Modelisation and numerical simulation of the Smoluchowski equation in perforated domains

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Outline

Outline

Introduction

The development of Alzeihmer's desease (AD)

- The agglomeration of β-Amyloid peptide ($A\beta$) : process associated with the development of AD.
- In some neurons, imbalance between production and clearance of $A\beta$ during aging.
- At elevated levels : produces pathological aggregates $\rightarrow$ accumulation of deposits known as **senile plaques**.

Smolushowski equation

- system of partial differential equations
- describes the evolving densities of diffusing particles that are prone to coagulate in pairs

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Smoluchwoski equation in polymerization 1/2

Binary reactions

- P_k, for $k \in \mathbb{N}$: polymer of size k, a set of k identical particle (monomers).
- With time, if 2 polymers are very close, they are likely to merge $\rightarrow$ creation of a new polymer
- By convention, only binary reactions

Coalescence of polymers size k and j :

$$P_k \quad + \quad P_j \qquad \rightarrow \qquad P_{k+j}$$

Restrictions of the model studied

- Assumptions : aggregation results only from Brownian movement or diffusion (thermal coagulation).
- We neglect other effects such as : multiple coagulation, condensation, fragmentation ...

Smoluchowski equation in polymerisation 2/2

Discrete diffusive coagulation equations

$$\frac{\partial u_i}{\partial t}(t,x) - d_i \triangle_x u_i(t,x) = Q_i(u) \quad \text{in } [0,\, T]x\Omega \tag{1}$$

$u_i(t,x) \geq 0$ (for $i \geq 1$) $\rightarrow$ **concentration of i-clusters**
clusters with i identical elementary particles.

$d_i \rightarrow$ **diffusion coefficient** of an i-cluster, $d_i > 0 \;\forall i \geq 1$.

Coagulation term

$$Q_i(u) = Q_{g,i}(u) - Q_{l,i}(u) \quad i \geq 1 \tag{2}$$

Coagulation term

$a_{i,j} \rightarrow$ **coagulation rates**, non nonnegative constants such that $a_{i,j} = a_{j,i}$ coefficient that represents the reaction in which an$i + j$-cluster is formed from an i and a j-cluster.

Gain

$$Q_{g,i} = \frac{1}{2} \sum_{j=1}^{i-1} a_{i-j,j} u_{i-j} u_j \tag{3}$$

Describes the creation of polymers of size i by coagulation of polymers of size j and $i - j$ (clusters of size $\leq i - 1$).

Loss

$$Q_{l,i} = u_i \sum_{j=1}^{\infty} a_{i,j} u_i u_j \tag{4}$$

Describes the depletion (reduction) of polymers of size i after coalescence with other polymers.

Outline

Parameters of the microscopic model

Domain

- $\Omega_0 \subset \mathbb{R}^3$: smooth bounded domain representing a portion of **cerebral tissue**
- $\overline{\Omega}_j \subset \Omega_0$ with $j = 1...N$: regular regions representing N **neurons**
- $\overline{\Omega}_i \cap \overline{\Omega}_j = \neq$ if $i \neq j$

$$\Omega := \Omega_0 \setminus \cup_{j=1}^{N} \overline{\Omega}_j$$

Concentration u

- $u = (u_1, ..., u_M)$: $M \in \mathbb{N}$ and $u_j = u_j(t, x), t \geq 0, x \in \Omega$
- $u_j(t, x)$ with $1 \leq j < M - 1$: concentration of an $A\beta$ assembly of j monomers.
- u_M : takes into account aggregation of more than M-1 monomers (M $=$maximum size of an assembly).

$A\beta$'s concentration in the monomeric form

$$
\begin{cases}
\frac{\partial u_1}{\partial t}(t,x) - d_1 \triangle_x u_1(t,x) - Q_{l,1} = 0 & \\
\nabla_x u_1 . n = 0 & \text{on } \partial\Omega_0 \\
\nabla_x u_1 . n = \Psi_j & \text{on } \partial\Omega_j,\ j = 1...N \\
u_1(0,x) = U_1 \geq 0 &
\end{cases}
\tag{5}
$$

- No Q_{gain} $\rightarrow$ we cannot form a monomer by coagulation.
- Homogeneous Neumann condition on $\partial\Omega_0$ $\rightarrow$ artificial isolation of the cerebral from its environment
- Non-homogeneous Neumann condition on $\partial\Omega_j$, $j = 1...N$ $\rightarrow$ production of $A\beta$ in the monomeric form at the level of neuron membranes
- $\Psi_j \neq 0$ $\rightarrow$ only neurons affected by the disease are taken into account

