g** : $3.5e-3$	▽ **p** : $4.2e-4$ **g** : $3.8e-3$
`Vb-Conf`	□ **p** : $4.7e-5$ **g** : $2.1e-4$	△ **p** : $1.3e-4$ **g** : $3.6e-3$	▽ **p** : $4.3e-4$ **g** : $2.4e-3$
`VCb`	□ **p** : $2.3e-5$ **g** : $1.1e-2$	△ **p** : $1.1e-4$ **g** : $3.9e-2$	▽ **p** : $3.9e-4$ **g** : $6.0e-2$
`Fb-SUSHI`	■ **p** : $1.1e-4$ **g** : $1.0e-2$	▲ **p** : $7.4e-5$ **g** : $1.4e-2$	▽ **p** : $6.9e-4$ **g** : $8.3e-2$

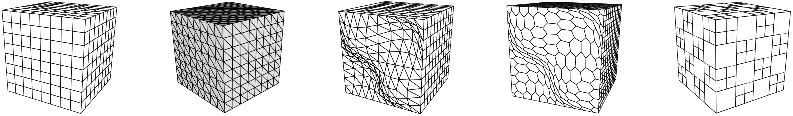




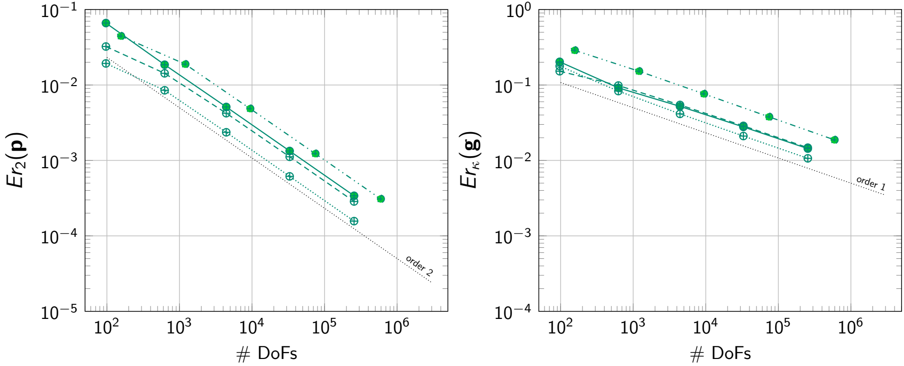


`Vb-DGA`	■	$\mathbf{p}: 1.3e-4$ $\mathbf{g}: 4.8e-4$	▲	$\mathbf{p}: 1.2e-4$ $\mathbf{g}: 3.5e-3$	▽	$\mathbf{p}: 4.2e-4$ $\mathbf{g}: 3.8e-3$	⬟	$\mathbf{p}: 4.2e-3$ $\mathbf{g}: 3.5e-4$
`Vb-Conf`	□	$\mathbf{p}: 4.7e-5$ $\mathbf{g}: 2.1e-4$	△	$\mathbf{p}: 1.3e-4$ $\mathbf{g}: 3.6e-3$	▽	$\mathbf{p}: 4.3e-4$ $\mathbf{g}: 2.4e-3$	⬠	$\mathbf{p}: 4.0e-4$ $\mathbf{g}: 3.0e-3$
`VCb`	□	$\mathbf{p}: 2.3e-5$ $\mathbf{g}: 1.1e-2$	△	$\mathbf{p}: 1.1e-4$ $\mathbf{g}: 3.9e-2$	▽	$\mathbf{p}: 3.9e-4$ $\mathbf{g}: 6.0e-2$	⬠	$\mathbf{p}: 1.9e-4$ $\mathbf{g}: 1.6e-2$
`Fb-SUSHI`	■	$\mathbf{p}: 1.1e-4$ $\mathbf{g}: 1.0e-2$	▲	$\mathbf{p}: 7.4e-5$ $\mathbf{g}: 1.4e-2$	▽	$\mathbf{p}: 6.9e-4$ $\mathbf{g}: 8.3e-2$	⬟	$\mathbf{p}: 3.9e-4$ $\mathbf{g}: 2.6e-2$



