

**Reaction-Diffusion Problem with Concentration Driven  
Deformation**

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Internship Work Supervised by

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Zürich, 30 / 9 / 2006

## 1. ABSTRACT

We are dealing with a model of reaction-diffusion phenomena of multi-spices mass in a closed surface. The problem is studied in three-dimensional situation. The transport of the spices should cause the surface to move and undergo swilling, shrinking and other complex deformations. We enclose this surface within a larger domain called “band”, we proceed by applying extension and projection techniques in order to use Particle Method for solving this problem in the band. We obtain then the corresponding projected values of fields on the moved surface.

## 2. MODEL IN EMBEDDING DOMAIN

Let us consider the interval of time  $]0, T[$  where  $T \in \mathbb{R}^+$ . We introduce the following notations:

- $\mathcal{S}(t)$  is a closed surface in  $\mathbb{R}^3$  at time step  $t \in [0, T]$ ,
- $\Omega(t)$  is a large domain in  $\mathbb{R}^3$  at time step  $t \in ]0, T[$  such that  $\mathcal{S}(t) \subset \Omega(t)$ ,
- $Q_T = \{(x, t), x \in \Omega(t) \text{ and } t \in ]0, T[ \}$ ,
- $\mathcal{S}_T = \{(x, t), x \in \mathcal{S}(t) \text{ and } t \in ]0, T[ \}$ ,
- $u, v : Q_T \rightarrow \mathbb{R}$ , the density of tow chemicals,
- $\mathbf{a} : Q_T \rightarrow \mathbb{R}^3$  the velocity field.

After applying the extension techniques, the model of mass transport is introduced in the large domain, it is governed by the following equations:

$$\left\{ \begin{array}{ll} \frac{\partial u}{\partial t} = D\delta\Delta u - \nabla \cdot (u\mathbf{a}) + \alpha u(1 - r_1 v^2) + v(1 - r_2 u) & \text{in } Q_T, \quad (2.1) \\ \frac{\partial v}{\partial t} = \delta\Delta v - \nabla \cdot (v\mathbf{a}) + \beta v(1 + \frac{\alpha r_1}{\beta} uv) + u(\gamma + r_2 v) & \text{in } Q_T, \quad (2.2) \\ \frac{\partial u}{\partial n} = 0 & \text{on } \partial\Omega, \quad (2.3) \\ \frac{\partial v}{\partial n} = 0 & \text{on } \partial\Omega, \quad (2.4) \\ u(., 0) = u^0 & \text{in } \Omega(0), \quad (2.5) \\ v(., 0) = v^0 & \text{in } \Omega(0). \quad (2.6) \end{array} \right.$$

The law of mass conservation is given by the equations (2.1) – (2.2), the equations (2.3) – (2.4) enforce the isolation at the boundaries. The initial conditions are given by (2.5) – (2.6). The values of the parameters  $\alpha$ ,  $\beta$  and  $\gamma$  are dictated by conservation relations between chemicals as explained in *R. A. Barrio et al: Math. Biol. 61. 483 (1999)*. In biological framework, the interaction parameter  $r_1$  is associated with a cubic coupling, and favors the formation of the striped patterns.

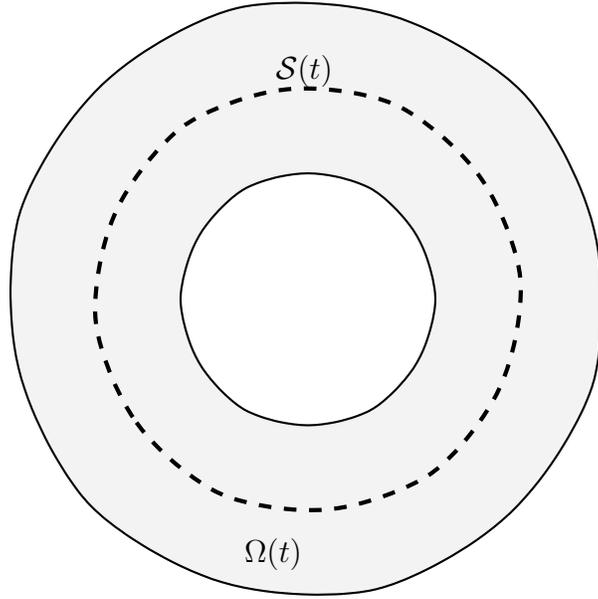


FIGURE 1. The surface  $\mathcal{S}$  is embedded in the large domain  $\Omega$  at time step  $t$