$A\beta$'s concentration in assemblies

For assemblies of size $1 < m \leq M - 1$:

$$\begin{cases} \frac{\partial u_m}{\partial t}(t,x) - d_m \triangle_x u_m(t,x) - Q_{l,m} = Q_{g,m} & \\ \nabla_x u_m . n = 0 & \text{on } \partial\Omega_0 \\ \nabla_x u_m . n = 0 & \text{on } \partial\Omega_j,\ j = 1...N \\ u_m(0,x) = 0 & \end{cases} \tag{6}$$

For assemblies of size M :

$$\begin{cases} \frac{\partial u_M}{\partial t}(t,x) - d_M \triangle_x u_M(t,x) = Q_{g,M} & \\ \nabla_x u_M . n = 0 & \text{on } \partial\Omega_0 \\ \nabla_x u_M . n = 0 & \text{on } \partial\Omega_j,\ j = 1...N \\ u_M(0,x) = 0 & \end{cases} \tag{7}$$

Special case : assembly size M
(takes into account all assemblies with size $\geq M$)

No Q_{loss} and $Q_{g,M} = \frac{1}{2} \sum_{\substack{j+k \geq M \\ k<M \\ j<M}} a_{j,k} u_j u_k$

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Weak formulation 1/2

For m = 1, non-homogeneous Neumann condition :

$$\int_\Omega \frac{\partial u_1}{\partial t} \cdot v - d_1 \int_\Omega \Delta u_1 \cdot v = \int_\Omega Q_1 v \quad \text{on } \Omega$$

Then, applying the Green theorem :

$$\int_\Omega \Delta u_1 \cdot v = - \int_\Omega \nabla u_1 \nabla v + \int_{\partial\Omega} \underbrace{(\partial_n u_1)}_{=\Psi_j \text{ on } \partial\Omega_j} v$$

$$\Longrightarrow \int_\Omega \frac{\partial u_1}{\partial t} \cdot v + d_1 \int_\Omega \nabla u_1 \cdot \nabla v = \int_\Omega Q_1 v + \int_{\partial\Omega_j} \Psi_j v \quad \text{on } \Omega$$

Weak formulation 2/2

For m = 2...M, homogeneous Neumann condition :

$$\int_\Omega \frac{\partial u_m}{\partial t} \cdot v + d_m \int_\Omega \nabla u_m \cdot \nabla v = \int_\Omega Q_m v \quad \text{on } \Omega$$

Final weak formulation :

$$\left\{ \begin{array}{l} \text{Finding } u_m \in V \text{ such that :} \\ a(u_m, v) = l_m(v) \forall v \in V \end{array} \right. \tag{8}$$

with :

$$\boxed{\begin{array}{lll} a(u_m, v) & = \int_\Omega \frac{\partial u_m}{\partial t} + d_m \int_\Omega \nabla u_m \cdot \nabla v & \text{for m=1...M} \\ l_m(v) & = \begin{cases} \int_\Omega Q_1 v + \int_{\partial\Omega_{j=1\dots N}} \Psi_j v, & \text{if } m = 1 \\ \int_\Omega Q_m v & \text{otherwise} \end{cases} & \end{array}} \tag{9}$$

Time discretisation

Implicit Euler scheme to approximate $\frac{\partial u_m}{\partial t}$ considering $u_m^n = u_m(t_n)$:

$$\frac{\partial u_m^{n+1}}{\partial t} \approx \frac{u_m^{n+1} - u_m^n}{\Delta t} \quad \text{with } \Delta t = t_{n+1} - t_n$$

Replacing $\frac{\partial u_m^{n+1}}{\partial t}$ in the weak formulation :

$$\boxed{\begin{aligned} a(u_m, v) &= \int_\Omega u_m^{n+1} \cdot v + \Delta t d_m \int_\Omega \nabla u_m^{n+1} \cdot \nabla v \\ l_m(v) &= \begin{cases} \int_\Omega u_m^n \cdot v + \Delta t \int_\Omega Q_1 v + \Delta t \int_{\partial\Omega_{j=1\ldots N}} \Psi_j v, & \text{if } m = 1 \\ \int_\Omega u^n \cdot v + \Delta t \int_\Omega Q_m v & \text{otherwise} \end{cases} \end{aligned}} \tag{10}$$

Galerkin Method

We consider a space V_h of finite dimension and define a base $(\phi_i)_{i=1..N_s}$ such that : $u_{h,m} = \sum_{i=1}^{N_s} x_{i,m}\phi_i$

Replacing u_m by u_h, m in the weak formulation, we obtain the following linear system :
For m=1...M

$$(M + \Delta t d_m K)X_m^{n+1} = \Delta t B^n + MX_m^n$$

with :

- M : the mass matrix
- K : the rigidity matrix
- B^n : the coagulation term at time t_n

Outline

Only diffusion

Parameters :
Figure 1

Result with one neuron and N=??