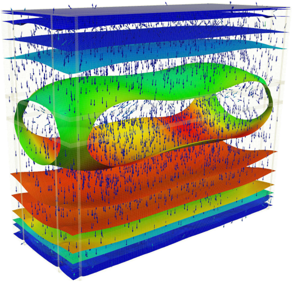


Vb-DGA	■	$\mathbf{p}: 1.3e-4$ $\mathbf{g}: 4.8e-4$	▲	$\mathbf{p}: 1.2e-4$ $\mathbf{g}: 3.5e-3$	▽	$\mathbf{p}: 4.2e-4$ $\mathbf{g}: 3.8e-3$	⬟	$\mathbf{p}: 4.2e-3$ $\mathbf{g}: 3.5e-4$	⊕	$\mathbf{p}: 3.4e-4$ $\mathbf{g}: 1.4e-2$
Vb-Conf	□	$\mathbf{p}: 4.7e-5$ $\mathbf{g}: 2.1e-4$	△	$\mathbf{p}: 1.3e-4$ $\mathbf{g}: 3.6e-3$	▽	$\mathbf{p}: 4.3e-4$ $\mathbf{g}: 2.4e-3$	⬠	$\mathbf{p}: 4.0e-4$ $\mathbf{g}: 3.0e-3$	⊕	$\mathbf{p}: 2.9e-4$ $\mathbf{g}: 1.5e-2$
VCb	□	$\mathbf{p}: 2.3e-5$ $\mathbf{g}: 1.1e-2$	△	$\mathbf{p}: 1.1e-4$ $\mathbf{g}: 3.9e-2$	▽	$\mathbf{p}: 3.9e-4$ $\mathbf{g}: 6.0e-2$	⬠	$\mathbf{p}: 1.9e-4$ $\mathbf{g}: 1.6e-2$	⊕	$\mathbf{p}: 1.6e-4$ $\mathbf{g}: 1.1e-2$
Fb-SUSHI	■	$\mathbf{p}: 1.1e-4$ $\mathbf{g}: 1.0e-2$	▲	$\mathbf{p}: 7.4e-5$ $\mathbf{g}: 1.4e-2$	▽	$\mathbf{p}: 6.9e-4$ $\mathbf{g}: 8.3e-2$	⬟	$\mathbf{p}: 3.9e-4$ $\mathbf{g}: 2.6e-2$	⊕	$\mathbf{p}: 3.1e-4$ $\mathbf{g}: 1.9e-2$



CDO groundwater flow module in *Code_Saturne*

An example of industrial applications of robust discretizations



Acknowledgment: R. Lamouroux (EDF), Y. Fournier (EDF)

The groundwater flow module in *Code_Saturne*

1. Solve the **Richards equation** to compute the hydraulic head distribution H

$$\partial_t \theta - \nabla \cdot \left(\underline{\underline{K}} \nabla H \right) = s_R$$

θ moisture content $[-]$

$\underline{\underline{K}}$ permeability tensor $[m/s]$

2. Build the **Darcy flux**: $\underline{q}_D := -\underline{\underline{K}} \nabla H$
3. Solve one or several **transport equations** to compute the distribution of a tracer concentration c:

$$\partial_t (\theta + \rho K_d) c + \nabla \cdot \left(c \underline{q}_D - \underline{\underline{D}} \nabla c \right) + \lambda (\theta + \rho K_d) c = s_T$$

where $\underline{\underline{D}} := (\alpha_t |\underline{q}_D| + d_m) \underline{\underline{Id}} + \frac{1}{|\underline{q}_D|} (\alpha_l - \alpha_t) \underline{q}_D \otimes \underline{q}_D$

ρ soil density $[kg/m^3]$

α_l, α_t dispersivity coef. $[m]$

d_m molecular diffusivity $[m^2/s]$

K_d distribution coef. $[m^3/kg]$

$h := H - \underline{g} \cdot \underline{x} / |\underline{g}|$ pressure head $[m]$

λ 1st order decay coef. $[kg.m^{-3}.s^{-1}]$

Modelling capabilities

↦ Heterogeneous and/or anisotropic permeabilities

↦ Saturated (θ is constant) or unsaturated (Van Genuchten or user-defined) soil model

CDO discretizations for the groundwater flow module

Case of **Vertex-based** schemes and a **saturated soil** modelling

1. Solve the steady linear Darcy equation

Find the hydraulic head $\mathbf{H} \in \mathcal{V}$ s.t.

$$\sum_{c \in C} \int_c \underline{\mathrm{L}}_{\mathcal{E}_c}(\mathsf{GRAD}(\mathbf{H})) \cdot \underline{\underline{K}}_c \cdot \underline{\mathrm{L}}_{\mathcal{E}_c}(\mathsf{GRAD}(\mathbf{z})) = \sum_{c \in C} \int_c s_R \cdot \mathrm{L}^0_{\mathcal{V}}(\mathbf{z}) \qquad \forall \mathbf{z} \in \mathcal{V}$$

Semi-discrete formulation: Time scheme is either Implicit Euler or Crank-Nicolson

