A NUMERICAL SCHEME FOR ROD-LIKE POLYMERS WITH FRAGMENTATION AND MONOMERS LENGTHENING

Erwan Hingant

Université de Lyon, CNRS UMR 5208, Université Lyon 1
Institut Camille Jordan
43 blvd. du 11 novembre 1918
F-69622 Villeurbanne cedex, France.

(hingant@math.univ-lyon1.fr)

December 19, 2011

Abstract

In this paper, we introduce a new numerical method to solve a Fokker-Planck-Smolukowsky equation arising in the simulation of dilute polymeric liquids. The very recent model, considered here and introduced in a former paper, deals with rod-like polymers with fragmentation and monomers lengthening arising in biology. We formulate a spectral decomposition leading to a set of lengthening-fragmentation equations. The resulting system is solved by integration along the caracteristic curves.

1 Introduction

In the present work we are concerned with the simulation of dilute polymeric liquids. Particularly, it deals with a model, introduced and analyzed in [5], that describes the dynamics of the configurational distribution of rod-like polymers with monomers addition and fragmentation submitted to a flow. This latter is relevant for biological polymer, especially when polymers are formed from proteins. For instance, the prion protein which forms rigid rod polymers during *in vivo* experiments.

For a complete description of the model we refer to [5]. Succintly, we assume a fluid surrounding monomers and polymers. Each polymers has a length, related

to the mass of monomers that form it, which increases by addition of monomers one-by-one at its both ends. A polymer can split into two new polymers and the stress induced by the flow modify the sensibility of a polymer to break. Moreover, polymers moves according to their angle and position due to the flow.

The key ingredient to study polymeric fluids is the stress tensor induced by polymers onto the fluid. The cornerstone, to compute this stress, is the probability of the configurational distribution equation on polymers which is of a Fokker-Planck-Smolukowsky equation. This latter has to be coupled with the monomers density, which drives the lengthening of polymers. Here, we propose a numerical scheme to approach the configurational density in the case of a steady shear flow. Other type of flow has been studied in similar problem, as planar flow in [4], and could be studied here in a similar way.

The second section of this parper is dedicated to establish the equations and to reduce the system from three to one dimension in space. The third is to develop the numerical sheme combining a spectral and a semi-lagrangian method. Finally, the fourth section is devoted to numerical experiments.

2 Equations being at stake

2.1 The system studied

Let $\Omega \subset \mathbb{R}^3$ be the flow-domain of polymers and monomers. The configurational distribution of polymers is given by the function $\psi(r, \eta, y, t)$ where $r \in \mathbb{R}_+$ describes the length of polymers, $\eta \in \mathbb{S}^2$ its orientation and $y \in \Omega$ the position in the flow-domain while the time is given by $t \geq 0$. The problem takes into account the monomers density given by $\phi(y, t)$ and the flow $u(y, t) \in \mathbb{R}^3$ is assumed to be a given incompressible velocity field. Polymers lengthen and split at non-negative rates, respectively denoted by τ and β. The polymerisation rate τ depends on the concentration ϕ of monomers at y and time t, on the size r and orientation η, eventually on the flow u. The fragmentation rate β depends on the size r, the orientation η and the gradient of the flow ∇u induces on the polymer. Moreover, when it splits at a size r, the two new polymers are of size r' and $r - r'$ with a probability given by the kernel κ.

Thus, from [5] equation on ψ reads,

$$\frac{\partial}{\partial t}\psi + (u \cdot \nabla_y)\,\psi + \mathcal{R}[\nabla u](\psi) + \mathcal{L}[\nabla u, u, \phi](\psi) = 0, \tag{1}$$

on $\mathbb{R}_+ \times \mathbb{S}^2 \times \Omega$ and $t > 0$. The operators $\mathcal{R}$ and $\mathcal{L}$, respectively for the Rotational motion and the Lengthening-fragmentation process, both defined by

$$\mathcal{R}[\nabla u](\psi) = -\nabla_\eta \cdot \Big(D\nabla_\eta \psi - \mathrm{P}_{\eta^\perp}\big(\nabla u\ \eta\big)\psi \Big), \tag{2}$$

where $D > 0$ stands for the rotational diffusion constant and

$$\mathcal{L}[\nabla u, u, \phi](\psi) = \frac{\partial}{\partial r}\big(\tau(\phi, r, \eta, u)\psi\big) + \beta(r, \eta, \nabla u)\psi + \\ - 2\int_r^\infty \beta(r', \eta, \nabla u)\kappa(r, r')\psi(t, y, r', \eta)\ dr', \tag{3}$$

where $\nabla_\eta \cdot$ and ∇_η are respectively the divergence and the gradient on the sphere. The projection operator to the tangent space on the sphere satisfies $\mathrm{P}_{\eta^\perp}(z) = z - (z \cdot \eta)\eta$, for any $z \in \mathbb{R}^3$. The size distribution kernel $\kappa : \mathbb{R}_+ \times \mathbb{R}_+ \mapsto \mathbb{R}_+$ must observe the following property,

$$\kappa(r', r) = 0, \text{ if } r' > r, \tag{4}$$

$$\kappa(r', r) = \kappa(r - r', r), \tag{5}$$

and

$$\int_0^r \kappa(r', r)\ dr' = 1, \tag{6}$$

to be consistent with the fact that a polymer split into two new polymers and the mass conservation after scission.

