Development of an Adaptive Mesh Refinement strategy for the Melodie software

simulating flow and radionuclide transport in porous media

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Joint work with Fayssal Benkhaldoun

IRSN - LAGA

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IRSN
INSTITUT
DE RADIOPROTECTION
ET DE SÛRETÉ NUCLÉAIRE
Faire avancer la sûreté nucléaire

UNIVERSITÉ PARIS 13 NORD

Outline

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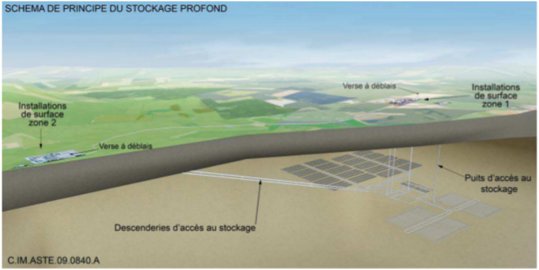
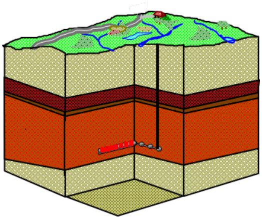
IRSN & BERIS

- IRSN : The French Institute for Radiological Protection and Nuclear Safety
  (**I**nstitut de **R**adioprotection et de **S**ûreté **N**ucléaire)
  is the national public expert in nuclear and radiological risks.

✓ BERIS : Safety Assessment and Research Section for Radioactive Waste Disposal Facilities
(**B**ureau d'**E**xpertise et de **R**echerche pour la sûreté des **I**nstallations de **S**tockage de déchets radioactifs)
is responsible for the safety assessment of above-ground radioactive waste disposal facilities and underground or deep geological disposal projects





The MELODIE computation code

- developed by IRSN since 1984 (Fortran 77/90)
- allows to simulate the flow and the transport of solutes in porous media, saturated or non-saturated, in 2d and 3d
- uses vertex-centered finite volume scheme

Mathematical models in MELODIE

- Water flow equation
  - Case of saturated media : continuity equation + Darcy's law

$$S\frac{\partial p}{\partial t} - \mathrm{div}(\mathbb{K}\nabla p) + q = 0$$

- p = hydraulic head
- $\mathbb{K}(x)$ = permeability tensor
- $\mathbf{v} = -\mathbb{K}\nabla p$ = Darcy's velocity

  - Case of non-saturated media : Richard equation
- Transport of solutes equation :
  - convection-diffusion-reaction equation

$$\omega R\frac{\partial c}{\partial t} - \mathrm{div}(\mathbb{D}\nabla c - \mathbf{v}c) - \lambda R\omega c + Q = 0$$

- c = radionuclide concentration
- $\mathbb{D}(\mathbf{v}, x)$ = diffusion-dispersion tensor
- ω = porosity, R = retardation factor
- λ = decay constant

Outline

Adaptive mesh refinement

- Motivation
  - to obtain more accurate solutions
  - to optimize the mesh and computation cost
  - etc.

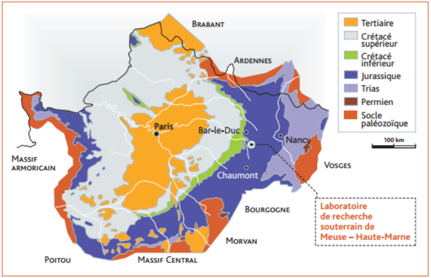


Figure 1 : Carte géologique simplifiée du bassin de Paris et localisation du site Meuse – Haute-Marne (d'après Andra, Dossier 2005 Argile – Document de synthèse, modifié).

Adaptive mesh refinement

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  - etc.
- Adaptive mesh refinement procedure

SOLVE → ESTIMATE → MARK → REFINE/ COARSEN

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- Several particularities of Melodie
  - linear and non-linear equations
  - 2 and 3 dimensions simulations
  - vertex-centered finite volume scheme

✓ guaranteed upper bound
✓ asymptotic exactness
✓ negligible evaluation cost

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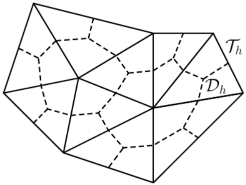
- Interested types of estimators
  - Residual estimators (Affif '06, Bergam '03, Verfürth '03, Amaziane '09)
  - Estimators based on H(div) flux reconstruction (Vohralik and co-workers)

H(div) flux reconstruction : recall the principles

(see Ern and Vohralik '10 ; Hilhorst and Vohralik '11 for time-depending problems)

