Simulating some interface problems with FreeFem++

(PhD subject: "*A FE approximation of a biofilm growth model*")

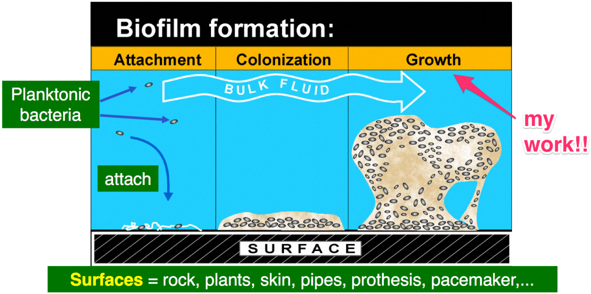
DINH Anh-Thi
under the guidance of
Linda EL ALAOUI & Adel BLOUZA

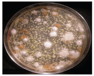
LAGA - University Paris 13

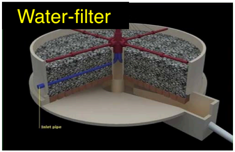
Seventh Workshop on FreeFem++
Wednesday, 16/12/15

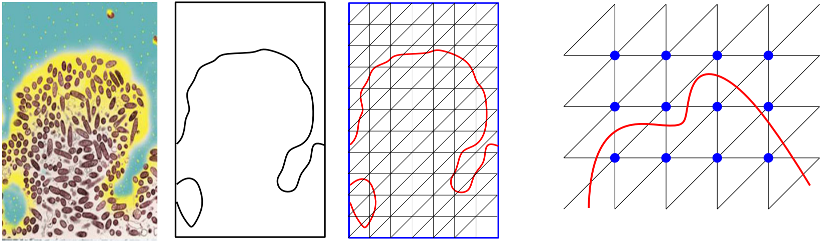
Contents

A biofilm is any group of microorganisms in which cells stick to each other on a surface.









- **Model** : the groth of biofilm.
- **What I want** : simulate the growth of the biofilm with time.
  - Generate only 1 mesh for the whole process.
  - The mesh doesn't fit the interface.
- **Method to use** : Unfitted-Nistche FEM[1] + Level set method.

[1] This method is introduced in Anita Hansbo and Peter Hansbo (2002). "An unfitted finite element method, based on Nitsche's method, for elliptic interface problems". In: 191, pp. 5537–5552.

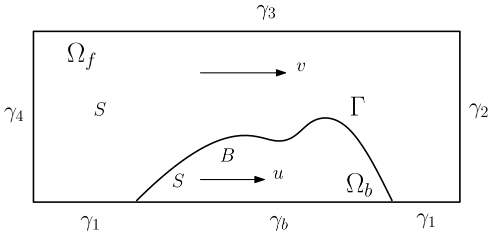
Problem model on $\Omega = \Omega_f \cup \Omega_b, \overline{\Omega}_f \cap \overline{\Omega}_b = \Gamma$

$$\begin{cases} \textbf{Substrate}\text{: } \partial_t S - \underbrace{\nabla \cdot (D_S^* \nabla S)}_{\text{diffusion}} + \underbrace{\mathbf{u}^* \cdot \nabla S}_{\text{advection}} + \underbrace{Bg^*(S)}_{\text{consumption}} & = 0 \quad \text{in } (0,T) \times \Omega_f \cup \Omega_b \\ \textbf{Bacteria}\text{: } \partial_t B - \underbrace{\nabla \cdot (D_B \nabla B)}_{\textit{diffusion}} + \underbrace{\mathbf{u}^* \cdot \nabla B}_{\text{advection}} - \underbrace{Bg^*(S)}_{\text{growth}} & = 0 \quad \text{in } (0,T) \times \Omega_b \\ \textbf{Biomass flow}\text{: } -\Delta\Phi + Bg^*(S) & = 0 \quad \text{in } (0,T) \times \Omega_f \cup \Omega_b \\ \textbf{Fluid flow}\text{: } \partial_t v - \nu \Delta v + \nabla p & = F \quad \text{in } (0,T) \times \Omega_f \end{cases}$$

with some boundary conditions and (especially) conditions on interface

$$[S] = 0, [D_S^* \nabla_{\mathbf{n}} S] = 0.$$
$$B = 0, \nabla_{\mathbf{n}} B = 0.$$

where $[\mu]$ is the jump of μ at the interface.



Consider only substrate (S) equation to explain the method.

