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INSTITUT
DE RADIOPROTECTION
ET DE SÛRETÉ NUCLÉAIRE

Faire avancer la sûreté nucléaire

Development of an adaptive mesh based on a posteriori error estimate for radionuclide transport modeling

MaNu

14 November 2017
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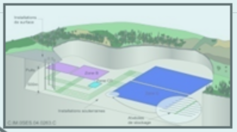
Plan

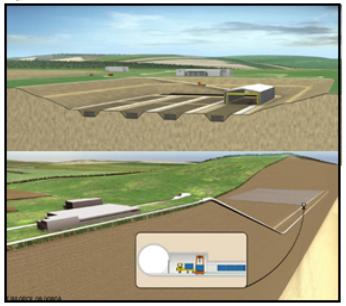
- Context
- MELODIE
- Refinement/Coarsening
- Numerical test cases
- Optimization
- Conclusion

DISPOSAL FACILITIES IN FRANCE

Managed by ANDRA (National agency for radioactive waste management)

Activity \ Period (1/2 life)	Short < 30 years	Long > 30 years
VLLW (1 - few Bq/g)	Morvilliers VLLW disposal site	
LLW (100 to 100 k Bq/g)	surface disposal sites : Manche site (CSM) Aube site (CSA)	Radium and graphite waste disposal site (project>2020)
ILW (100 k to 100 M Bq/g)		under investigation (June 28th 2006 law)
HLW (10 billion Bq/g)	the future Cigeo facility	



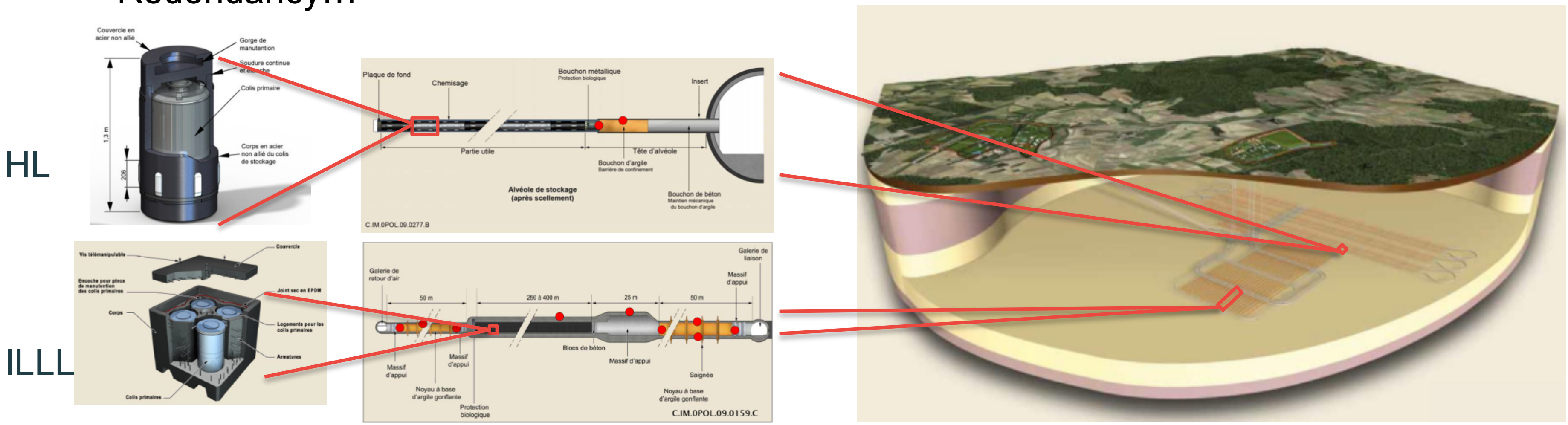


- Run from 1969 to 1994
- 500 000 m^3 of waste stored
- 12 ha of surface area
- Institutional control during 300 yrs **(containment and isolation required)**

- Started in 1992
- ~30 ha surface area
- Capacity : 1 000 000 m^3
- Nuclear production period covered ~50 yr
- Safety based on multiple barriers

…THE FUTURE CIGEO (2014 DGD CONCEPT)

- **A classical Nuclear Facility…**
  - Multi-barrier (« matrix-pack », seals, host-rock)
  - Redondancy…



- **… though quite a special one**
  - No existing one (studies since early 1980's)
  - Very long exploitation period (> century)
  - Very Long time scales (uncertainty on phenomenology)
  - Large spatial scales.

