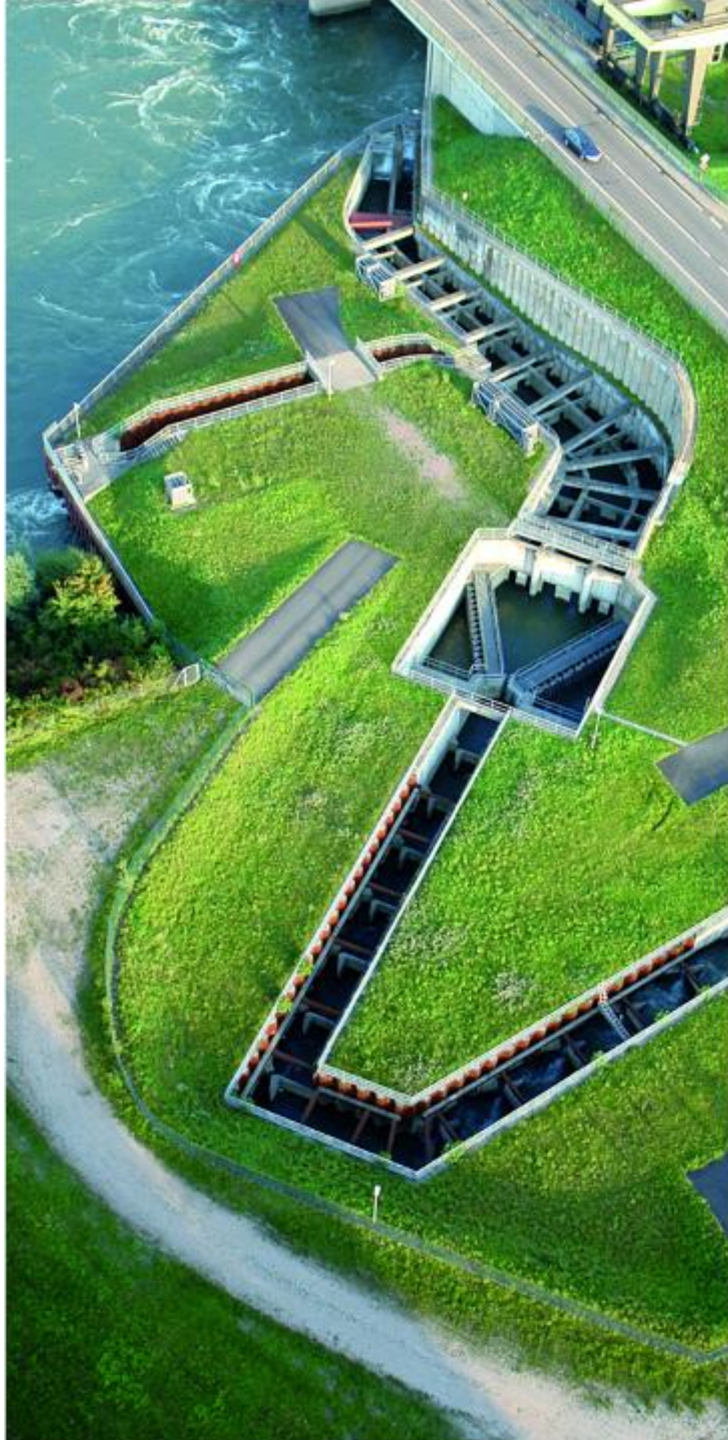
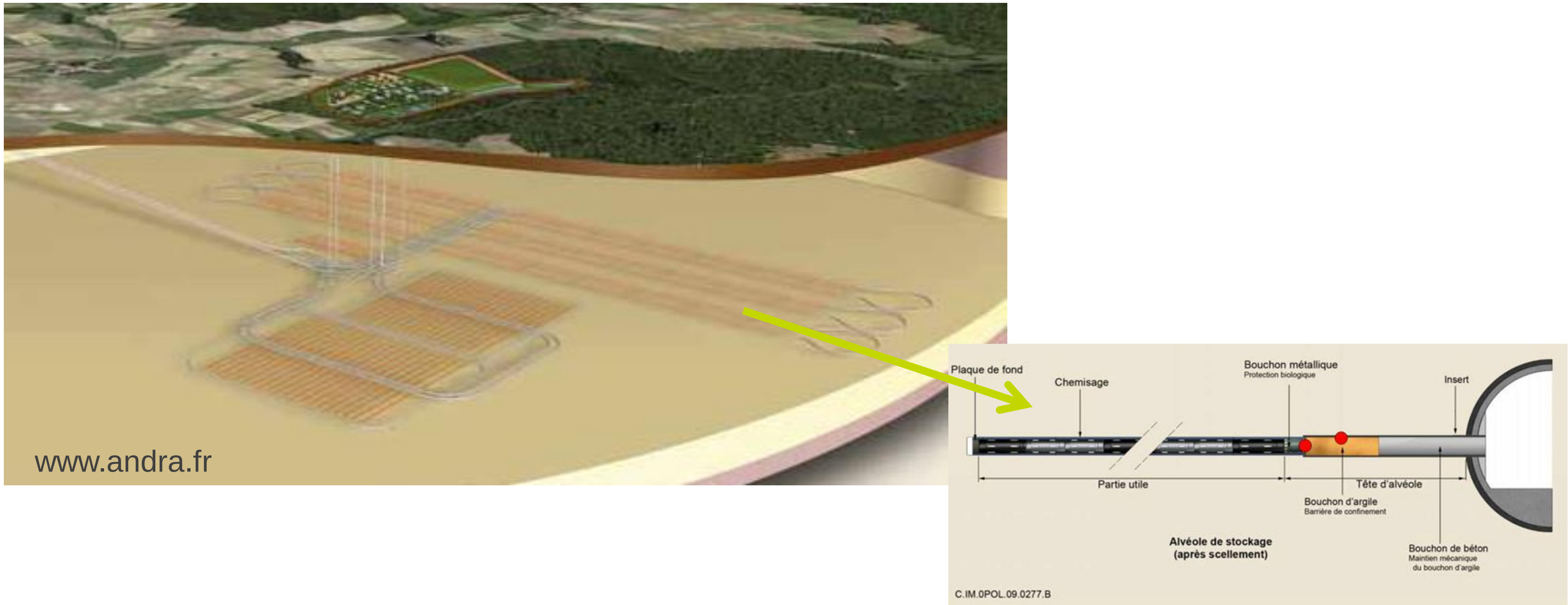
First results with Compatible Discrete Operator for nuclear waste storage applications