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2. Compute Darcy quantities

$\mapsto$ $\mathbf{q}_c = -\mathrm{H}^{\mathcal{E}_c}_K \cdot \mathsf{GRAD}(\mathbf{H}) \in \mathbb{R}^{\#E_c}$ where $[\![\mathbf{a}_1, \mathrm{H}^{\mathcal{E}_c}_K(\mathbf{a}_2)]\!]_{\mathcal{E}_c} := \int_c \mathrm{L}_{\mathcal{E}_c}(\mathbf{a}_1)\cdot\underline{\underline{K}}\cdot \mathrm{L}_{\mathcal{E}_c}(\mathbf{a}_2)$

$\mapsto$ Define $\underline{\underline{D}}_c$ using the Darcy velocity in each cell: $\underline{q}_c := \frac{1}{|c|}\int_c \underline{\mathrm{L}}_{\widetilde{\mathcal{F}}_c}(\mathbf{q}_c)\in\mathbb{R}^3$

Semi-discrete formulation: Time scheme is either Implicit Euler or Crank-Nicolson

CDO discretizations for the groundwater flow module

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3. Solve the transport equation(s)

Set $R := \theta+\rho K_d$. Find the concentration $\boldsymbol{\xi}\in\mathcal{V}$ s.t.

$$\sum_{c\in C}\int_c \underbrace{d_t\mathrm{L}^0_{\mathcal{V}_c}(\boldsymbol{\xi})\cdot R\cdot\mathrm{L}^0_{\mathcal{V}_c}(\mathbf{z})}_{unsteady} + \underbrace{\underline{\mathrm{L}}_{\mathcal{E}_c}(\mathrm{GRAD}(\boldsymbol{\xi}))\cdot\underline{\underline{D}}_c\cdot\underline{\mathrm{L}}_{\mathcal{E}_c}(\mathrm{GRAD}(\mathbf{z}))}_{diffusion}$$

$$+\underbrace{\mathrm{T}_{\mathbf{q}_c}(\mathrm{GRAD}(\boldsymbol{\xi}))\cdot\mathrm{L}_{\mathcal{V}_c}(\mathbf{z})}_{\text{advection}} + \underbrace{\mathrm{L}^0_{\mathcal{V}_c}(\boldsymbol{\xi})\cdot\lambda R\cdot\mathrm{L}^0_{\mathcal{V}_c}(\mathbf{z})}_{reaction} = \sum_{c\in C}\int_c s_R\cdot\mathrm{L}^0_{\mathcal{V}}(\mathbf{z}) \qquad \forall\mathbf{z}\in\mathcal{V}$$

$\mathrm{T}_{\mathbf{q}_c}$ is the convection operator (upwind, Peclet-weighted, centered. . .)

Semi-discrete formulation: Time scheme is either Implicit Euler or Crank-Nicolson

Context

↦ Design and safety studies related to nuclear waste storage facilities

- ANDRA (National Agency for the Management of Radioactive Wastes) is in charge of this subject
- ASN (Nuclear Safety Agency) is the authority in charge of the control
- EDF as a major contributor wants to have its own expertise on this subject

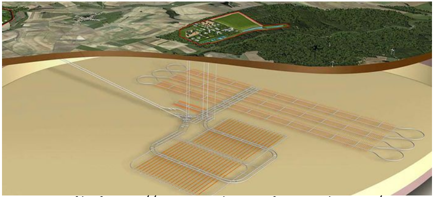
CIGEO: The nuclear waste storage facility

↦ Management of the **High-Activity** Long-Life (HALL) wastes

- 0.2% of all radioactive wastes but 94% of the radioactivity
- Up to $10,000m^3$ of storage for HALL

↦ Management of the **Medium-Activity** Long-Life (MALL) wastes

- 3% of all radioactive wastes but 6% of the radioactivity
- Up to $75,000m^3$ of storage for MALL



`credit:https://www.connaissancedesenergies.org/`

↦ Storage depth: $500m$

↦ Storage area: $15km^2$

↦ More than 100 years of operating life

↦ Estimated cost: 25B euros

Reference: ANDRA (https://www.andra.fr)