To define proper boundary conditions in space, we have to consider the in-flow part of the boundary $\Gamma = \partial\Omega$. This is defined by

$$\Gamma_{in} = \{y \in \Gamma : u \cdot \vec{n} < 0\}, \tag{7}$$

where $\vec{n}$ is the outward normal vector to the boundary. We complete equation (1) with boundary conditions

$$\psi = \psi_{in} \text{ over } \Gamma_{in} \quad \text{and} \quad \psi(r,\eta,y,t)\big|_{r=0} = 0, \tag{8}$$

at any time $t \geq 0$, with ψ_{in} a given data. Initial condition at time $t = 0$, where ψ^0 a given function, reads

$$\psi(r,\eta,y,t)\big|_{t=0} = \psi^0(r,\eta,y). \tag{9}$$

Let us now introduced the density equation of free monomers in Ω, see [5] for more details, it reads

$$\frac{\partial}{\partial t}\phi + (u\cdot\nabla_y)\,\phi - d\Delta_y\phi = -\int_{\mathbb{S}^2\times\mathbb{R}_+} \tau(\phi,r,\eta,u)\psi\; dr d\eta, \tag{10}$$

on Ω and $t > 0$ with $d > 0$ the diffusion constant. The source term take into account the polymerization of monomers into polymers. This equation is completed by boundary conditions

$$\phi = \phi_{in} \text{ over } \Gamma_{in} \quad \text{and} \quad \nabla_y\phi\cdot\vec{n} = 0 \text{ over } \Gamma\backslash\Gamma_{in}, \tag{11}$$

at any time $t \geq 0$, where ϕ_{in} is given. Finally, initial contition reads

$$\phi(y,t)\big|_{t=0} = \phi^0(y), \tag{12}$$

with ϕ^0 a given data.

2.2 Space reduction

Here we are going to reduce the problem (1)-(10) to a 1-dimensional problem in space. For that purpose, we consider a stationary shear flow given by the velocity field $u(y) = (\gamma y_2, 0, 0)^T$ in $\Omega = (0, L_1)\times(0, L_2)\times(0, L_3)$ with $L_1, L_2, L_3 > 0$ and the shear rate $\gamma > 0$. The jacobian matrix of u is a constant matrix denoted by

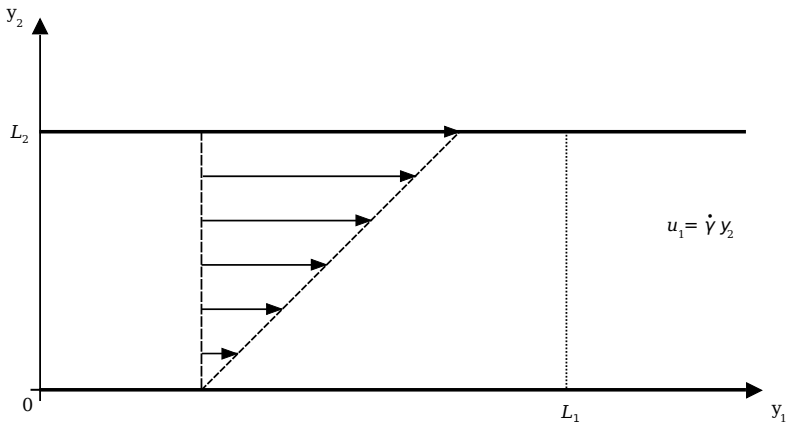


Figure 1: Shear flow: intersection with plane $y_3 = c \in (0, L_3)$.

M_γ such that

$$M_\gamma := \nabla u(y) = \begin{pmatrix} 0 & \gamma & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \tag{13}$$

This shear flow suggests to find solutions depending only of the second component of y. For that, we consider an alternative problem on $\psi(r, \eta, x, t)$ the configurational density of polymer at $x \in (0, X)$ and $\phi(x, t)$ the density of monomer, with $X > 0$ the size of the one-dimensional physical space. With respect to this density, taking $v_\gamma(x) = (\gamma x, 0, 0)^T$, we are interested in the following equations on polymers,

$$\frac{\partial}{\partial t}\psi + \mathcal{R}[M_\gamma](\psi) + \mathcal{L}[M_\gamma, v_\gamma, \phi](\psi) = 0, \tag{14}$$

on $\mathbb{R}_+ \times \mathbb{S}^2 \times (0, X)$ and $t > 0$. Meanwhile, the monomers density satisfies

$$\frac{\partial}{\partial t}\phi - d\frac{\partial^2}{\partial x^2}\phi = -\int_{\mathbb{R}_+ \times \mathbb{S}^2} \tau(\phi, r, \eta, v_\gamma)\psi \; dr d\eta, \tag{15}$$

on $(0, X)$ and $t > 0$. These equations are complete with the boundary conditions

$$\frac{\partial}{\partial x}\phi(x, t)\big|_{x=0,X} = 0 \text{ and } \psi(r, \eta, x, t)\big|_{r=0} = 0, \tag{16}$$

at any time $t \geq 0$, with initial conditions

$$\psi(r, \eta, x, t)\big|_{t=0} = \psi^0(r, \eta, x) \text{ and } \phi(x, t)\big|_{t=0} = \phi^0(x), \tag{17}$$

where ψ^0 and ϕ^0 are given.