Parameters :
$U_0 =$, $\Psi =$, $d_m =$, $a_i, j =$ Figure ...

Convergence studies

Computational domain: $\Omega = [-0.5; 0.5] \times [-0.5; 0.5] \times [0; 1]$

Initial condition:

$$\begin{bmatrix} u \\ v \\ w \\ \eta \end{bmatrix} = \begin{bmatrix} cos\left(\pi x - \frac{\pi}{4}\right) sin\left(\pi y - \frac{\pi}{4}\right) \\ -sin\left(\pi x - \frac{\pi}{4}\right) cos\left(\pi y - \frac{\pi}{4}\right) \\ 0 \\ 1 \end{bmatrix}$$

Convergence studies: divergence free

$\mathcal{O}2$ (**N=1**)	$\mathcal{O}(L_1)$		$\mathcal{O}(L_2)$		$\mathcal{O}(L_\infty)$	
8.94E-03	9.3167E-02	-	4.7585E-02	-	2.0916E-02	-
5.36E-03	3.4633E-02	1.9	1.7711E-02	1.9	7.7751E-03	1.9
3.83E-03	1.7973E-02	1.9	9.1864E-03	2.0	4.0131E-03	2.0
2.98E-03	1.0984E-02	2.0	5.6113E-03	2.0	2.4419E-03	2.0

$\mathcal{O}3$ (**N=2**)	$\mathcal{O}(L_1)$		$\mathcal{O}(L_2)$		$\mathcal{O}(L_\infty)$	
8.94E-03	6.3636E-03	-	3.3567E-03	-	1.7099E-03	-
5.36E-03	1.4233E-03	2.9	7.4921E-04	2.9	3.7861E-04	3.0
3.83E-03	5.2460E-04	3.0	2.7610E-04	3.0	1.3905E-04	3.0
2.98E-03	2.4831E-04	3.0	1.3062E-04	3.0	6.5434E-05	3.0

$\mathcal{O}4$ (**N=3**)	$\mathcal{O}(L_1)$		$\mathcal{O}(L_2)$		$\mathcal{O}(L_\infty)$	
8.94E-03	1.3029E-03	-	6.8714E-04	-	4.5625E-04	-
5.36E-03	1.8287E-04	3.8	9.5818E-05	3.9	6.5249E-05	3.8
3.83E-03	4.9274E-05	3.9	2.5704E-05	3.9	1.7244E-05	4.0
2.98E-03	1.8384E-05	3.9	9.5611E-06	3.9	6.3443E-06	4.0

Convergence studies: NON-divergence free

$\mathcal{O}2$ (**N=1**)	$\mathcal{O}(L_1)$		$\mathcal{O}(L_2)$		$\mathcal{O}(L_\infty)$	
8.94E-03	9.3301E-02	-	4.7647E-02	-	2.1148E-02	-
5.36E-03	3.4648E-02	1.9	1.7716E-02	1.9	7.8523E-03	1.9
3.83E-03	1.7975E-02	1.9	9.1864E-03	2.0	4.0512E-03	2.0
2.98E-03	1.0984E-02	2.0	5.6106E-03	2.0	2.4647E-03	2.0

$\mathcal{O}3$ (**N=2**)	$\mathcal{O}(L_1)$		$\mathcal{O}(L_2)$		$\mathcal{O}(L_\infty)$	
8.94E-03	9.6634E-03	-	4.9852E-03	-	2.6242E-03	-
5.36E-03	2.1862E-03	2.9	1.1255E-03	2.9	6.0363E-04	3.0
3.83E-03	8.1014E-04	3.0	4.1625E-04	3.0	2.2272E-04	3.0
2.98E-03	3.8443E-04	3.0	1.9725E-04	3.0	1.0511E-05	3.0