Find $S \in V$ such that,

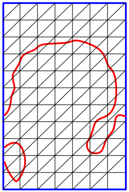
$$-\nabla\cdot(D_S^*\nabla S) + \mathbf{u}^*\cdot\nabla S + Bg^*(S) = 0. \quad (1)$$

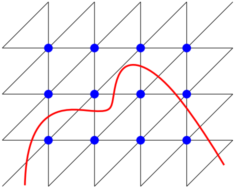
Find $S \in V$ such that,

$$a(S,\varphi) = L(\varphi),\ \forall\varphi\in V. \quad (2)$$

Find $S_h \in V_h$ such that,

$$a_h(S_h,\varphi_h) = L(\varphi_h),\ \forall\varphi_h\in V_h. \quad (3)$$





- FE space $V_h = \text{span}\{\Phi_i\} \Rightarrow$ Numerical solution $u_h = \sum_i u_i\Phi_i$.
- Strong problem (1) $\Leftarrow$ Weak problem (2) $\Leftarrow$ Discrete problem (3).
- **Question 1** : which FE we need to build to solve the discrete problem (3) when the interface changes?
- **Question 2** : How to implement with FreeFEM++? (*How to tell the computer do what the theory says?*)

The discrete problem (3),

$$a_h(S_h, \varphi_h) = L(\varphi_h), \, \forall \varphi_h \in V_h^\Gamma.$$

where

$$V_h^\Gamma := \{v_h \in L^2(\Omega) : v_h|_{\Omega_i} \in H^1(\Omega_i), v_h \in \mathbf{P}^1(K), \forall K \in \mathcal{K}_h^1 \cup \mathcal{K}_h^2\}$$

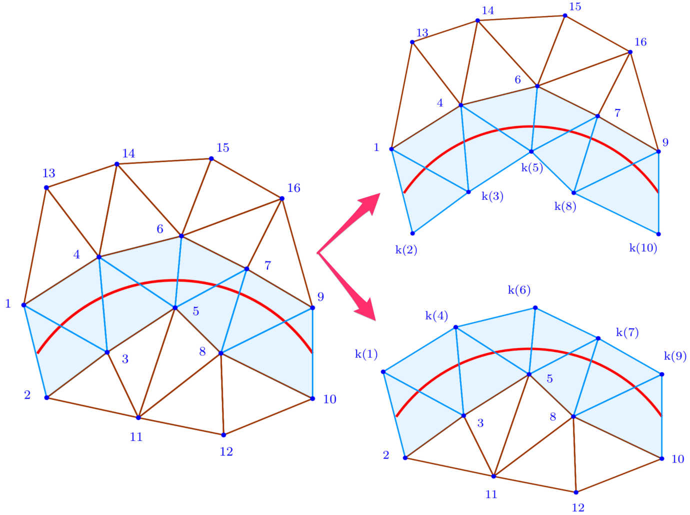
And construct a form a_h as

$$a_h(S_h, \phi) := \sum_{K \in \mathcal{K}_h^1 \cup \mathcal{K}_h^2} \left((D_S^* \nabla S_h, \nabla \phi)_K - ((\nabla \cdot u^*) S_h, \phi)_K - (S_h u^*, \nabla \phi)_K + (Bg^*(S_h), \phi)_K \right)$$

$$+ \sum_{e \in \Gamma_h} \underbrace{\left(- \underbrace{([\![S_h]\!], \{D_S^* \nabla_n \phi\})_e}_{\text{symmetrization}} - \underbrace{(\{D_S^* \nabla_n S_h\}, [\![\phi]\!])_e}_{\text{consistency}} + \underbrace{(\lambda [\![S_h]\!], [\![\phi]\!])_e}_{\text{penalization}} \right)}_{\text{The key point of the method}}$$

Define a basis of V_h^Γ

Idea : **each standard** basis function around interface $\xrightarrow[]{\textit{replaced by}}$ **2 new** basis functions restricted to Ω_1 and Ω_2



Theorem

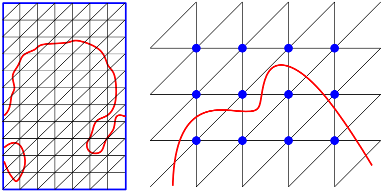
- **Consistency** : *Strong solution S of* (1) *also satisfies the discrete problem* (3).
- **Error & Convergence** :

$$|||S - S_h||| \leq Ch^{\mathbf{1}} \left(\|S\|^2_{H^2(\Omega_1)} + \|S\|^2_{H^2(\Omega_2)} \right)^{1/2}$$

$$\|S - S_h\|_{L^2(\Omega)} \leq Ch^{\mathbf{2}} \left(\|S\|^2_{H^2(\Omega_1)} + \|S\|^2_{H^2(\Omega_2)} \right)^{1/2}$$

where $|||v|||^2 := \|\{\nabla_n v\}\|^2_{-1/2,h,\Gamma} + \|[\![v]\!]\|^2_{1/2,h,\Gamma} + \|v\|^2_{H^1(\Omega_1 \cup \Omega_2)}$

Algorithm with FreeFem++



By using FreeFem++,

- **Step 1**: Generate the mesh
- **Step 2**: P_1-FE space, standard basic functions, standard nodes.
- **Step 3**: Identify the location of interface (triangles and nodes around the interface)
- **Step 4**: Build stiffness matrix and load vector.
- **Step 5**: Solve the problem
- **Step 6**: Update the interface and go back to **Step 3** for the next time step.
- Finish.

