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***2D simulation of chemotactic bacteria aggregation***

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## 2D simulation of chemotactic bacteria aggregation

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Thème 4 — Simulation et optimisation  
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Projet M3N

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**Abstract:** We start from a mathematical model which describes the collective motion of bacteria taking into account the underlying biochemistry. This model was first introduced by Keller-Segel [1]. A new formulation of the system of partial differential equations is obtained by the introduction of a new variable (this new variable is similar to the quasi-Fermi level in the framework of semiconductor modelling). This new system of P.D.E. is approximated via a mixed finite element technique. The solution algorithm is then described and finally we give some preliminary numerical results. Especially our method is well adapted to compute the concentration of bacteria.

**Key-words:** biophysics, chemotaxis, numerical simulation, mixed finite element

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# Simulation bidimensionnelle de l'aggrégation des bactéries

**Résumé :** Nous partons d'un modèle mathématique qui décrit le déplacement collectif de bactéries et qui prend en compte la biochimie sous-jacente. Ce modèle a été introduit initialement par Keller-Segel [1]. Une nouvelle formulation du système d'équations aux dérivées partielles est obtenue par l'introduction d'une variable similaire au quasi-niveau de Fermi de la modélisation des semi-conducteurs. Le nouveau système est approché par une technique d'éléments finis mixtes. On décrit ensuite l'algorithme de résolution et donnons quelques résultats numériques préliminaires. La méthode présentée est particulièrement adaptée au calcul de concentrations de bactéries

**Mots-clés :** biophysique, chemotaxis, simulation numérique, éléments finis mixtes

# 1 Problem Formulation

The equations for the collective motion of the bacteria can be derived (with no free parameters) from the underlying biochemistry. The basic equations for the bacterial density  $\rho$  and the attractant concentration  $c$  are (see [1][2][3][4])

$$\frac{\partial \rho}{\partial t} = D_b \nabla^2 \rho - \nabla \cdot (k\rho \nabla c) + a\rho \quad (1)$$

$$\frac{\partial c}{\partial t} = D_c \nabla_c^2 c + \alpha\rho \quad (2)$$

where

$D_b$  is the bacterial diffusion constant

$k$  is the chemotactic coefficient (or chemotactic sensitivity)

$a$  is the rate of bacterial division

$\alpha$  is the rate of attractant production

$D_c$  is the chemical diffusion constant.

The terms in equation (1) include the diffusion of bacteria, chemotactic drift and division of bacteria. Equation (2) expresses the diffusion and production of attractant.

In [2] for example, typical numerical values are given for the various parameters,

$$\begin{aligned} D_b &= 7 \cdot 10^{-6} \text{ cm}^2/\text{s}, & D_c &= 10^{-5} \text{ cm}^2/\text{s}, \\ k &= 10^{-16} \text{ cm}^5/\text{s}, & \alpha &= 10^3 \text{ /s/bacteria.} \end{aligned}$$

Taking a bacterial density  $\rho = 10^6/\text{cm}^3$  the length scale is about 260 microns and the time scale 100s.

In some semi-solid media (like agar), the diffusion of bacteria is much slower than attractant diffusion which motivate to drop the term with time derivative in equation (2). This limit case is also convenient for asymptotic behaviour when considering other media. Notice that for other applications, the diffusion of attractants is neglected, this is the case for angiogenesis, see [5] and the references therein.

In addition, cells divide much more slowly than the dynamics take place (the time scale for cell division is about 2 hours) so that we can take  $a = 0$  in (1) for an entry level model. The model used for the numerical simulations is then the following

$$\frac{\partial \rho}{\partial t} = D_b \nabla^2 \rho - \nabla \cdot (k\rho \nabla c) \quad (3)$$

$$0 = D_c \nabla_c^2 c + \alpha\rho \quad (4)$$

which we re-write (for convenience)

$$-\text{div}(D_c \text{grad } c) - \alpha\rho = 0 \quad (5)$$

$$\frac{\partial \rho}{\partial t} - \text{div}(D_b \text{grad } \rho - k\rho \text{grad } c) = 0. \quad (6)$$

This last formulation ((5)-(6)), strongly looks like a classical model of transient drift-diffusion of electrons in semiconductor media (nevertheless the term which corresponds here to the attractant production is with an opposite sign). The attractant concentration  $c$  corresponds to the electrostatic potential ( $\varphi$ ), the bacterial density  $\rho$  to the electron density ( $n$ ), the chemotactic coefficient  $k$  to the electron mobility ( $\mu_n$ ). As in semiconductor modelling framework, a new formulation of system ((5)-(6)) will be obtained by introduction of a variable which is similar to the electron quasi-Fermi level and denoted by  $\varphi_n$ .

Note that we can find in the paper [2], one other formulation of eq. (4)

$$0 = D_c \nabla_c^2 + \alpha \rho e^{-\rho/\rho^*} \quad (7)$$

which can be used when modelling the following fact: when the bacterial density becomes too high, the bacteria consume all the food sources (succinate and oxygen) in their local environment and cease producing the attractant aspartate. The parameter  $\rho^*$  is the cutoff bacterial density.

One of the problem that has attracted biologists and mathematicians is to understand pattern formation in such models. The most noticeable, and complex also is the aggregation of bacteria [6][7][8] [2][4]. In this paper we investigate this pattern based on a mixed finite element method. We begin with another formulation based on quasi-Fermi levels, then we describe the finite element algorithm and we present in a fourth section some numerical results.

## 2 New Formulation of the ‘‘Chemotaxis Model’’

First of all we can introduce a scaling on the  $c$  variable (attractant concentration) via the parameter  $q$ .

$$C = \frac{\tilde{C}}{q} \quad (8)$$

The system (5)-(6), becomes

$$- \operatorname{div}(D_c \operatorname{grad} \tilde{c}) - q\alpha\rho = 0 \quad (9)$$

$$\frac{\partial \rho}{\partial t} - \operatorname{div} \left[ D_b \operatorname{grad} \rho - \frac{k}{q} \rho \operatorname{grad} \tilde{c} \right] = 0 \quad (10)$$

(+  $\frac{\partial \tilde{c}}{\partial t}$  could be added to the left hand side of (9) if the transient equation for the attractant diffusion was considered). We introduce a new variable  $\varphi_n$  by setting

$$\rho = \rho(\tilde{c}, \varphi_n) = \rho_0 e^{\frac{\tilde{c} + \varphi_n}{z}} \quad (11)$$

where

- $\rho_0$  is a constant (which corresponds to a given bacterial density, the variable  $\tilde{c}$  and  $\varphi_n$  (or their sum) are then equal to zero)

- $z = \frac{q D_b}{k}$ .

This class of variables is useful because we expect high values of  $\rho$  (collapse) and the potential  $\varphi_n$  is a more reasonable quantity. The system of equations can now be written as

$$- \operatorname{div}(D_c \operatorname{grad} \tilde{c}) - \tilde{\alpha} \rho(\tilde{c}, \varphi_n) = 0 \quad (12)$$

$$\frac{\partial \rho(\tilde{c}, \varphi_n)}{\partial t} - \operatorname{div}(\tilde{k}\rho(\tilde{c}, \varphi_n) \operatorname{grad} \varphi_n) = 0 \quad (13)$$

where

$$\tilde{k} = k/q, \quad \tilde{\alpha} = \alpha q$$

The system of equation (12)-(13) where the unknowns are  $\tilde{c}$  and  $\varphi_n$  will be used for the numerical approximation. This system has to be completed with appropriate boundary condition on  $\tilde{c}$  and  $\varphi_n$  and initial condition for the bacterial density  $\rho$ .

Eq. (12) is similar to the Poisson equation and eq. (13) to the electron continuity equation in the semiconductor framework.

### 3 Mixed Finite Element Approximation and Solution Algorithm

#### 3.1 Numerical approximation (M.F.E.)

Following [9][10][11][12], and assuming that Dirichlet boundary condition on a part of the boundary ( $\Gamma_d$ ) – of the computational domain  $\Omega$  – and Neumann boundary condition on the complementary boundary part ( $\Gamma_n$ ) hold for the variables  $\tilde{c}$  and  $\varphi_n$ , we introduce the flux variables

$$\vec{V} = D_c \operatorname{grad} \tilde{c} \quad , \quad \vec{J}_\rho = \tilde{k}\rho(\tilde{c}, \varphi_n) \operatorname{grad} \varphi_n \quad , \quad (14)$$

and an equivalent formulation of the system (12)-(13)

$$\left\{ \begin{array}{ll} -\operatorname{div} \vec{V} - \tilde{\alpha}\rho(\tilde{c}, \varphi_n) = 0 & \text{in } \Omega \quad (15) \\ \vec{V} = D_c \operatorname{grad} \tilde{c} & \text{in } \Omega \quad (16) \\ \vec{V} \cdot \vec{n} = D_c \cdot f_{1n} & \text{on } \Gamma_{n1} \quad (17) \\ \tilde{c} = f_{1d} & \text{on } \Gamma_{d1} \quad (18) \end{array} \right.$$

$$\left\{ \begin{array}{ll} \frac{\partial \rho(\tilde{c}, \varphi_n)}{\partial t} - \operatorname{div} \vec{J}_\rho = 0 & \text{in } \Omega \quad (19) \\ \vec{J}_\rho = \tilde{k}\rho(\tilde{c}, \varphi_n) \operatorname{grad} \varphi_n & \text{in } \Omega \quad (20) \\ \vec{J}_\rho \cdot \vec{n} = \tilde{k}\rho f_{2n} & \text{on } \Gamma_{n2} \quad (21) \\ \varphi_n = f_{2n} & \text{on } \Gamma_{d2} \quad (22) \end{array} \right.$$

$f_{1d}$  and  $f_{1n}$  are given boundary conditions on  $\tilde{c}$  (respectively of Dirichlet and Neumann type), and  $f_{2d}$  and  $f_{2n}$  similarly for  $\varphi_n$ .

The system we have to consider is now made up of four equations (15) (16) (19) (20) with the four unknowns ( $\tilde{c}, \vec{V}, \varphi_n, \vec{J}_\rho$ ).

We consider now the following Sobolev spaces

$$H(\operatorname{div}) = \{w | w \in (L^2(\Omega))^2, \operatorname{div} w \in L^2(\Omega)\} \quad (23)$$



$$V_{0,i} = \{w | w \in H(\text{div}), \quad w \cdot n = 0 \text{ on } \Gamma_{n,i}\} \quad (24)$$

Then, for sufficiently smooth data we can obtain the following equivalent dual mixed variational formulation of the original problem.

$$\text{Find } \begin{cases} \vec{V} \in H(\text{div}), & \tilde{c} \in L^2(\Omega) \\ \vec{J}_\rho \in H(\text{div}), & \varphi_n \in L^2(\Omega) \end{cases} \text{ such that}$$

$$\left\{ \begin{aligned} & - \int_{\Omega} \text{div } \vec{V} \cdot v_1 \, dx - \int_{\Omega} \tilde{\alpha} \rho(\tilde{c}, \varphi_n) \cdot v_1 \, dx = 0 \quad \forall v_1 \in L^2(\Omega) \end{aligned} \right. \quad (25)$$

$$\left\{ \begin{aligned} & \int_{\Omega} [D_c]^{-1} \vec{V} \cdot \vec{w}_1 \, dx + \int_{\Omega} \tilde{c} \cdot \text{div } \vec{w}_1 \, dx - \int_{\Gamma_{d1}} f_{1d} \cdot \vec{w}_1 \cdot \vec{n} \, d\Gamma = 0 \quad \forall \vec{w}_1 \in V_{0,1} \end{aligned} \right. \quad (26)$$

$$\left\{ \begin{aligned} & \vec{V} \cdot \vec{n} = D_c f_{1n} \text{ on } \Gamma_{n,1} \end{aligned} \right. \quad (27)$$

$$\left\{ \begin{aligned} & \int_{\Omega} \frac{\partial \rho(\tilde{c}, \varphi_n)}{\partial t} \cdot v_2 \, dx - \int_{\Omega} \text{div } \vec{J}_\rho \cdot v_2 \, dx = 0 \quad \forall v_2 \in L^2(\Omega) \end{aligned} \right. \quad (28)$$

$$\left\{ \begin{aligned} & \int_{\Omega} [\tilde{k} \rho(\tilde{c}, \varphi_n)]^{-1} \vec{J}_\rho \cdot \vec{w}_2 \, dx + \int_{\Omega} \varphi_n \cdot \text{div } \vec{w}_2 \, dx - \int_{\Gamma_{d2}} f_{2d} \cdot \vec{w}_2 \cdot \vec{n} \, d\Gamma = 0 \quad \forall \vec{w}_2 \in V_{0,2} \end{aligned} \right. \quad (29)$$

$$\left\{ \begin{aligned} & \vec{J}_\rho \cdot \vec{n} = \tilde{k} \rho(\tilde{c}, \varphi_n) \cdot f_{2n} \text{ on } \Gamma_{n,2} \end{aligned} \right. \quad (30)$$

For the numerical applications (as often it happens) we will have  $f_{1n} \equiv f_{2n} \equiv 0$  so that we look for  $\vec{V}$  and  $\vec{J}_\rho$  in  $V_{0,1}$  and  $V_{0,2}$  respectively.