- Problem : find $p \in H^1_0(\Omega)$, $\begin{cases} -\mathrm{div}(\mathbb{K}\nabla p) = f & \text{in } \Omega \quad \subset \mathbb{R}^{d=2,3} \\ p = 0 & \text{on } \partial\Omega \end{cases}$
- FV-FE scheme :



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Remark : the flux $-\mathbb{K}\nabla p \in \mathrm{H}(\mathrm{div},\Omega)$ but $-\mathbb{K}\nabla p_h$ is not

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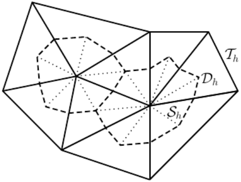

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- Flux reconstruction (exploits the local conservativity) : $\mathbf{t}_h \in \mathrm{RTN}_0(\mathcal{S}_h) \subset \mathrm{H}(\mathrm{div},\Omega)$ and

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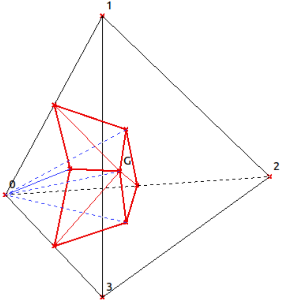

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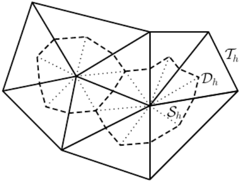

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$$(\mathrm{div}\ \mathbf{t}_h, 1)_D = (f,1)_D, \quad \forall D \in \mathcal{D}_h^{\mathrm{int}}$$

- Error estimator :

$$|||u - u_h|||^2 \leq \sum_{D \in \mathcal{D}_h} \Bigg(\underbrace{m_D \| f - \mathrm{div}\ \mathbf{t}_h \|_D}_{\text{residual error}} + \underbrace{\left\| \mathbb{K}^{\frac{1}{2}} \nabla p_h + \mathbb{K}^{-\frac{1}{2}} \mathbf{t}_h \right\|_D}_{\text{flux error}} \Bigg)^2$$

Local mesh refinement

- Conditions on the mesh : conforming and shape-regular

REFINEMENT + COMPLETION

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- Refinement methods (see e.g. Morin, 2008)
  - Regular refinement : an element is cut into 2^d smaller elements

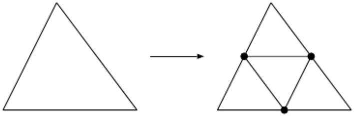
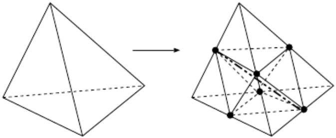


FIGURE: 2d : 4 new elements



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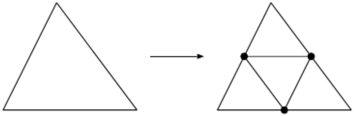

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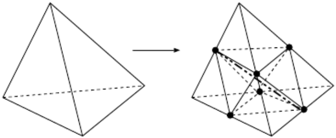

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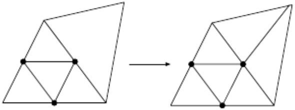

FIGURE: a completion method

Local mesh refinement

- Conditions on the mesh : conforming and shape-regular

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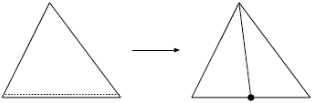
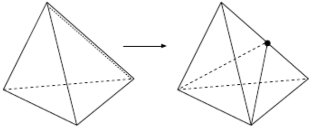
- Refinement methods (see e.g. Morin, 2008)
  - Regular refinement : an element is cut into 2^d smaller elements
  - Refinement by bisection : an element is always bisect into 2 smaller elements



Refinement of a triangle



Refinement of a tetrahedron

Local mesh refinement

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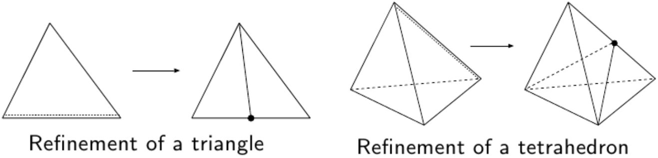
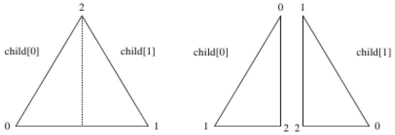
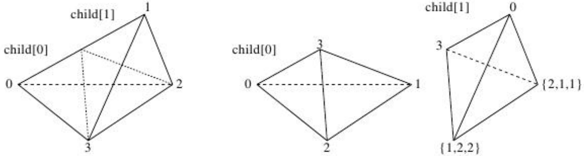


The newest vertex bisection : assigns the refinement edge of 2 children and preserves the shape regularity

Refinement edge, recursive algorithm and hierarchical mesh

- Refinement edge (see e.g. Kossaczky)