A solution of this reduced equation can be seen as solution of the above mentioned problem. Indeed, one can construct a solution of the original problem by taking appropriate ψ_{in} and ϕ_{in} solution of the above on dimensional problem with respect to the same initial conditions.

3 Approximation of the solution

In this section we are going to discretize the problem (14)-(28) with boundary conditions (16) and initial value (17) to approach numerically the solution. First a spectral method, used for instance in [4], is developed according to the spherical variable leading to a system of partial differential equations on spectral coefficients. The system is of type polymerization-fragmentation equations on the length r, with x considered as a parameter. The latter is solved thanks to a semi-lagrangian method.

3.1 Spectral method on the sphere

The spectral method consists in defined an orthogonal basis on $\mathbb{S}^2$, and a convenient base one is the spherical harmonics, eigenvectors of the laplacien on the sphere. To do that, let P_l^m be the associated Legendre polynomial of degree $l \geq 0$ and order $0 \leq m \leq l$. Real spherical harmonics, denoted by $S_{p,l,m}$, for $p = 0, 1$ and $p \leq m \leq l$, are defined as follows

$$S_{p,l,m}(\theta, \phi) = P_l^m\left(cos(\theta)\right) cos(m\varphi - p\pi/2), \tag{18}$$

for any $\theta \in (0, \pi)$ and $\phi \in (0, 2\pi)$. We use a second notation for the normalized real spherical harmonics, $Y_{p,l,m} = N_{l,m} S_{p,l,m}$, with

$$N_{l,m} = \sqrt{\frac{(2l+1)(l-m)!}{2\pi(1+\delta_{m0})(l+m)!}}, \tag{19}$$

such that

$$\int_{\mathbb{S}^2} Y_{p,l,m} Y_{q,k,j} \, d\eta = \delta_{(p,l,m),(q,k,j)}. \tag{20}$$

Then, we approximate the configurational probability density ψ in terms of spherical harmonics by

$$\psi_L = \sum_{p=0}^{1} \sum_{l=0}^{L} \sum_{m=p}^{2l} \alpha_{p,l,m}(t,r,x) Y_{p,2l,m}(\eta) \tag{21}$$

with harmonics of even order in l at each point $x \in (0,L)$. Indeed, there is no way to identify a polymer of orientation η and $-\eta$, thus we are interested in even harmonics, which is satisfied if and only if l is even.
In order to simplify some notation we defined two subset of $\mathbb{N}^2$,

$$\mathcal{N}_p = \{(k,j) : k \geq 0 \text{ and } p \leq m \leq l\}, \tag{22}$$

for relevant spectral coefficients and

$$\mathcal{M}_{l,m} = \{(k,j) : |k-l| \leq 2 \text{ and } |j-m| \leq 2\}, \tag{23}$$

Spherical harmonics satisfy two properties of interest in our study. First, as mentioned, they are eigenvectors of the laplacien on the sphere,

$$-\Delta_\eta Y_{p,l,m} = l(l+1) Y_{p,l,m}. \tag{24}$$

when $(l,m) \in \mathcal{N}_p$ for $p = 0, 1$. Second, for a shear flow, we have

$$\nabla_\eta \cdot \Big(\mathrm{P}_{\eta^\perp}\big(M_\gamma \eta\big) Y_{p,l,m} \Big) = (-1)^{1-p} \dot{\gamma} \sum_{(k,j) \in \mathcal{N}_{1-p} \cap \mathcal{M}_{l,m}} \frac{N_{l,m}}{N_{k,j}} \, a_{lk}^{mj} \, Y_{1-p,k,j}. \tag{25}$$

This is obtain using Table 14.4-1 in [3], precised in Table 1, for the definition of coefficients a_{lk}^{mj}. The goal is to write a system of equations on the $\alpha_{p,l,m}$, for that we assume that ψ_L is a solution of (14). For a sake of simplicity, we assume that β and τ are independent of η. Moreover, τ is taken independent of v_γ, we deal with $\beta(r) \equiv \beta(r,\eta,M_\gamma)$ (M_γ being a constan matrix) and $\tau(\phi,r) \equiv \tau(\phi,r,\eta,v_\gamma)$. After injecting the solution ψ_L in equation on polymers, multiplying by $Y_{p,2l,m}$ for any relevant $(2l,m) \in \mathcal{N}_p$ with $p = 0, 1$ and integrating over $\mathbb{S}^2$, this leads to a coupled system on $\alpha_{p,l,m}$ with $p = 0, 1$, $0 \leq l \leq L$ and $p \leq m \leq 2l$,