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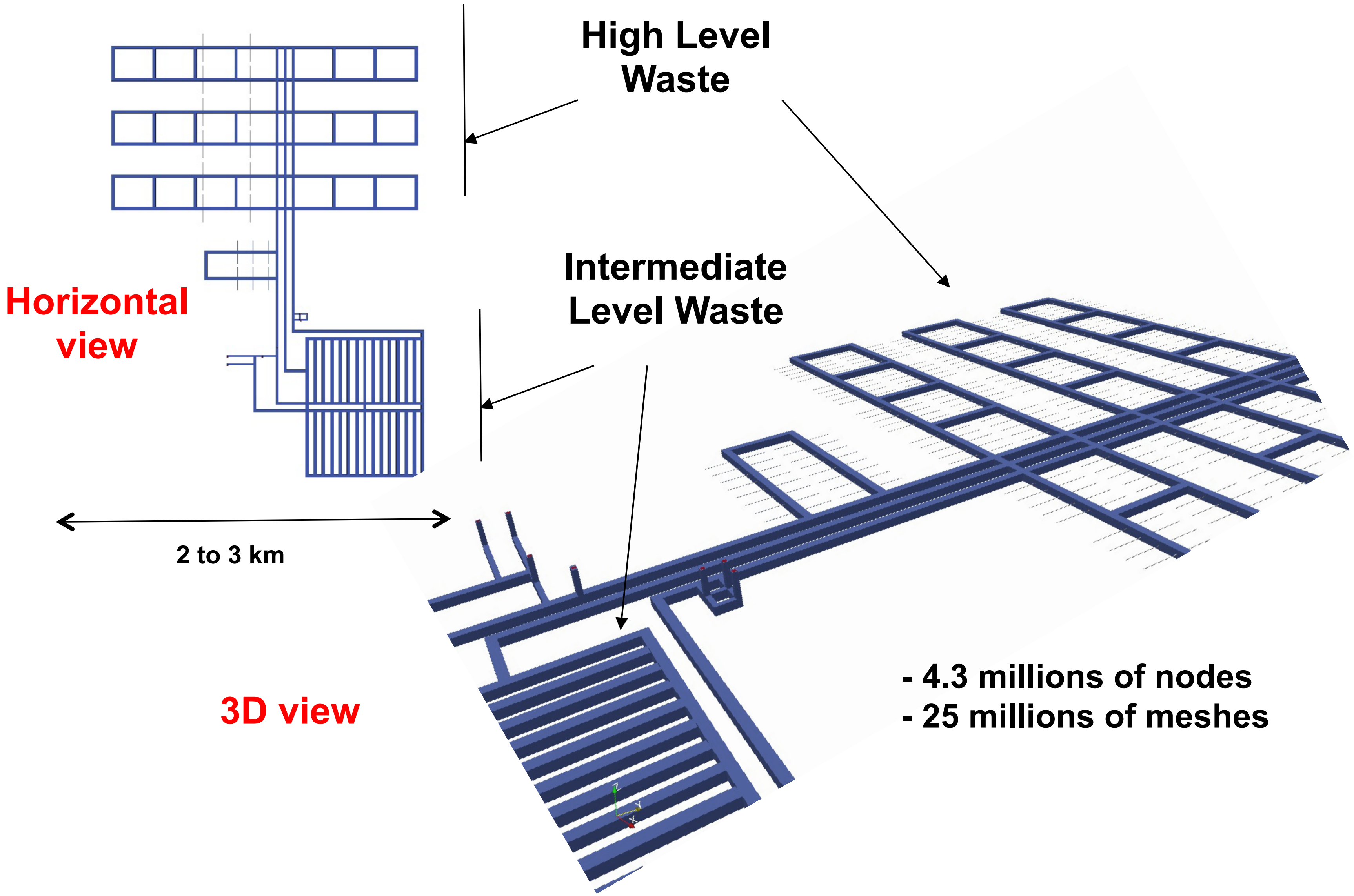
CIGEO PROJECT



- 4.3 millions of nodes
- 25 millions of meshes

MELODIE 5.1

(Modèle d'Evaluation à Long terme des Déchets Irradiants Enterrés)

- **MELODIE v5.1 – A software allowing to model flow and transport in porous saturated and unsaturated media in 2D et 3D**
  - Currently in an optimization step → Adaptive mesh based on an a posteriori estimator
  - Expertise tool for HLW disposals facilities (historical use of the software), as well as for surface repositories (more recent)

- **OBJECTIVES**
  - ✓ to have a tool for the assessment of the safety demonstration of a storage
  - ✓ To model the behavior of a storage in global way
  - ✓ To assess the impact on population

- **REQUIREMENTS**
  - ✓ To seek a envelop character of the phenomena
  - ✓ To fix the operational limits

- **MEANS**
  - ✓ classification and simplification of the phenomena
  - ✓ search for means of validation of the hypotheses

Conceptual model (1)

- Equation of the water flow

  - In saturated medium, the continuity equation (mass conservation) and Darcy's law are applied

$$\vec{U} = -K\,\overrightarrow{\text{grad}}\,h$$

$$\text{div}(K\,\overrightarrow{\text{grad}}\,h) = S_s \frac{\partial h}{\partial t} + q$$

K : permeability tensor (m.unit of time^{-1})
h : hydraulic charge (m)
U : Darcy velocity (m/unit of time)
Ss : specific storage coefficient of the aquifer in (m^{-1})
q : **volumetric flow rate injected or withdrawn per unit of rock volume (unit of time^{-1}).**

  - In unsaturated medium Richard's equation is applied:

$$\text{div}(K(\psi)\,\overrightarrow{\text{grad}}\,h) = S(\psi) \frac{\partial h}{\partial t} + q$$

K (ψ): permeability tensor, function of moisture content or capillary pressure (m/unit of time)

S (ψ): specific moisture capacity of the aquifer (m^{-1}) function of capillary pressure (m.unit of time^{-1})

Conceptual model (2)

- Transport equation

$$div(D\ grad\ A\ - U\ A) = \omega\, R\, \frac{\partial A}{\partial t} + \lambda\, \omega\, R\ \ A$$

ω : porosity (-)
A : activity field (Bq,m^{-3})
U : Darcy velocity(m/unit of time)
D : diffusion-dispersion tensor (m^2 ,unit of $time^{-1}$)

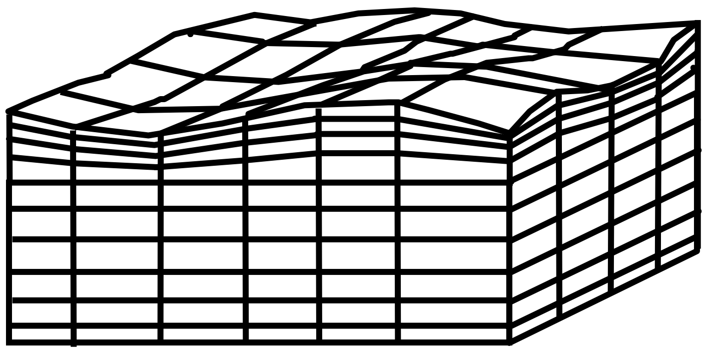
$$R = 1 + \frac{1-\omega}{\omega}\ \rho_s Kd$$

R : Delay coefficient (Kd approach) due to adsorption on the solid phase and retention in the immobile fluid phase. It corresponds to a coefficient multiplier of the porosity, which modifies the apparent speed of transfer of the elements.

λ : radioactive decay constant of an element (unit of time-1)

Space approximation

- To solve this system, it is advisable to **transform the partial differential equation into a finished number of algebraic equations**, corresponding to the number of nodes of a grid, which spatially discretize the field studied.