As in [9][12][13][14] the previous formulation (25)–(27) and (28)–(30) allows us to realize easily a discrete approximation via mixed finite elements.

We retain the lowest order M.F.E. of Raviart-Thomas ( $R_0^T$ ) for implementation. After a triangulation  $\mathcal{T}_h$  of the computational domain  $\Omega \subset \mathbb{R}$ , we define the following finite dimensional spaces

$$L_h = \{v_h \in L^2(\Omega) | \forall K \in \mathcal{T}_h, \quad v_h|_K = \text{constant}\} \quad , \quad (31)$$

$$V_h = \{w_h \in H(\text{div}) | \forall K \in \mathcal{T}_h, \quad w_h(x, y)|_K = \begin{vmatrix} \alpha_K \\ \beta_K \end{vmatrix} + \gamma_K \begin{vmatrix} x \\ y \end{vmatrix}\}. \quad (32)$$

We assume also that  $\Gamma_{n,i}$  ( $i = 1, 2$ ) is obtained by union of edges of triangles which belong to the mesh  $\mathcal{T}_h$  and that

$$V_{0,i,h} = V_{0,i} \cap V_h. \quad (33)$$

Then the discrete formulation of the problem follows directly from (25)–(30) by replacing  $L^2(\Omega)$  by  $L_h$  and  $V_{0,i}$  by  $V_{0,i,h}$ .

### 3.2 Solution algorithm

Referring again to the publications related to semiconductor area [9][11][12] [13][14], various algorithms are described for a “stationary” version of system (25)–(30) (i.e. without  $\frac{\partial \rho}{\partial t}$  term !). Let us recall here the major characteristics of these numerical schemes.

- association to each (stationary) equation (primal variable) of the system of an “artificial” transient equation,

- semi-implicit (Peaceman Rachford, Douglas Rachford) or implicit (Backward-Euler) time discretization schemes for the “artificial” evolution equations. Use of local time steps,
- relaxation on the equations at each time step,
- for each time step, and for each equation of the system, solution of the nonlinear problem by Newton-Raphson technique.

The fact that we associate an “evolution” equation and the use of implicit or semi-implicit schemes is an other way to consider augmented Lagrangian techniques for the solution of saddle point problems [15] arising from the mixed formulation. Local time steps are closely connected with the penalty functions in the framework of Augmented Lagrangian techniques.

Special features of such an approach are relative simplicity and ease of implementation of model extensions. It is easy to add one equation to the system without need of deep changes in the algorithm architecture. Equations are handled successively in the algorithmic process. This numerical scheme, specially when using backward Euler for time discretization, has appeared to be rather efficient for semiconductor device (drift diffusion model and standard applied potentials). One can think reasonably that if the coupling between the equations of the system is not “too strong” then the relaxation on the equations do not penalize strongly the (speed of) convergence of the iterates towards the stationary solution of the whole system. This is certainly what happens in the static drift diffusion model for regimes not so far from the equilibrium state.

Nevertheless this solution technique failed when applied to energy-transport models for semiconductors [6] [7]. One equation (relative to electron temperature) has been added to the drift diffusion model and the constitutive relation for the current density has been slightly modified. The previous numerical scheme works correctly only for solutions very close to the equilibrium state. In order to recover the algorithmic behaviour, for typical load range, similar to the behaviour, obtained when using the drift diffusion model, one has to consider simultaneously (couple) the equations relative to the electron current continuity and the energy [7]. The implementation of such numerical scheme in a little bit more complicated but seems a necessity to insure the convergence of the iterative procedure.

In past few years we are also interested by the numerical simulation of the transient behaviour (physical transient) of a semiconductor device governed by the drift diffusion model (numerical simulation of the switching of a diode). The model is very close to the “chemotaxis model”.

After the semi-discretization in time, using fully implicit scheme, we have to deal with a sequence of “quasi-static” problems which are similar to the static drift diffusion problem himself, but generally easier to solve because the nonlinearities involved are of lower amplitude. The degree of nonlinearity may be controlled in practice by the physical time step. For “very small time step” the operator governing the transient tends to the identity operator (linear operator) and for sufficiently large time steps, the operator corresponds to the static drift diffusion (fully non linear operator).

The first attempt for the numerical simulation of the transient behaviour was to apply the most efficient scheme developed for the static drift diffusion model at each “quasi static” problem obtained via the semi-discretization in time of the transient model. As the time step (physical time step) becomes smaller and smaller the convergence of the iterates becomes more and more difficult to obtain and solution of quasi-static problems is not reached. The whole algorithm failed to converge. The only plausible explanation to this algorithm behaviour is that, as the time step (physical time step) becomes smaller, the coupling between the equations (Poisson equation

and continuity equations) becomes stronger, and the relaxation strategy (decoupling) used in the numerical algorithm is no more adapted. A more implicit scheme has to be used for the solution of the quasi-static problems. The fully implicit scheme (on the system and not on each equation of the system) has been implemented and convergence was restored.

We describe now an adaptation of this numerical scheme as simply as possible.

A) Semi-discretization in time (physical time), by a fully implicit scheme (Backward-Euler)

The solution of the problem represents an approximation of the transient solution at different times  $T_{n+1} = T_n + \delta t$  ( $n = 0, 1, 2, 3, \dots$ ); the time step  $\delta t$  may be adapted if needed. The formulation of the sequence of quasi-static problems is the following:

Find  $(\tilde{c}^{n+1}, \vec{V}^{n+1}, \varphi_n^{n+1}, \vec{J}_\rho^{n+1})$  solution of

$$-\operatorname{div} \vec{V}^{n+1} - \tilde{\alpha} \rho(\tilde{c}^{n+1}, \varphi_n^{n+1}) = 0 \quad (34)$$

$$\int_{\Omega} [D_c]^{-1} \vec{V}^{n+1} \cdot w_1 \, dx + \int_{\Omega} c^{n+1} \operatorname{div} w_1 \, dx - \int_{\Gamma_{d1}} f_{1d} w_1 \cdot n \, d\Gamma = 0, \quad \forall w_1 \in V_{0,1,h} \quad (35)$$

$$-\operatorname{div} \vec{J}_\rho + \frac{1}{\delta t} [\rho(\tilde{c}^{n+1}, \varphi_n^{n+1}) - \rho(\tilde{c}^n, \varphi_n^n)] = 0 \quad (36)$$

$$\int_{\Omega} [\tilde{k} \rho(\tilde{c}^{n+1}, \varphi_n^{n+1})]^{-1} \vec{J}_\rho \cdot w_2 \, dx + \int_{\Omega} \varphi_n^{n+1} \cdot \operatorname{div} w_2 \, dx - \int_{\Gamma_{d2}} f_{2d} w_2 \cdot n \, d\Gamma = 0, \quad \forall w_2 \in V_{0,2,h}. \quad (37)$$

B) Each quasi-static problem (index  $n$ ) is solved via artificial transient [12][14]. The index of time discretization is here  $k$  (Backward Euler scheme on the system of equation)

$$\tilde{c}^{k+1} - \tilde{c}^k - \Delta t_1(x) \operatorname{div} \vec{V}^{k+1} - \Delta t_1(x) \cdot \tilde{\alpha} \rho(\tilde{c}^{k+1}, \varphi_n^{k+1}) = 0 \quad (38)$$

$$\int_{\Omega} [D_0]^{-1} \vec{V}^{k+1} \cdot w_1 \, dx + \int_{\Omega} c^{k+1} \operatorname{div} w_1 \, dx - \int_{\Gamma_{d1}} f_{1d} w_1 \cdot n \, d\Gamma = 0, \quad \forall w_1 \in V_{0,1,h} \quad (39)$$

$$\varphi_n^{k+1} - \varphi_n^k - \Delta t_2(x) \operatorname{div} \vec{J}_\rho^{k+1} + \Delta t_2(x) \cdot \frac{1}{\partial t} [\rho(\tilde{c}^{k+1}, \varphi_n^{k+1}) - \rho^n] = 0 \quad (40)$$

$$\int_{\Omega} [\tilde{k} \rho(\tilde{c}^{k+1}, \varphi_n^{k+1})] \vec{J}_\rho^{k+1} \cdot w_2 \, dx + \int_{\Omega} \varphi_n^{k+1} \cdot \operatorname{div} w_2 \, dx - \int_{\Gamma_{d2}} f_{2d} w_2 \cdot n \, d\Gamma = 0, \quad \forall w_2 \in V_{0,2,h} \quad (41)$$

In (40)  $\rho^n$  is given ( $\rho^n = \rho(\tilde{c}^n, \varphi_n^n)$ ); In this process indexed with  $k$ , we can take  $\tilde{c}^0 = \tilde{c}^n$  and  $\varphi_n^0 = \varphi_n^n$ . The unknowns are here  $(\tilde{c}^{k+1}, \vec{V}^{k+1}, \varphi_n^{k+1}, \vec{J}_\rho^{k+1})$ . When the convergence with respect to  $k$  is obtained, then the current solution gives  $(\tilde{c}^{n+1}, \vec{V}^{n+1}, \varphi_n^{n+1}, \vec{J}_\rho^{n+1})$ .

As we use the lowest order Raviart-Thomas element, the equations (38) and (40) lead to scalar relation on each elements  $T$  of the triangulation  $\mathcal{T}_h$  (it is natural in this approximation to take the “local time steps”  $\Delta t_1$  and  $\Delta t_2$  constant on each element  $T$ ).

C) At each step  $k$ , we have a non linear problem to solve. We use Newton-Raphson technique, the index of iteration is now denoted by  $\ell$ . We set:

$$\vec{U} = \begin{pmatrix} \tilde{c} \\ \vec{V} \\ \varphi_n \\ \vec{J}_\rho \end{pmatrix} = \begin{pmatrix} U_1 \\ U_2 \\ U_3 \\ U_4 \end{pmatrix} \quad (42)$$

Equations (38) and (39) can formally be written as

$$E_1(\tilde{c}, \vec{V}, \varphi_n, \cdot) = E_1(U_1, U_2, U_3, U_4) = E_1(\vec{U}) = 0.$$

$$E_2(\tilde{c}, \vec{V}, \cdot, \cdot) = E_2(U_1, U_2, U_3, U_4) = E_2(\vec{U}) = 0$$

and so on, and finally the system (38)–(41) may be synthetized by

$$\vec{E}(\vec{U}) = 0. \quad (43)$$

The Newton-Raphson rule applied to (43) gives

$$\left[ \frac{\partial E_i}{\partial U_j} \right]_{\ell} \delta \vec{U}^{\ell} = -\vec{E}(\vec{U})^{\ell}, \quad \delta \vec{U}^{\ell} = \vec{U}^{\ell+1} - \vec{U}^{\ell} \quad (44)$$

or equivalently

$$\vec{U}^{\ell+1} = \vec{U}^{\ell} - \left[ \frac{\partial E_i}{\partial U_j} \right]_{\ell}^{-1} \vec{E}(\vec{U})^{\ell} \quad (45)$$

where

$$\left[ \frac{\partial E_i}{\partial U_j} \right]_{\ell} \text{ is the jacobian matrix of the application } \vec{E} \text{ evaluated at step } \ell.$$

The Newton-Raphson technique leads to a sequence of linear systems (indexed by  $\ell$ ). In our context of approximation (M.F.E.- $RT_0$ ) the size of each linear system is approximatively

$$2 \times (NT + NA)$$

where  $NT$  is the number of triangles of the triangulation  $\mathcal{T}_h$ , and  $NA$  is the number of edges of the mesh.

On can reduce the size of linear system by eliminating the primal variables (i.e.,  $\tilde{c}$  and  $\varphi_n$ ).