$$\frac{\partial}{\partial t}\alpha_{p,l,m} + \tau(\phi,r)\frac{\partial}{\partial r}\alpha_{p,l,m} + f_l(\phi,r)\alpha_{p,l,m} + \gamma G_{p,l,m}(\boldsymbol{\alpha}) = 2\int_r^\infty \beta(r')\kappa(r,r')\alpha_{p,l,m}(r',x,t)\ dt, \quad (26)$$

with $f_l(\phi,r) = 2l(2l+1)D + \beta(r) + \frac{\partial}{\partial r}\tau(\phi,r)$, $\boldsymbol{\alpha}$ corresponding to the vector of componments the $\alpha_{p,l,m}$ and

$$G_{p,l,m}(\boldsymbol{\alpha}) = \sum_{p'=0}^{1}\sum_{l'=0}^{L}\sum_{m'=p'}^{2l'} G_{(p,l,m);(p',l',m')}\alpha_{p',l',m'}. \quad (27)$$

where coefficients $G_{(p,l,m);(p',l',m')}$ are derived in the Appendix. On the other hand, equation on the approach density of monomers ϕ_L, reads now

$$\frac{\partial}{\partial t}\phi_L - d\frac{\partial^2}{\partial x^2}\phi_L = -2\sqrt{\pi}\int_{\mathbb{R}_+} \tau(\phi,r)\alpha_{0,0,0}(r,x,t)\ dr, \quad (28)$$

since,

$$\int_{\mathbb{S}^2} Y_{p,l,m}d\eta = \begin{cases} 2\sqrt{\pi} & \text{if } (p,l,m) = (0,0,0), \\ 0 & \text{else.} \end{cases} \quad (29)$$

In the following section, we formulate a semi-lagrangian method to solve the system on $\alpha_{p,l,m}$.

3.2 Integration along the caracteristics curves

The approximation with spectral method on the sphere leads to a system of $(2L+1)(L+1)$ differential equations on each $\alpha_{p,l,m}$ with $p = 0, 1$ and $l = 0, \ldots, L$ and $m = p, \ldots, 2l$ where each equations on $\mathbb{R}_+ \times \mathbb{S}^2 \times (0, X)$ are given by (30). This system is of course coupled to the monomers advection-diffusion equation (28). The method used is similar to the one developped by O. Angulo in [1, 2]. First, let $R_{max} > 0$ and approximate the system with a finite size on $r \in (0, R_{max})$.

$a_{l,l-2}^{m,m-2}$	$=$	$\dfrac{(l-2)(l+m)(l+m-1)(l+m-2)(l+m-3)(1-\delta_{m0})}{4(2l+1)(2l-1)}$
$a_{l,l}^{m,m-2}$	$=$	$\dfrac{3(l+m)(l+m-1)(l-m+1)(l-m+2)(1-\delta_{m0})}{4(2l-1)(2l+3)}$
$a_{l,l+2}^{m,m-2}$	$=$	$-\dfrac{(l+3)(l-m+1)(l-m+2)(l-m+3)(l-m+4)(1-\delta_{m0})}{4(2l+1)(2l+3)}$
$a_{l,l}^{m,m}$	$=$	$-\dfrac{m}{2}$
$a_{l,l-2}^{m,m+2}$	$=$	$-\dfrac{(l-2)(1+\delta_{m0})}{4(2l+1)(2l-1)}$
$a_{l,l}^{m,m+2}$	$=$	$-\dfrac{3(1+\delta_{m0})}{4(2l-1)(2l+3)}$
$a_{l,l+2}^{m,m+2}$	$=$	$\dfrac{(l+3)(1+\delta_{m0})}{4(2l+1)(2l+3)}$
All other $a_{l,l'}^{m,m'}$ are zero		

Table 1: Tabulation of the $a_{l,l'}^{m,m'}$ from Table 14-4.1 in [3].

Equations on $\alpha_{p,l,m}$ read now,

$$\frac{\partial}{\partial t}\alpha_{p,l,m} + \tau(\phi,r)\frac{\partial}{\partial r}\alpha_{p,l,m} + f_l(\phi,r)\alpha_{p,l,m} + \gamma G_{p,l,m}(\boldsymbol{\alpha}) = 2\int_r^{R_{max}} \beta(r')\kappa(r,r')\alpha_{p,l,m}(r',x,t)\,dt, \quad (30)$$

over $(0,R_{max})\times(0,X)$ and $t\geq 0$.
Let $R(t,x;t_0,r_0)$ be the caracteristic curve starting in r_0 at time t_0 at $x\in(0,X)$ solution of the problem

$$\begin{cases} \dfrac{d}{dt}R(t,x;t_0,r_0) = \tau\left(\phi(x,t),R(t,x;t_0,r_0)\right), & \text{for } t>t_0, \\ R(t_0,x;t_0,r_0) = r_0. \end{cases} \quad (31)$$

We define the solutions along the characteristic starting at (t_0, r_0) by $\tilde{\alpha}_{p,l,m}(t, x; t_0, r_0) = \alpha_{p,l,m}(R(t, x; t_0, r_0), x, t)$ satisfying

$$\frac{d}{dt}\tilde{\alpha}_{p,l,m} = 2\int_{R(t,x;t_0,r_0)}^{R_{max}} \beta(r')\kappa(R(t, x; t_0, r_0), r')\alpha_{p,l,m}(r', x, t)\, dr' - \\ - f_l(\phi(x,t), R(t, x; t_0, r_0))\tilde{\alpha}_{p,l,m} - \dot{\gamma}G_{p,l,m}(\tilde{\boldsymbol{\alpha}}), \quad (32)$$

such that $\tilde{\alpha}_{p,l,m}(t_0, x; t_0, r_0) = \alpha_{p,l,m}(r_0, x, t_0)$. Noting again that x is a parameter, the system have to be solved for any $x \in (0, X)$.