- The differential operators characterizing the system of equations call upon physical parameters such as: permeability, porosity, dispersivity, diffusion.... **These parameters are viewed as uniforms on each element.** The values of these parameters are assigned to all elements.

Discretization of equations

Finite Element method FE

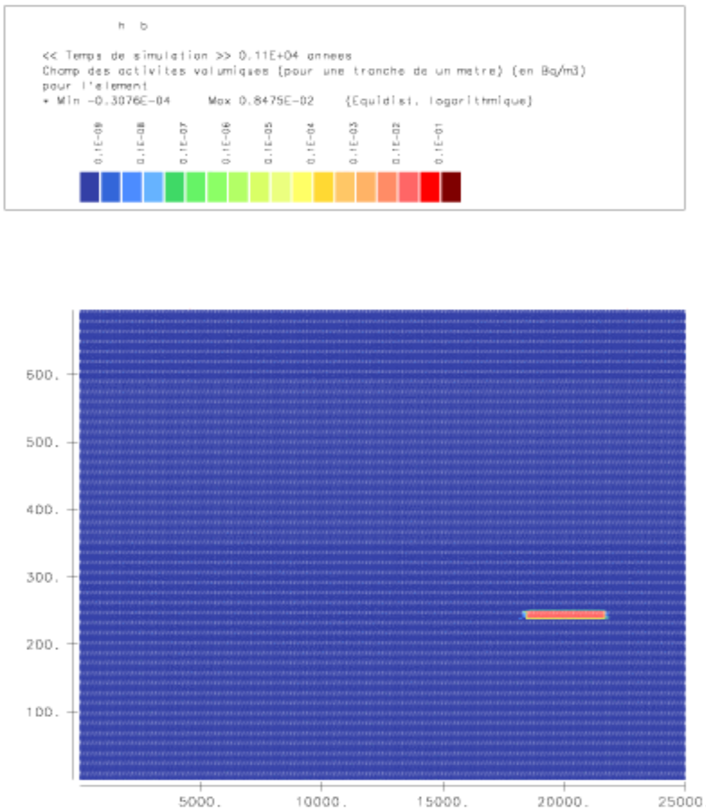
- Very well adapted for the diffusive problems
- Unspecified grid
- Numerical oscillations due to the advective term
- Negative values of the concentration - instability

Finite Volumes - Finite Elements FVFE

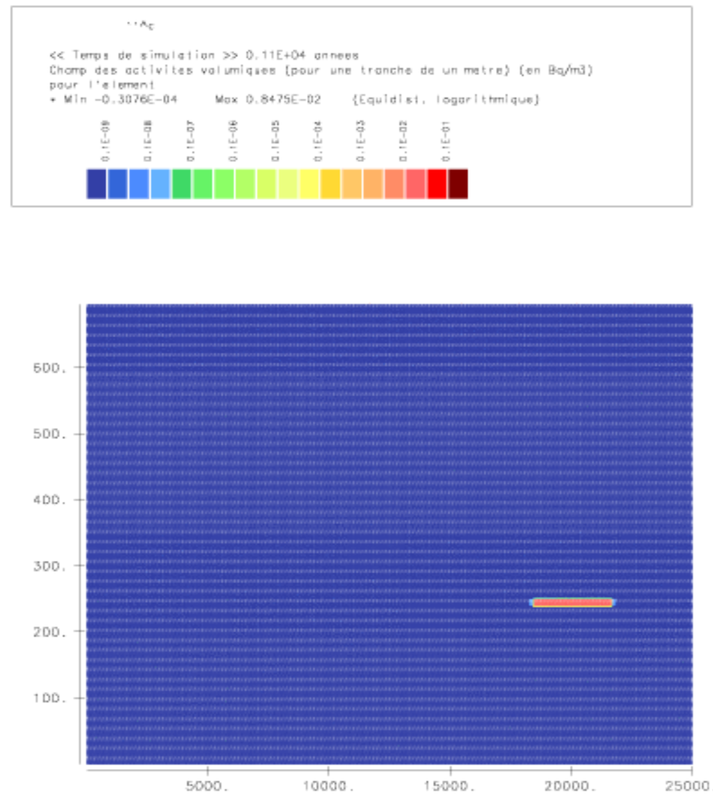
- Finite volume method for the advective term and finite element method for the diffusive term
- Respect of the principle of maximum with conditions on the meshes
- Stability of calculation
- Local mass conservation
- Numerical diffusion
- Strong requirements on the mesh