A challenging long-term safety study for CIGEO

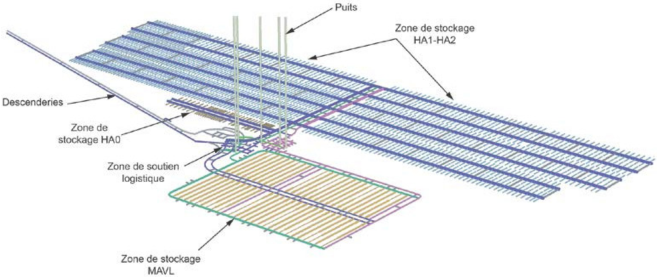
Key figures

↦ **Large geometry with many small objects**:
  - Dimensions in Km: $\sim 3 \times 5 \times 0.5$
  - Catch geometric details ($\sim 0.1m$) around storage cells
  - ~ 1500 **storage cells**

↦ Long-term study: **Evolution over 1M years**

↦ Several scenarii to analyze

Aims: Study the validity of the design of the storage facilty by estimating the quantity of RNs released in the biosphere



Credits: ANDRA

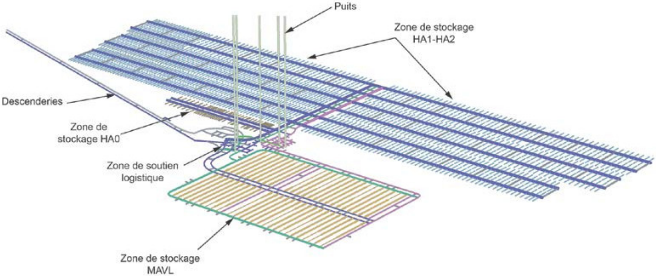
A challenging long-term safety study for CIGEO

Key figures

- ↦ **Large geometry with many small objects**:
  - Dimensions in Km: $\sim 3 \times 5 \times 0.5$
  - Catch geometric details ($\sim 0.1m$) around storage cells
  - ~ 1500 **storage cells**
- ↦ Long-term study: **Evolution over 1M years**
- ↦ Several scenarii to analyze

- Up to 1B mesh cells
- Adaptative time stepping strategy

Aims: Study the validity of the design of the storage facilty by estimating the quantity of RNs released in the biosphere

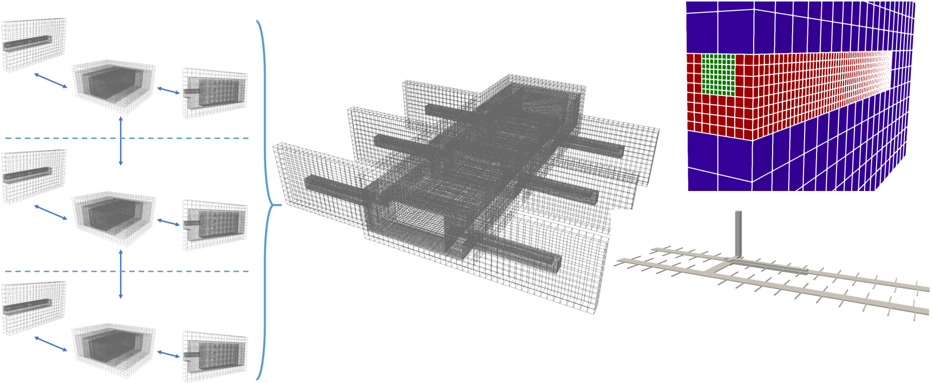


Credits: ANDRA

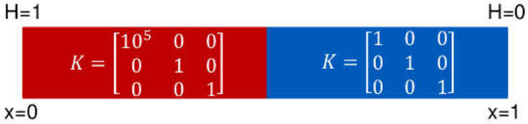
1 Billion mesh cells built on-the-fly in less than 10mn

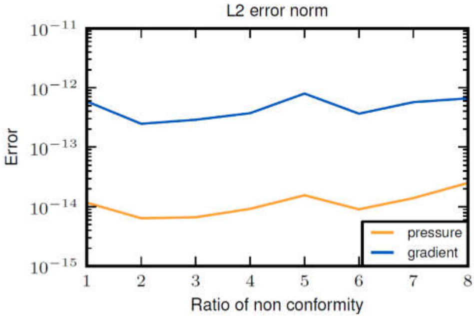
Mesh building strategy

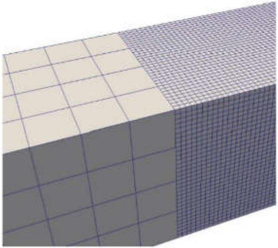
- ↦ Strictly speaking not the CIGEO geometry but the same level of complexity
- ↦ Use the **parallel joining algorithm** of *Code_Saturne* to assemble the final geometry from a small set of elementary meshes after duplication and translation
  - Take advantage of the redundancy of the geometry: storage cells and galleries



