A posteriori error estimates and mesh adaptation for porous media

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Workshop

« *A posteriori* error estimates and mesh adaptivity
for evolutionary and nonlinear problems »

Outline

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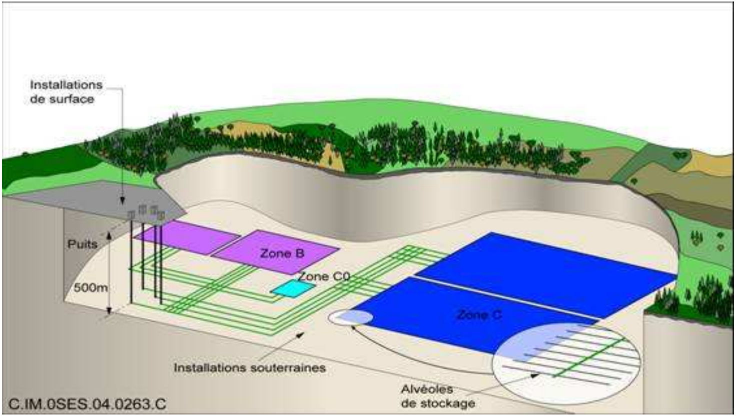
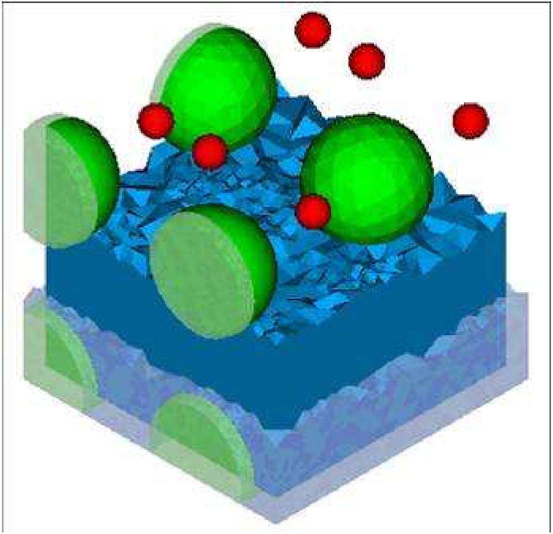
The need for adaptivity at CEA-DM2S/SFME/LSET

- Application domains :



geological porous media (waste disposal)



« technological » porous media (concrete or polymer deterioration)

The need for adaptivity at CEA-DM2S/SFME/LSET

- Physical models :
  - hydraulics (diffusive and convective transport)
  - non–linear multi-phase diffusive transport
  - non–linear diffusive and reactive transport (with tough kinetic terms)
- Major concerns :
  - evaluating and controlling the numerical error (safety studies)
  - optimizing CPU time/mesh size/accuracy trade–offs
  - tracking fronts (saturation, precipitation)

The need for adaptivity at CEA-DM2S/SFME/LSET

- Methodology :
  - unstructured meshes (complex geometric models, geological layers, heterogeneous models at the microscopic scale)
  - finite–volume methods
  - massively parallel simulations with load balancing
  - last but not least : *a posteriori* error estimation fitted to the physical model and the numerical scheme
- Implementation :
  - Experimental code (DDFV scheme, mainly linear diffusion models)
  - Shared tools implemented in Trio–U's numerical kernel (geometric adaptation, load balancing)
  - Dedicated tools implemented in application codes (FV schemes, error estimation, non–conformity compliance, ...)

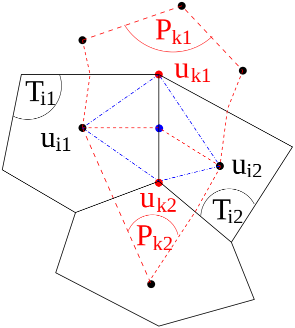
Outline

1. Introduction : The need for adaptivity at CEA-DM2S/SFME/LSET
2. A posteriori error estimation for the DDFV scheme
3. AMR implementation details
4. Conclusion : Ongoing works

A posteriori error estimation for the DDFV scheme

The Discrete Duality Finite Volume (DDFV) scheme has been designed to solve anisotropic heterogeneous diffusion equations on arbitrary meshes. Hermeline JCP 2003, Domelevo Omnes M2AN 2005, $\cdots$

The unknowns of the scheme are located at the center and at the vertices of the mesh. The diffusion equation is integrated on primal and dual cells.



$$-\int_C \nabla \cdot K\nabla u = -\int_{\partial C} (K\nabla u)\cdot n = \int_C f$$

To evaluate the fluxes, one uses the natural "four points" gradient formula on the diamond cells.
Equivalent discrete variational formulation

$$\sum_j \int_{D_j} (K\nabla u)_j \cdot \nabla v_j = \int_\Omega f v^*$$

Symmetric scheme - Numerical analysis easy and general

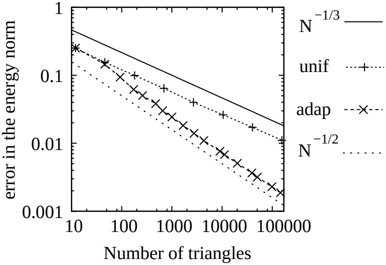
A posteriori error estimation for the DDFV scheme