As a matter of fact, if we consider the first and third rows of relation (44), we can express explicitey the primal variables ( $\tilde{c}^{\ell+1}, \varphi_n^{\ell+1}$ ) as functions of the dual variables  $\vec{V}^{\ell+1}$  and  $\vec{J}_{\rho}^{\ell+1}$  by

$$[A] \begin{bmatrix} \tilde{c}^{\ell+1} - \tilde{c}^{\ell} \\ \varphi_n^{\ell+1} - \varphi_n^{\ell} \end{bmatrix} = \begin{bmatrix} \Delta t_1 \cdot \text{div } \delta \tilde{V}^{\ell} \\ \Delta t_2 \text{div } \delta \tilde{J}_{\rho}^{\ell} \end{bmatrix} - \begin{bmatrix} E_1(\vec{U}^{\ell}) \\ E_3(\vec{U}^{\ell}) \end{bmatrix}. \quad (46)$$

The matrix  $[A]$  is given by

$$[A] = \begin{bmatrix} 1 - \Delta t_1 \tilde{\alpha} \rho'_{\tilde{c}}|_{\ell} & -\Delta t_1 \tilde{\alpha} \rho'_{\varphi_n}|_{\ell} \\ \frac{\Delta t_2}{\delta t} \rho'_{\tilde{c}}|_{\ell} & 1 + \frac{\Delta t_2}{\delta t} \rho'_{\varphi_n}|_{\ell} \end{bmatrix}. \quad (47)$$

By the definition of  $\rho$  in (11), the derivatives of  $\rho$  with respect to  $\tilde{c}$  and  $\varphi_n$  are the same and the determinant of  $A$  can be evaluated as

$$\det A = 1 + \rho'_{\tilde{c}} \left( \frac{\Delta t_2}{\delta t} - \Delta t_1 \cdot \tilde{\alpha} \right). \quad (48)$$

We can eventually act on the physical time step  $\delta t$  or the local time steps  $\Delta t_1$  and  $\Delta t_2$  in order to keep  $\det A \neq 0$  or even  $> 0$ .

Let us denote by  $B$  the inverse of matrix  $A$

$$B = A^{-1}. \quad (49)$$

Then the following relations are obtained for  $\tilde{c}^{\ell+1}$  and  $\varphi_n^{\ell+1}$

$$\left. \begin{aligned} \tilde{c}^{\ell+1} - \tilde{c}^\ell = \delta\tilde{c}^\ell &= B_{11}\Delta t_1 \operatorname{div} \tilde{V}^{\ell+1} - B_{11}[\tilde{c}^\ell - \tilde{c}^k - \Delta t_1 \tilde{\alpha}\rho^\ell] \\ &+ B_{12}\Delta t_2 \operatorname{div} \tilde{J}_\rho^{\ell+1} - B_{12} \left[ \varphi_n^\ell - \varphi_n^k + \frac{\Delta t_2}{\delta t} (\rho^\ell - \rho^n) \right] \end{aligned} \right\} \quad (50)$$

$$\left. \begin{aligned} \varphi_n^{\ell+1} - \varphi_n^\ell = \delta\varphi_n^\ell &= B_{21}\Delta t_1 \operatorname{div} \tilde{V}^{\ell+1} - B_{21}[\tilde{c}^\ell - \tilde{c}^k - \Delta t_1 \tilde{\alpha}\rho^\ell] \\ &+ B_{22}\Delta t_2 \operatorname{div} \tilde{J}_\rho^{\ell+1} - B_{22} \left[ \varphi_n^\ell - \varphi_n^k + \frac{\Delta t_2}{\delta t} (\rho^\ell - \rho^n) \right]. \end{aligned} \right\} \quad (51)$$

These relations (50) and (51) are then used within the second and fourth rows of (45). Finally the linear system we have to solve is relative to the unknowns  $\tilde{V}^{\ell+1}$  and  $\tilde{J}_\rho^{\ell+1}$  only (i.e. of maximum size  $2.NA$ ). When the convergence with respect to  $\ell$  is reached then the solution at step  $k$  of the whole process is obtained.

## 4 Numerical Applications

We take for  $\Omega$  the rectangular domain  $L \times \ell$  and we suppose that at  $T = 0$  we have a uniform

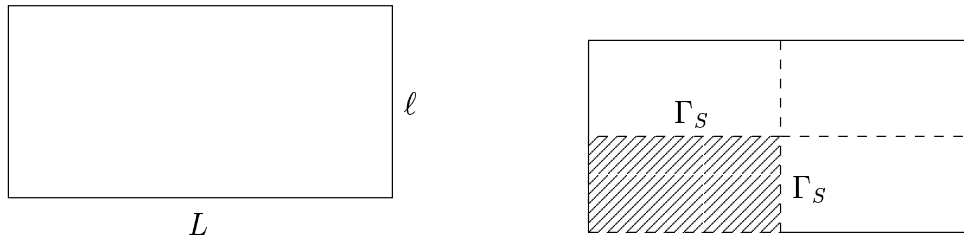


Figure 1: *Simulation Domain and reduction by symmetry.*

distribution of bacteria with density  $\rho_0$ .

From the definition of  $\rho$  in (11) it is natural to take at initial time

$$\tilde{c} + \varphi_n = 0. \quad (52)$$

By analogy with the drift diffusion model for semiconductor the variable  $\tilde{c}$  is similar to the electrostatic potential which is defined up to an additive constant. We can fix this constant by taking the value 0. On the other hand we want to ensure in the following numerical approximation, the mass conservation (or volume conservation) for the bacteria. From eq. (13) this will be the case if we take the following boundary condition on  $\varphi_n$

$$\frac{\partial \varphi_n}{\partial n} = 0 \quad \text{on } \Gamma = \partial\Omega. \quad (53)$$

In short, we can take at initial time

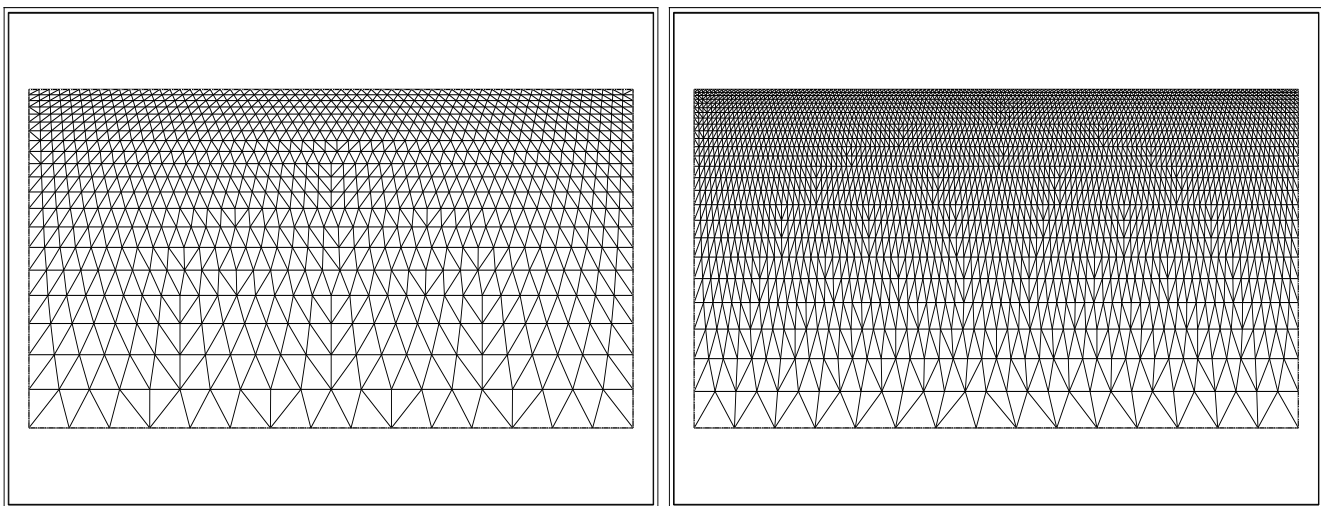
$$\rho = \rho_0 \text{ and } \tilde{c} = \varphi_n \equiv 0 \quad (54)$$

and the boundary condition

$$\left. \begin{array}{l} \tilde{c}|_{\Gamma} = 0 \\ \frac{\partial \varphi_n}{\partial n} |_{\Gamma} = 0 \end{array} \right\} \quad (55)$$

Of course, by reason of symmetry we can consider only a quarter of the simulation domain  $\Omega$ , namely  $(L/2, \ell/2)$ , then we have to take the following boundary conditions on the boundaries of symmetry  $\Gamma_S$

$$\left. \begin{array}{l} \frac{\partial \tilde{c}}{\partial n} = 0 \quad \text{on } \Gamma_S, \\ \text{and } \frac{\partial \varphi_n}{\partial n} = 0 \quad \text{on } \Gamma_S. \end{array} \right\} \quad (56)$$



(a) Mesh 1 (1775 triangles)

(b) Mesh 2 (5433 triangles)

Figure 2: MESHES. *The meshes are adapted to the geometries by deformation .*

In all numerical experimentations, two meshes have been used in order to see if the transient may be strongly affected by the spatial discretization. Fig (2) show the first mesh (with 1775 triangles) and the second mesh (with 5433 triangles)

The bacterial density is also assumed to be larger than a prescribed minimum value  $\rho_{min}$  (projection). We choose in our simulations,

$$\rho_{min} = 10^{-10}/cm^3. \quad (57)$$

#### 4.1 Numerical results with $\Omega = \text{square}$

In this part, we take  $L = \ell = 0.5cm$ ;

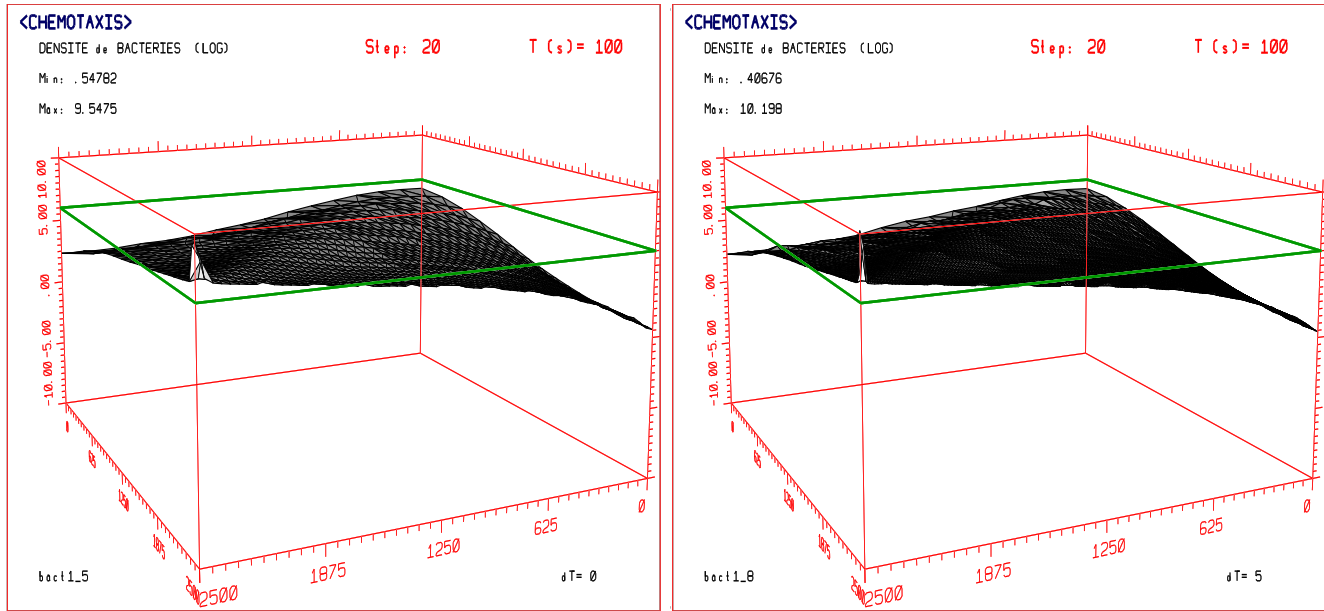
The physical parameters are those given in section 1. The model for attractant diffusion and production is given by (4). In (8) the scaling factor  $q$  is taken (as in other applications) as  $10^{-12}$ . The initial uniform distribution of bacteria is taken  $\rho_0 = 10^6/cm^3$ .