Verification testcase

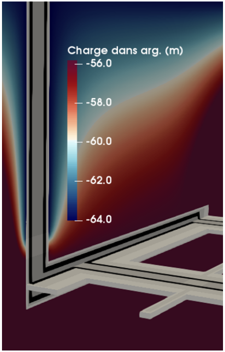


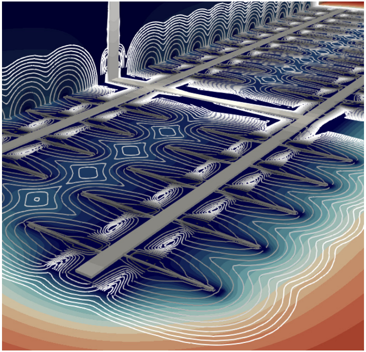




- Strong heterogeneity (10^5 ratio)
- Polyhedral cells: up to 1:64 cell–cell visibility
- Check the consistency on a linear solution

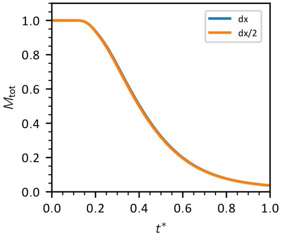
Study of the migration of radionuclides (RNs)

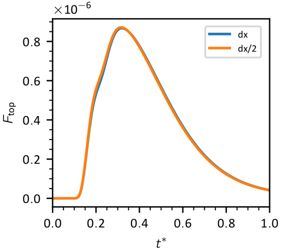




Slices in the 500M mesh

- ↦ `Left`: Hydraulic head distribution in the clay
- ↦ `Right`: RN concentration near the galleries





Influence of the **mesh refinement** on the quantities of interest

- ↦ `Left`: Adimensional total quantity of RN
- ↦ `Right`: Outflow flux of RN

Performances

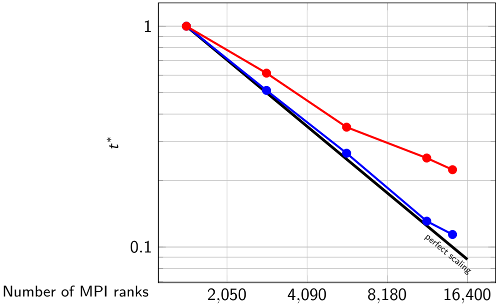
Massively parallel simulation on EDF cluster (GAIA)

- Building a **1B DoFs system takes less than 1s** per iteration (11520 cores)

Case: 3200 iterations on the 500M cell mesh

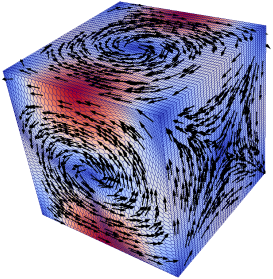
↦ Simulation time is **less than 6 hours** with 11520 cores (MPI)

- 5% of the time dedicated to build linearsystems
- 85% of the time dedicated to solve linear systems:
  - CG + BoomerAMG multigrid solver from the Hypre library for solving the hydraulic head
  - GMRES + Jacobi for solving the radionuclide concentration



Strong scaling of the most time consuming steps.

Stokes equations with CDO Face-based schemes



Joint work with A. Ern & R. Milani (PhD)

CDO-Fb schemes for Stokes

Find $(\underline{u}, p) \in H^1_0(\Omega)^3 \times L^2_0(\Omega)$ (zero-mean value) s.t.

$$\begin{cases} -\underline{\Delta}\, \underline{u} + \underline{\text{grad}}\, p &= \underline{f} & \text{in } \Omega \\ \text{div}\, \underline{u} &= 0 & \text{in } \Omega \\ \underline{u} &= \underline{u}_{\partial\Omega} & \text{on } \partial\Omega \end{cases}$$

↦ Two keys operators:

- The gradient reconstruction operators for the velocity for the term $-\underline{\Delta}\, \underline{u}$
- The divergence operator $\text{div}\, \underline{u}$ (adjoint to $\underline{\text{grad}}\, p$)

↦ Velocity space $\widehat{\underline{\mathcal{U}}}$: **hybrid space with DoFs at faces and cells**

- One DoF per each component at faces and cells defined as mean-values
- $\mathsf{R}_{\widehat{\underline{\mathcal{U}}}}(\underline{u}) := (\{\pi_{\mathrm{f}}(\underline{u})\}_{\mathrm{f}\in\mathrm{F}}, \{\pi_{\mathrm{c}}(\underline{u})\}_{\mathrm{c}\in\mathrm{C}})$
- Cell DoFs can be eliminated using static condensation