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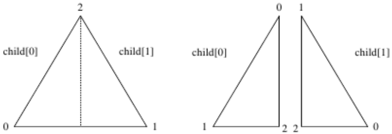
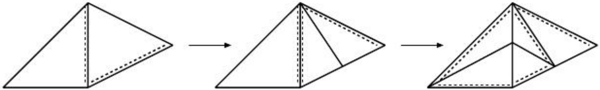
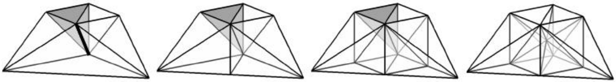


- Recursive algorithm





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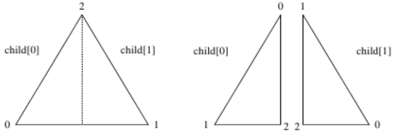
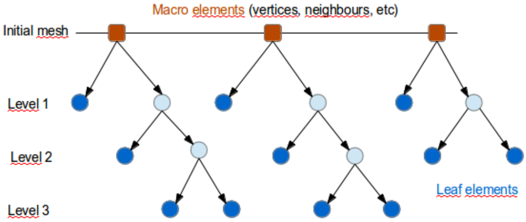


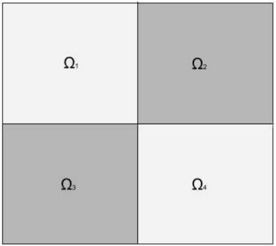
- Recursive algorithm
- Hierarchical mesh (see e.g. ALBERTA document)



Outline

Test with an analytical solution

(see e.g. VOHRALIK '11)



- Problem :

$$\begin{aligned} -\mathrm{div}(\mathbb{K}\nabla p) &= 0 && \text{in } \Omega = (-1,1)^2 \\ p &= p_{ex} && \text{on } \partial\Omega \end{aligned}$$

- Heterogeneous permeability

$$\mathbb{K} = \begin{cases} 1.\mathbb{I}_2 & \text{if } x \in \Omega_{1,4} \\ 100.\mathbb{I}_2 & \text{else.} \end{cases}$$

- Solution
$p \in H^{1+\alpha}(\Omega),\ \alpha = 0.127,\ a_i, b_i =$ const.

$$p(r,\theta) = r^\theta (a_i \sin(\alpha\theta) + b_i \cos(\alpha\theta))$$

Test with an analytical solution

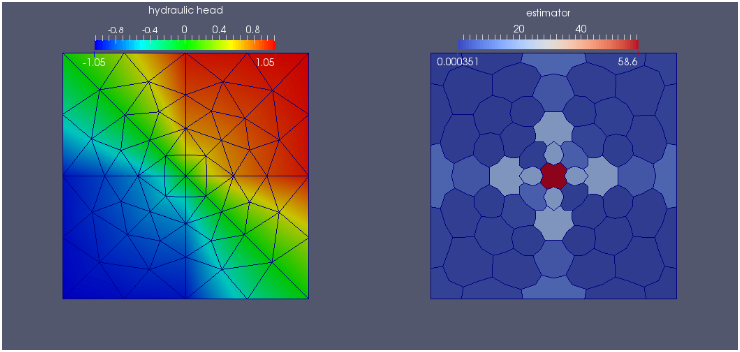


FIGURE: Solution on the coarse mesh

Test with an analytical solution

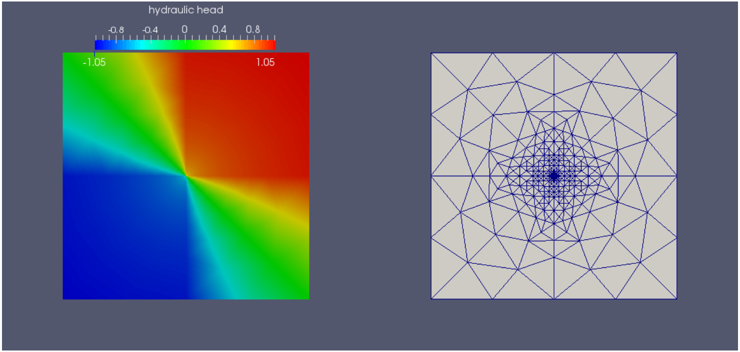


FIGURE: Solution on the adaptive mesh

Test with an analytical solution

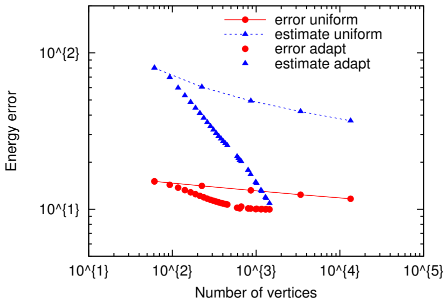


FIGURE: Error vs estimator

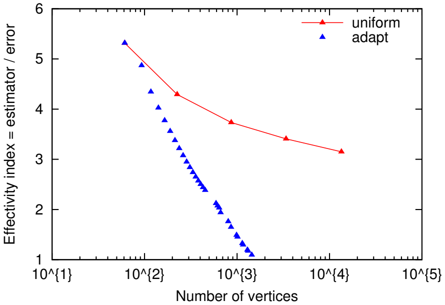


FIGURE: Effectivity index

A more realistic configuration

(see Amaziane et al., '14)