Omnes, Penel and Rosenbaum, SIAM J. Numer. Anal. 2009
Tools used for the estimation :

- Equivalence with a nonconforming FE scheme with $P1$ basis functions on the diamonds ; continuity only at the midpoints of the diamond edges ;
- continuous Hodge decomposition of the error broken gradient ;
- the conforming part is treated classicaly FE tools and involves normal jumps of the computed gradients through diamond edges ;
- the non-conforming part is evaluated thanks to the discrete orthogonality of discrete gradient and curls and involves tangential jumps of the gradient through diamond edges ;
- there are terms coming from both primal and dual cells ;
- Poincaré-type and trace inequalities in star-shaped non-convex polygonals with explicit expressions of the constants (Carstensen and Funken, East-West J. Numer. Math. 2000 ; Nicaise, SIAM J. Numer. Anal. 2005 ; Verfürth, M2AN 1999)
- Fully computable data oscillation terms (Higher order terms when regular)

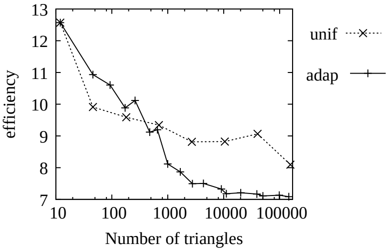
A posteriori error estimation for the DDFV scheme

Test on an L-shaped domain with a singular (H^{1+s} with $s < 2/3$) solution



The optimal order of convergence is recovered

Since then, adaptations of M. Vohralík's work have been implemented to yield better efficiencies



Outline

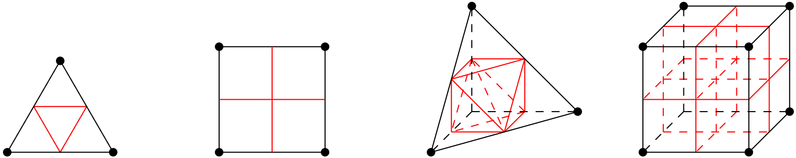
AMR implementation details

- Geometrical issues
  - implemented in a numerical kernel shared with several codes
  - using subdivision as refinement scheme (mesh quality conservation)
  - using hierarchical data structures (with cell genealogy)
  - providing dynamic load balancing in parallel contexts
- Numerical issues
  - implemented in application codes
    - MPCube at CEA-Saclay (SFME/LSET)
    - Trio–U at CEA–Grenoble (SSTH/LDAL)
  - Stationary case :
    - compliance with non–conforming meshes
    - *a posteriori* error estimates adapted to numerical and physical choices
  - Transient case : theoretical work in progress...

$\Longrightarrow$ Main objective : factorizing code as much as possible

AMR implementation details : geometrical tools

- cell refinement by regular subdivision



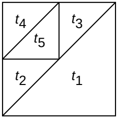
  - mesh quality conservation :-)
  - algebraic refinement :-)
  - non–conforming generated meshes :-(

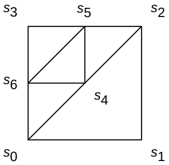
- hierarchical mesh data structures
  - mandatory for mesh coarsening
  - easier field interpolation after mesh adaptation
  - clean interation with fast multigrid solvers

- dynamic load balancing
  - geometric adaptation : no load balance
  - numerical resolution : load balance through partitionning and redistribution of the cell–adjacency graph

AMR implementation details : numerical tools

- MPCube's cell–centered finite volumes method

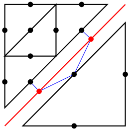




  - rather simple, thanks to the relative independance of the scheme to the real shape of cells :-)
  - care must be taken to consistency and convergence orders !

    (cf. C. Lepotier (CEA-SFME/LSET) and ANR project VF–Sitcom)

- Trio–U's Finite Volumes–Élements method ($\approx$ Crouzeix–Raviart FEM)



  - use of Mortar Finite Elements
  - rather simple implementation thanks to dedicated tools already implemented in the numerical kernel

AMR implementation details : available tools

- Experimental code from E. Laucoin's PhD and S. Veys's DRT
  - good performance trade–off between resolution and adaptation (95% vs 1.2% of computation time)
  - show the importance of fine–grain load balancing
- Experimental code from P. Omnes
  - using DDFV Finite Volumes
  - implements well–suited error estimates
- *A posteriori* error estimation for stationary diffusion problem using Diamond Finite Volumes
  - theoretical work from M. Vohralík (Numer. Math. 2008)
  - integration took a 2 month internship (I. Chettab)

Outline

Ongoing works

- N. Chalhoub's PhD thesis (supervision by A. Ern and M. Vohralík) on non-stationary convection-diffusion problems (numerical tests with DDFV)
- A. H. Le's PhD thesis (supervision by F. Benkhaldoun) on stationary Stokes (DDFV) and non-linear diffusion (TPFA on admissible meshes)
- Anisotropic mesh adaptation ?
- Errors due to the Schwarz and iterative solvers