

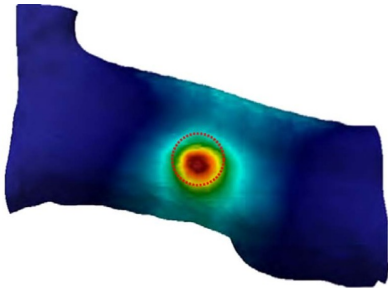
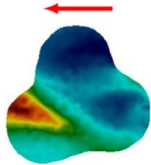
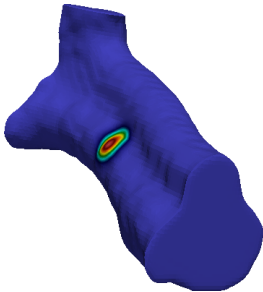
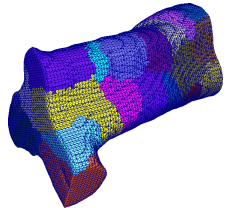
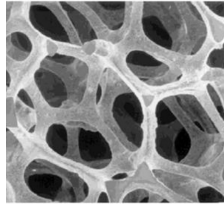
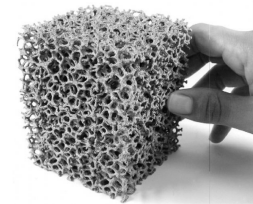
Éléments finis et équation de transfert radiatif

Yann Favennec

avec aussi B. Rousseau, D. Le Hardy, A. Badri, P. Jolivet,
O. Balima, F. Dubot, D. Rouse, H. Digonnet, S. Guévelou, ...

(22 novembre 2017)

Objectif 1



0,10

0,0031

1. Le Hardy et al. "3D numerical modelling of the propagation of radiative intensity through a X-ray tomographed ligament." *Journal of Quantitative Spectroscopy and Radiative Transfer* 194 (2017): 86-97.



Problème radiatif

search $I(\mathbf{x}, \mathbf{s}) : \mathcal{D} \times \mathcal{S}^{n-1} \mapsto \mathbb{R}^+$

$$\mathbf{s} \cdot \nabla I(\mathbf{x}, \mathbf{s}) + (\kappa + \sigma_s)I(\mathbf{x}, \mathbf{s}) = \sigma_s \int_{\mathcal{S}^{n-1}} \Phi(\mathbf{s}, \mathbf{s}')I(\mathbf{x}, \mathbf{s}') \, d\mathbf{s}' + \kappa I_b(T)$$

+ B.C.

Features :

- ▶ Advection (transport)
- ▶ Reaction
- ▶ no "diffusion"
- ▶ integro-diff eq.

Regularité

$$I(\mathbf{x}, \mathbf{s}) \in H^1(\mathcal{D}) \times L^2(\mathcal{S}^{n-1})$$

Éléments finis

Ingrédients

- ▶ Introduction d'une formulation variationnelle
- ▶ Approximation de l'espace fonctionnel / maillage
- ▶ Intégrales
- ▶ Résolution d'un système linéaire

Historique

- ▶ Reddy, 1978 : 1D
- ▶ Fiveland, 1994 : DOM-FEM

Versions

- ▶ Galerkin – moindres carrés - SUPG
- ▶ Espace / Angulaire
- ▶ coulage EF avec DOM – harmoniques sphériques ...

discrétisation angulaire

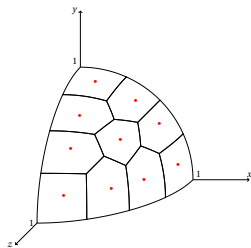
Quadrature :

$$\int_S I(\mathbf{x}, \mathbf{s}) \, d\mathbf{s} = \sum_{m=1}^{N_d} I_m(\mathbf{x}) w_m,$$

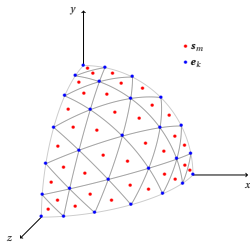
ETR semi-discrète

$$\mathcal{R}_m \left(\{I_n\}_{n=1}^{N_d} \right) = (\mathbf{s}_m \cdot \nabla + \beta(\mathbf{x})) I_m(\mathbf{x}) - \sigma_s(\mathbf{x}) \sum_{n=1}^{N_d} \mathbf{w}_n I_n(\mathbf{x}) \Phi_{m,n} - \kappa(\mathbf{x}) I_b(\mathbf{x}) = 0$$