The quadratic coupling  $r_2$  produces spot patterns. The velocity field  $\mathbf{a}$  is given by the orthogonal extension in  $\Omega(t)$  of the vector  $\bar{\mathbf{a}}$  defined on  $\mathcal{S}(t)$  by the relation:

$$\bar{\mathbf{a}} = C u \mathbf{n}, \quad (2.7)$$

where  $C$  is a positive constant and  $\mathbf{n}$  is the outer normal unit vector on  $\mathcal{S}(t)$ .

As mentioned above, the conservation of mass introduced in the framework of large domain is an extension of the model given in the surface  $\mathcal{S}$ :

$$\left\{ \begin{array}{ll} \frac{\partial u}{\partial t} = D\delta\Delta_{\mathcal{S}}u - \nabla_{\mathcal{S}} \cdot (u\bar{\mathbf{a}}) + \alpha u(1 - r_1 v^2) + v(1 - r_2 u) & \text{in } \mathcal{S}_T, \\ \frac{\partial v}{\partial t} = \delta\Delta_{\mathcal{S}}v - \nabla_{\mathcal{S}} \cdot (v\bar{\mathbf{a}}) + \beta v(1 + \frac{\alpha r_1}{\beta} uv) + u(\gamma + r_2 v) & \text{in } \mathcal{S}_T, \\ u(\cdot, 0) = u^0 & \text{in } \mathcal{S}(0), \\ v(\cdot, 0) = v^0 & \text{in } \mathcal{S}(0). \end{array} \right.$$

Here  $\nabla_{\mathcal{S}}$  is the intrinsic gradient and  $\Delta_{\mathcal{S}}$  is the intrinsic Laplacian or Laplacian-Beltrami operator. The intrinsic gradient is just the projection onto  $\mathcal{S}$  of the regular 3D gradient while the Laplace-Beltrami is the projected divergence of it.

### 3. GENERAL STEPS

We choose the spherical surface domain  $\mathcal{S}$  with center  $O = (0, 0, 0)$  and radius  $R$ . The surface  $\mathcal{S}$  is given by the zero level of the signed distance function  $\Phi$  which is given by Hamilton-Jacobi equation:

$$\frac{\partial \Phi}{\partial t} = \mathbf{a} \nabla \Phi. \quad (3.1)$$

The function  $\Phi$  is also governed by the Eikonal equation:

$$\|\nabla \Phi\| = 1. \quad (3.2)$$

We begin by enclosing the interface within a larger, annular domain “band”:

$$|\Phi| \leq h. \quad (3.3)$$

where  $2h$  is the large of the band.

We then proceed via:

- (1) Initialize a level set function  $\Phi$  to represent the interface  $\mathcal{S}$  while ensuring that there are sufficiently many computational node points between  $\mathcal{S}$  and the computational boundary.
- (2) Compute the reaction-diffusion value in (2.1) – (2.2) by using PSE and update  $u$  and  $v$ .
- (3) Calculate the normal vector  $\mathbf{n}$  by using  $\mathbf{n} = \frac{\nabla \Phi}{\|\nabla \Phi\|}$ .
- (4) Calculate the normal velocity  $\mathbf{a}$  in a band about  $\mathcal{S}$  according to (2.7). Extend the normal velocity orthogonally from the interface  $\mathcal{S}$ .
- (5) Move the particle according to the convection term.
- (6) Reinitialize the level set.
- (7) Repeat (2)-(6) for each step of the time discretization.