↦ Pressure space $\mathcal{P}$: **DoF at cells**

- Defined as the mean-cell value
- $\mathsf{R}_{\mathcal{P}}(p) := \{\pi_{\mathrm{c}}(p)\}_{\mathrm{c}\in\mathrm{C}}$

where $\pi_{\mathrm{f}}(q) := \frac{1}{|\mathrm{f}|}\int_{\mathrm{f}} q$ for $\mathrm{f} \in \mathrm{F}$ and $\pi_{\mathrm{c}}(q) := \frac{1}{|\mathrm{c}|}\int_{\mathrm{c}} q$ for $\mathrm{c} \in \mathrm{C}$

Two key operators

1. Cellwise **velocity gradient reconstruction** operator: $\underline{\underline{\mathrm{G}}}_{\mathrm{c}}$

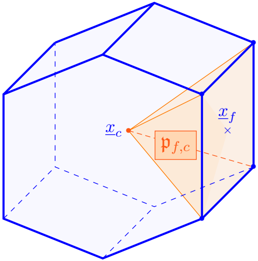
$\mapsto$ Piecewise constant tensor in each pyramid $\{\mathfrak{p}_{f,c}\}_{f \in F_c} := \mathfrak{P}_{F,c}$

- $\underline{\underline{\mathrm{G}}}_{\mathrm{c}} : \widehat{\underline{\mathcal{U}}}_{\mathrm{c}} \to \mathbb{P}_0(\mathfrak{P}_{F,c})^{dxd}$
- $\underline{\underline{\mathrm{G}}}_{\mathrm{c}}(\hat{\mathbf{\underline{u}}}) := \bar{\underline{\underline{\mathrm{G}}}}_{\mathrm{c}}(\hat{\mathbf{\underline{u}}}) + \beta \dfrac{|f|}{|\mathfrak{p}_{f,c}|} \Big((\mathbf{\underline{u}}_f - \mathbf{\underline{u}}_c) - \bar{\underline{\underline{\mathrm{G}}}}_{\mathrm{c}}(\hat{\mathbf{\underline{u}}})(\underline{x}_f - \underline{x}_c) \Big) \otimes \underline{\nu}_{f,c}$
- Consistency part: $\bar{\underline{\underline{\mathrm{G}}}}_{\mathrm{c}}(\hat{\mathbf{\underline{u}}}) := \dfrac{1}{|c|} \sum_{f \in F_c} |f| (\mathbf{\underline{u}}_f - \mathbf{\underline{u}}_c) \otimes \underline{\nu}_{f,c}$

2. Cellwise **divergence** operator: D_{c}

$\mapsto$ Piecewise constant in each cell

- $\mathrm{D}_{\mathrm{c}} : \widehat{\underline{\mathcal{U}}}_{\mathrm{c}} \to \mathcal{P}_{\mathrm{c}} \equiv \mathbb{P}_0(c)$
- $\mathrm{D}_{\mathrm{c}}(\hat{\mathbf{\underline{u}}}) := \mathrm{tr}(\bar{\underline{\underline{\mathrm{G}}}}_{\mathrm{c}}(\hat{\mathbf{\underline{u}}})) = \dfrac{1}{|c|} \sum_{f \in F_c} |f| (\mathbf{\underline{u}}_f - \mathbf{\underline{u}}_c) \cdot \underline{\nu}_{f,c}$



Discrete formulation of the Stokes equations

Find $(\underline{\hat{\mathbf{u}}}, \mathbf{p}) \in \underline{\widehat{\mathcal{U}}} \times \mathcal{P}$ s.t.

$$\begin{aligned}
\sum_{\mathrm{c}\in\mathrm{C}} \int_{\mathrm{c}} \underline{\underline{\mathsf{G}}}_{\mathrm{c}}(\underline{\hat{\mathbf{u}}}) : \underline{\underline{\mathsf{G}}}_{\mathrm{c}}(\underline{\hat{\mathbf{w}}}) - \int_{\mathrm{c}} \mathbf{p}_{\mathrm{c}} \mathsf{D}_{\mathrm{c}}(\underline{\hat{\mathbf{w}}}) &= \sum_{\mathrm{c}\in\mathrm{C}} \int_{\mathrm{c}} \underline{f} \cdot \underline{\hat{\mathbf{w}}}_{\mathrm{c}}, && \forall \underline{\hat{\mathbf{w}}} \in \underline{\widehat{\mathcal{U}}} \\
\sum_{\mathrm{c}\in\mathrm{C}} \int_{\mathrm{c}} \mathbf{q}_{\mathrm{c}} \mathsf{D}_{\mathrm{c}}(\underline{\hat{\mathbf{u}}}) &= 0, && \forall \mathbf{q} \in \mathcal{P}
\end{aligned}$$