3.3 Numerical scheme

There, we give the method to solve reformulated problem. First, let $L > 0$ fixed, the order of approximation over the spherical harmonics. Then, let us discretize the space by $X_i = i\Delta x$, $i = 0 \dots I$ with $\Delta x = X/I$ and the size by $R_j = j\Delta r$, $i = 0 \dots J$ with $\Delta r = R_{max}/J$. Now we assume that the numerical approximation of the solution is known at a time t_n and denote by P_i^n the approximation of $\phi(X_i, t_n)$ and $A^n_{p,l,m;i;j}$ of $\alpha_{p,l,m}(R_j, X_i, t_n)$. It is now possible to compute $A^{n+1}_{p,l,m;j;i}$ and P_i^{n+1} for any relevant (p, l, m), $i = 0, \dots, I$ and $j = 0, \dots, J$. First, we determine the next time $t_{n+1} = t_n + \Delta t_n$ with the time step

$$\Delta t_n = \frac{\Delta r}{\max_{0\le j\le J;\ 0\le i\le I} \tau(P_i^n, R_j)}. \quad (33)$$

As the space variable x is taking as a parameter, fix the size by choosing $i \in (0, \dots, I)$ and forgetting the notation i to be lighter, we now compute the $A^{n+1}_{p,l,m;j}$ (keeping in mind that it is at point X_i). We defined S_j^n the size point such that (S_j^n, t_n) and (R_j, t_{n+1}) be numerically on the same characteristic curve, given by

$$S_0^n = 0, \quad S_j^n = R_j - \Delta t_n \tau(P_i^n, R_j)\ 1 \le j \le J, \quad S_{J+1}^n = R_J. \quad (34)$$

It is nessecary to interpolate the solution at time t_n onto the points S_j^n denoted by $B^n_{p,l,m;j}$ and it is given by a linear interpolation,

$$B^n_{p,l,m;j} = A^n_{p,l,m;j-1} + (S_j^n - R_{j-1})\frac{A^n_{p,l,m;j} - A^n_{p,l,m;j-1}}{\Delta r},\ 1 \le j \le J, \quad (35)$$

and set $B^n_{p,l,m;0} = A^n_{p,l,m;0}$ and $B^n_{p,l,m;J+1} = A^n_{p,l,m;J}$. Finally, we obtain the $A^{n+1}_{p,l,m;j}$ by discretization of (32)

$$\begin{aligned} A^{n+1}_{p,l,m;j} = \; & B^n_{p,l,m;j} - \Delta t_n f_l(P^n_i, R_j) A^{n+1}_{p,l,m;j} - \gamma \Delta t_n G_{p,l,m}(\mathbf{B}^n_j) + \\ & + 2\Delta t_n \left((R_j - S^n_j)\beta(S^n_j)\kappa(S^n_j, S^n_j) B^n_{p,l,m;j} + \sum_{q=j}^{J} \beta(R_q)\kappa(S^n_j, R_q) A^n_{p,l,m;q} \, \Delta r \right), \end{aligned} \tag{36}$$

for $1 \leq j \leq J$ and $A^{n+1}_{p,l,m;0} = 0$ where $\mathbf{B}^n_j$ is vector of all the $B^n_{p,l,m;j}$. We do that for any space point X_i. We have to finish by P^{n+1}_i, solving

$$(I - \Delta t_n M)\, P^{n+1} = K^n, \tag{37}$$

where M is the Neumann diffusion matrix and K^n is given by approaching the source terms in (28), given by

$$K^n_i = P^n_i - 2\sqrt{\pi}\Delta t_n \sum_{j=0}^{J} \tau(P^n_j, R_j) A^{n+1}_{0,0,0;i;j} \Delta r. \tag{38}$$

This ends the method to solve the approximate problem.

4 Numerical experiments

In this section, we propose a numerical convergence analysis and some simulations. In order to analyzed the convergence of the scheme let us defined some technical tools and notations. First for the monomers density we denoted by $\phi_\Delta x$ the approximation of the solution with a space discretization $X_i = i\Delta x$, $i = 0, \cdots, I$. The ℓ^2-norm is given by

$$||\phi_{\Delta x}(\cdot, T)||_{\ell^2(0,I)} = \sum_{i=0}^{I} P^N_i \Delta x, \tag{39}$$

where N is the last time step such that $t_N = T$. We now defined the relative error by

$$E_\phi(\Delta x) = \frac{||\phi_{\Delta x}(\cdot, T) - \phi_{2\Delta x}(\cdot, T)||_{\ell^2}}{||\phi_{2\Delta x}(\cdot, T)||_{\ell^2}}. \tag{40}$$

and the order,

$$O_\phi(\Delta x) = \frac{\log\left(E_\phi(2\Delta x)/E_\phi(\Delta x)\right)}{\log 2}. \tag{41}$$

This is the definition used to compute the order of convergence in space on the solution ϕ.