Vincent Stobiac EDF R&D – LNHE
Jérôme Bonelle EDF R&D – MFEE



PURPOSE OF THE STORAGE : LONG TERM SAFETY

- **The flow of radionuclides reaching the biosphere should be as low as reasonably achievable**

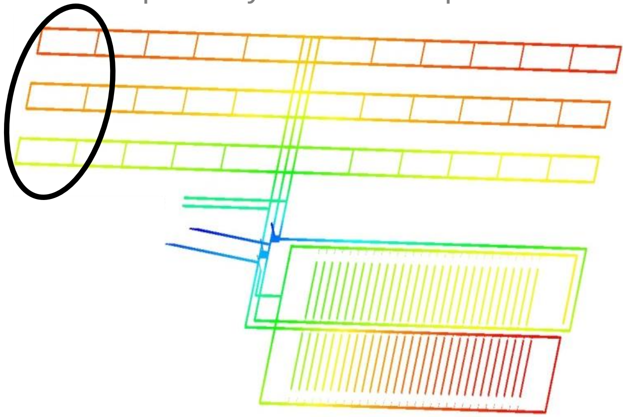


- **Two possible pathways:**
  - Migration through artificial tunnels (convection due to higher permeabilities);
  - Migration through natural clay (diffusion).

PREVIOUS STUDY : IMPACT OF DENSIFIED STORAGE

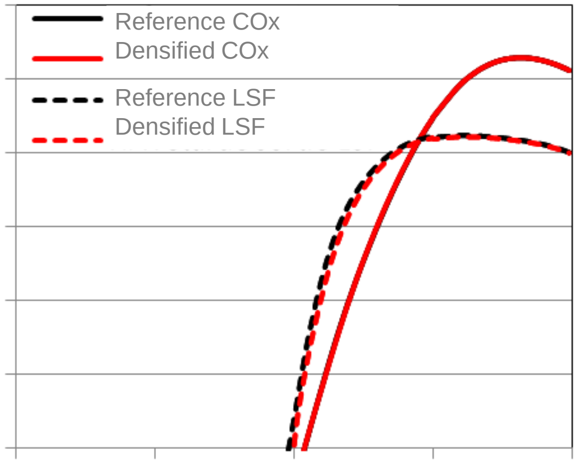
- **Densification of one section of the storage:**
  - Meshes of 350 millions of tetrahedra generated in 24h (big memory node of cluster);
  - Computation done in 22h on 768 cores.