#### 4. NUMERICAL METHOD

Let  $\Omega$  denote an open domain in  $\mathbb{R}^3$ . We introduce the notations:

- $x_k^0 \in \mathbb{R}^3$ : the initial location of the particle  $k$ ,
- $\omega_k^0$ : the initial volume of the particle  $k$ .

We define traveling particles by setting  $x_k(t) = X(t; x_k^0, 0)$  the solution of the problem:

$$\begin{cases} \frac{\partial X(t)}{\partial t} = \mathbf{a}(X(t), t), & \text{in } \Omega \times ]0, T[, \\ X(0) = X_k^0, & \text{in } \Omega. \end{cases} \quad (4.1)$$

$$\quad (4.2)$$

We denote by  $J(t; \zeta, s)$  the determinant of the change of variable:  $\zeta \rightarrow X(t; \zeta, s)$  and we set  $\omega_k(t) = J(t; x_k^0, 0)\omega_k^0$ . We have:

$$\frac{\partial \omega_k(t)}{\partial t} = \text{div}(\mathbf{a}(x_k(t), t))\omega_k(t). \quad (4.3)$$

##### 4.1. Function approximation by particles.

We approximate a continuous function  $f(x) : \mathbb{R}^3 \rightarrow \mathbb{R}$  by particles. We follow the three steps:

- Step 1: Integral representation:

$$f(x) = \int_{\Omega} f(y)\delta(y-x)dy, \forall x, y \in \Omega,$$

the term  $\delta$  is the Dirac function.

- Step 2: Integral mollification:

$$f_{\epsilon}(x) = \int_{\Omega} f(y)\eta_{\epsilon}(y-x)dy,$$

the term  $\eta_{\epsilon}$  is the mollification kernel regularizing the Dirac function:  $\lim_{\epsilon \rightarrow 0} \eta_{\epsilon} = \delta$ .

- Step 3: Integral discretization:

Using the location and the volume of the particles respectively as nodes and weights, we obtain a quadrature formula:

$$\int_{\Omega} g(x)dx = \sum_{k \in I} \omega_k g(x_k(t)), \quad I \subset \mathbb{Z}^n. \quad (4.4)$$

Then we get:

$$f_{\epsilon}^h(x_k, t) = \sum_{l \in I} \omega_l f_l(t)\eta_{\epsilon}(x_k - x_l(t)). \quad (4.5)$$

## 4.2. Approximation of Laplace Operator.

The development of Laplace operator is given by:

$$\Delta f(x) = \epsilon^{-2} \int_{\Omega} (f(y) - f(x)) \eta_{\epsilon}(y - x) dy + O(\epsilon^r), \quad (4.6)$$

we obtain the following approximation:

$$\Delta_{\epsilon} f(x) = \epsilon^{-2} \int_{\Omega} (f(y) - f(x)) \eta_{\epsilon}(y - x) dy. \quad (4.7)$$

By applying the discretization by quadrature formula of the above integral we have:

$$\Delta_{\epsilon}^h f(x_k, t) = \epsilon^{-2} \sum_{l \in I} \omega_l (f_l(t) - f_k(t)) \eta_{\epsilon}(x_l(t) - x_k(t)). \quad (4.8)$$

## 4.3. Space discretization of the reaction diffusion problem.

In order to solve the system of equations (2.1)-(2.6) we use a space discretization by particles. We obtain the approximate values of the positions, the volumes and the strengths of the particles by solving of the following system:

$$\left\{ \begin{array}{l} \frac{dx_k}{dt} = \mathbf{a}(x_k(t), t), \quad (4.9) \\ \frac{d\omega_k(t)}{dt} = \text{div} \mathbf{a}(x_k(t), t) \omega_k(t), \quad (4.10) \\ \frac{du_k(t)}{dt} + \text{div}(\mathbf{a}(x_k(t), t) u_k(t)) - D \delta \epsilon^{-2} \sum_{l \in I} \omega_l (u_l(t) - u_k(t)) \eta_{\epsilon}(x_l(t) - x_k(t)) \\ \quad = \alpha u_k(t) (1 - r_1 v_k(t)^2) + v_k(t) (1 - r_2 u_k(t)) \quad (4.11) \\ \frac{dv_k(t)}{dt} + \text{div}(\mathbf{a}(x_k(t), t) v_k(t)) - \delta \epsilon^{-2} \sum_{l \in I} \omega_l (v_l(t) - v_k(t)) \eta_{\epsilon}(x_l(t) - x_k(t)) \\ \quad = \beta v_k(t) \left( 1 + \frac{\alpha r_1}{\beta} u_k(t) v_k(t) \right) + u_k(t) (\gamma + r_2 v_k(t)) \quad (4.12) \\ x_k(0) = x_k^0, \quad \omega_k(0) = \omega_k^0, \quad u_k(0) = u_0(x_k^0), \quad v_k(0) = v_0(x_k^0) \quad (4.13) \end{array} \right.$$

## 5. APPLICATIONS

### 5.1. Case of heigh velocity.

In this test case we observe the evolution of a dumbbell surface. The initial values of concentrations are randomly distributed, we choose the constant value in relation (2.7) as  $C = 1$ .

Interparticle spacing  $h = 0.02$ .

Core size  $\epsilon = 1h$ .

Cutoff =  $3\epsilon$ .

The larger band (half width) = 2 Cutoff.

The inner band (half width) = 1 Cutoff.

Time stepping = 0.01 for time step  $\leq 56000$  and 0.001 for time step  $> 56000$ .

Reinitialization method: Hamilton-Jacobi.

Extension method: Hamilton-Jacobi.

$r_1 = 0.02$ .

$r_2 = 0.2$ .

$\alpha = 0.899$ .

$\beta = -0.910$ .

$\gamma = -0.899$ .

$\delta = 0.0171$ .

$D = 0.516$ .

The large velocity cases topology change in the surface at time step: 80000. It should be worth to note that the swilling deformation observed in the results corresponds to the positive value of the constant  $C$ . A swilling deformation should be expected when we choose a shrinking value for  $C$ .