↦ Very close to HHO ($k = 0$) schemes

- Only the stabilization of the gradient reconstruction for the velocity differs

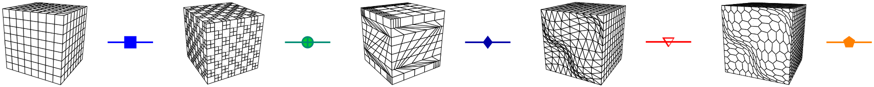
↦ Convergence analysis performed in Di Pietro et al. *'16* with $k = 0$ holds

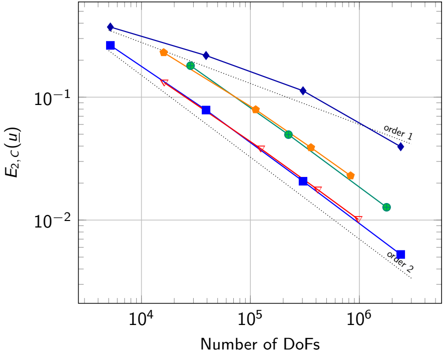
- **Inf-sup stable** discretization
- Order of convergence for the velocity: **2 in L^2 norm**
- Order of convergence for the pressure: **1 in L^2 norm**

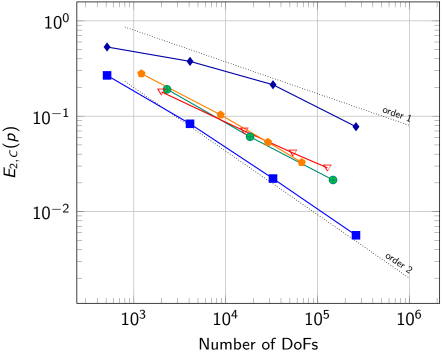
↦ Discrete velocity field is **cellwise divergence free**

Testcase: Steady Taylor-Green vortices

$$\underline{u} := \begin{pmatrix} -2c_x.s_y.s_z \\ s_x.c_y.s_z \\ s_x.s_y.c_z \end{pmatrix},\ p := -6\pi s_x.s_y.s_z \text{ with } c_* := \cos(2\pi *) \text{ and } s_* := \sin(2\pi *)$$







$E_{2,C}(\underline{u}) := \frac{|||\pi_C(\underline{u}) - \hat{\underline{\mathbf{u}}}|||_C}{|||\pi_C(\underline{u})|||_C}$ and $E_{2,C}(p) := \frac{|||\pi_C(p) - \mathbf{p}|||_C}{|||\pi_C(p)|||_C}$ where $|||\cdot|||_C^2 := \sum_{c\in C} |c||\cdot|^2$

Ongoing works & Perspectives

CDO Face-based schemes for the incompressible Navier–Stokes equations

Milani's PhD

Coming soon (implemented but need more tests)

- ↦ Coupling the velocity field arising from the Stokes/Navier–Stokes equations with the transport of tracers
- ↦ Alternatives to the monolithic (saddle-point) approach for the velocity/pressure coupling
  - Augmented-Lagrangian Uzawa algorithm
  - Artifical compressibility algorithm with the possibility to get higher-order time steppings

To be done

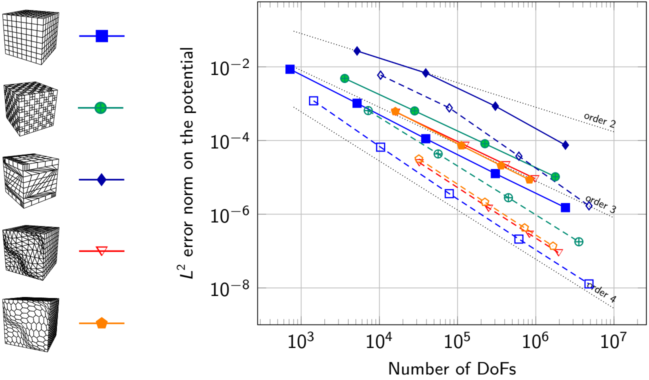
- ↦ Improve the convection scheme in Navier–Stokes to get a better kinetic energy balance
- ↦ Improvement: Pressure-robust discretization of the momentum RHS (cf. Di Pietro et al. *'16*)

HHO schemes in *Code_Saturne*

High-order schemes to get better accuracy on coarse meshes

↦ HHO(k=1 & k=2) schemes are available in *Code_Saturne* (parallel MPI+OpenMP)