$\mathcal{O}4$ (**N=3**)	$\mathcal{O}(L_1)$		$\mathcal{O}(L_2)$		$\mathcal{O}(L_\infty)$	
8.94E-03	1.4103E-03	-	7.2876E-04	-	3.9854E-04	-
5.36E-03	1.9756E-04	3.8	1.0153E-05	3.9	5.6671E-05	3.8
3.83E-03	5.3161E-05	3.9	2.7238E-05	3.9	1.4968E-05	4.0
2.98E-03	1.9817E-05	3.9	1.0134E-06	3.9	5.5062E-06	4.0

Convergence studies: divergence-free error

div-free

$h(\Omega)$	$\epsilon_{L_2}\mathcal{O}(2)$	$\epsilon_{L_2}\mathcal{O}(3)$	$\epsilon_{L_2}\mathcal{O}(4)$
8.94E-03	0.0000E-00	5.1383E-16	1.3726E-15
5.36E-03	0.0000E-00	6.0425E-16	1.1620E-15
3.83E-03	0.0000E-00	4.7411E-16	9.9785E-16
2.98E-03	0.0000E-00	4.5329E-16	7.7298E-16

NON div-free

$h(\Omega)$	$\epsilon_{L_2}\mathcal{O}(2)$	$\epsilon_{L_2}\mathcal{O}(3)$	$\epsilon_{L_2}\mathcal{O}(4)$
8.94E-03	8.9549E-02	6.7913E-04	1.3485E-04
5.36E-03	1.0477E-03	1.4317E-04	1.5366E-05
3.83E-03	4.9002E-04	5.0082E-05	4.2957E-06
2.98E-03	2.8251E-04	2.2798E-05	1.6770E-06

Nonlinear convective terms

Horizontal plane $x - y$

$$\begin{aligned} (u, v, w) &= (x, y, x) \times (0, 0, 1) \\ \eta &= 1 \end{aligned}$$

Nonlinear convective terms

Vertical plane $x - z$

$$
\begin{aligned}
(u, v, w) &= (x, y, x) \times (0, 1, 0) \\
\eta &= 1
\end{aligned}
$$

Horizontal viscous terms

Finite volume discretization

$$\nabla_i^2 \mathbf{u}_k = \frac{1}{|P_i|} \int_{P_i} \nabla \cdot \nabla_h \mathbf{u}_k \, dA = \frac{1}{|P_i|} \int_{\partial P_i} \nabla_h \mathbf{u}_k \cdot \mathbf{n}_j \, ds.$$

Viscous numerical flux (Gassner et al., *JCP*,2017):

$$\nabla_h \mathbf{u}_k \cdot \mathbf{n}_j = \frac{1}{2} \left(\nabla \mathbf{u}_k^+ + \nabla \mathbf{u}_k^- \right) \cdot \mathbf{n}_j + \frac{1}{\delta_j \sqrt{\frac{1}{2}\pi}} \left(\mathbf{u}_k^+ - \mathbf{u}_k^- \right)$$

Horizontal viscous terms

First problem of Stokes ($\nu^h = 10^{-3}$)

Figure: Horizontal velocity distribution for the first problem of Stokes at time $t = 0.3\ s$ (left) and $t = 0.5\ s$. The initial flow velocity is (u,v,w)=(1,0,0) with $\eta = 1$.

Horizontal viscous terms

First problem of Stokes ($\nu^h = 10^{-3}$)

Figure: Horizontal velocity distribution for the first problem of Stokes at time $t = 0.3\ s$ (left) and $t = 0.5\ s$. The initial flow velocity is (u,v,w)=(1,0,0) with $\eta = 1$. Different order of accuracy are shown.

Nonhydrostatic flow

Computational domain: $\Omega = [0; 10]^3$

$$
\begin{aligned}
(u, v, w) &= 0 \\
\eta &= 0.02x - 0.1
\end{aligned}
$$

Nonhydrostatic flow

Computational domain: $\Omega = [0;10]^3$

$$
\begin{aligned}
(u, v, w) &= 0 \\
\eta &= 0.02x - 0.1
\end{aligned}
$$

Outline

Conclusions and outlook

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- high order reconstruction for the velocity field on unstructured Voronoi meshes;
- decoupled horizontal and vertical divergence-free reconstruction procedure;
- applications to hydrostatic and nonhydrostatic flows.

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- high order reconstruction for the velocity field on unstructured Voronoi meshes;
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Outlook

- sediment transport;
- turbulence model.

Thank you!

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