Example of hydraulic head profile



$$\nabla(K.\nabla H) = 0 \quad \Longrightarrow \quad q = -K.\nabla H$$

Diffusive and convective exit fluxes

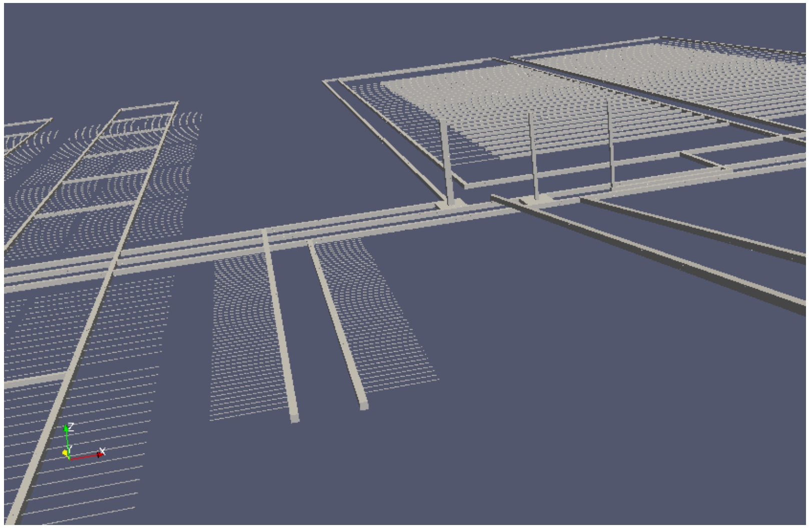


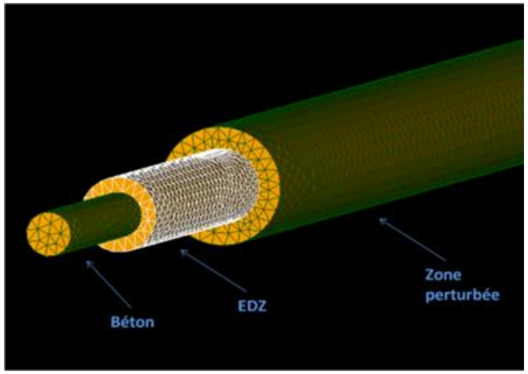
$$\frac{\partial(\theta c)}{\partial t} = \nabla.(D.\nabla c) - \nabla.(qc)$$

- **Anisotropic and heterogeneous problem difficult to solve:**
  - Methodology reaches tetrahedral meshing limits;
  - Anisotropy and heterogeneity cannot be treated simultaneously in *Code_Saturne*.

REQUIRED IMPROVEMENTS

- **Non-conforming hexahedral meshing approach:**
  - Geometry too complex for conforming hexahedral mesh;
  - Non-conformity will reduce the number of elements.

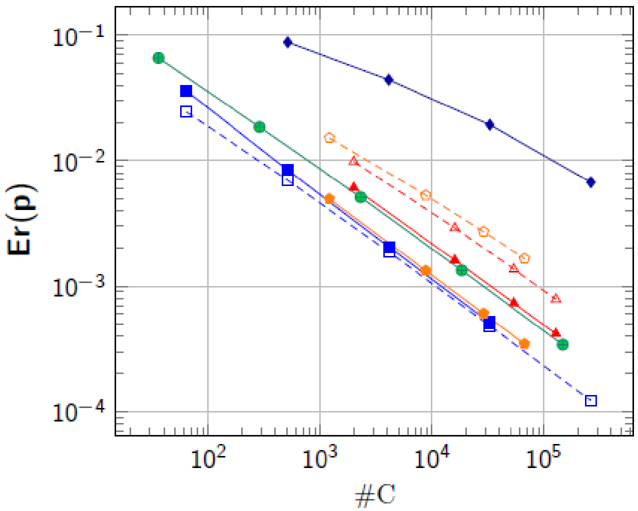


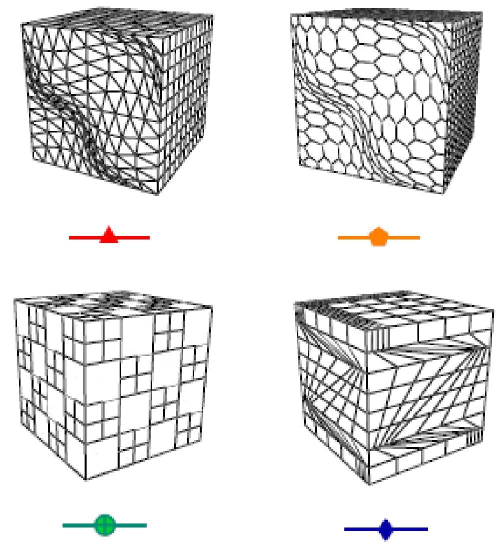


- **A robust method for heterogeneous anisotropic problem:**
  - High permeability ratio (up to 10^7) and low dispersion ratio (lower than 10);
  - Should manage non-conforming mesh.

NEW COMPATIBLE DISCRETE OPERATOR SCHEMES

- **Effective method on polyhedral meshes for advection-diffusion equations:**





- Integration of the CDO method in *Code_Saturne*:
  - Done by Jérôme BONELLE and Pierre CANTIN (see also poster).