- for scalar-valued diffusion problem (Milani's internship)
- for vector-valued diffusion problem (AMIES project with Montpellier U. – D. Castenon & D. Di Pietro)



↦ **Work in progress**: Stokes equations (to be integrated) and scalar-valued advection (internship): AMIES project with Montpellier U. – D. Castenon & D. Di Pietro

HHO schemes in **code_aster**

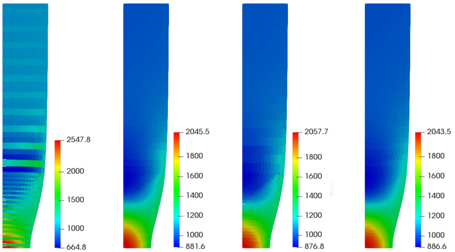
M. Abbas (EDF), A. Ern (Paris-Est U.) & N. Pignet's PhD (EDF)

↦ Applications:

- Hyper-elasticity
- Finite elastoplastic deformations with logarithmic strain

↦ WIP: Integration in **code_aster**

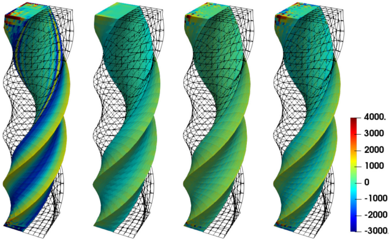
Necking of a 2D rectangular bar



(g) Q2 (h) UPG (i) HHO(1 ;1) (j) HHO(2 ;2)

Trace of the Cauchy stress tensor $\underline{\underline{\sigma}}$ (in MPa) at the quadrature points on the final configuration

Torsion of a square section bar



(a) Q2 (b) UPG (c) HHO(1 ;2) (d) HHO(2 ;3)

Trace of the Cauchy stress tensor $\underline{\underline{\sigma}}$ (in MPa) at the quadrature points for a rotation of 2π

↦ HHO supports large deformations

↦ No volumetric locking for HHO (primal formulation) and UPG (mixed formulation)

Perspectives

1. **CDO-ALE** (Arbitrary Lagrangian Eulerian) approach for free-surface flows
    - Joint work with C. Demay (EDF), J. Dorsz (EDF internship) and M. Ferrand (EDF)
2. **Magneto-Hydrodynamics** for ferro-fluids in transformers
    - Joint work with O. Moreau (EDF)
3. $H(div)$-**conforming reconstruction** on polyhedral meshes.
    - Joint work with H. Cheng (Monash U.) and J. Droniou (Monash U.)
4. **ANR project FAST4HHO**: solve efficiently linear system arising from robust polyhedral discretizations.
    - Joint work with CERFACS, EDF, Montpellier U. and IRIT
    - D. Di Pietro (Montpellier U.), Y. Fournier (EDF), F. Hülsemann (EDF), C. Kruse (CERFACS), P. Matalon (Montpellier U.), P. Mycek (CERFACS), U. Ruede (CERFACS), D. Ruiz (IRIT Toulouse) and F. Vilar (Montpellier U.)
    - **Next talk !**

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    - **Next talk !**

All CDO & HHO developments are freely available. Download and test it !

Code_Saturne website: `https://www.code-saturne.org`

Published works related to CDO schemes

Articles

- Analysis of Compatible Discrete Operator schemes for elliptic problems on polyhedral meshes, *Bonelle & Ern* (M2AN), 2013
- Analysis of Compatible Discrete Operator Schemes for the Stokes Equations on Polyhedral Meshes, *Bonelle & Ern* (IMA JNA), 2014
- Low-order reconstruction operators on polyhedral meshes: Application to Compatible Discrete Operator schemes, *Bonelle, Di Pietro & Ern* (CAGD), 2015
- Vertex-based Compatible Discrete Operator schemes on polyhedral meshes for advection-diffusion equations, *Cantin & Ern* (CMAM), 2016
- A vertex-based scheme on polyhedral meshes for advection–reaction equations with sub-mesh stabilization, *Cantin, Bonelle, Burman & Ern*(CaMwA), 2016
- An edge-based scheme on polyhedral meshes for vector advection-reaction equations, *Cantin & Ern*, (M2AN), 2017
- New polyhedral discretisation methods applied to the Richards equation: CDO schemes in *Code_Saturne*, *Bonelle, Fournier & Moulinec*, (CaF), 2018

Phd thesis

- Compatible Discrete Operator schemes on polyhedral meshes for elliptic and Stokes equations, *Bonelle's PhD*, 2014
- Approximation of scalar and vector transport problems on polyhedral meshes, *Cantin's PhD*, 2016

Thank you for your attention!