FIGURE 2. The Dumbbell at time step: 0

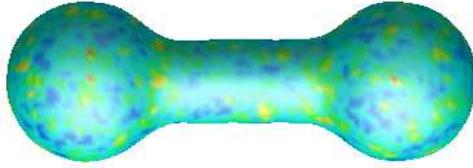


FIGURE 3. The Dumbbell at time step: 36000

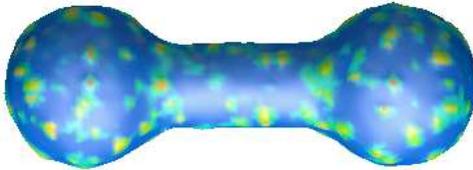


FIGURE 4. The Dumbbell at time step: 56000

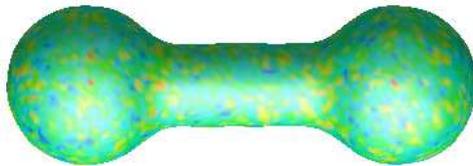


FIGURE 5. The Dumbbell at time step: 64000

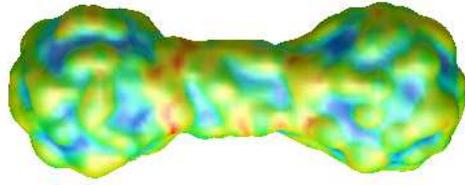


FIGURE 6. The Dumbbell at time step: 68000

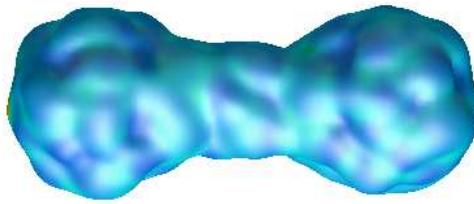


FIGURE 7. The Dumbbell at time step: 76000

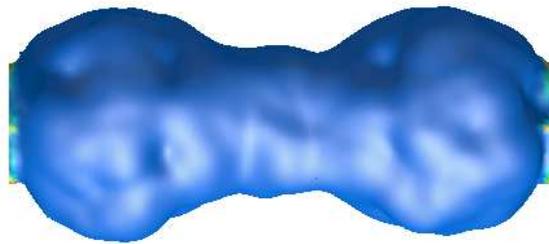


FIGURE 8. The crashed Dumbbell at time step: 82000

## 5.2. Case of low velocity.

By taking the same case with  $C = 0.1$  and time stepping = 0.001. The dumbbell surface presents the following deformations:

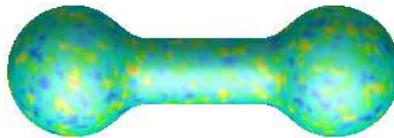


FIGURE 9. The Dumbbell at time step: 30000



FIGURE 10. The Dumbbell at time step: 65000

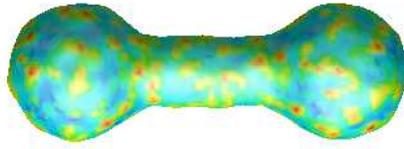


FIGURE 11. The Dumbbell at time step: 95000

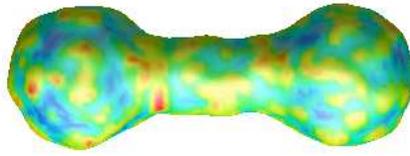


FIGURE 12. The Dumbbell at time step: 130000

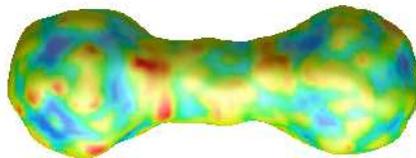


FIGURE 13. The Dumbbell at time step: 160000

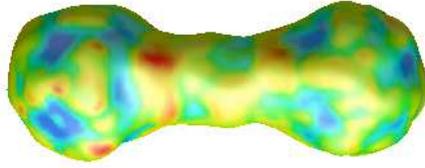


FIGURE 14. The Dumbbell at time step: 195000

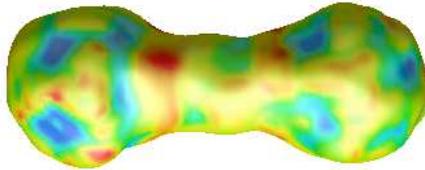


FIGURE 15. The Dumbbell at time step: 225000

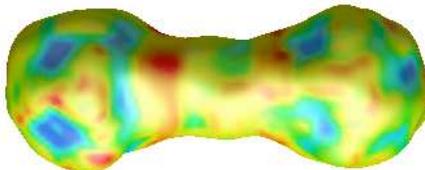


FIGURE 16. The Dumbbell at time step: 235000

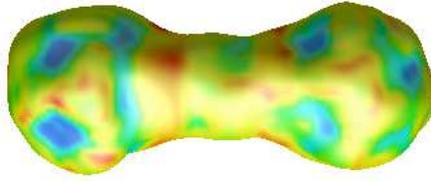


FIGURE 17. The Dumbbell at time step: 255000

An other numerical computing of the above test case with a spherical surface is also carried out, it exhibits a compared behavior. From the observation of the results we conclude that the numerical scheme used in this calculation is not unconditionally stable.

This work is in the prolongation of the former studies in Institute of Computational Science, ETH Zürich, intended for the observation of the evolution of the deforming surface under curvature effects. As perspective it should be important to compare the tow approaches (curvature driven growth and concentration driven growth) for the derivation of criteria making it possible to determine the stable or unstable character movement.

As proposed idea, it should be instructive if we can carry out a new numerical computing of the deforming surface under the combined effects (curvature and concentrations).

#### ACKNOWLEDGEMENTS

I want to thanks Prof. Ivo Sbalzarini from Computational Biophysics Lab, Prof. Petros Koumoutsakos, Michael Bergdorf and Charalampos Haris Damalos from the Institute of Computational Science, ETH Zürich for the fruitful discussions and remarks and for allowing use of supercomputing facilities.