Second, we compute the convergence in size according to the solution ψ, configurational probability density of polymers. Let $\psi_{\Delta r}$ be the approximation of ψ with a size discretization $R_j = j\Delta r$, $j = 0, \cdots, J$. A generalyzed Parseval theorem gives

$$||f||^2_{L^2(\mathbb{S}^2)} = \sum_{p=0}^{1} \sum_{l=0}^{\infty} \sum_{m=p}^{l} |f_{p,l,m}|^2, \tag{42}$$

when

$$f = \sum_{p=0}^{1} \sum_{l=0}^{\infty} \sum_{m=p}^{l} f_{p,l,m} Y_{p,l,m}. \tag{43}$$

This follows from orthogonality of the spherical harmonics. Now, we are able to use the following norm

$$||\psi_{\Delta r}(\cdot, T)||_{\ell^\infty(\ell_2)} = \max_{j=0,\ldots,J} \left[\left(\sum_{i=0}^{I} \sum_{p=0}^{1} \sum_{l=0}^{L} \sum_{m=p}^{2l} |A^N_{p,l,m;i;j}|^2 \Delta x \right)^{1/2} \right] \tag{44}$$

where N is the last time step such that $t_N = T$. The relative error is given by

$$E_\psi(\Delta r) = \frac{||\psi_{\Delta r}(\cdot, T) - \psi_{2\Delta r}(\cdot, T)||_{\ell^\infty(\ell^2)}}{||\psi_{2\Delta r}(\cdot, T)||_{\ell^\infty(\ell^2)}}. \tag{45}$$

This is the relative error used to compute the order of convergence and the order O_ψ is defined as in (41).

For numerical simulations, we have choosen particular coefficient, as in [6]. The framentation rate is assumed to be linear in r, thus $\beta(r) = \beta_0 r$ with $\beta_0 > 0$. The polymerization rate is choosen as a constant mass action, *i.e.* $\tau(\phi, r) = \tau_0 \phi$, with

$\tau_0 > 0$. The parameters use in our simulation are given in table 2 and the initial conditions have been taken as below

$$\psi^0(r, \eta, x) = 4e^{-\frac{(x-0.4)^2+(r-0.4)^2}{0.01}}, \tag{46}$$

taking uniformly distribute in η and

$$\phi^0(x) = \frac{1}{2} + \frac{1}{2}e^{-\frac{(x-0.5)^2}{0.5}}. \tag{47}$$

Parameter	Unit	Parameter	Unit
τ_0	0.01	β_0	0.05
$\dot{\gamma}$	0.1	D	0.01
d	0.001	X	1
R_{max}	1	T	10

Table 2: Parameters use for simulations

The results on numerical convergence, with the method presented here, are shown in table 3 and 4. The order of convergence according to the space on ϕ is 2 (see table 3) meanwhile the one in size is 1 (see table 4). These resul numerically.

Nb of points I	Norm	Relative error	Order
10	$939.61 \cdot 10^{-3}$	—	—
20	$939.83 \cdot 10^{-3}$	$2.64 \cdot 10^{-3}$	—
40	$939.26 \cdot 10^{-3}$	$6.60 \cdot 10^{-4}$	1.999
80	$939.12 \cdot 10^{-3}$	$1.63 \cdot 10^{-4}$	2.021
160	$939.08 \cdot 10^{-3}$	$4.05 \cdot 10^{-5}$	2.005
320	$939.07 \cdot 10^{-3}$	$1.01 \cdot 10^{-5}$	2.001
640	$939.07 \cdot 10^{-3}$	$2.53 \cdot 10^{-6}$	2.001

Table 3: Convergence analysis according to x on ϕ. We used a degree of spherical harmonics $L = 7$ and a discretization in size given by $J = 100$. The error and order are given by the norm (39)

We finish by showing results of simulation. Figure 2 represents the density of

Nb of points J	Norm	Relative error	Order
20	1.3910	—	—
40	1.4055	$8.80 \cdot 10^{-2}$	—
80	1.4215	$4.57 \cdot 10^{-2}$	0.95
160	1.4261	$2.06 \cdot 10^{-2}$	1.15
320	1.4278	$9.54 \cdot 10^{-3}$	1.11
640	1.4284	$4.78 \cdot 10^{-3}$	1.00
1280	1.4286	$2.35 \cdot 10^{-3}$	1.02
2560	1.4287	$1.17 \cdot 10^{-3}$	1.01

Table 4: Convergence analysis according to r on ψ. We used a degree of spherical harmonics $L = 4$ and a discretization in space given by $I = 20$. The error and order are given by the norm (44)

monomers and the mass of polymers according to x,

$$x \mapsto \int_{\mathbb{R}_+ \times \mathbb{S}^2} r\psi_L \, dr d\eta, \tag{48}$$

at initial conditions and final time ($T = 0$).