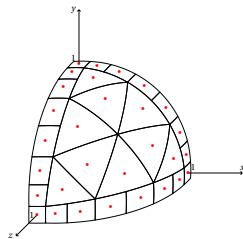
couples (s_m, w_m)



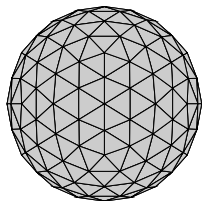
S_8



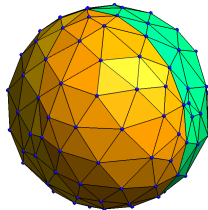
T_6



SqT_{83}



icosahedron niveau 2



maillage de la sphere

Streamline Upwind Petrov-Galerkin²

- ▶ Espace fonctionnel

$$\mathcal{V}_m^h = \{v \in L^2(\Omega^h) \text{ and } \mathbf{s}_m \cdot \nabla v \in L^2(\Omega^h)\}.$$

- ▶ Multiplication de (E_m) par la fonction de fonction test

$$f_m(v_h) = v_h + \gamma \mathbf{s}_m \cdot \nabla v_h \quad v_h \in V_h^{\text{SUPG}}$$

avec $\gamma(\mathbf{x}) = \gamma(h_i, N_d, \kappa, \sigma_s)$ ³

- ▶ Intégration en espace sur tout le domaine \mathcal{D}
- ▶ Inclusion des conditions aux limites par la méthode de Green.

2. G. Kanschat et al., eds. Numerical methods in multidimensional radiative transfer. Springer, 2009

3. M. Avila et al., CMAME, 2011

FEM $\triangleright\triangleright$ Variational formulation

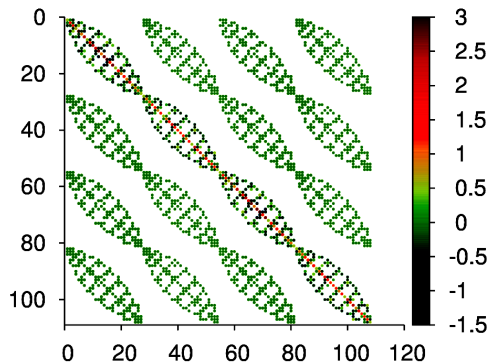
$$\left\| \begin{array}{l} \text{Find } \{I_m^h \in \mathcal{V}_m^h\}_{m=1}^{N_d} \text{ such that} \\ a_{m,m}(I_m^h, w^h) + \sum_{\substack{n=1 \\ n \neq m}}^{N_d} a_{m,n}(I_n^h, w^h) = l_m(w^h) \quad \forall w^h \in \mathcal{V}_m^h(w^h), \quad \forall m = 1, \dots, N_d \end{array} \right.$$

avec

$$\begin{aligned} a_{m,m}(I_m^h, w^h) = & - \int_{\Omega^h} \mathbf{s}_m \cdot \nabla w^h (I_m^h - \gamma \mathbf{s}_m \cdot \nabla I_m^h) \, d\mathbf{x} + \int_{\partial\Omega_m^+} \mathbf{s}_m \cdot \mathbf{n} w^h I_m^h \, d\mathbf{x} \\ & + \int_{\Omega^h} (\beta I_m^h - \mathbf{w}_m \Phi_{m,m} \sigma_s I_m^h) (w^h + \gamma \mathbf{s}_m \cdot \nabla w^h) \, d\mathbf{x}, \end{aligned}$$

$$a_{m,n \neq m}(I_n^h, w^h) = - \int_{\Omega^h} \mathbf{w}_n \Phi_{m,n} \sigma_s I_n^h (w^h + \gamma \mathbf{s}_m \cdot \nabla w^h) \, d\mathbf{x},$$

$$l_m(w^h) = - \int_{\partial\Omega_m^-} \mathbf{s}_m \cdot \mathbf{n} w^h I_{in} \, d\mathbf{x} + \int_{\Omega^h} \kappa I_b (w^h + \gamma \mathbf{s}_m \cdot \nabla w^h) \, d\mathbf{x}.$$



solveurs

- ▶ block-based : Source itérée (Jacobi), Gauss-Seidel, SOR
- ▶ matrice complète : GMRES, BICGStab