- Background : broad class of compatible, mimetic or structure-preserving schemes
  - Roots: Tonti (1974), Bossavit (1988) (E&M)
  - Related works: VEM (Virtual Element Method), DEC (Discrete Exterior Calculus)

- State of the art method for anisotropic and heterogeneous problems
  - Well understood theoretical basis.

CDO : DISCRETIZATION PROCESS

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

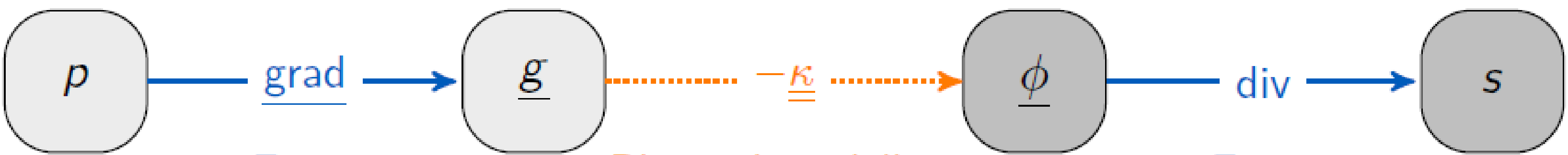
Topological laws $\begin{cases} \underline{g} = \underline{\operatorname{grad}}(p) \\ \operatorname{div}(\underline{\phi}) = s \end{cases}$

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

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

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

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



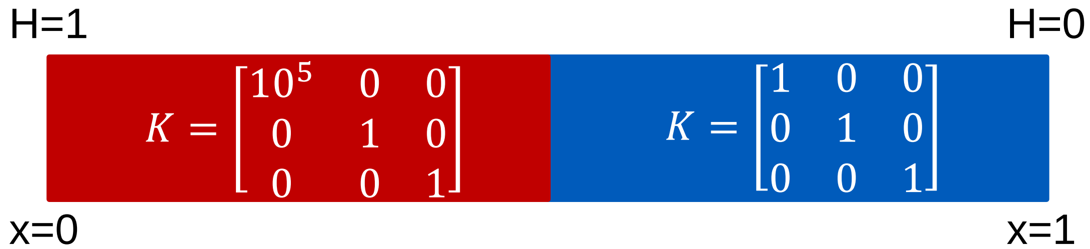
Exact — Physical modelling — Exact

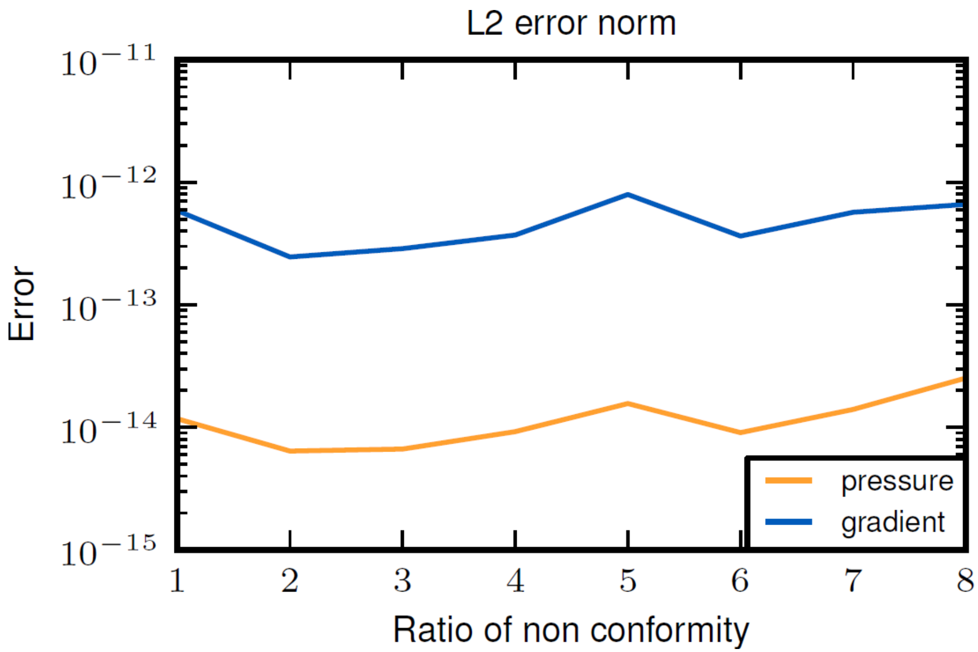
Potential evaluated at a point	Gradient evaluated along a line	Flux evaluated across a surface	Density evaluated in a volume