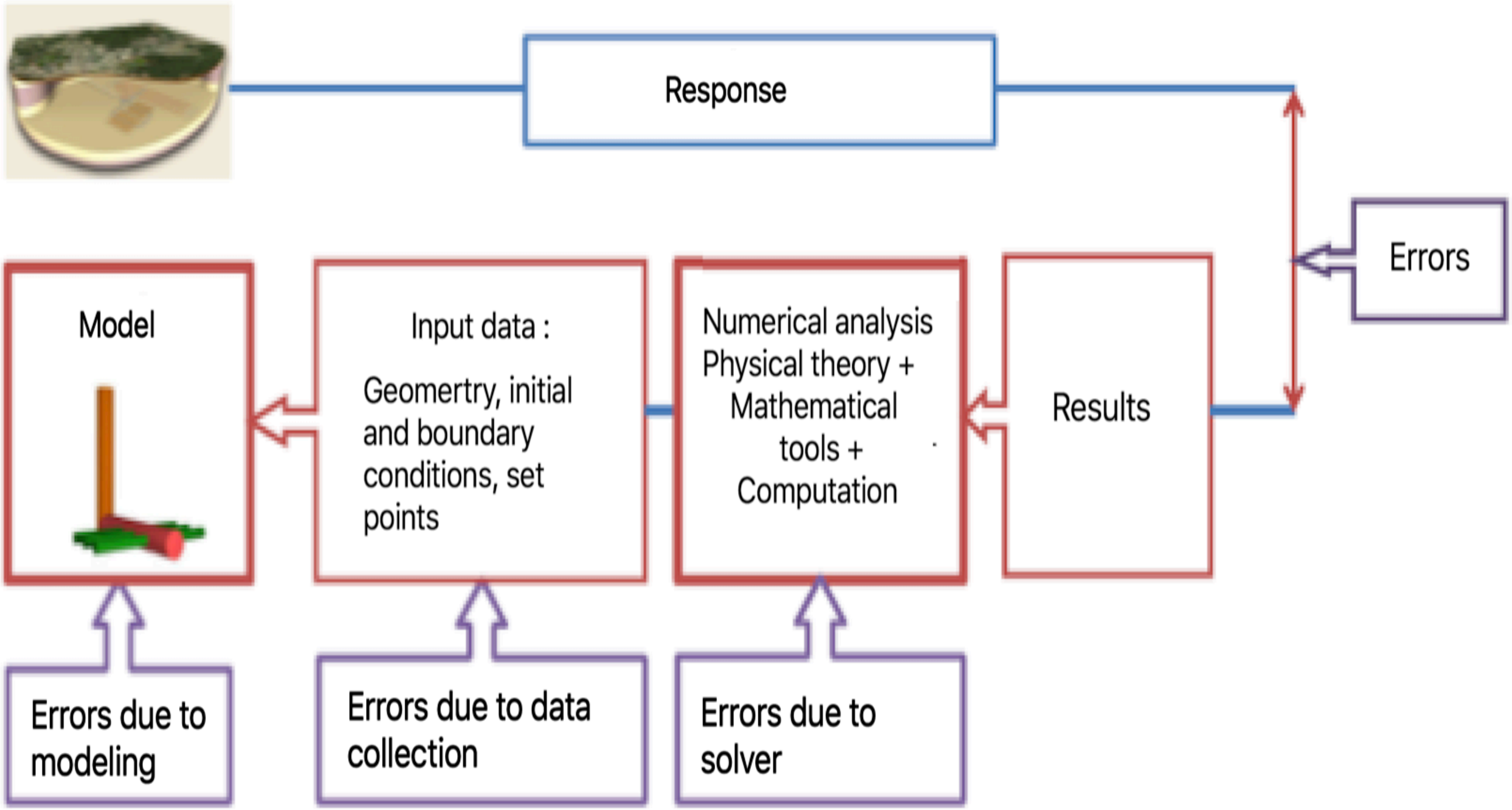
Discretization of equations – COUPLEX benchmark

FE method

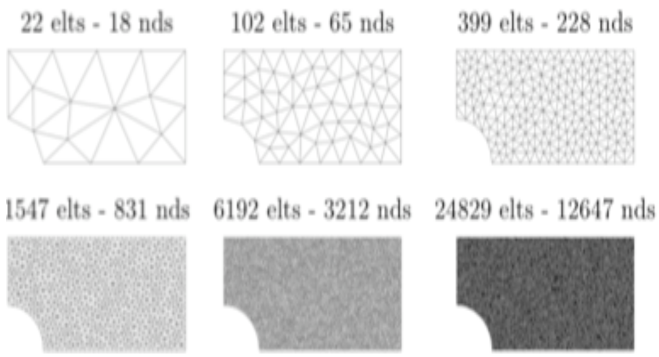


FVFE method





How to control error due to discretization?



To reduce the impact of these errors, there is a well known way which consists in refining the mesh by using smaller elements.

- ✓ The amplitude of the error decreases

- ✓ Increase the calculation time
- ✓ Example: if we divide the size of the elements by two, we multiply the total number of nodes by 8 (in 3D) and the computation time by a few hundred.

Rigorous quantitative procedures must be in place to quantify errors.

Pb: identify areas of singular behavior + refine so that the overall error is evenly distributed across the entire domain

➢ **A posteriori error estimate**

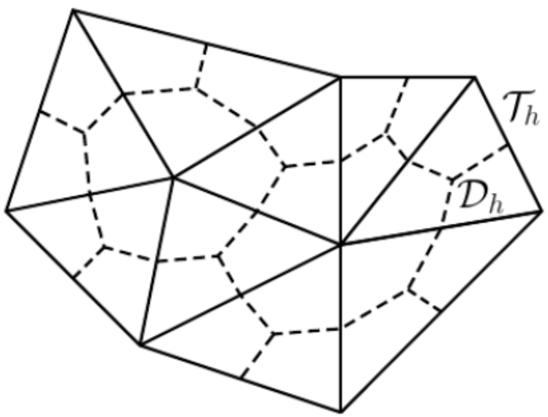
Flux reconstruction:

Transport equation

$$-\nabla \cdot (\mathbb{K}\nabla p) = f, \qquad (1)$$

$$\omega R \frac{\partial c}{\partial t} - \nabla \cdot (\mathbb{D}\nabla c - \vec{U} c) - \lambda \omega R c = S, \qquad (2)$$

FVFE method



$$-\sum_{\gamma \subset \partial D_i} \int_\gamma \mathbb{K}\nabla p_h \cdot \vec{n}_\gamma \mathrm{d}s = \int_{D_i} f \, \mathrm{d}x,$$

$$\int_{D_i} \omega R \frac{c_h^n - c_h^{n-1}}{\tau_n} \, \mathrm{d}x - \sum_{\gamma \subset \partial D_i} \left\{ \int_\gamma \mathbb{D}\nabla c_h^n \cdot \vec{n}_\gamma \mathrm{d}s - \int_\gamma \vec{U}_h c_h^{n-1} \cdot \vec{n}_\gamma \mathrm{d}s \right\}$$

$$- \int_{D_i} \lambda \omega R c_h^n \, \mathrm{d}x = \int_{D_i} S \, \mathrm{d}x,$$

$$\vec{U}_h = -\mathbb{K}\nabla p_h$$

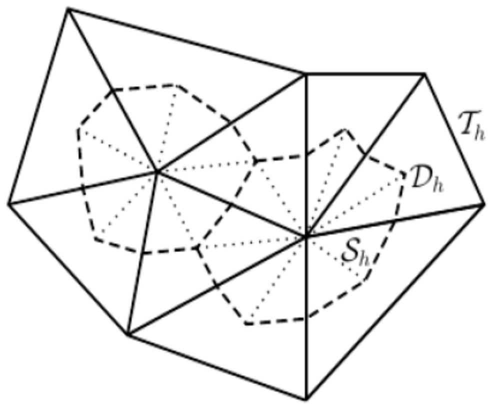
Flux reconstruction:

Transport equation

$$-\nabla \cdot (\mathbb{K}\nabla p) = f, \qquad (1)$$

$$\omega R\frac{\partial c}{\partial t} - \nabla \cdot (\mathbb{D}\nabla c - \vec{U}c) - \lambda\omega Rc = S, \qquad (2)$$

FVFE method



Find $p_h \in C(\overline{\Omega}) \cap P_1(\mathcal{T}_h) \subset H_0^1(\Omega)$,

$-\langle \mathbb{K}\nabla p_h, 1\rangle_{\partial D} = (f, 1)_D, \quad \forall D \in \mathcal{D}_h^{\mathrm{int}}$

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

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

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

A posteriori error estimate : M. Vohralik

A posteriori error estimate for transport equation

$$|||p - p_h||| \leq \left\{ \sum_{D \in \mathcal{D}_h^*} (\eta_{R,D} + \eta_{DF,D})^2 \right\}^{\frac{1}{2}},$$

$$\eta_{DF,D} := \|a^{\frac{1}{2}} \nabla p_h + a^{-\frac{1}{2}} \mathbf{t}_h\|_D \qquad D \in \mathcal{D}_h^*,$$

$$\eta_{R,D} := m_{D,a} \|f - \nabla \cdot \mathbf{t}_h\|_D \qquad D \in \mathcal{D}_h^*,$$

$$\eta_{tm}^n := \left\{ \int_{t^{n-1}}^{t^n} \sum_{D \in \mathcal{D}_h^n} ||\mathbb{D}^{\frac{1}{2}} \nabla (c_{h,\tau} - c_h^n) - \mathbb{D}^{-\frac{1}{2}} \vec{U}_h (c_{h,\tau} - c_h^n)||_D^2(t) \mathrm{d}t \right\}^{1/2}$$

$$\eta_{sp}^n := \left\{ \tau_n \sum_{D \in \mathcal{D}_h^n} m_{\mathbb{D},D}^2 ||S - \omega R \frac{\partial c_{h,\tau}}{\partial t} + \lambda \omega R c_h^n - \nabla \cdot \theta_h^n||_D^2 \right\}^{1/2} +$$

$$\left\{ \tau_n \sum_{D \in \mathcal{D}_h^n} ||\mathbb{D}^{\frac{1}{2}} \nabla c_h^n - \mathbb{D}^{-\frac{1}{2}} \vec{U} c_h^n + \mathbb{D}^{-\frac{1}{2}} \theta_h^n||_D^2 \right\}^{1/2}$$

$$|||c - c_{h,\tau}|||_X \leq \left\{ \sum_{n=1}^{N} \{(\eta_{sp}^n)^2 + (\eta_{tm}^n)^2\} \right\}^{1/2}$$

Adaptive Algorithm

Stationary Pb

i. Let a given initial mesh

ii. Solve the problem on the initial mesh

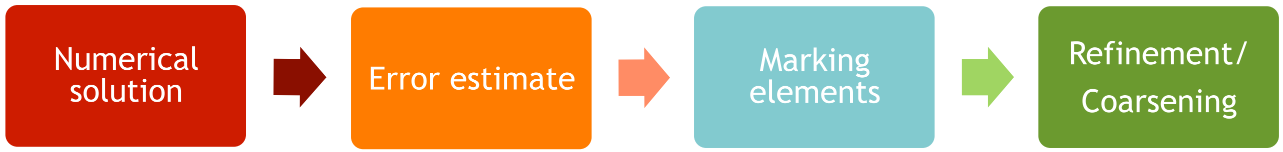
iii. Calculate the a posteriori error estimate for this mesh

iv. If the calculation of this estimator does not satisfy the stopping criterion, then choose the elements to refine, build the new mesh and go back to step ii.

Non-Stationary Pb

a. The refinement process must combine the control of space step and time step

b. Coarsening in some areas of the mesh must be considered when the solution evolves in time



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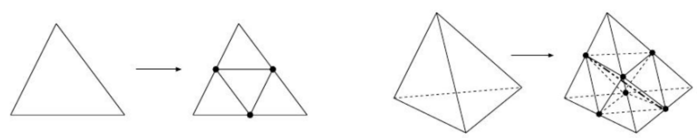
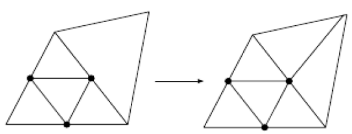
Technique of refinement/coarsening

Two refinement strategies to preserve the regularity in the mesh

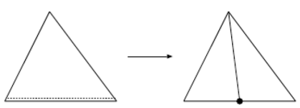
A. Regular refinement : divide the elements into 4 (in 2D) or 8 (in 3D) by joining the midpoints of the edges



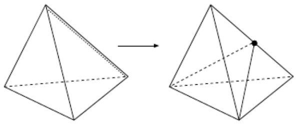


a completion method

B. Longest edge bisection : divide the elements by joining the middle of the longest edge to the opposite vertex to this edge.