The figures(3,4) represent the distribution of bacteria density within the domain of simulation at times 100s and 2000s and for the two meshes. The coordinates  $(x_1, x_2)$  are given in  $\mu m$  on the figures and a log scale is used for representation of the density  $\rho$  (range from  $10^{-10}$  to  $10^{+10}$  ( $cm^{-3}$ )). The initial constant value  $\rho_0$  is marked on the figures.

The total amount of bacteria remain constant along the evolution process:

$$\int_{\Omega} \rho dx = C^{te} = \int_{\Omega} \rho_0 dx = \rho_0 \times Area(\Omega)$$

For this example, the bacteria migrate towards the center of the square. Something like a Dirac mass at this center is obtained after a certain amount of time (see fig.(4)) A  $P^1$ -smoothing is applied (for visualization of solution) to the raw data obtained from the mixed finite element approximation. The primal variables  $\tilde{c}, \varphi_n$  and associated quantities (as bacteria density) are constant on each triangle of the mesh. As such an action (smoothing) reduce strongly the function peaks, a special treatment (only for visualization) is applied on the smoothed function in order to retrieve peak values.



(a) With mesh 1 (1775 triangles)

(b) With mesh 2 (5433 triangles)

Figure 3: BACTERIA CONCENTRATION, (LOG. SCALE). Computational domain:square  $0.25cm \times 0.25cm$ . Distribution after 100s. Initial Concentration is marked, observer position near  $(x_{max}, y_{max})$ .

In order to follow quantitatively what happens to the bacterial density distribution, we can analyse the solution at a given time T in the following way:

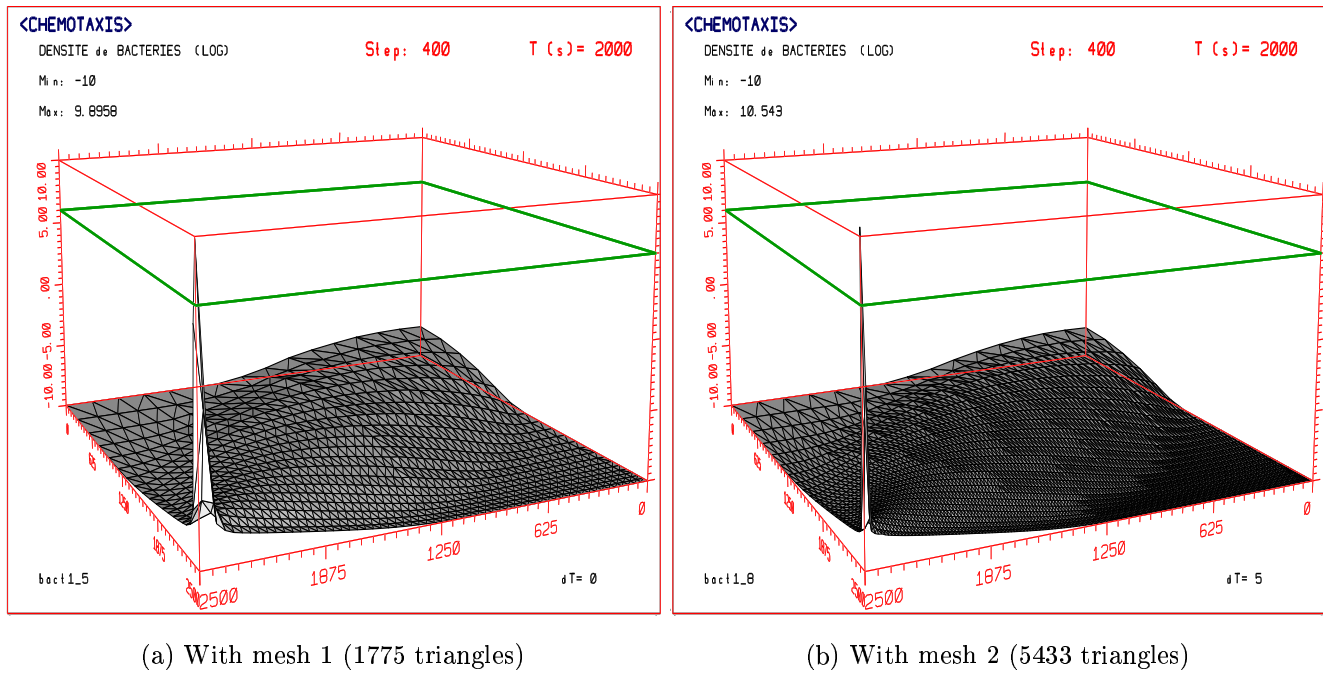


Figure 4: BACTERIA CONCENTRATION, (LOG. SCALE). Computational domain: square  $0.25\text{cm} \times 0.25\text{cm}$ . Distribution after 2000s. Initial Concentration is marked, observer position near  $(x_{max}, y_{max})$ .

1. We control the value of the total bacterial mass (which remains constant during the evolution process)

$$Total\_Mass = \int_{\Omega} \rho dx = \sum_J \rho(J) * Area(J) \quad (J \text{ triangle of the mesh})$$

2. We consider a threshold value ( $\rho_{th}$  - typically we choose  $\rho_{th} = \rho_0$ ) for the density  $\rho$  and only triangles for which the density is larger or equal than  $\rho_{th}$  will be taken into consideration in the following. First of all, we begin to attach the attribute “not marked” to all the triangles.
3. -Determination of the  $i^{th}$  local maxima

- We look for the triangle  $J_i$  such that

$$\rho(J_i) \geq \rho(J) \quad \forall J$$

where  $J \in$  list of “not marked” triangles and such that  $\rho(J) \geq \rho_{th}$

- If the triangle  $J_i$  does not exist  $\implies EXIT$  (GoTo END)
- The triangle  $J_i$  is “marked”
- We determine all the triangles  $J_{i,k}$  in the (connected) neighbourhood of  $J_i$  such that
  - $\rho(J_{i,k}) \geq \rho_{th}$
  - $J_{i,k}$  “not marked”



All these triangles  $J_{i,k}$  (including  $J_i$ ) form a connected domain  $\Omega_i$

$$\Omega_i = J_i \bigcup_k J_{i,k}$$

- We evaluate and print several quantities
  - $J_i$  = number of the triangle where the local maximum(i) occur
  - $Conc$  = density value (local maximum)
  - $XG(J_i), YG(J_i)$  = coordinates of the center of gravity for triangle  $J_i$
  - $N(i)$  = number of triangles in  $\Omega_i$
  - $Local\_Mass(i) = \int_{\Omega_i} \rho dx$
  - $Contrib(J_i) = \rho(J_i) \times Area(J_i)$
  - $Percent(i) = \frac{Local\_Mass(i)}{Total\_Mass} \times 100$
  - $Percent\_max\_local(i) = \frac{Contrib(J_i)}{Local\_Mass(i)} \times 100$
  - $Percent\_max\_total(i) = \frac{Contrib(J_i)}{Total\_Mass} \times 100$
- All triangles in  $\Omega_i$  are “marked”
- Return to 3 for the determination of next local max.
- END
  - At this point, a certain number ( $I$ ) of local maxima has been found
  - $N$  = the total number of triangles considered =  $\sum_i N(i)$
  - $Troncated\_Mass = \sum_i Local\_Mass(i)$
  - $Troncated\_Mass\_Percent = \frac{Troncated\_Mass}{Total\_Mass} \times 100$

### Analysis of the solution on Mesh 2 at 100s and 2000s

```

----- Mesh 2
... Process time : 100.0 s Total bacteria mass: 6.25000E+04 Threshold value: 1.00000E+06
----- Local max number: 1
*** J1 = 5433 Conc: 1.577E+10 (XG,YG)= ( 2.489E-01, 2.493E-01) (cmXcm)
Number of triangles N(1)= 1532
Local_Mass(1) = 5.26292E+04 Percent(1) = 84.20681 %
Contrib( 5433)= 2.82386E+04 Percent_max_local(1)= 53.65572 % Percent_max_total(1)= 45.18177 %
----- Global results -----
Number of local maxima : 1 Total number of triangles N= 1532
Troncated_Mass : 5.26292E+04 Troncated_Mass_Percent : 84.20681 %

----- Mesh 2
... Process time : 2000.0 s Total bacteria mass: 6.25001E+04 Threshold value: 1.00000E+06
----- Local max number: 1
*** J1 = 5433 Conc: 3.490E+10 (XG,YG)= ( 2.489E-01, 2.493E-01) (cmXcm)
Number of triangles N(1)= 1
Local_Mass(1) = 6.25001E+04 Percent(1) = 99.99998 %
Contrib( 5433)= 6.25001E+04 Percent_max_local(1)= 100.00000 % Percent_max_total(1)= 99.99998 %
----- Global results -----
Number of local maxima : 1 Total number of triangles N= 1
Troncated_Mass : 6.25001E+04 Troncated_Mass_Percent : 99.99998 %

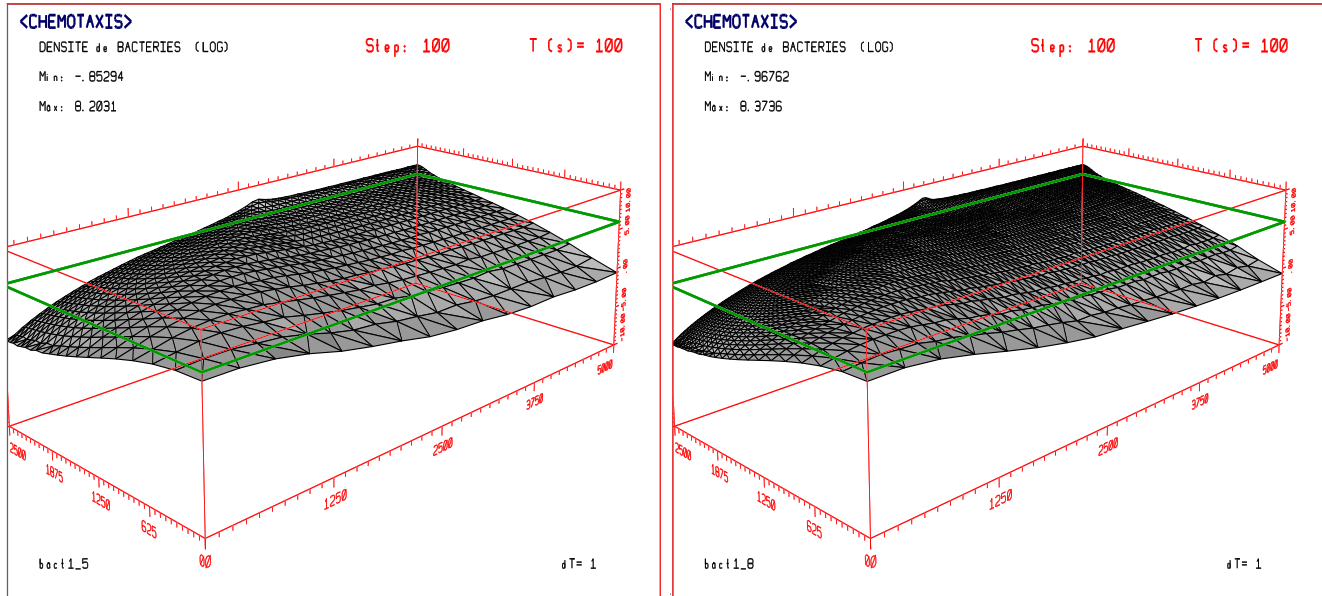
```

We can see (qualitatively) on figure (4) the formation of a Dirac Mass at the center of the square. Quantitatively, we can see from the solution analysis at 600s that only one triangle (the smallest part in our MFE approximation) contribute to the total Mass. As early as the process time reached 100s, this triangle contained more than 45% of the total mass of bacteria.

## 4.2 Numerical results with $\Omega = \text{rectangle}$ with small aspect ratio

In this part, we take  $L = 1.\text{cm}$   $\ell = 0.5\text{cm}$ ;

The figures(5,6) represent the distribution of bacteria density within the domain of simulation at times 100s and 600s and for the two meshes.



(a) With mesh 1 (1775 triangles)

(b) With mesh 2 (5433 triangles)

Figure 5: BACTERIA CONCENTRATION,(LOG. SCALE). Computational domain:rectangle  $0.50\text{cm} \times 0.25\text{cm}$ . Distribution after 100s. Initial Concentration is marked, observer position near  $(x_{min}, y_{min})$ .