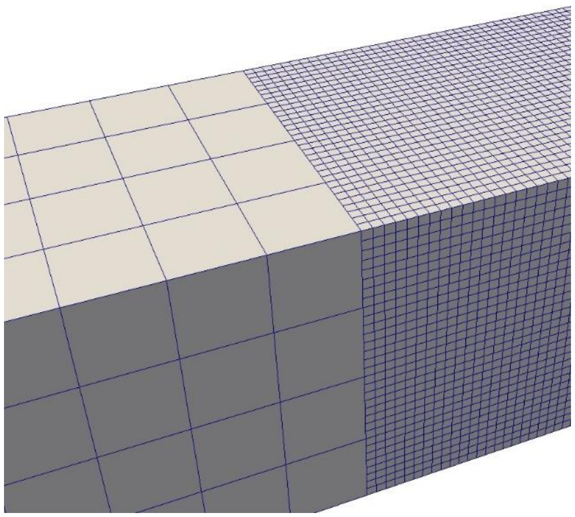
- **Three families of CDO schemes depending on where potential DoFs are located:**
  - Vertex, cell or face-based schemes

PERMEABILITY GRADIENT TEST CASE

- **Saturated and steady 1D flow throughout anisotropic soils:**
  - Non-conformity of the mesh at the interface.