## APPENDIX.

In this test case we choose the diffusion tensor with coefficient values: 0.001, 0.002 respectively instead of (0.00000521 , 0.00021) as it was proposed in the above applications. By taking the same case with  $C = 0.1$  and time stepping = 0.001. The dumbbell surface presents the following deformations:

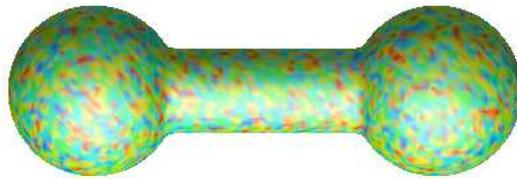


FIGURE 18. The Dumbbell at time step: 0 (View: Top)



FIGURE 19. The Dumbbell at time step: 0 (View: front)

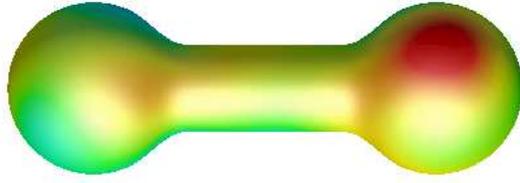


FIGURE 20. The Dumbbell at time step: 15000 (View: Top)

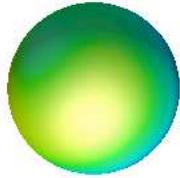


FIGURE 21. The Dumbbell at time step: 15000 (View: front)

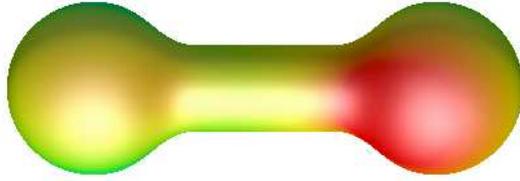


FIGURE 22. The Dumbbell at time step: 65000 (View: Top)



FIGURE 23. The Dumbbell at time step: 115000 (View: front)

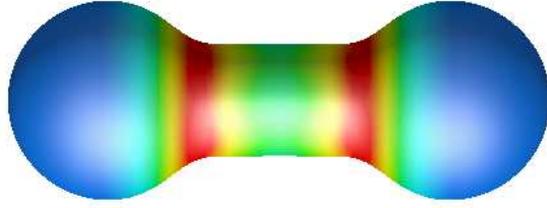


FIGURE 24. The Dumbbell at time step: 125000 (View: Top)



FIGURE 25. The Dumbbell at time step: 125000 (View: front)

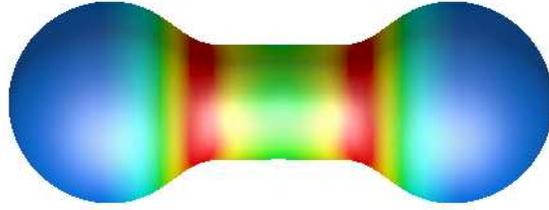


FIGURE 26. The Dumbbell at time step: 130000 (View: Top)



FIGURE 27. The Dumbbell at time step: 130000 (View: front)

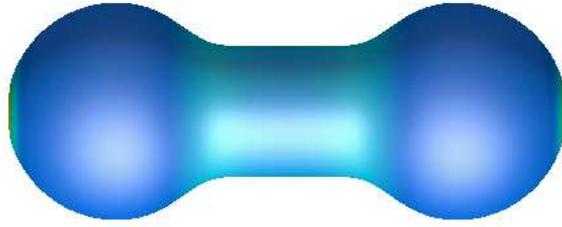


FIGURE 28. The Dumbbell at time step: 165000 (View: Top)

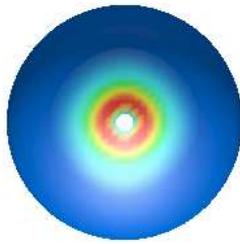


FIGURE 29. The Dumbbell at time step: 215000 (View: front)