### Analysis of the solution on meshes 1 and 2 at time 100s

```

----- Mesh 1
... Process time : 100.0 s Total bacteria mass: 1.25000E+05 Threshold value: 1.00000E+06
----- Local max number: 1
*** J1 = 1115 Conc: 1.597E+08 (XG,YG)= ( 2.710E-01, 2.487E-01) (cmXcm)
Number of triangles N(1)= 605
Local_Mass(1) = 1.11694E+05 Percent(1) = 89.35488 %
Contrib( 1115)= 2.55813E+03 Percent_max_local(1)= 2.29031 % Percent_max_total(1)= 2.04651 %
----- Global results -----
Number of local maxima : 1 Total number of triangles N= 605
Troncated_Mass : 1.11694E+05 Troncated_Mass_Percent : 89.35488 %

----- Mesh 2
... Process time : 100.0 s Total bacteria mass: 1.25000E+05 Threshold value: 1.00000E+06
----- Local max number: 1
*** J1 = 3372 Conc: 2.365E+08 (XG,YG)= ( 2.746E-01, 2.493E-01) (cmXcm)
Number of triangles N(1)= 2107
Local_Mass(1) = 1.11937E+05 Percent(1) = 89.54935 %
Contrib( 3372)= 8.46726E+02 Percent_max_local(1)= 0.75643 % Percent_max_total(1)= 0.67738 %
----- Global results -----
Number of local maxima : 1 Total number of triangles N= 2107
Troncated_Mass : 1.11937E+05 Troncated_Mass_Percent : 89.54935 %

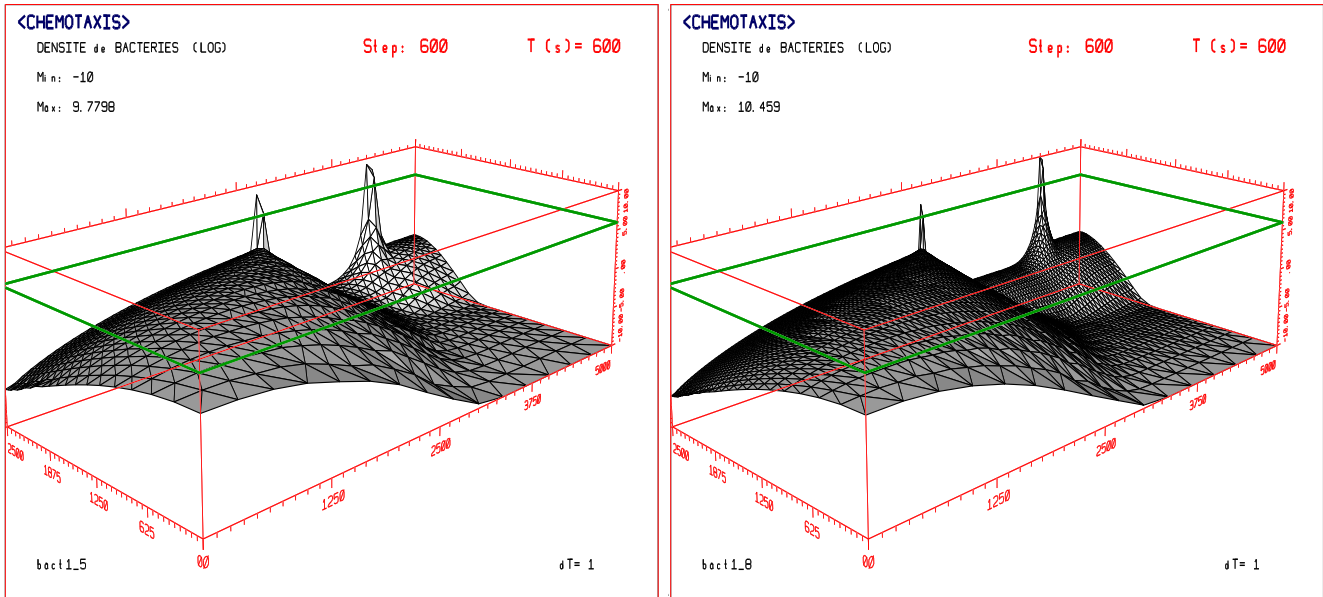
```

### Analysis of the solution on meshes 1 and 2 at time 600s

```

----- Mesh 1
... Process time : 600.0 s Total bacteria mass: 1.25000E+05 Threshold value: 1.00000E+06

```



(a) With mesh 1 (1775 triangles)

(b) With mesh 2 (5433 triangles)

Figure 6: BACTERIA CONCENTRATION, (LOG. SCALE). Computational domain: rectangle  $0.50\text{cm} \times 0.25\text{cm}$ . Distribution after 600s. Initial Concentration is marked, observer position near  $(x_{min}, y_{min})$ .

```

----- Local max number: 1
*** J1 = 1146   Conc: 6.023E+09 (XG,YG)= ( 2.794E-01, 2.487E-01) (cmXcm)
    Number of triangles N(1)=      1
    Local_Mass(1) = 9.64805E+04 Percent(1)           = 77.18437 %
    Contrib( 1146)= 9.64805E+04 Percent_max_local(1)= 100.00000 %   Percent_max_total(1)= 77.18437 %
----- Local max number: 2
*** J2 = 1636   Conc: 1.780E+09 (XG,YG)= ( 4.302E-01, 2.487E-01) (cmXcm)
    Number of triangles N(2)=      1
    Local_Mass(2) = 2.85119E+04 Percent(2)           = 22.80950 %
    Contrib( 1636)= 2.85119E+04 Percent_max_local(2)= 100.00000 %   Percent_max_total(2)= 22.80950 %
----- Global results -----
    Number of local maxima : 2 Total number of triangles N=      2
    Troncated_Mass : 1.24992E+05 Troncated_Mass_Percent : 99.99388 %

----- Mesh 2
... Process time :   600.0 s Total bacteria mass: 1.25000E+05   Threshold value: 1.00000E+06
----- Local max number: 1
*** J1 = 3372   Conc: 2.876E+10 (XG,YG)= ( 2.746E-01, 2.493E-01) (cmXcm)
    Number of triangles N(1)=      1
    Local_Mass(1) = 1.02971E+05 Percent(1)           = 82.37659 %
    Contrib( 3372)= 1.02971E+05 Percent_max_local(1)= 100.00000 %   Percent_max_total(1)= 82.37659 %
----- Local max number: 2
*** J2 = 5028   Conc: 6.145E+09 (XG,YG)= ( 4.386E-01, 2.493E-01) (cmXcm)
    Number of triangles N(2)=      2
    Local_Mass(2) = 2.20225E+04 Percent(2)           = 17.61800 %
    Contrib( 5028)= 2.20013E+04 Percent_max_local(2)= 99.90358 %   Percent_max_total(2)= 17.60101 %
----- Global results -----
    Number of local maxima : 2 Total number of triangles N=      3
    Troncated_Mass : 1.24993E+05 Troncated_Mass_Percent : 99.99458 %

```

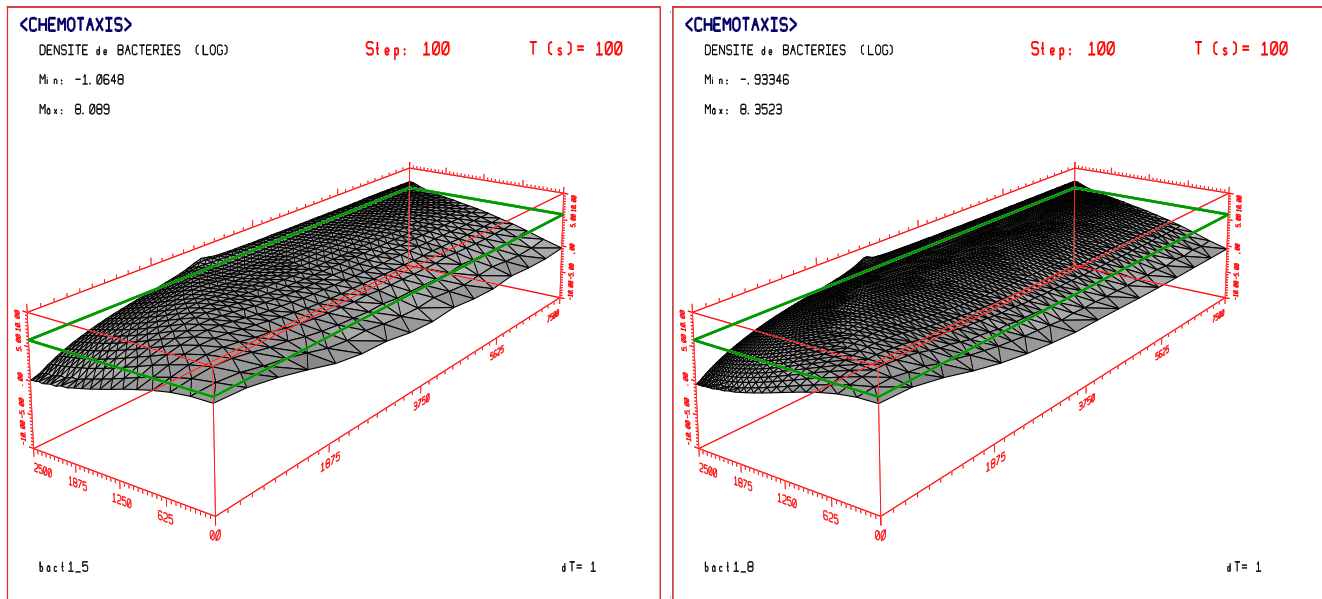
At  $T = 100\text{s}$  we begin to see the first local maxima -see fig.(5)-, but only a few percentage of the total mass is located on the triangle which presents the maximum bacterial density. We can see on the quantitative analysis that the localization of local maxima and concentration values at

these points remain mesh dependent. We can also remark from the analysis at  $T = 600s$  that the distortion between mass repartition (at local maxima) is amplified when the mesh is refined.

### 4.3 Numerical results with $\Omega = \text{rectangle with large aspect ratio}$

In this part, we take  $L = 1.5\text{cm}$   $\ell = 0.5\text{cm}$ ;

The figures(7,8,9) represent the distribution of bacteria density within the domain of simulation at times 100s, 250s and 600s and for the two meshes.



(a) With mesh 1 (1775 triangles)

(b) With mesh 2 (5433 triangles)

Figure 7: BACTERIA CONCENTRATION, (LOG. SCALE). Computational domain:rectangle  $0.75\text{cm} \times 0.25\text{cm}$ . Distribution after 100s. Initial Concentration is marked, observer position near  $(x_{min}, y_{min})$ .