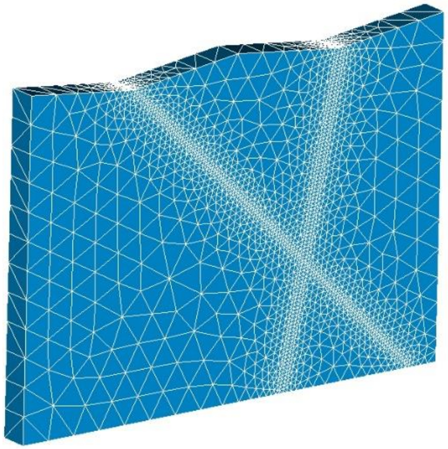


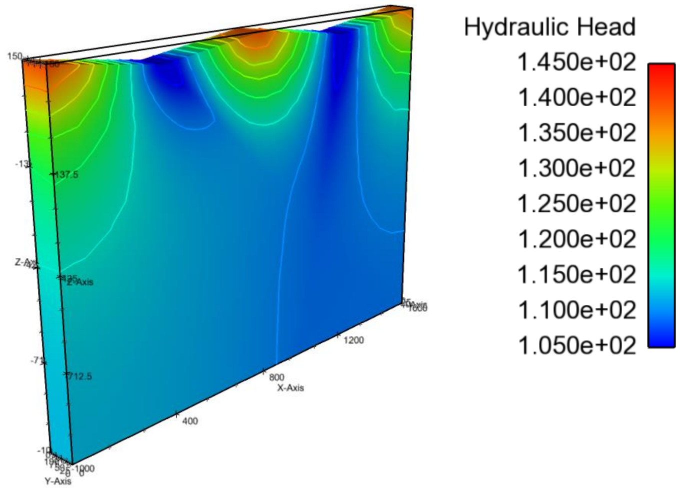


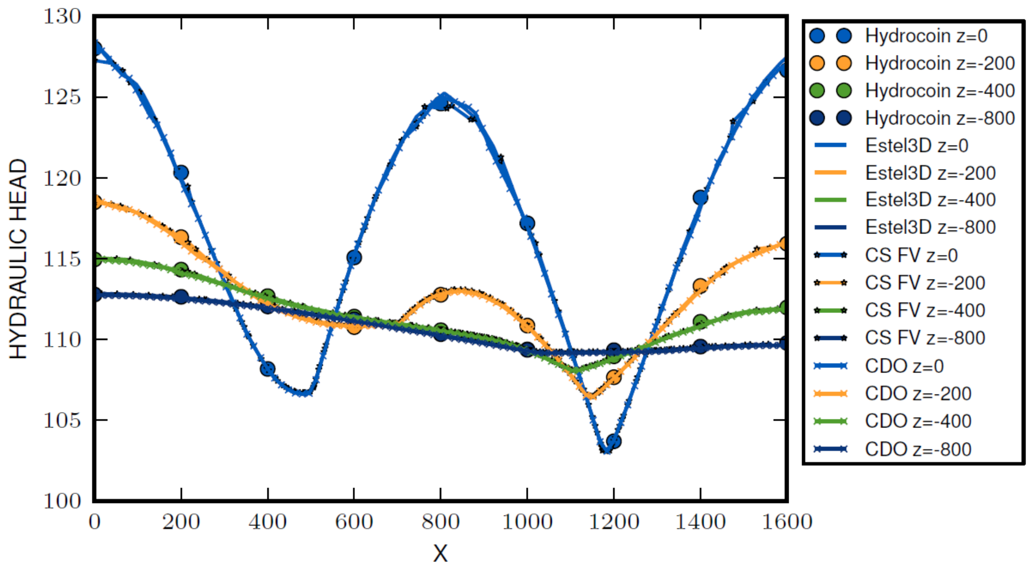


HYDROCOIN TEST CASE

- **Fully saturated domain with two fractures (permeability ratio of 100):**

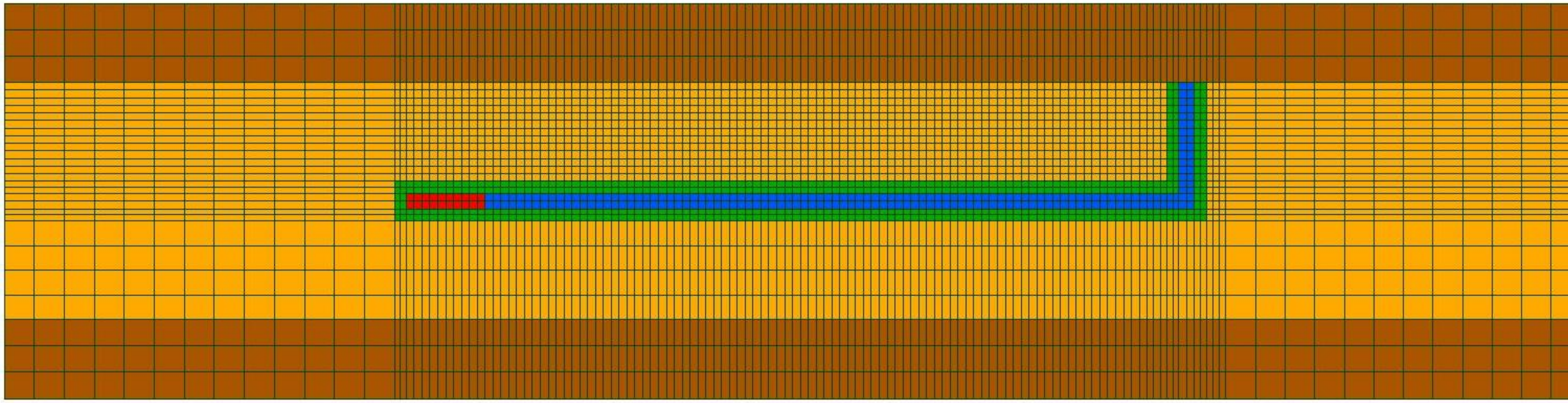