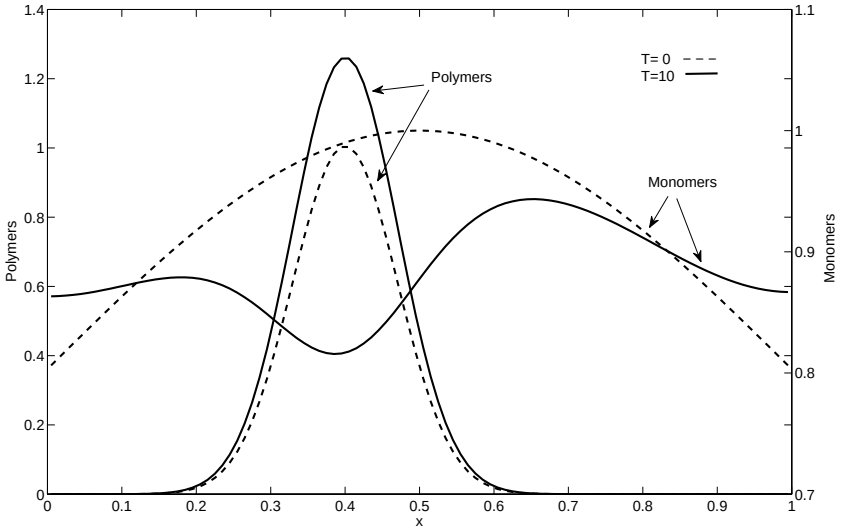


Figure 2: Mass of polymers and density of monomers according to x.

Figure 3 represents the size distribution of polymers at time T, given by the map

$$r \mapsto \int_{\Omega \times \mathbb{S}^2} \psi_L \, d\eta dx. \tag{49}$$

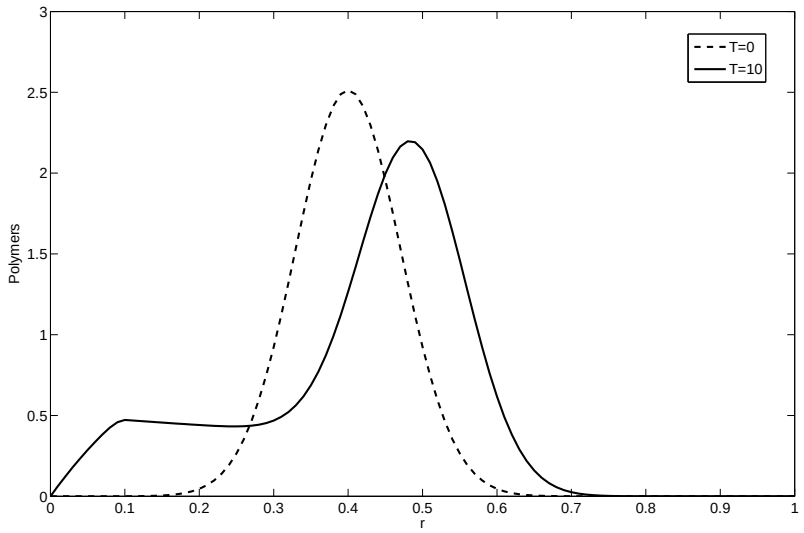


Figure 3: Size distribution of polymer, integrate over the sphere and the space.

Meanwhile, figure 4 is the configurational probability density of polymers at a point (x_0, r_0) and time T,

$$\eta \mapsto \psi_L(r_0, \eta, x_0, T) \tag{50}$$

These figures gives and idea of how the solutions behave.

5 Discussion

In this paper, we propose a combine method to solve efficiently the problem introduced in [5]. We prove numerical convergence of the scheme proposed and we show some simulations provide by this method. The method presented here is a first step ahead more general coefficients. The good results obtain here indicate that this way is to take into account as a numerical approach of this new problem.

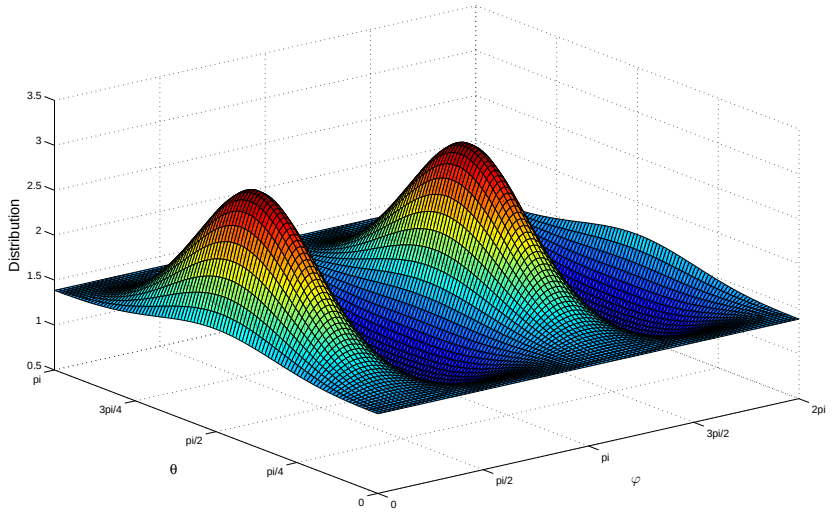


Figure 4: Probability configuration of polymers at $x = 0.4$ and $r = 0.4$ for $\theta \in (0, \pi)$ and $\varphi \in (0, 2\pi)$.