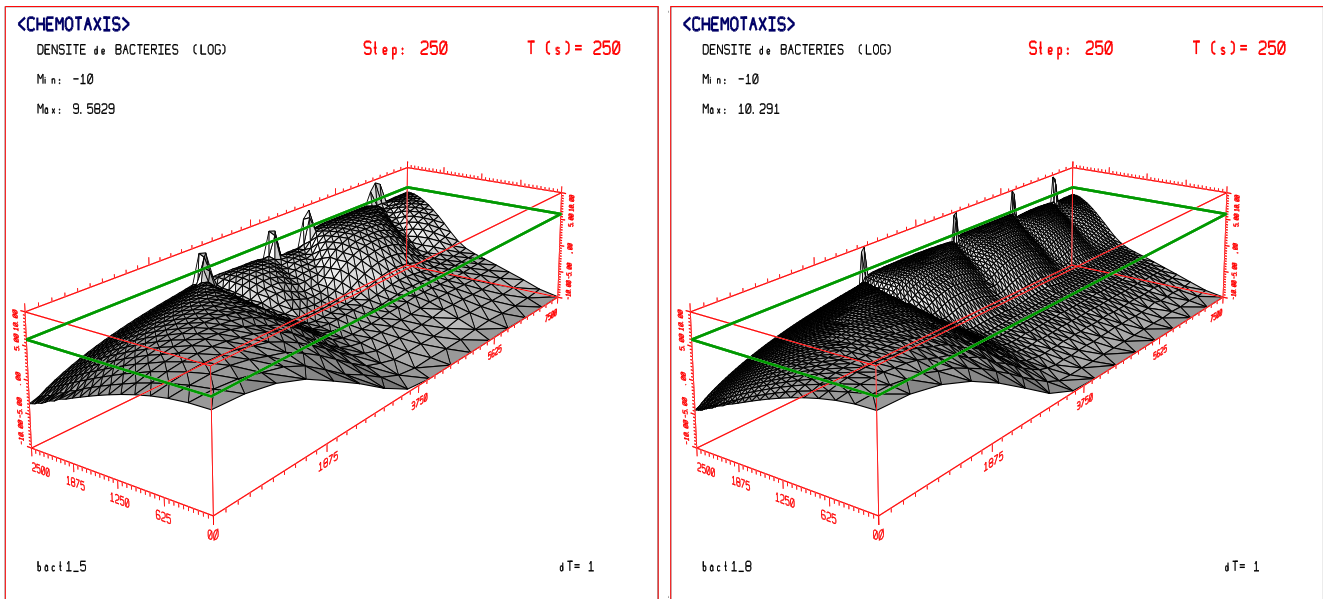
#### Solution analysis on mesh 1 and 2 at 100s (respectively)

```

----- Mesh 1
... Process time : 100.0 s Total bacteria mass: 1.87500E+05 Threshold value: 1.00000E+06
----- Local max number: 1
*** J1 = 830 Conc: 1.228E+08 (XG,YG)= ( 2.740E-01, 2.474E-01) (cmXcm)
Number of triangles N(1)= 656
Local_Mass(1) = 1.69660E+05 Percent(1) = 90.48521 %
Contrib( 830)= 3.01108E+03 Percent_max_local(1)= 1.77478 % Percent_max_total(1)= 1.60591 %
----- Global results -----
Number of local maxima : 1 Total number of triangles N= 656
Troncated_Mass : 1.69660E+05 Troncated_Mass_Percent : 90.48521 %

----- Mesh 2
... Process time : 100.0 s Total bacteria mass: 1.87500E+05 Threshold value: 1.00000E+06
----- Local max number: 1
*** J1 = 2500 Conc: 2.252E+08 (XG,YG)= ( 2.730E-01, 2.493E-01) (cmXcm)
Number of triangles N(1)= 2314
Local_Mass(1) = 1.69736E+05 Percent(1) = 90.52596 %
Contrib( 2500)= 1.20953E+03 Percent_max_local(1)= 0.71259 % Percent_max_total(1)= 0.64508 %
----- Global results -----
Number of local maxima : 1 Total number of triangles N= 2314
Troncated_Mass : 1.69736E+05 Troncated_Mass_Percent : 90.52596 %

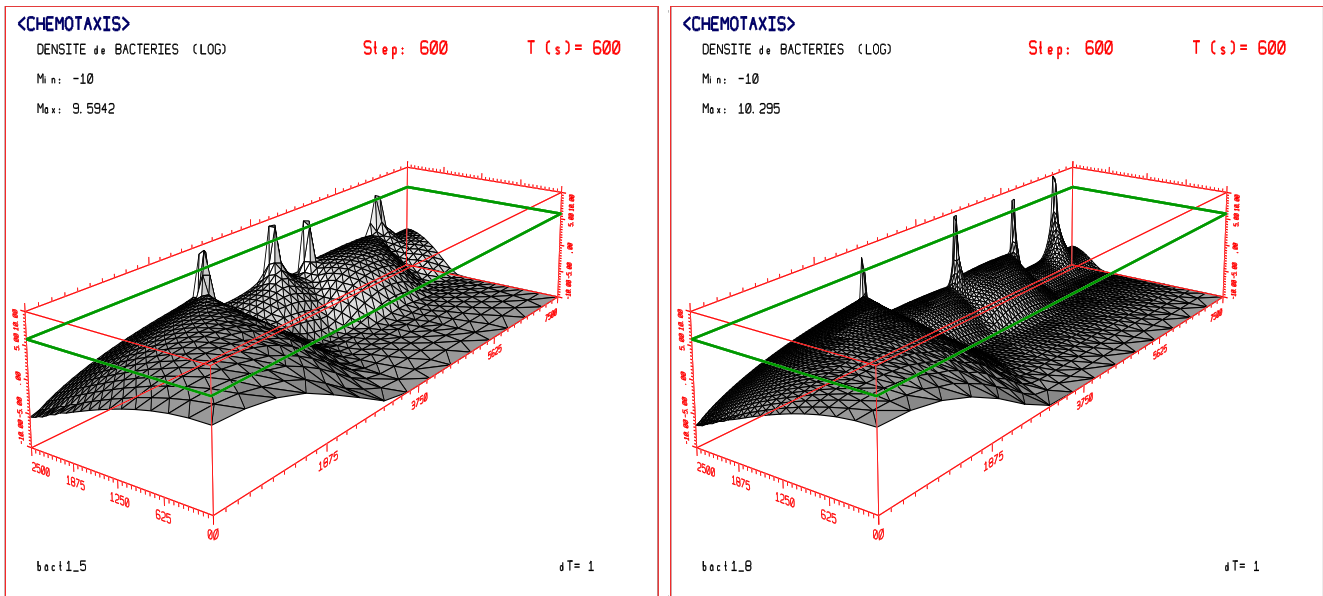
```



(a) With mesh 1 (1775 triangles)

(b) With mesh 2 (5433 triangles)

Figure 8: BACTERIA CONCENTRATION, (LOG. SCALE). Computational domain: rectangle  $0.75\text{cm} \times 0.25\text{cm}$ . Distribution after 250s. Initial Concentration is marked, observer position near  $(x_{min}, y_{min})$ .



(a) With mesh 1 (1775 triangles)

(b) With mesh 2 (5433 triangles)

Figure 9: BACTERIA CONCENTRATION, (LOG. SCALE). Computational domain: rectangle  $0.75\text{cm} \times 0.25\text{cm}$ . Distribution after 600s. Initial Concentration is marked, observer position near  $(x_{min}, y_{min})$ .

Solution analysis on mesh 1 and 2 at 600s (respectively)

----- Mesh 1

```

... Process time : 600.0 s Total bacteria mass: 1.87500E+05 Threshold value: 1.00000E+06
----- Local max number: 1
*** J1 = 869 Conc: 3.928E+09 (XG,YG)= ( 2.808E-01, 2.487E-01) (cmXcm)
Number of triangles N(1)= 2
Local_Mass(1) = 9.71086E+04 Percent(1) = 51.79124 %
Contrib( 869)= 9.43845E+04 Percent_max_local(1)= 97.19479 % Percent_max_total(1)= 50.33838 %
----- Local max number: 2
*** J2 = 1685 Conc: 1.777E+09 (XG,YG)= ( 6.704E-01, 2.487E-01) (cmXcm)
Number of triangles N(2)= 1
Local_Mass(2) = 4.26938E+04 Percent(2) = 22.77004 %
Contrib( 1685)= 4.26938E+04 Percent_max_local(2)= 100.00000 % Percent_max_total(2)= 22.77004 %
----- Local max number: 3
*** J3 = 1297 Conc: 1.189E+09 (XG,YG)= ( 4.945E-01, 2.487E-01) (cmXcm)
Number of triangles N(3)= 1
Local_Mass(3) = 2.85685E+04 Percent(3) = 15.23651 %
Contrib( 1297)= 2.85685E+04 Percent_max_local(3)= 100.00000 % Percent_max_total(3)= 15.23651 %
----- Local max number: 4
*** J4 = 1146 Conc: 7.957E+08 (XG,YG)= ( 4.191E-01, 2.487E-01) (cmXcm)
Number of triangles N(4)= 1
Local_Mass(4) = 1.91198E+04 Percent(4) = 10.19721 %
Contrib( 1146)= 1.91198E+04 Percent_max_local(4)= 100.00000 % Percent_max_total(4)= 10.19721 %
----- Global results -----
Number of local maxima : 4 Total number of triangles N= 5
Troncated_Mass : 1.87491E+05 Troncated_Mass_Percent : 99.99500 %

----- Mesh 2
... Process time : 600.0 s Total bacteria mass: 1.87500E+05 Threshold value: 1.00000E+06
----- Local max number: 1
*** J1 = 2500 Conc: 1.971E+10 (XG,YG)= ( 2.730E-01, 2.493E-01) (cmXcm)
Number of triangles N(1)= 1
Local_Mass(1) = 1.05869E+05 Percent(1) = 56.46339 %
Contrib( 2500)= 1.05869E+05 Percent_max_local(1)= 100.00000 % Percent_max_total(1)= 56.46339 %
----- Local max number: 2
*** J2 = 4575 Conc: 5.821E+09 (XG,YG)= ( 5.927E-01, 2.493E-01) (cmXcm)
Number of triangles N(2)= 1
Local_Mass(2) = 3.12662E+04 Percent(2) = 16.67531 %
Contrib( 4575)= 3.12662E+04 Percent_max_local(2)= 100.00000 % Percent_max_total(2)= 16.67531 %
----- Local max number: 3
*** J3 = 3667 Conc: 4.727E+09 (XG,YG)= ( 4.571E-01, 2.493E-01) (cmXcm)
Number of triangles N(3)= 1
Local_Mass(3) = 2.53862E+04 Percent(3) = 13.53927 %
Contrib( 3667)= 2.53862E+04 Percent_max_local(3)= 100.00000 % Percent_max_total(3)= 13.53927 %
----- Local max number: 4
*** J4 = 5264 Conc: 4.649E+09 (XG,YG)= ( 6.981E-01, 2.493E-01) (cmXcm)
Number of triangles N(4)= 1
Local_Mass(4) = 2.49685E+04 Percent(4) = 13.31652 %
Contrib( 5264)= 2.49685E+04 Percent_max_local(4)= 100.00000 % Percent_max_total(4)= 13.31652 %
----- Global results -----
Number of local maxima : 4 Total number of triangles N= 4
Troncated_Mass : 1.87490E+05 Troncated_Mass_Percent : 99.99449 %

```

For the present example, the two meshes give the same number of local maxima (4), but localization and relative weight to the total mass contributions are slightly different. Are the patterns too mesh sensitive? Perhaps mesh adaption may be needed in the evolution process when density gradients begin to become significant.

#### 4.4 Numerical results with limited attractant production

The model of attractant production is given via eq. (7),

$$\alpha \rho e^{-\rho/\rho^*}$$

where the parameter  $\rho^*$  is the cutoff bacterial density. For the numerical results presented in the following, we have considered only the rectangle  $\Omega$  defined by  $L = 1.5\text{cm}$ ,  $\ell = 0.5\text{cm}$  and used the Mesh 2 (5433 triangles).

When taking into account the fact that the production of attractants may be bounded, the behaviour of bacterial density distribution during the process is quite different.

In the previous simulations (attractant production modelled via  $\alpha\rho$ ), when a peak of concentration appears within the evolution process, it remains at the same (or nearly the same) place during all the process. The bacteria density decreases around these peaks.

In the present simulations, the first concentration peak travels towards the center of the domain ( upper right corner of the computational domain), “eating” successively all the other local peaks of bacterial concentration. High densities values are not localized only over one mesh element.

With the values  $\rho^* = 50\rho_0$ ,  $\rho^* = 100\rho_0$ ,  $\rho^* = 500\rho_0$ , the center of  $\Omega$  is reached more or less quickly. With  $\rho^* = 1000\rho_0$ , the peak of concentration does not reach the center, the progression is stopped after the last local peak has been “eaten”. After this positioning, the concentration of bacteria “far” to the peak decreases continuously but very slowly. We have to take large time steps (physical time steps) in order to have significant variations of the variables and consequently of the density  $\rho$  in the numerical scheme and reach as quick as possible something like a “stationary solution”.