Build a stiffness matrix

Thanks to the command `levelset` in FreeFem++, we can express the idea in theoritical part into FreeFem++ to build the stiffness matrix A and the load vector F

$$AU = F.$$

Sample code,

```
varf b1(S,v) = int2d(Th,levelset=phi)(...) //in Omega_1
      + on(...); //boundary conditions
varf b2(S,v) = int2d(Th,levelset=-phi)(...) //in Omega_2
      + on(...); //boundary conditions
```

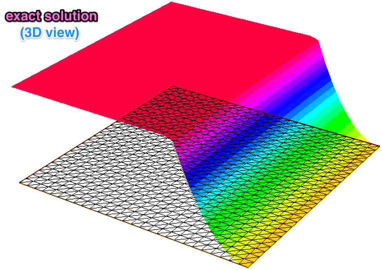
$$\Omega = [0,1] \times [0,1],$$
$$\Gamma = \{\xi\} \times [0,1]\,(0 < \xi < 1),$$
$$\Omega_1 = [0,\xi] \times [0,1],$$
$$\Omega_2 = [\xi,1] \times [0,1]$$

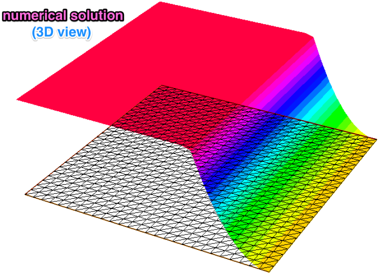
$$\begin{cases} -\nabla \cdot (k\nabla u) & = f, \text{ in } \Omega \\ [\![u]\!] & = 0, \text{ on } \Gamma \\ [\![k\nabla u \cdot \mathbf{n}]\!] & = 0, \text{ on } \Gamma. \end{cases}$$

The exact solution is

$$u(x,y) = \begin{cases} \frac{x^2}{k_1} & (x \le \xi) \\ \frac{x^2-\xi^2}{k_2} + \dfrac{\xi^2}{k_1} & (x > \xi) \end{cases}$$

The parameters:
$k_1 = \mathbf{0.1}$, $k_2 = \mathbf{1000}$,
$\lambda = \mathbf{10^5}, \xi = \mathbf{0.3}, f = -2.$





[2] Nelly Barrau et al. (2012). "A robust variant of NXFEM for the interface problem". In: *Comptes Rendus Mathematique* 350.15-16, pp. 789–792.

Validation of the code : Sinha's test case[3]

$$\Omega = [0,2] \times [0,1],$$
$$\Gamma = \{\xi\} \times [0,1]\,(0 < \xi < 1),$$
$$\Omega_1 = [0,\xi] \times [0,1],$$
$$\Omega_2 = [\xi,2] \times [0,1]$$

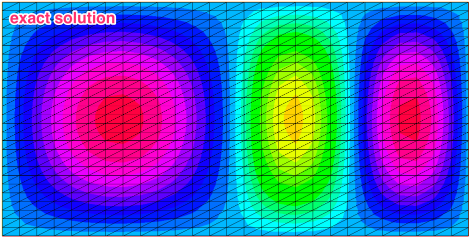
$$\begin{cases} -\nabla \cdot (k \nabla u) & = f, \text{ in } \Omega \\ [\![u]\!] & = 0 \text{ on } \Gamma \\ [\![k \nabla u \cdot \mathbf{n}]\!] & = 0 \text{ on } \Gamma \\ u & = 0 \text{ on } \partial\Omega \end{cases}$$

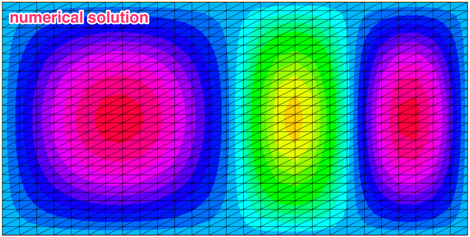
The exact solution is

$$u_{\text{ex}}(x,y) = \begin{cases} u_1 := \sin(\pi x)\sin(\pi y) \\ u_2 := -\sin(2\pi x)\sin(\pi y) \end{cases}$$

$$f = \begin{cases} f_1 := 2\sin(\pi x)\pi^2 \sin(\pi y) \\ f_2 := -\frac{5}{2}\sin(2\pi x)\pi^2 \sin(\pi y) \end{cases}$$

The parameters:
$k_1 = \mathbf{1}, k_2 = \mathbf{1/2}$,
$\lambda = \mathbf{10^5}, \xi = \mathbf{1}$.