Refinement of a triangle



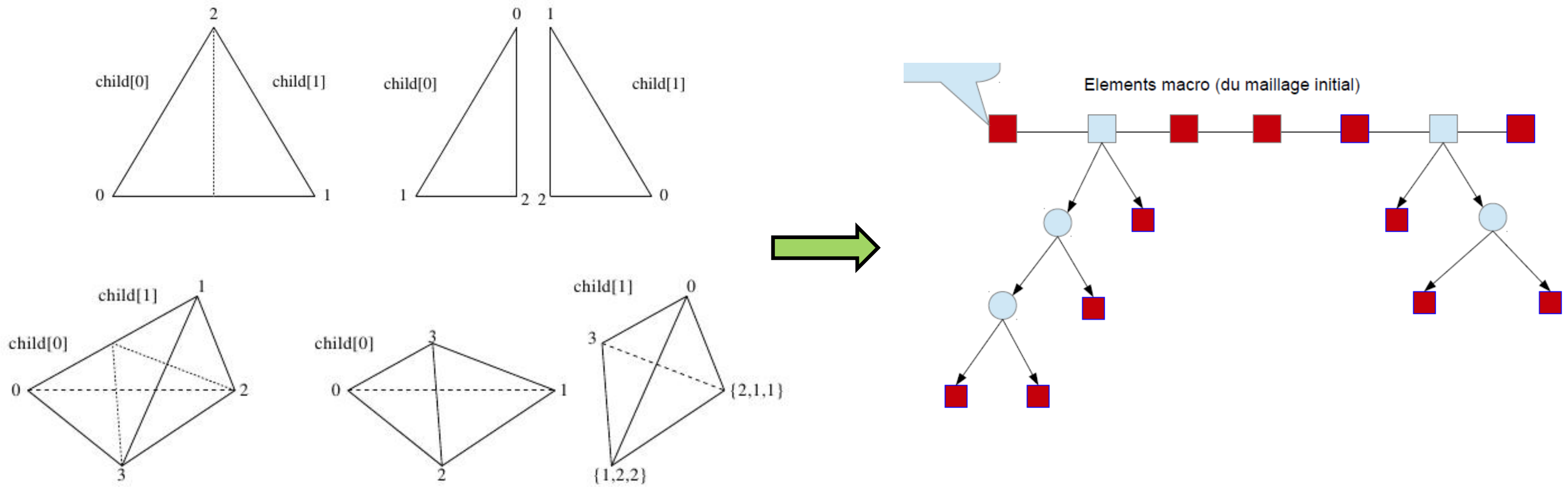
Refinement of a tetrahedron

(a) Bisect a triangle (b) Completion

a completion method

MELODIE test cases

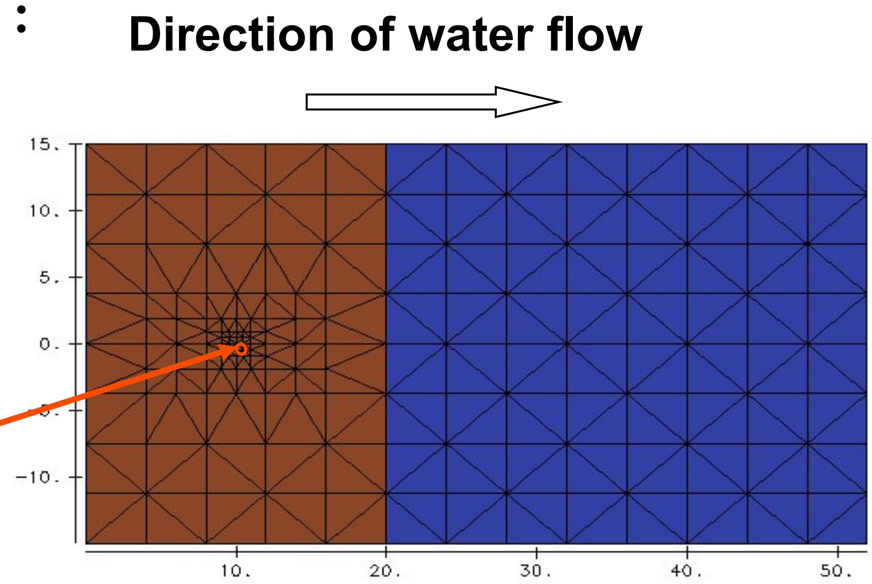
Refinement strategy



Heterogeneous and anisotropic model (1)

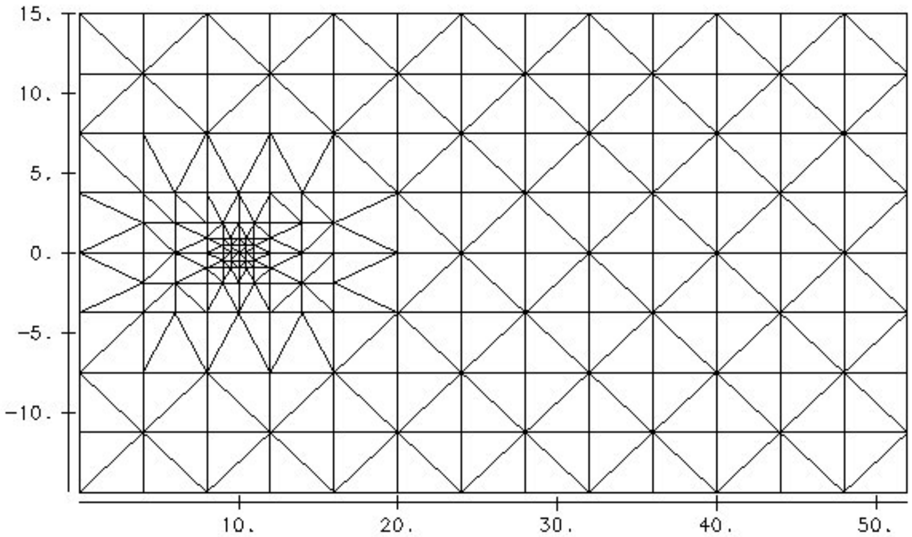
Flow boundary condition :
Hydraulic head =
left side : 30 m
right side : 0 m