In the following analysis reports, we add the percentage of area represented by the triangles retained for numerical integration (ie triangles where the density is  $\geq \rho_{th}$ , threshold value)

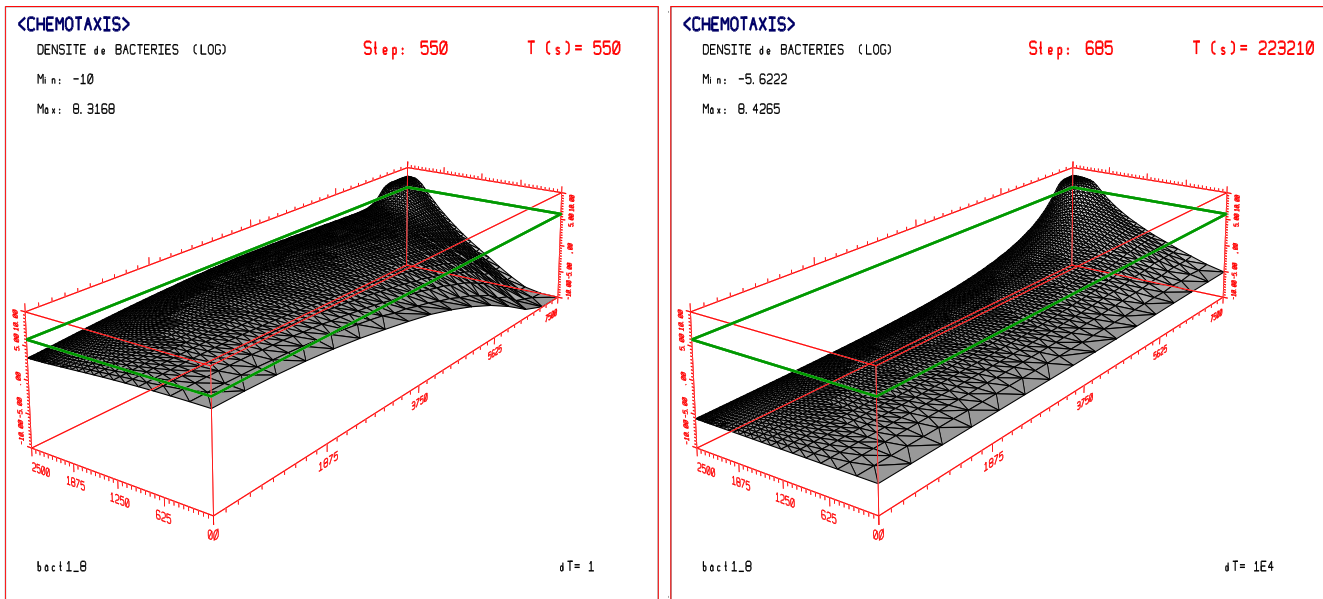
### Quantitative results for $\rho^* = 50\rho_0$

```
----- Mesh 2
... Process time : 550.0 s Total bacteria mass: 1.87500E+05 Threshold value: 1.00000E+06
----- Local max number: 1
*** J1 = 5379 Conc: 2.074E+08 (XG,YG)= ( 7.233E-01, 2.493E-01) (cmXcm)
Number of triangles N(1)= 277 Area % = 1.3118
Local_Mass(1) = 1.79917E+05 Percent(1) = 95.95565 %
Contrib( 5379)= 1.11379E+03 Percent_max_local(1)= 0.61906 % Percent_max_total(1)= 0.59402 %
----- Global results -----
Number of local maxima : 1 Total number of triangles N= 277 Area % : 1.3118
Troncated_Mass : 1.79917E+05 Troncated_Mass_Percent : 95.95565 %
```

```
----- Mesh 2
... Process time :223220.0 s Total bacteria mass: 1.87500E+05 Threshold value: 1.00000E+06
----- Local max number: 1
*** J1 = 5432 Conc: 2.670E+08 (XG,YG)= ( 7.484E-01, 2.486E-01) (cmXcm)
Number of triangles N(1)= 199 Area % = 1.0750
Local_Mass(1) = 1.87157E+05 Percent(1) = 99.81688 %
Contrib( 5432)= 1.40406E+03 Percent_max_local(1)= 0.75021 % Percent_max_total(1)= 0.74883 %
----- Global results -----
Number of local maxima : 1 Total number of triangles N= 199 Area % : 1.0750
Troncated_Mass : 1.87157E+05 Troncated_Mass_Percent : 99.81688 %
```

### Quantitative results for $\rho^* = 500\rho_0$

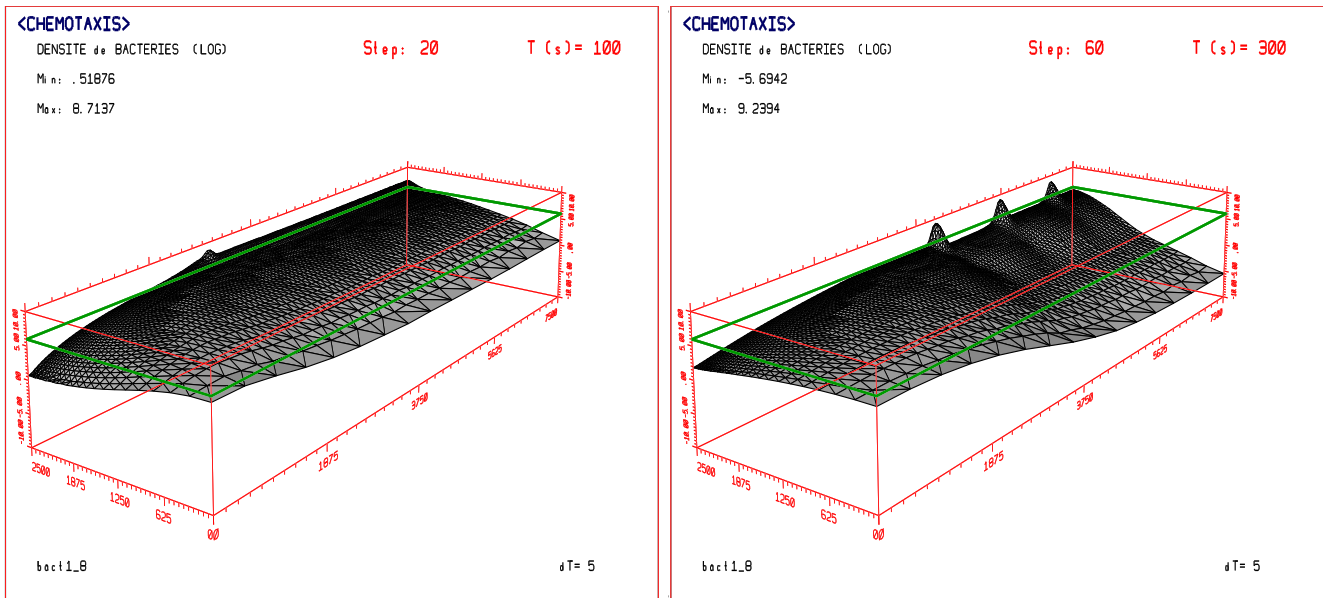
```
-----
... Process time : 100.0 s Total bacteria mass: 1.87500E+05 Threshold value: 1.00000E+06
----- Local max number: 1
*** J1 = 2622 Conc: 5.173E+08 (XG,YG)= ( 2.930E-01, 2.493E-01) (cmXcm)
Number of triangles N(1)= 2441 Area % = 15.4336
Local_Mass(1) = 1.63828E+05 Percent(1) = 87.37489 %
Contrib( 2622)= 2.77833E+03 Percent_max_local(1)= 1.69589 % Percent_max_total(1)= 1.48178 %
----- Global results -----
Number of local maxima : 1 Total number of triangles N= 2441 Area % : 15.4336
Troncated_Mass : 1.63828E+05 Troncated_Mass_Percent : 87.37489 %
-----
```



(a) High concentration localization after 550s

(b) Distribution after large simulation time

Figure 10: BACTERIA CONCENTRATION, (LOG. SCALE). Computational domain: rectangle  $0.75\text{cm} \times 0.25\text{cm}$ . Bounded production of attractants ( $\rho^* = 50\rho_0$ ), observer position near  $(x_{min}, y_{min})$ .



(a) High concentration localization after 100s

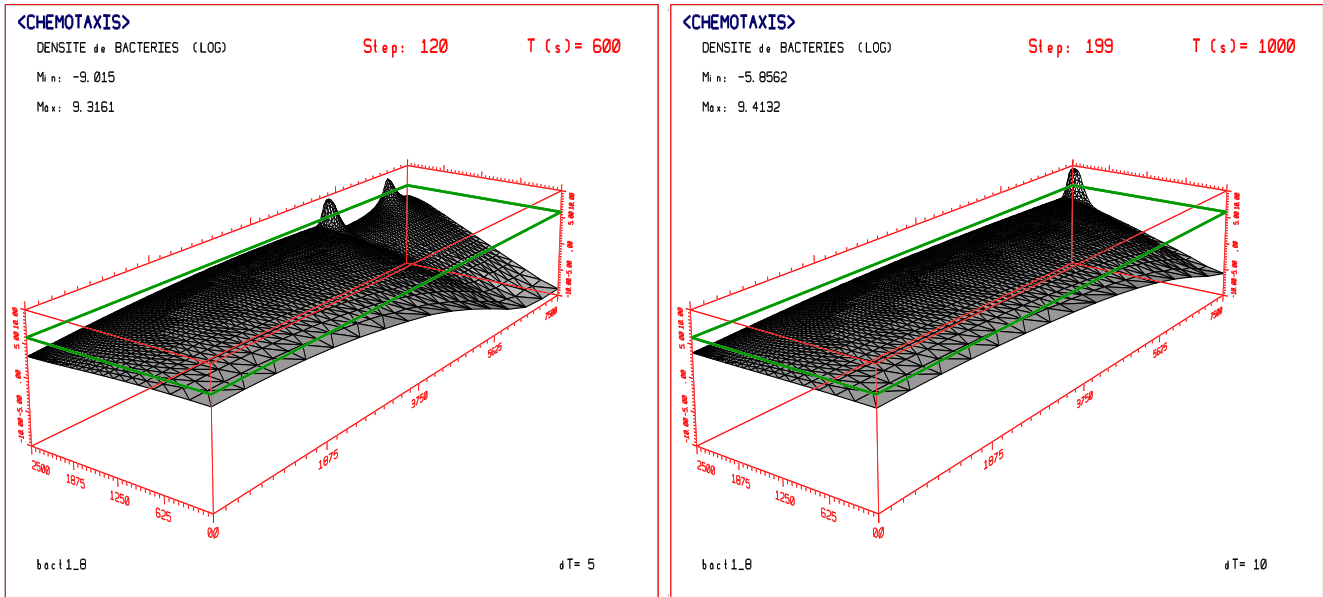
(b) High concentration localization after 300s

Figure 11: BACTERIA CONCENTRATION, (LOG. SCALE). Computational domain: rectangle  $0.75\text{cm} \times 0.25\text{cm}$ . Bounded production of attractants ( $\rho^* = 500\rho_0$ ), observer position near  $(x_{min}, y_{min})$ .

```

... Process time : 300.0 s Total bacteria mass: 1.87500E+05 Threshold value: 1.00000E+06
----- Local max number: 1
*** J1 = 3358 Conc: 1.735E+09 (XG,YG)= ( 4.138E-01, 2.486E-01) (cmXcm)
    
```





