A Becker-Döring model with irreversible fragmentation and injection

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Model: polymerization of biomolecules

We are interested in polymerization of biomolecules such as fibrin clots formation. Fibrin polymers go through a coagulation process (fibrin polymerisation) and fragmentation processes, the latter of which is irreversible (fibrin digestion by plasmin [6]). It is thus natural to consider *open systems* in which monomers arise from a reaction cascades (e.g. fibrinogen conversion to fibrin protein). The infinite reactions taking place are the following:

$$\begin{cases} \emptyset \xrightarrow{\lambda} (1) \\ (1) + (i) \xrightarrow{a_i} (i+1) \\ (i) \xrightarrow{b_i} (i-1) \\ (2) \xrightarrow{b_2} \emptyset \end{cases}$$

where (i) represents the concentration of clusters of size i.

Equations

From the law of mass action, the infinite system of ordinary differential equations associates to the reaction scheme is:

$$\begin{cases} \dfrac{d}{dt}C_1(t) = \lambda - \displaystyle\sum_{j=1}^{+\infty} a_j C_1(t) C_j(t) - a_1 C_1(t)^2, \\ \dfrac{d}{dt}C_i(t) = J_{i-1}(t) - J_i(t), \qquad i \geq 2, \end{cases} \tag{1}$$

where, for all $i \geq 1$,

$$J_i(t) = a_i C_1(t) C_i(t) - b_{i+1} C_{i+1}(t), \tag{2}$$

and $C_i(t)$ denotes the concentration of i-particles clusters per unit of volume at time t.

Notion of solution

Definition: *Let $T \in (0, +\infty]$. A solution $C = (C_i)_{i\geq 1}$ of (1) on $[0,T)$ is a sequence of non-negative functions satisfying the following conditions for all $i \geq 1$, $t \in [0,T)$,*

(i) $C_i \in \mathcal{C}^0([0,t))$, $\displaystyle\sum_{j=1}^{+\infty} a_j C_j \in \mathrm{L}^1(0,t)$,

(ii) and there holds

$$\begin{cases} C_1(t) = C_1(0) + \lambda t - \displaystyle\int_0^t C_1(s) \sum_{j=1}^{+\infty} a_j C_j(s) - a_1 C_1(s)^2 ds, \quad i = 1 \\ C_i(t) = C_i(0) + \displaystyle\int_0^t \left[J_{i-1}(s) - J_i(s)\right] ds, \qquad i \geq 2. \end{cases}$$

We define the following Banach spaces in which solutions will lie. Let $\alpha \geq 0$, we define the following subspaces of $\ell^1(\mathbb{R})$,

$$X_\alpha := \left\{ x = (x_k)_{k\geq 1} \in \mathbb{R}^{\mathbb{N}} \ : \ \|x\|_{X_\alpha} := \sum_{k=1}^{+\infty} k^\alpha |x_k| < +\infty \right\},$$

and we denote X_α^+ its positive cone.

Well-posedness

Let $\alpha \in [0,1]$. Since our equations do not preserve mass, we can consider a larger space for the existence. Following the proofs in [1], and a refined version in [5], we obtain the well-posedness under the following hypothesis on kinetics coefficients:

(H1) There exists $a \geq 0$ such that $0 \leq a_i \leq a i^\alpha$ and $b_i \geq 0$ for all $i \geq 1$.

Theorem: *Let $C^{init} \in X_\alpha^+$. Under the hypothesis (H1), there exists at least one solution $C \in \mathcal{C}^0([0,+\infty), X_\alpha^+)$ to (1) with initial data $C(0) = C^{init}$.*

We also prove moments propagation, meaning that if there exists $\mu \geq \alpha$ such that $C^{init} \in X_\mu^+$, then for all $T > 0$, $\|C\|_{\mathrm{L}^\infty(0,T)} \in X_\mu^+$.