Éléments finis pour l'ETR

1 Les bases

Discrétisation angulaire

Discrétisation spatiale : SUPG

2 Allons plus loin

HPC : EF Vectoriels & calcul //

Gestion de la spécularité

3 Applications

Matériaux hétérogènes

Inversion

géométrie complexe

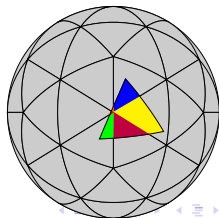
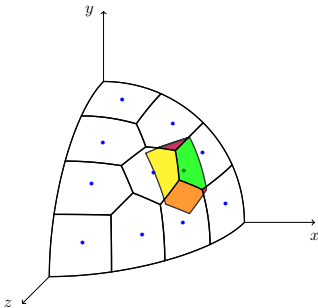
4 conclusion

Condition de réflexion

par ex. spéculaire :

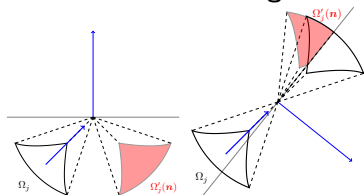
$$I_m^{\vee}(\mathbf{x}) = \rho(\mathbf{s}_m \cdot \mathbf{n}) \sum_{i=1}^{N_d} \delta_{m,j}(\mathbf{n}) I_j(\mathbf{x})$$
$$\implies \sum_{j \neq m} \left[\dots + \int_{\partial \mathcal{D}^{m-}} \delta_{m,j}(\mathbf{n}) I_j v(\mathbf{s}_m \cdot \mathbf{n}) d\Gamma \right]$$

Méthode de partitionnement : $\delta_{m,j}(\mathbf{n}) = \frac{\text{mes}(\Omega_m \cap \Omega_j)}{\text{mes}(\Omega_m)}$

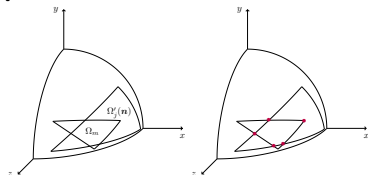


Specularity \gg Partitioning method⁴

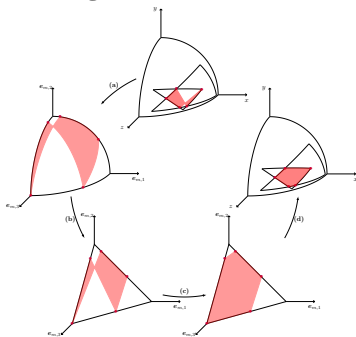
1. reflexion of solid angles



2. computation of intersection points



3. computation of the intersection area with nodes re-ordering



Mixed (vectorial) Finite Elements

From :

- ▶ Solid mechanics⁵
- ▶ CFD with FEM

Problem in vectorial aspect

- ▶ search for vector of Intensity \mathbb{I} using RTE in vectorial form :

$$\mathbb{S} \cdot \nabla \mathbb{I} + \beta \mathbb{I} - \Theta \mathbb{I} = \kappa I_b \mathbb{1}$$

utilizing vectorial trial function $\mathbb{V} + \gamma \mathbb{S} \cdot \nabla \mathbb{I}$

- ▶ weak form based on tensor product :

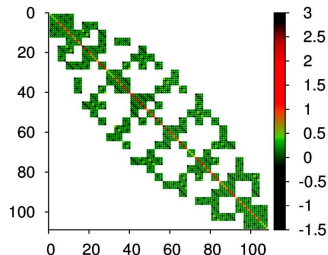
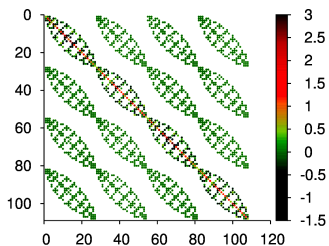
$$\int_{\mathcal{D}} [\mathbb{S} \cdot \nabla \mathbb{I} + \beta \mathbb{I} - \Theta \mathbb{I} - \kappa I_b \mathbb{1}]^T (\mathbb{V} + \gamma \mathbb{S} \cdot \nabla \mathbb{I}) = 0$$

- ▶ Output is single equation unlike normal SUPG where we had N_d equations.