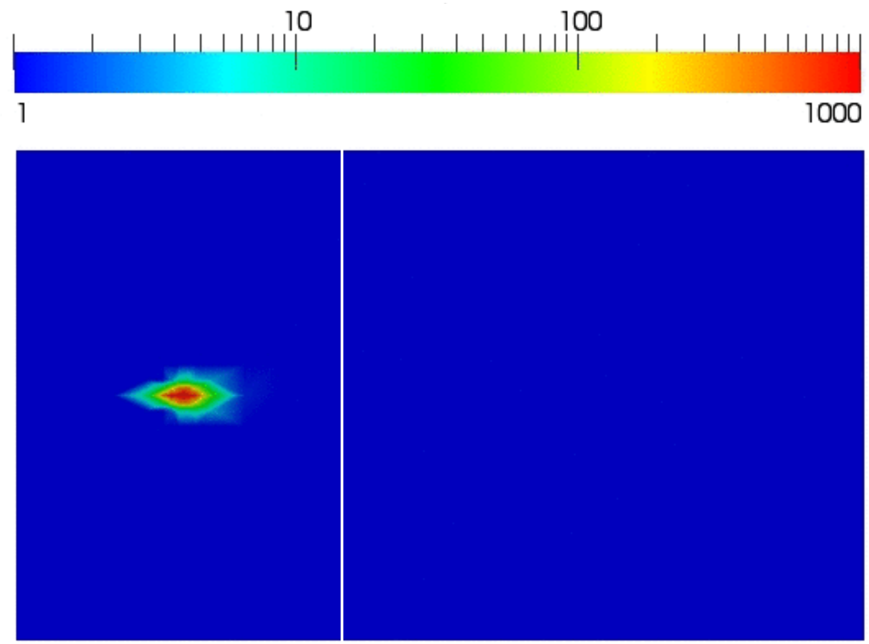
Injection pulse condition :
Duration : 0.01 unit of time
Quantity : 600 Bq



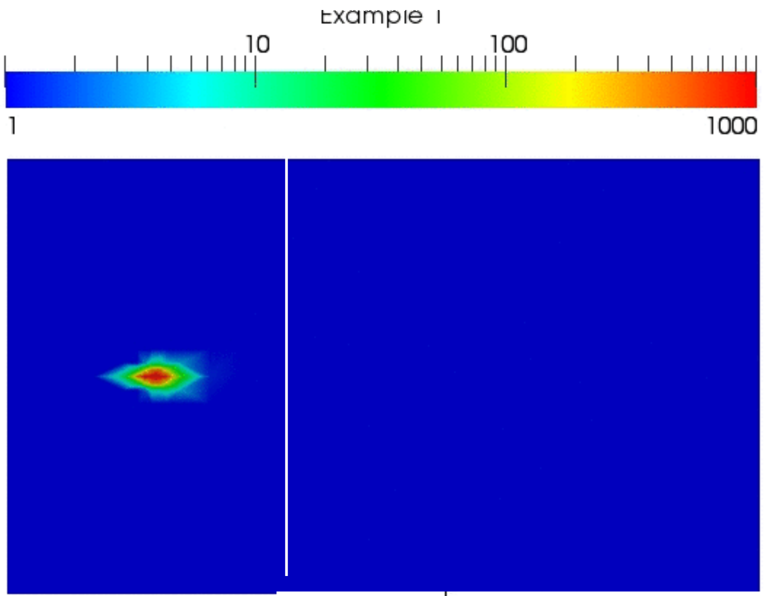
	Permeability X	Permeability Y	Porosity	Dispersion α_l	Dispersion α_t	Diffusion
(brown)	5.	5.	0.1	1.	5.e-4	0
(blue)	1.	1.	0.05	0.5	0.5	0

Results of the simulation (2)

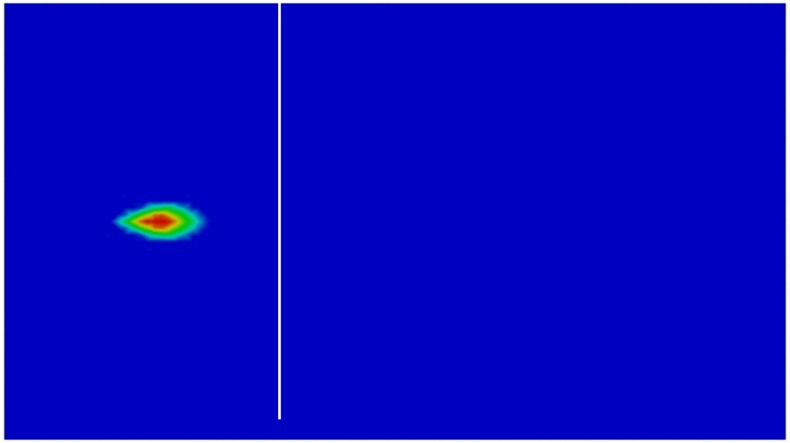


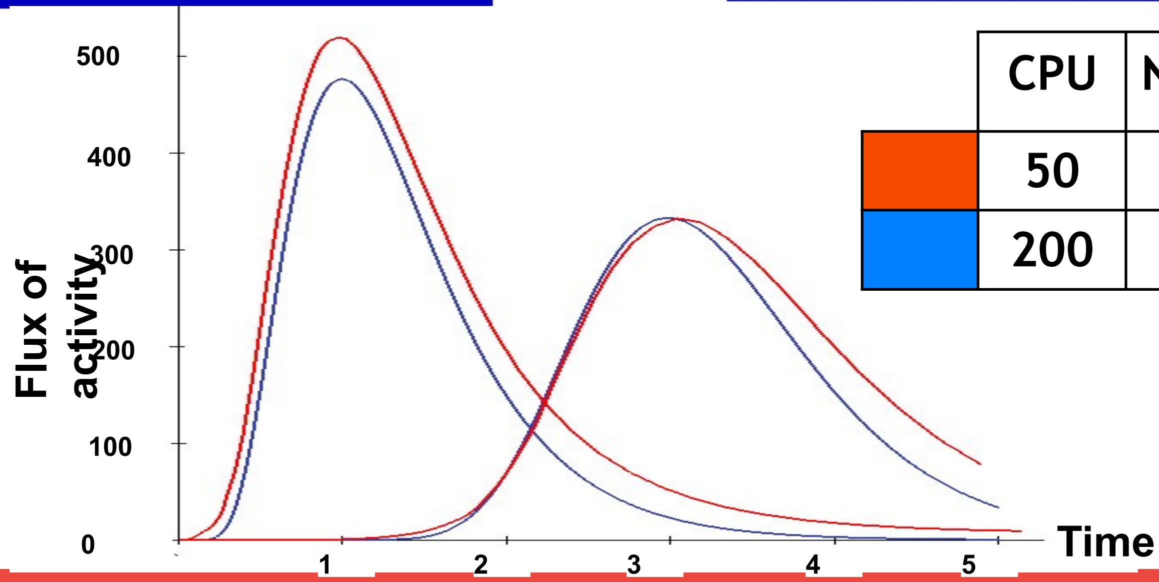


Comparison with uniform static mesh (3)