Theorem: *Let $C^{init} \in X_\alpha^+$, and $T \in (0, +\infty]$. Under the hypothesis (H1), there exists at most one solution C on $[0,T)$ to (1) with initial condition $C(0) = C^{init}$ such that*

$$C \in \mathrm{L}^\infty([0,t], X_\alpha^+) \text{ and } \sum_{i=1}^{+\infty} i^{2\alpha} C_i \in \mathrm{L}^1(0,t) \text{ for all } t \in (0,T).$$

Long-time bahviour: steady-states

By steady-state we understand a constant solution C, in particular, $\sum_{i=1}^{+\infty} a_i C_i < \infty$. The family of steady-state is defined from the following equations:

$$J_i = J \text{ and } \lambda - \sum_{j=1}^{+\infty} a_j C_1(t) C_j(t) - a_1 C_1(t)^2 = 0. \tag{3}$$

For $J = 0$, we obtain the detailed balance coefficients Q_i defined by $Q_1 = 1$ and $b_{i+1} Q_{i+1} = a_i Q_i$, for all $i \geq 1$. We remark that, for $J > 0$, there is no steady-states.

From these coefficients, we define two others significant quantities. The first quantity is the *critical monomer density*, denoted z_s, it is defined as the radius of convergence of the power series $\sum a_i Q_i z^i$. The second quantity is the *critical production threshold* defined as follows:

$$\lambda_s := \sup_{z \leq z_s} \sum_{j=1}^{+\infty} a_j Q_j z^{j+1} + a_1 z^2.$$

(H2) $\left(\dfrac{Q_{i+1}}{Q_i}\right)_{i\geq 1}$, $\left(\dfrac{a_{i+1}}{a_i}\right)_{i\geq 1}$ converge, $a_i \geq \underline{a} > 0$ and $b_i \geq \underline{b} > 0$,

Theorem (Steady-states): *Under the assumption (H2), we have the two following possibilities:*

(i) *(Sub-critical) If $\lambda \leq \lambda_s$, then the detailed balance $(Q_i z^i)_{i\geq 1}$ is a steady-state and*
  (a) *either $b_i \leq i a_i$ for $i \gg 1$, then there are no others,*
  (b) *either $b_i > i^\nu a_i$ for $i \gg 1$ and $\nu > 1$, then there is an infinity of additional steady-states ($J < 0$).*

(ii) *(Super-critical) Else $\lambda > \lambda_s$, and then there exists no steady-state.*

Long-time behaviour: local stability

From the lack of Lyapunov function, we use the linearised equations in order to prove local stability. To do so, we analyse the spectral properties of the linearised operator, which can be represented as a perturbation of the one studied in [2].

(H3) There exists $\beta \in [0,1]$ and $b > 0$ such that $b_i \leq b i^\beta$ for all $i \geq 1$,

(H4) $\frac{8b}{\sqrt{z}} \sqrt{\sum_{i=1}^{+\infty} i^{2\beta} Q_i z^i} \sup_{k\geq 1} \left(\sum_{j=k+1}^{+\infty} Q_j z^j\right) \left(\sum_{j=1}^{k} \frac{1}{a_j Q_j z^j}\right) < 1.$

Hypothesis (H4) reduce to λ small for linear and constant coefficients.

Theorem (Local exponential convergence): Assume (H1)-(H4). Let $\lambda < \lambda_s$, C_1^{init} and ν small enough. Let $C = (C_i)_{i\geq 1}$ a solution of (1) with initial condition C^{init}. Then there exists some $K, \varepsilon > 0$ and some $\mu_* > 0$ such that if

$$\sum_{i=1}^{+\infty} \exp(\nu i) |C_i^{init} - Q_i z^i| \leq \varepsilon,$$

then

$$\sum_{i=1}^{+\infty} \exp(\nu i) |C_i(t) - Q_i z^i| \leq K \exp(-\mu_* t), \ \forall t \geq 0.$$

Numerical simulations

The idea to numerically simulate the conservative truncation (meaning $J_n = 0$) is to see the truncation as some discretization of a particular PDE for some size step Δx, in which the size of the aggregates x is a continuous variable. The aforementioned PDE is the following:

$$\frac{\partial C(t,x)}{\partial t} = -\frac{\partial J(t,x)}{\partial x}, \text{ in } [0,T] \times (1,n),$$

with

$$J(t,x) = -a(x) Q(x) C(t,1)^{x+1/2} \frac{\partial}{\partial x} \left(\frac{C(t,x)}{Q(x) C(t,1)^x}\right),$$

To which we add boundary conditions. Then we develop a coarse-grain scheme, consisting of sub-sampling the clusters at some given size, preserving the asymptotics of the system, meaning that we compute

$$C_{n_j}^k \approx C(t^k, n_j),$$

where $(n_j)_{j=1,\dots,K}$ is an increasing sequence of integers. Numerically, we solve the linear system

$$(I + \Delta t W^k) C^{k+1} = C^k + \beta^k,$$

which is unconditionally stable in Δt and Δx_j. The scheme is based on the flux approximation method in [3], and the scheme in [4].