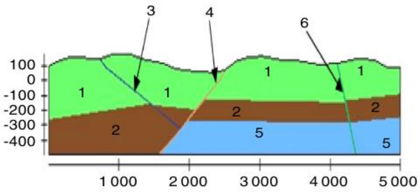


Figure: A heterogeneous porous medium

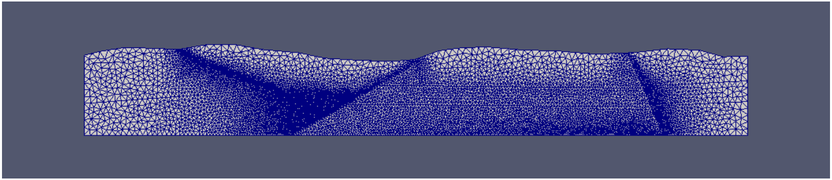
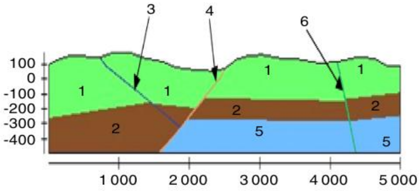


Figure: Initial mesh with 8.217 vertices

A more realistic configuration

(see Amaziane et al., '14)



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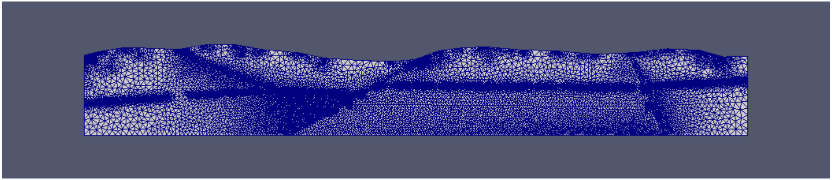
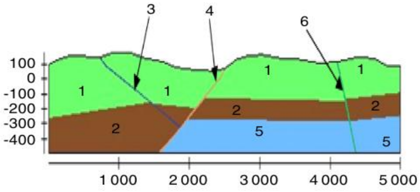


Figure: Adaptive mesh with 34.435 vertices

A more realistic configuration

(see Amaziane et al., '14)



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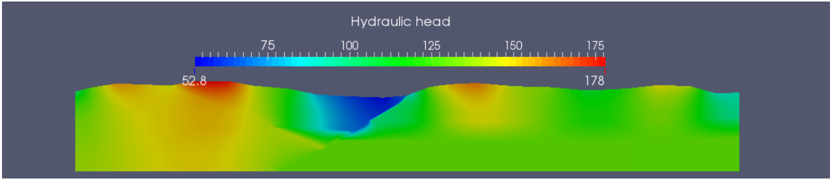

Figure: Solution on the adaptive mesh

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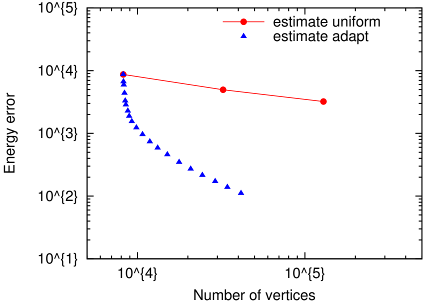

FIGURE: Estimator

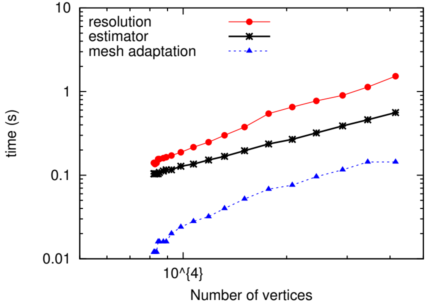

FIGURE: Time

Outline

Discussion and Conclusion

- Conclusion
  - Estimators based on H(div) flux reconstruction
  - Refinement by bisection
  - Newest vertex bisection
  - Recursive algorithm and hierarchical mesh

- Works in progress ...
  - Algebraic error and stop criteria
  - Implementation of estimator for non-linear equation
  - Refinement edge of initial elements (ok in 2d but difficult in 3d)