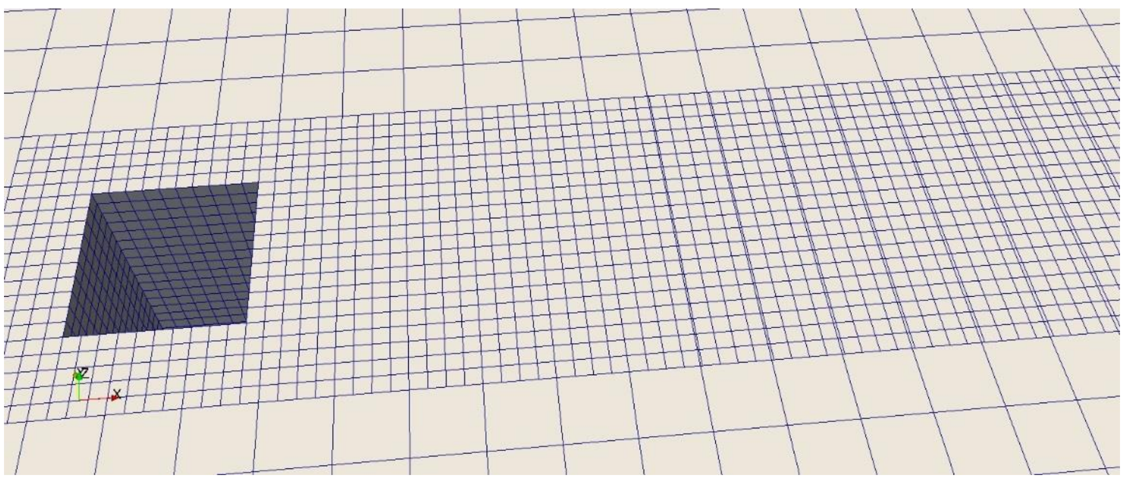


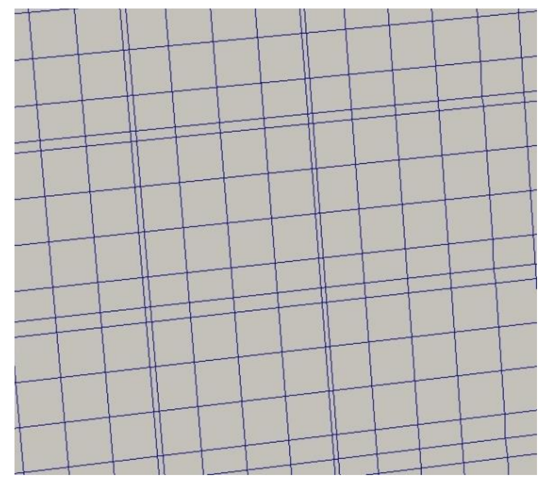
STORAGE TEST CASE WITH SIMPLIFIED GEOMETRY

- **Isotropic permeabilities to compare with *Code_Saturne*.**



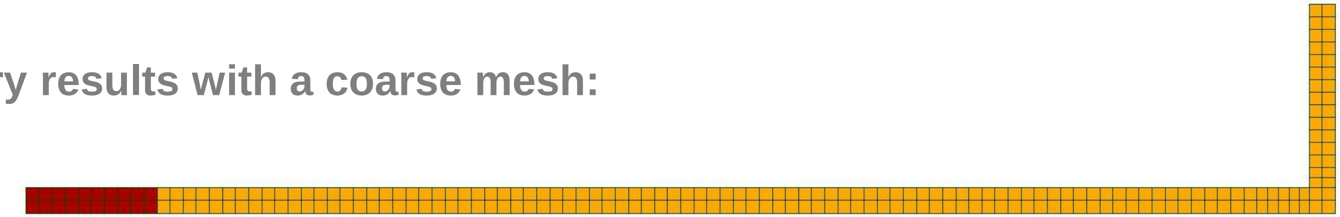
- **Both conforming and non-conforming hexahedral meshes are tested:**