Acknowledgment

The author gratefully acknowledge Ionel S. Ciuperca and Laurent Pujo-Menjouet for many thoughtful and constructive suggestions to improve the paper. The author thanks Liviu I. Palade for very helpful discussions on the model.
This works was supported by ANR grant MADCOW no. 08-JCJC-0135-CSD5.

Appendix

Here we derive terms involving in the system of partial differential equations on spectral coefficeints. First, the time derivative is given by

$$\int_{\mathbb{S}^2} \frac{\partial}{\partial t} \psi_L Y_{p,2l,m} \, d\eta = \frac{\partial}{\partial t} \alpha_{p,l,m}(r, x, t). \tag{51}$$

Then the diffusion over the sphere provides

$$\begin{aligned}
&\int_{\mathbb{S}^2} \nabla_\eta \cdot (D\nabla_\eta \psi_L)\, Y_{p,2l,m}\, d\eta \\
&= \sum_{p'=0}^{1} \sum_{l'=0}^{L} \sum_{m'=p'}^{2l'} \alpha_{p',l',m'} D \int_{\mathbb{S}^2} (\Delta_\eta Y_{p',2l',m'})\, Y_{p,2l,m}\, d\eta \\
&= 2l(2l+1) D \alpha_{p,l,m}.
\end{aligned} \tag{52}$$

The drift on the sphere, regarding (25), leads to

$$\begin{aligned}
&\int_{\mathbb{S}^2} \nabla_\eta \cdot \Big(\mathrm{P}_{\eta^\perp}\big(M_\gamma \eta\big) \psi_L \Big) Y_{p,2l,m}\, d\eta \\
&= \gamma \sum_{p'=0}^{1} \sum_{l'=0}^{L} \sum_{m'=p'}^{2l'} \alpha_{p',l',m'} \int_{\mathbb{S}^2} \nabla_\eta \cdot \Big(\mathrm{P}_{\eta^\perp}\big(M_\gamma \eta\big) Y_{p',2l',m'} \Big) Y_{p,2l,m}\, d\eta \\
&= \gamma \sum_{p'=0}^{1} \sum_{l'=0}^{L} \sum_{m'=p'}^{2l'} \left((-1)^{1-p'} \sum_{(k,j) \in \mathcal{N}_{1-p'} \cap \mathcal{M}_{2l',m'}} \frac{N_{2l',m'}}{N_{k,j}} a_{2l'k}^{m'j}\, \delta_{(1-p',k,j);(p,2l,m)} \right) \alpha_{p',l',m'} \\
&= \gamma \sum_{p'=0}^{1} \sum_{l'=0}^{L} \sum_{m'=p'}^{2l'} G_{(p,l,m);(p',l',m')} \alpha_{p',l',m'},
\end{aligned} \tag{53}$$

such that

$$G_{(p,l,m);(p',l',m')} = (-1)^p \delta_{1-p',p} \frac{N_{2l',m'}}{N_{2l,m}} a_{2l'2l}^{m'm}, \tag{54}$$

by definition of a_{kl}^{jm}.
Finally, due to the fact that the fragmentation and the orientation remains independant on η,

$$\int_{\mathbb{S}^2} \mathcal{L}[M_\gamma, v_\gamma, \phi](\psi) Y_{p,2l,m}\, d\eta = \mathcal{L}[M_\gamma, v_\gamma, \phi](\alpha_{p,l,m}). \tag{55}$$

References

[1] O. Angulo and J. López-Marcos. Numerical integration of a size-structured cell population model in an environment of changing substrate concentration. In *Proceedings of the international conference on Computational methods in sciences and engineering*, pages 28–32, 2003.

[2] O. Angulo, J. López-Marcos, and M. López-Marcos. A semi-lagrangian method for a cell population model in a dynamical environnement. *Math. Model. Nat. Phenom.*, 3(1):1–3, 2008.

[3] R. B. Bird, C. F. Curtiss, R. C. Armstrong, and O. Hassager. *Dynamics of Polymeric Liquids. Vol. 2: Kinetic Theory.* John Wiley & Sons, New-York, 1987.

[4] C. Chauvière and A. Lozinski. Simulation of complex viscoelastic flows using the fokkerplanck equation: 3D FENE model. *J. Non-Newtonian Fluid Mech.*, 122:201–214, 2004.

[5] I. S. Ciuperca, E. Hingant, L. I. Palade, and L. Pujo-Menjouet. Fragmentation and monomer lengthening of rod-like polymers, a relevant model for prion proliferation. *Discrete Contin. Dyn. Syst. Ser. B*, to appear, 2011.

[6] M. Greer, L. Pujo-Menjouet, and G. Webb. A mathematical analysis of the dynamics of prion proliferation. *Journal of theoretical biology*, 242(3):598–606, 2006.