<u>**uniform static mesh**</u>





	CPU	Nb cells
	50	3 000
	200	13 000

Profiling MELODIE code

Test case : 2D Permanent flow

NbEl	NbNo	NbIT (starting GC)	%			
			Estim.	Pecaln	Refinement	Hier. Mesh.
8	9	4	58	15	10	5,76
98	64	15	57	18	8	5,7
1058	576	37	48	30	8	5,23
10082	5184	104	43	38	6	5,16
99458	50176	341	24	63	2,5	6,56
245000	123201	683	15	71	1	8,44

- ✓ Pecaln = GC solver
- ✓ Hierarchical mesh = saving the results.

Test case : 3D Permanent flow

NbEl	NbNo	NbIT (starting GC)	%			
			Estim.	PecaIn	Refinement	Hier. Mesh.
48	27	7	85,91	5	1,14	4,57
1296	343	16	85,82	5,89	0,77	4
10368	2197	28	84,66	6,78	0,86	4,17
93750	17576	63	82	8,62	0,67	3,82
384000	68921	89	77	11	3,58	4,88

- In 3D, the estimator takes a long time;
  - ✓ In the computation of the flow th;
  - ✓ Construction of the local mesh;
  - ✓ Construction of normal vectors

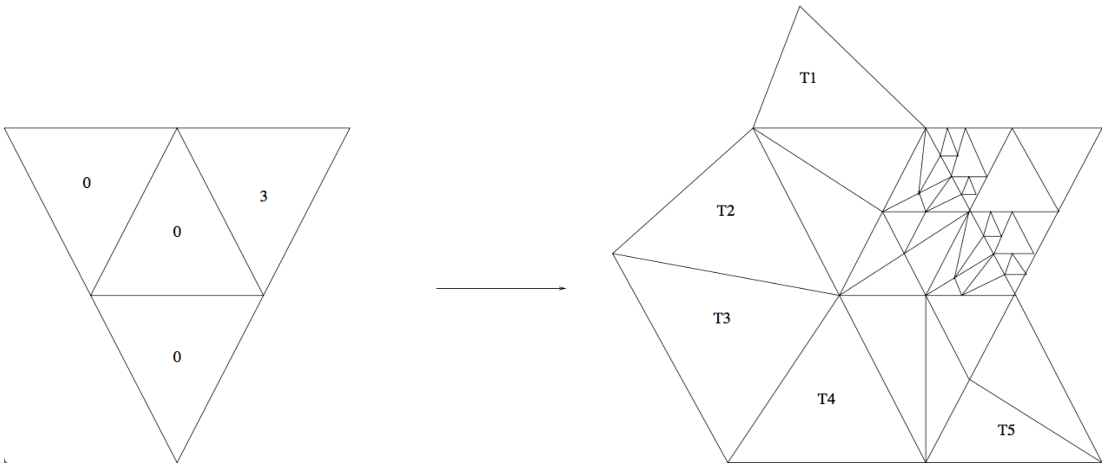
Test case : 2D Transient flow

NbEl	NbNo	%			
		Estim.	TecaIn	Refinement	Hier. Mesh
8	9	64,8	17,15	6,31	3,97
98	64	64,94	19,75	4,51	5,10
1058	576	64,8	17,90	7,26	2,5
10082	5184	64,31	27,47	1,43	3,4
99458	50176	62,4	22,95	3,3	6
245000	123201	55,4	23,4	0,08	17,45

✓ TecaIn = GC solver;

Optimization

Refinement strategy



- Cuting mesh into 4 triangles
- Doing conformity using Longest edge bisection

Table: Comparison between the NewestVB and AdaptNVB approaches. CPU times are in seconds.

NewestVB approach

iter	DoFs	η	ϵ_1	ϵ_2	f_η	CPU
1	128	103.3915	15.836	0.30586	6.5289	0.679
12	942	44.08	8.8284	0.074364	4.993	0.074
45	4608	9.7158	6.5221	0.027443	1.2734	2.575
Total						**112.741**

AdaptNVB approach

iter	DoFs	η	ϵ_1	ϵ_2	f_η	CPU
1	240	103.3915	15.836	0.30586	6.5289	0.671
6	1040	42.7369	10.677	0.081534	4.0027	0.918
29	7296	6.9263	5.104	0.022277	1.357	3.995
Total						**56.647**

Table: Comparison between the conventional and nested approaches. CPU times are in seconds.

Conventional approach

iter	DoFs	η	ϵ_1	ϵ_2	f_η	CPU
1	240	103.3915	15.836	0.30586	6.5289	0.71
6	2256	42.0556	10.298	0.079115	4.0838	1.45
20	9903	10.617	5.2289	0.020684	2.0305	5.5
Total						**60.691**

Nested approach

iter	DoFs	η	ϵ_1	ϵ_2	f_η	CPU
1	1046	103.3915	15.836	0.30586	6.5289	0.39
3	3054	37.5234	9.6343	0.065962	3.8948	1.5
10	10082	7.9307	5.5007	0.024378	1.4418	6.8
Total						**35.13**

Conclusion

- 2D and 3D flow and transport in porous saturated and unsaturated media.
- Refinement/coarsening mesh using a posteriori error estimate.

Perspective

- Optimizing the algorithm of the a posteriori error estimate computation.
- Parallelization of 2D and 3D codes using domain decomposition.