Mixed (vectorial) Finite Elements ⁶

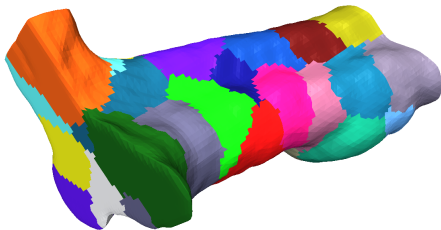
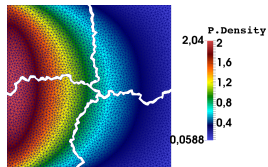
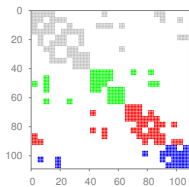
Permutation of unknowns :

$$\llbracket (\mathbf{x}_n, \mathbf{s}_k) \forall n, \forall k \implies \llbracket (\mathbf{x}_n, \mathbf{s}_k) \forall k, \forall n$$



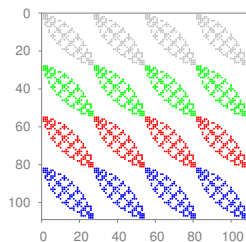
- ▶ Weakens the coupling : short banded matrix
- ▶ One step building + one step solving

Méthode de décomposition \triangleright (de) domaine

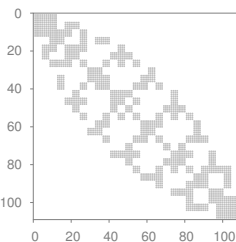


Méthode de décomposition \triangleright angulaire

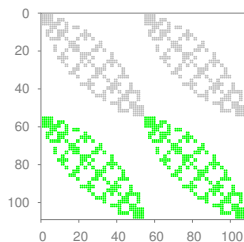
e.g. $N_d = 4$



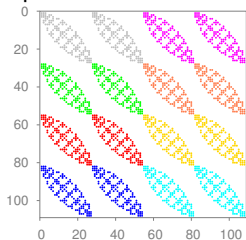
4 proc



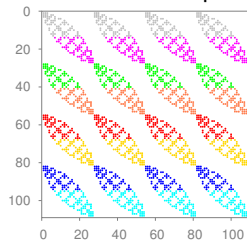
1 proc



2 proc

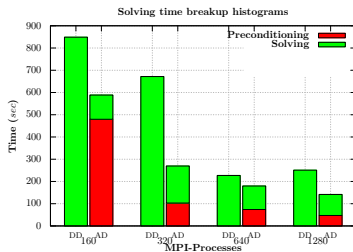
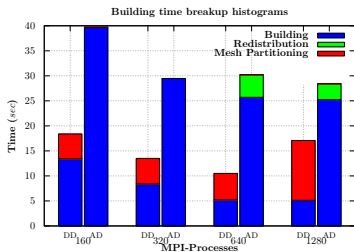
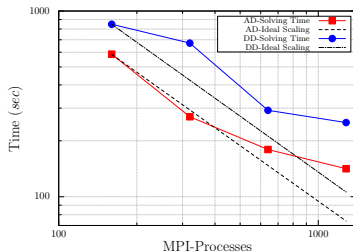
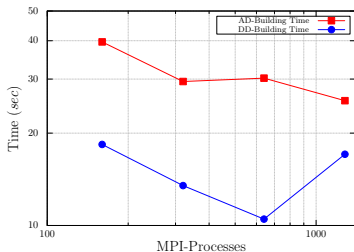


8 proc



8 proc after redistrib.

3D – 320 dir – 107 484 nodes – P1 \Rightarrow ndof=34 10⁶



Contents

1 Les bases

Discrétisation angulaire

Discrétisation spatiale : SUPG

2 Allons plus loin

HPC : EF Vectoriels & calcul //

Gestion de la spécularité

3 Applications

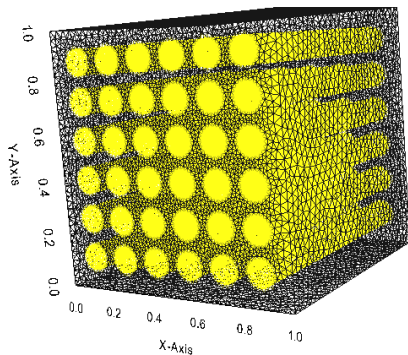
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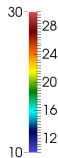
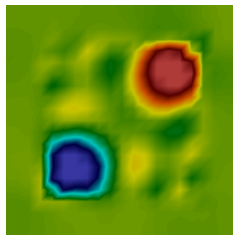
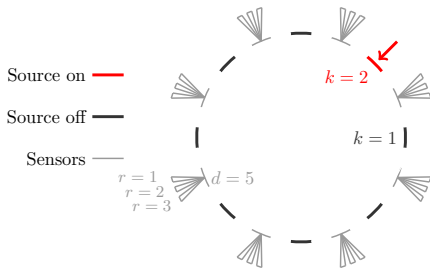
4 conclusion