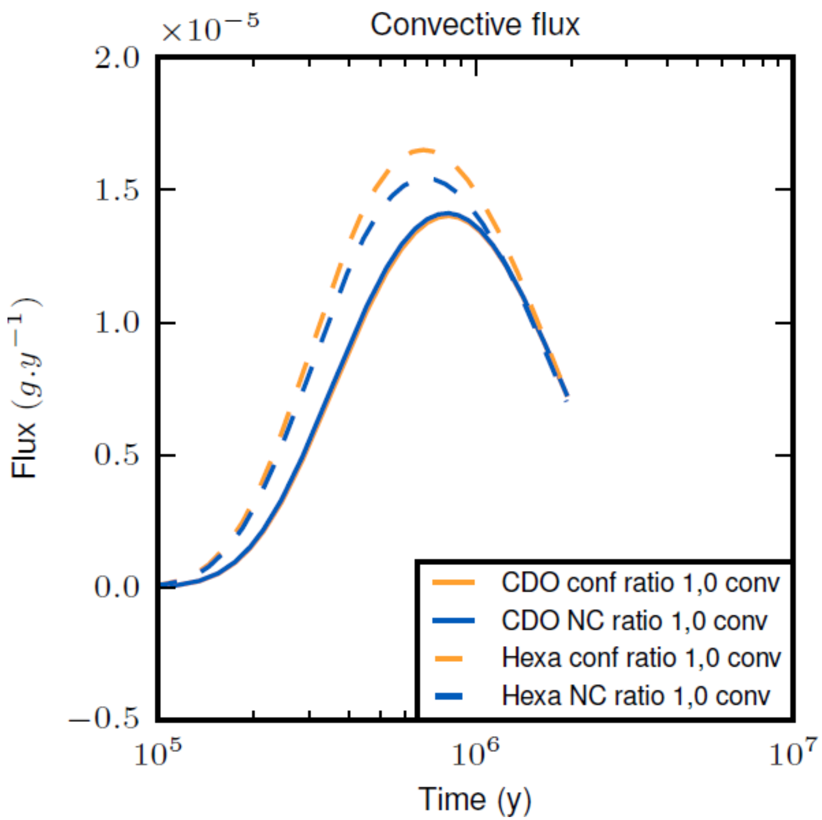


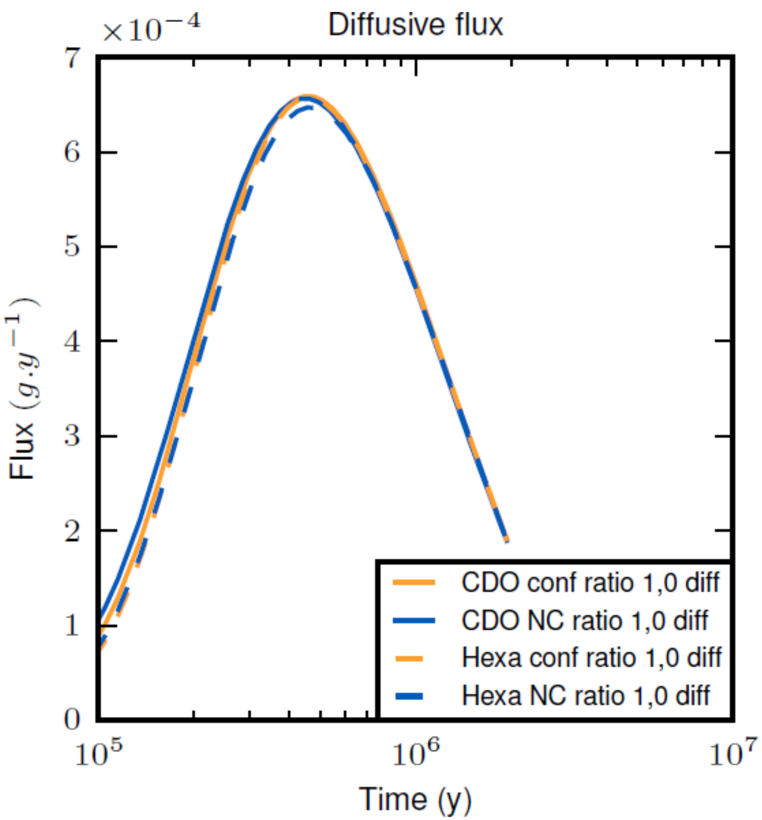


STORAGE TEST CASE WITH SIMPLIFIED GEOMETRY

- **Preliminary results with a coarse mesh:**

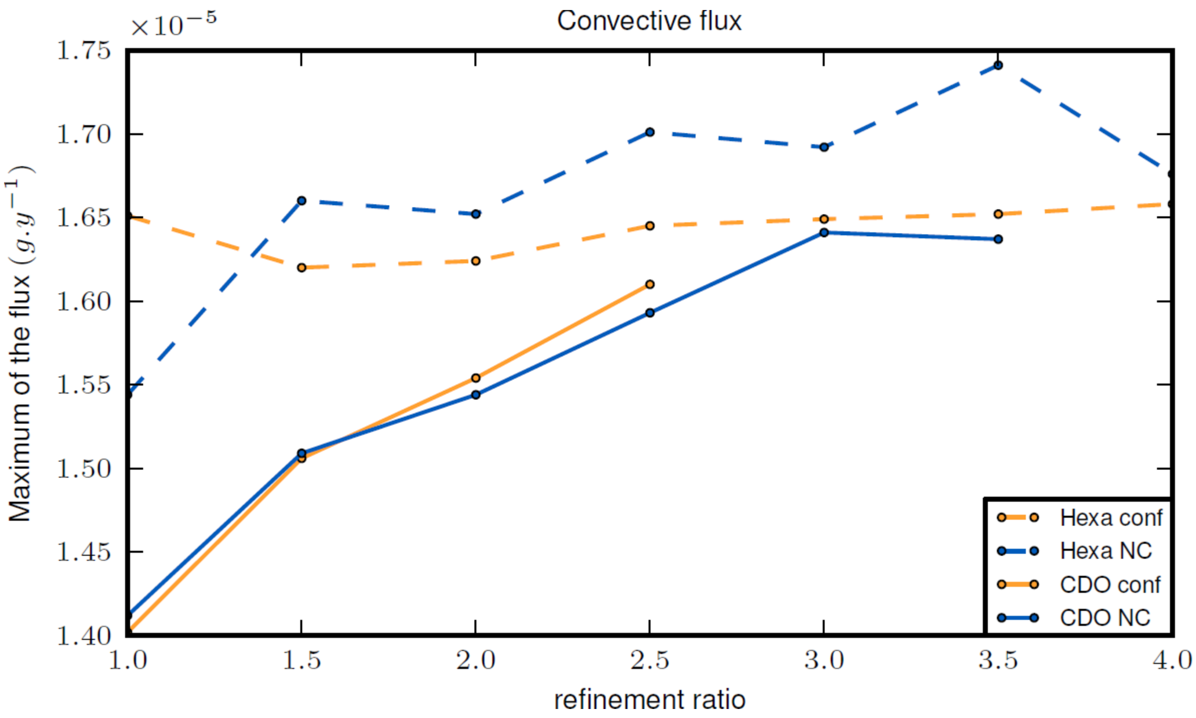






STORAGE TEST CASE WITH SIMPLIFIED GEOMETRY

- **Impact of the mesh size:**



- **Total number of elements:**
  - Conforming hexahedral mesh: from 140 000 to 6,9 millions.
  - Non-conforming hexahedral mesh: from 45 000 to 2,2 millions.

CONCLUSIONS

- **Encouraging results with CDO on hydrogeological flows:**
  - Able to handle high heterogeneity and anisotropy;
  - Robust to non-conforming mesh.

- **Work in progress:**
  - Comparison of initialization strategies;
  - Quantification of maximal non-conformity.

- **Next steps:**
  - MPI parallel computing in CDO;
  - Performance tests on large meshes (up to the complete repository architecture);
  - Extension to other flows…