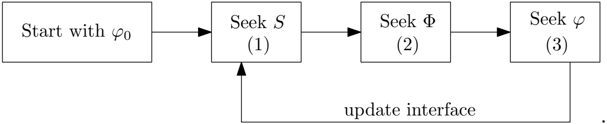


[3] Rajen Kumar Sinha and Bhupen Deka (2005). "An unfitted finite-element method for elliptic and parabolic interface problems". eng. In: *IMA journal of numerical analysis* 27.3, pp. 529–549.

$$\begin{cases} \textbf{Substrate}: \ \partial_t S - \underbrace{\nabla \cdot (D_S^* \nabla S)}_{\text{diffusion}} + \underbrace{\mathbf{u}^* \cdot \nabla S}_{\text{advection}} + \underbrace{Bg^*(S)}_{\text{consumption}} & = 0 \quad \text{in } (0,T) \times \Omega_f \cup \Omega_b \\ \textbf{Biomass flow}: \ -\Delta \Phi + Bg^*(S) & = 0 \quad \text{in } (0,T) \times \Omega_f \cup \Omega_b \end{cases}$$

We track the interface via level set function φ at every time step by using following algorithm

$$\partial_t \varphi + \nabla \Phi \cdot \nabla \varphi = 0.$$




```
... //code for solving Phi

Vh dxpot = dx(pot);
Vh dypot = dy(pot);
phinew = convect([dxpot,dypot],-dt,phi); //find the new interface function
phi = phinew; //update the levelset function
```

Validation of the code

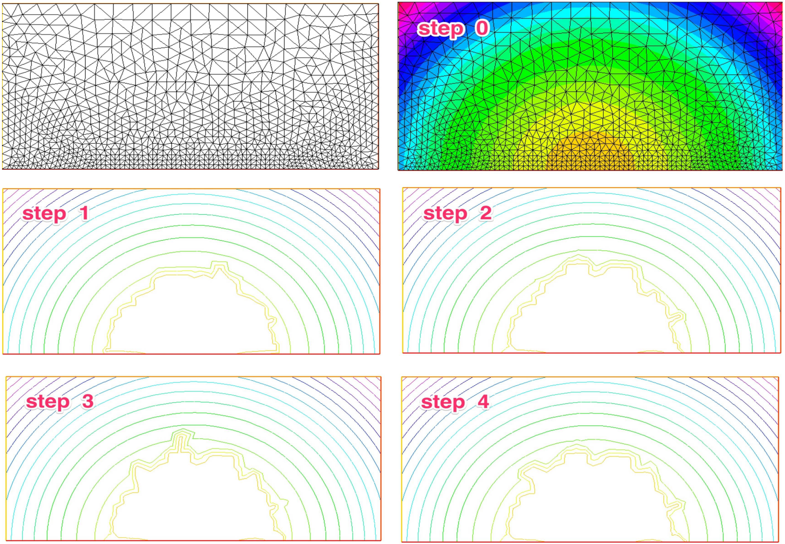


Figure: The level set function φ.

Validation of the code

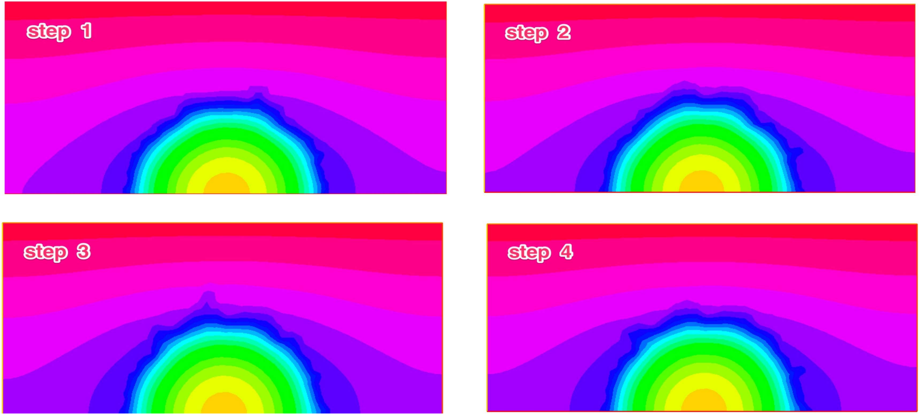


Figure: Plot of substrate concentration.

Conclusion

Forthcoming work:

- Numerical analysis of the full nonlinear system (work in progress)
- Work on the realistic data from experiments.