(a) High concentration localization after 600s

(b) High concentration localization after 1000s

Figure 12: BACTERIA CONCENTRATION, (LOG. SCALE). Computational domain: rectangle  $0.75\text{cm} \times 0.25\text{cm}$ . Bounded production of attractants ( $\rho^* = 500\rho_0$ ), observer position near  $(x_{min}, y_{min})$ .

```

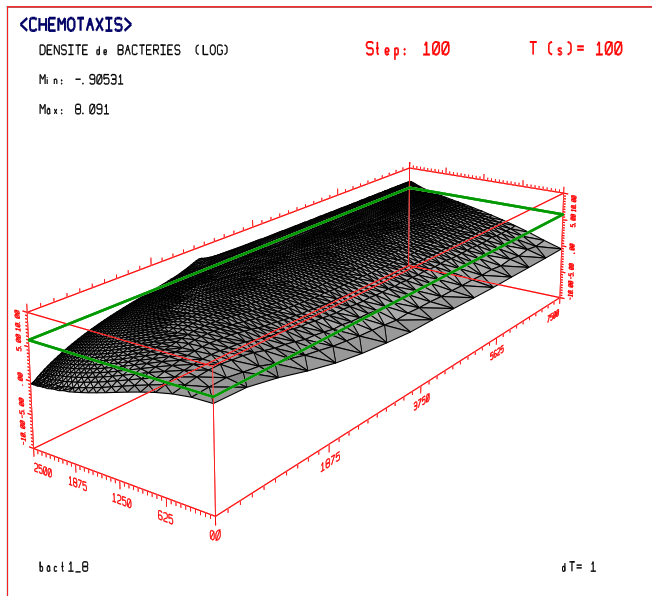
Number of triangles N(1)= 57 Area % = 0.2050
Local_Mass(1) = 9.84080E+04 Percent(1) = 52.48427 %
Contrib( 3358)= 9.09209E+03 Percent_max_local(1)= 9.23918 % Percent_max_total(1)= 4.84911 %
----- Local max number: 2
*** J2 = 4338 Conc: 1.342E+09 (XG,YG)= ( 5.601E-01, 2.486E-01) (cmXcm)
Number of triangles N(2)= 51 Area % = 0.1813
Local_Mass(2) = 5.36993E+04 Percent(2) = 28.63965 %
Contrib( 4338) = 7.56914E+03 Percent_max_local(2)= 14.09541 % Percent_max_total(2)= 4.03688 %
----- Local max number: 3
*** J3 = 5207 Conc: 8.238E+08 (XG,YG)= ( 6.881E-01, 2.493E-01) (cmXcm)
Number of triangles N(3)= 55 Area % = 0.1963
Local_Mass(3) = 2.53662E+04 Percent(3) = 13.52863 %
Contrib( 5207) = 4.42463E+03 Percent_max_local(3)= 17.44302 % Percent_max_total(3)= 2.35980 %
----- Local max number: 4
*** J4 = 2925 Conc: 1.193E+06 (XG,YG)= ( 3.433E-01, 2.493E-01) (cmXcm)
Number of triangles N(4)= 102 Area % = 0.3556
Local_Mass(4) = 7.28307E+02 Percent(4) = 0.38843 %
Contrib( 2925)= 6.40780E+00 Percent_max_local(4)= 0.87982 % Percent_max_total(4)= 0.00342 %
----- Global results -----
Number of local maxima : 4 Total number of triangles N= 265 Area % : 0.9383
Troncated_Mass : 1.78202E+05 Troncated_Mass_Percent : 95.04099 %
-----
... Process time : 600.0 s Total bacteria mass: 1.87499E+05 Threshold value: 1.00000E+06
----- Local max number: 1
*** J1 = 4240 Conc: 2.070E+09 (XG,YG)= ( 5.425E-01, 2.493E-01) (cmXcm)
Number of triangles N(1)= 63 Area % = 0.2316
Local_Mass(1) = 1.56721E+05 Percent(1) = 83.58472 %
Contrib( 4240)= 1.11202E+04 Percent_max_local(1)= 7.09557 % Percent_max_total(1)= 5.93081 %
----- Local max number: 2
*** J2 = 5250 Conc: 8.198E+08 (XG,YG)= ( 6.963E-01, 2.486E-01) (cmXcm)
Number of triangles N(2)= 53 Area % = 0.1891
Local_Mass(2) = 2.57054E+04 Percent(2) = 13.70959 %
Contrib( 5250)= 4.29516E+03 Percent_max_local(2)= 16.70921 % Percent_max_total(2)= 2.29076 %
----- Global results -----
Number of local maxima : 2 Total number of triangles N= 116 Area % : 0.4207

```

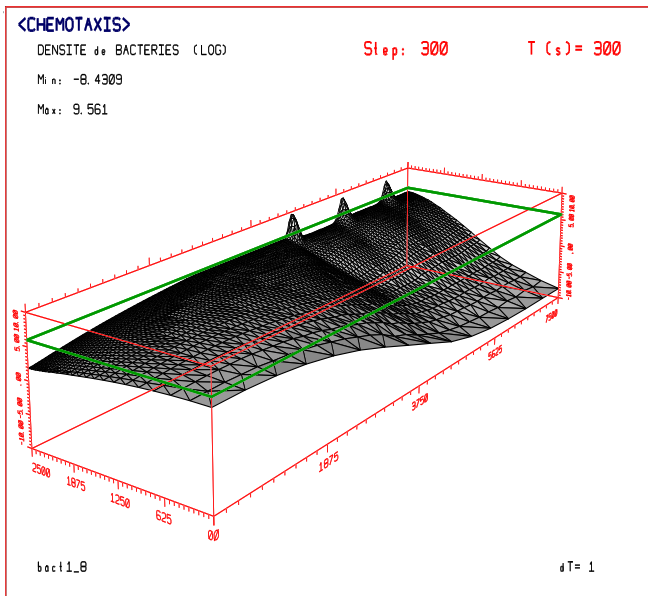
```

Troncated_Mass : 1.82426E+05 Troncated_Mass_Percent : 97.29431 %
-----
... Process time : 1000.0 s Total bacteria mass: 1.87500E+05 Threshold value: 1.00000E+06
----- Local max number: 1
*** J1 = 5432 Conc: 2.589E+09 (XG,YG)= ( 7.484E-01, 2.486E-01) (cmXcm)
Number of triangles N(1)= 39 Area % = 0.1455
Local_Mass(1) = 1.83725E+05 Percent(1) = 97.98692 %
Contrib( 5432)= 1.36181E+04 Percent_max_local(1)= 7.41218 % Percent_max_total(1)= 7.26297 %
----- Global results -----
Number of local maxima : 1 Total number of triangles N= 39 Area % : 0.1455
Troncated_Mass : 1.83725E+05 Troncated_Mass_Percent : 97.98692 %

```



(a) High concentration localization after 100s



(b) High concentration localization after 300s

Figure 13: BACTERIA CONCENTRATION, (LOG. SCALE). Computational domain: rectangle  $0.75\text{cm} \times 0.25\text{cm}$ . Bounded production of attractants ( $\rho^* = 1000\rho_0$ ), observer position near  $(x_{min}, y_{min})$ .

Quantitative results for  $\rho^* = 1000\rho_0$ , "Stationary solution".

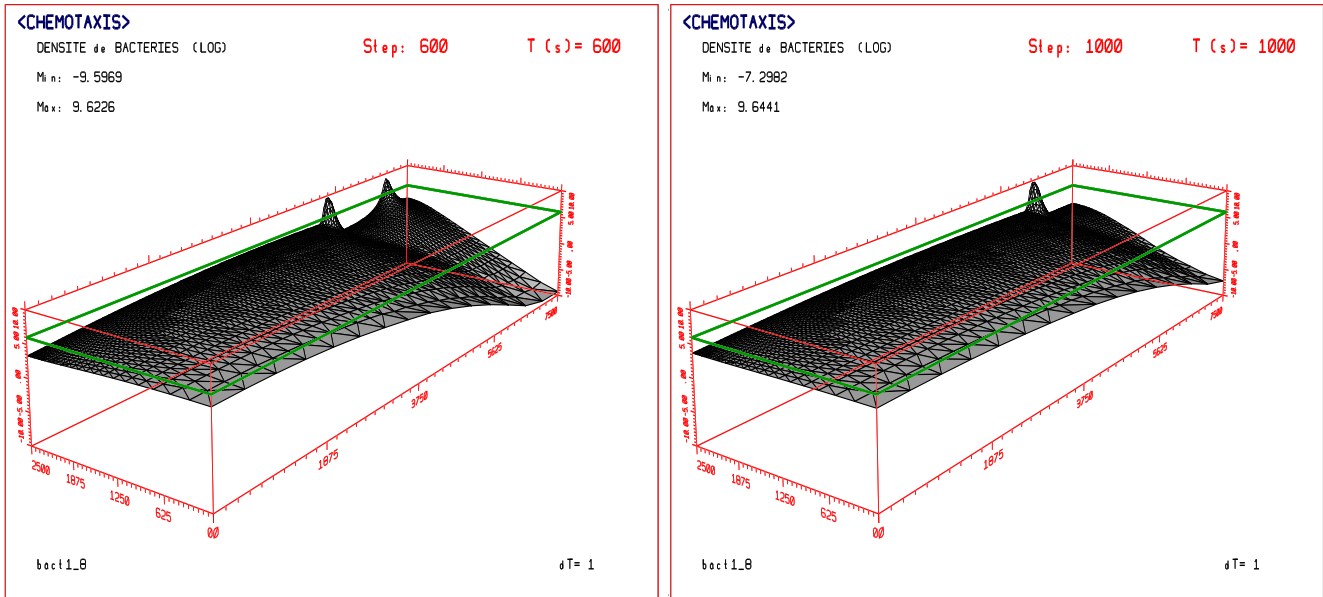
```

-----
... Process time :***** s Total bacteria mass: 1.87534E+05 Threshold value: 1.00000E+06
----- Local max number: 1
*** J1 = 4953 Conc: 4.422E+09 (XG,YG)= ( 6.479E-01, 2.493E-01) (cmXcm)
Number of triangles N(1)= 38 Area % = 0.1325
Local_Mass(1) = 1.87473E+05 Percent(1) = 99.96752 %
Contrib( 4953)= 2.37528E+04 Percent_max_local(1)= 12.67000 % Percent_max_total(1)= 12.66588 %
----- Global results -----
Number of local maxima : 1 Total number of triangles N= 38 Area % : 0.1325
Troncated_Mass : 1.87473E+05 Troncated_Mass_Percent : 99.96752 %

```

## Conclusion

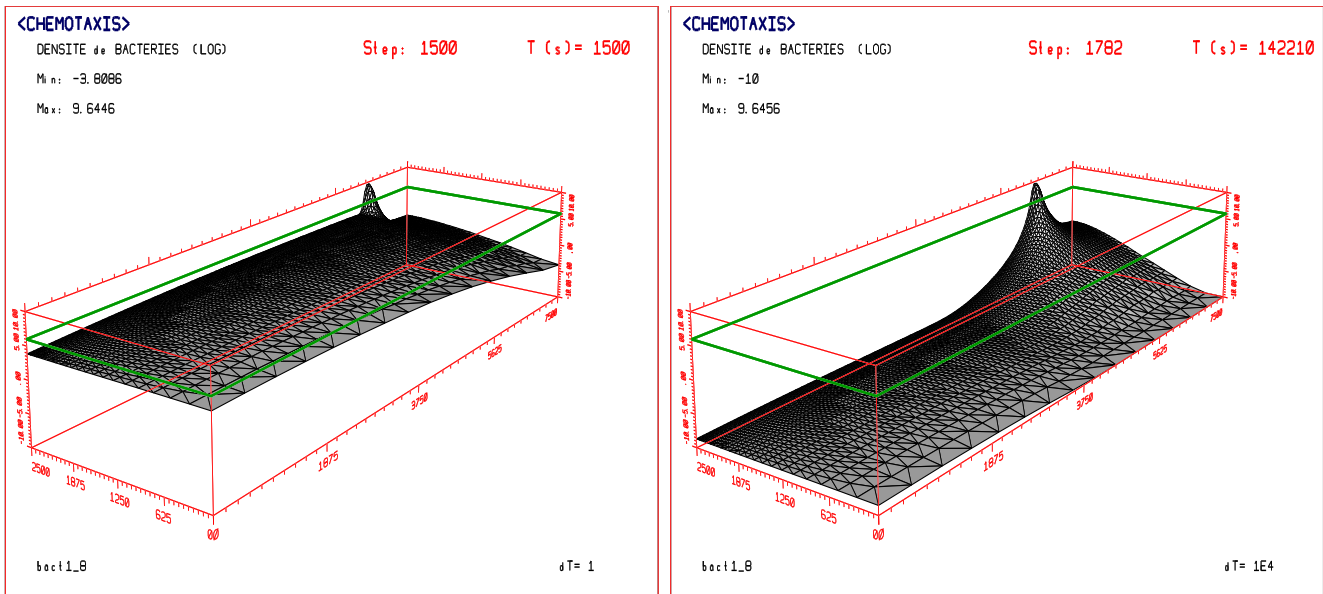
We have presented here a computational scheme which allows the simulation of chemotactic bacteria aggregation. As theoretically predicted, the density redistribution during the evolution process



(a) High concentration localization after 600s

(b) High concentration localization after 1000s

Figure 14: BACTERIA CONCENTRATION, (LOG. SCALE). Computational domain: rectangle  $0.75\text{cm} \times 0.25\text{cm}$ . Bounded production of attractants ( $\rho^* = 1000\rho_0$ ), observer position near  $(x_{min}, y_{min})$ .



(a) High concentration localization after 1500s

(b) Distribution after a long time

Figure 15: BACTERIA CONCENTRATION, (LOG. SCALE). Computational domain: rectangle  $0.75\text{cm} \times 0.25\text{cm}$ . Bounded production of attractants ( $\rho^* = 1000\rho_0$ ), observer position near  $(x_{min}, y_{min})$ .

appears to be strongly dependent on the model used for the source (production) of attractants. With the first model (source of attractants proportional to the bacterial density  $\rho$ ), several isolated

peaks of bacterial concentration may appear -concentration localized over only one element, which is something like a Dirac mass at discrete level- and remain more or less at the same place along the evolution process.

Introducing a cutoff value in the production of attractants, the first peak of bacterial concentration travels to the center of the domain, “eliminating” all the secondary peaks. After a certain amount of time, high densities values remain localized on small part of the domain (0.1 to 1 %) but not only over one mesh element.

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