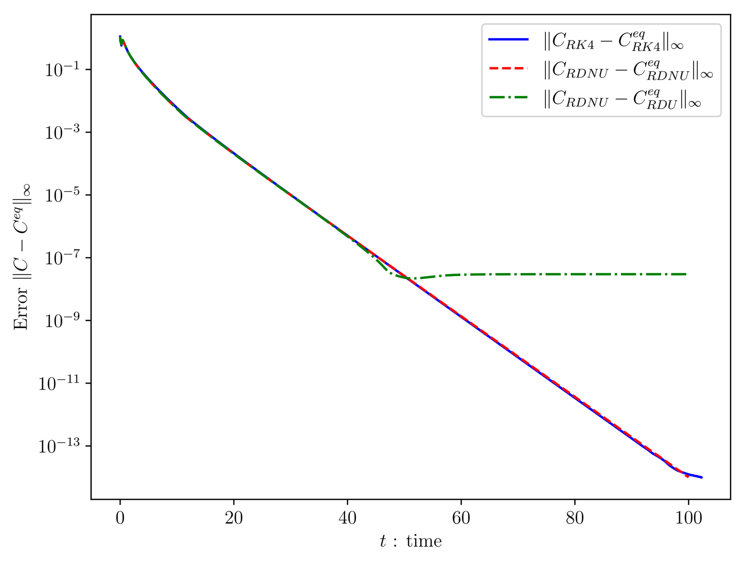

Figure 1. Convergence towards equilibrium for different sub-samplings of clusters.

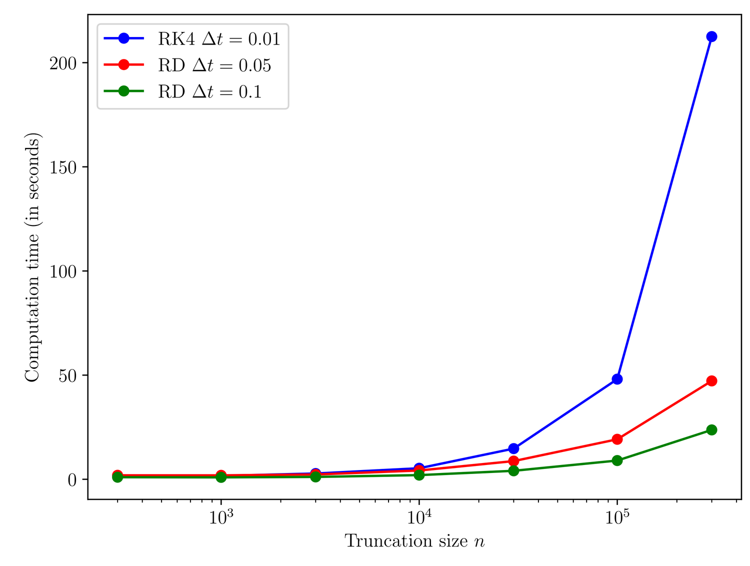

Figure 2. Comparison of computation time.

The difference in Figure 1 comes from (3), which is rewritten for the uniform and non-uniform mesh below, which do not have the same solutions.

$$\lambda - \sum_{i=1}^{N-1} a_i Q_i z^{i+1} - a_1 z^2 = 0 \text{ and } \lambda - \sum_{j=1}^{K-1} a_{n_j} \Delta x_{n_{j+1/2}} Q_{n_j} \tilde{z}^{n_j+1} - a_{n_1} \tilde{z}^2 = 0$$

Perspectives

- Prove uniqueness without moment control.
- Sub-critical case: long-time behaviour with an infinity of steady-states.
- Super-critical case: long-time behaviour of the solution, numerical simulations.

References

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