Application ▷▷ Heterogeneous material

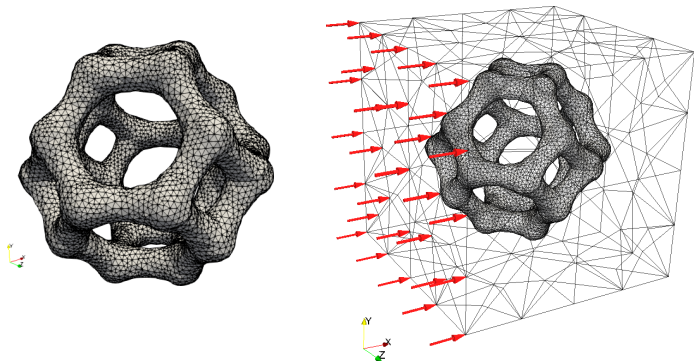


- ▷ Test case meshes and geometry, radiative property σ ■ = 0.1 ■ = 10.0, radiative property κ ■ = 10.0 ■ = 0.1.

Application ▷▷ Optical tomography (Inverse problem)

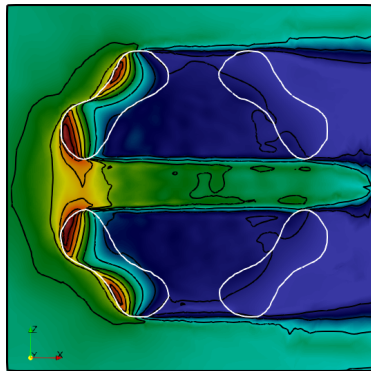
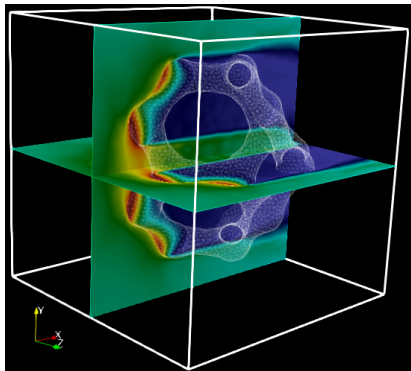


Application ▷▷ Complex geometry

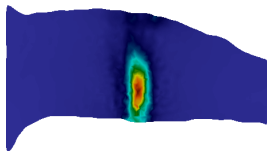
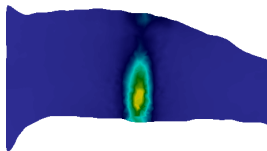
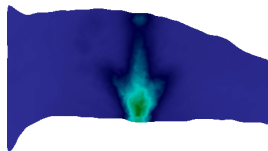
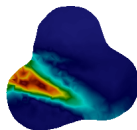
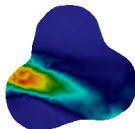
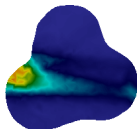
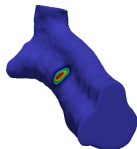
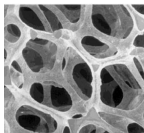
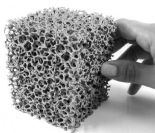


▷ The k-cell and the immersed mesh with collimated boundary conditions. Left: the k-cell skeleton, right: the k-cell with air mesh and boundary conditions.

Application \triangleright Complex geometry



Application \gg Specular reflections taken into account^{8 9}



$N_d = 20$

$N_d = 80$

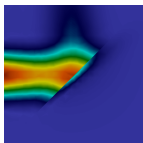
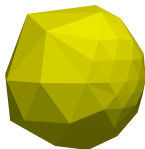
$N_d = 320$

8. X-Ray tomography performed at the European Synchrotron Radiation Facilities (Grenoble, France) on the ID19 beamline

9. Le Hardy et al., JQSRT, 2017

Travaux en cours et futurs

- ▶ adaptation de maillage pour x et pour s
- ▶ angular FEM
- ▶ réflexions internes et réfraction



Avantages et inconvénients

- ▶ approche systématique
- ▶ utilisation de bibliothèques
 - ▶ **EF** : FreeFem++, deal.II, Fenics
 - ▶ **solveurs** : PETSc
 - ▶ **mailleurs et remailleurs** : gmsh, mmg
 - ▶ **decomposition domaine** : METIS, ...
- ▶ communauté scientifique
- ▶ couplages
- ▶ système linéaire
- ▶ inversion : $\text{prop}(x)$