Simulation of Structured Population in a Stirred Tank

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Stirred Crystallizer

Parameters of the particles:
\[ \xi_1 = L: \text{the crystal length} \quad (\xi_2 = w: \text{the plastic deformation energy, \ldots}) \]
Parameters of the particles:
\(\xi_1\): the cell biomass \((\xi_2\): the nutrient storage pool in a cell, \ldots\)
Phenomena in the Crystallizer

**Fluid dynamics:**
- polydisperse suspension
- turbulence
- sedimentation
- transport of the dissolved substance
- temperature/heating/cooling

**Population dynamics:**
- growth
- breakage (splitting)
- nucleation
- dissolving
**The Population**

- **Number density** $F(t, \xi)$: number of particles with $\xi_i^l \leq \xi_i \leq \xi_i^u$ $(1 \leq i \leq N)$ at time $t$ is $\int_{\xi_1^l}^{\xi_1^u} \cdots \int_{\xi_N^l}^{\xi_N^u} F(t, \xi) \, d\xi$.

- **Growth and breakage:**

  $$F_t + \nabla_\xi \cdot (w(c, \xi) F) = -\delta(\xi) F + \int_\Omega k(\xi, \zeta) \delta(\zeta) F(t, \zeta) \, d\zeta,$$

  Growth

  Splitting

  $\xi \in \Omega = [\xi_1^{\text{min}}, \xi_1^{\text{max}}] \times \cdots \times [\xi_N^{\text{min}}, \xi_N^{\text{max}}]$,

  $w$: the growth rate, $\delta$: the splitting rate.

- **Balance of the dissolved substance:**

  $$c_t = -\int_\Omega a(\zeta, c, F) F(t, \zeta) \, d\zeta$$
The Integration Kernel for Crystals

\[ k(L, L') \]

\[ \xi =: L \in \mathbb{R} \text{ is the crystal length.} \]
The Integration Kernel for Bacteria

\[ k(. , y) \]

number density

size

\[ \xi =: x \in \mathbb{R} \text{ is the cell biomass} \]
**Stirred Crystallizer**

- \( F \) and \( c \) are functions of the spatial coordinates \( x \):
  \[
  F = F(t, \xi, x), \quad c = c(t, x).
  \]

- Fluid in the crystallizer is an incompressible polydisperse suspension of the crystals with averaged density \( \rho = \rho(c, F) \) and viscosity \( \nu = \nu(c, F) \).

- Spatial transport of \( F \) and \( c \) by the fluid volume velocity \( \mathbf{v} \). Further phenomena to consider: the inertia, the Brownian motion and the sedimentation of the particles.

- The population dynamics at every point \( x \).
The Coupled System

The flow \( (\rho = \rho(c, F), \nu = \nu(c, F)) \):

\[
\begin{align*}
(\rho v)_t + (v \nabla)(\rho v) &= \nabla(\nu(\nabla v + (\nabla v)^T)) - \nabla p + f, \\
\nabla \cdot v &= 0,
\end{align*}
\]

Balance of the particles:

\[
F_t = -\nabla_x \cdot (v F') - \nabla_\xi \cdot (w F) - \delta F + \int_\Omega k(\cdot, \zeta) \delta(\zeta, x) F(t, \zeta, x) \, d\zeta
\]

Balance of the dissolved substance:

\[
c_t = -\nabla_x \cdot (vc - D\nabla c) - \int_\Omega a(\zeta, c, F') F(t, \zeta, x) \, d\zeta
\]

+ the temperature
Features/Difficulties

- **High Dimensionality**: 3d geometrical space is extended with the parameter space of the population model (at least 1d). Biological population models can be high-dimensional ($\geq 5d$).

- **Different dimensionality** of the coupled equations: 3d for the transport of the dissolved substance and the temperature, $(3 + N)d$ for the particles involved in the population dynamics.

- **Integral terms** in the population dynamics models lead to non-local coupling of the grid points: need of special numerical methods.
Numerical methods

- Flow and transport equations
  - special implicit FV discretizations
  - linearization, MG-methods, ILU smoothers

- Population dynamics
  - FV-discretizations *(our choice)*:
    - high-resolution discr. of the convection term
    - efficient integration methods
  - Otherwise: method of moments, special test functions *(lower flexibility)*

- Coupling
  - by operator splitting *(more methods, greater error)*
  - one large system *(greater computational complexity)*
Integration Methods

\[ \phi(\xi) = \int_{\Omega} K(\xi, \zeta) F(\zeta) \, d\zeta \]

- **Exact integration in the general case:** Computational complexity \( O(n^2) \), where \( n \) is the number of grid points.
- If \( K(\xi, \zeta) = K_1(\xi)K_2(\zeta) \), the complexity is \( O(n) \).
- **Panel Clustering** (by Hackbusch and Novak):
  \[
  K(\xi, \zeta) \approx \sum_{i=1}^{L(n)} K_{1,i}(\xi)K_{2,i}(\zeta),
  \]
  (for ex. by Taylor expansion) on adaptively constructed subdomains of \( \Omega^2 \). Complexity \( O(n \ln^2 n) \) in the 1d case.
- **Method of primitive functions** (by T. Fischer).
Panel Clustering

Block structure of $\Omega \times \Omega$ for polynomial degree 6

$$k(\cdot, \zeta) \approx \sum_{d_1=0}^{D_1} \sum_{d_2=0}^{D_2} c_{d_1,d_2} P_{d_1}(\xi) P_{d_2}(\zeta)$$

on each clusterblock. ($P_d$ is a Legendre-polynomial of degree $d$.) The block structure, $D_1$ and $D_2$ depend on $n$ to provide the error of the same order as for the discretization of the convection term.
Problem of the panel clustering: high complexity if the kernel is not smooth enough.

\[ k(\xi, \zeta) = \begin{cases} 
\phi(\xi) \cdot \psi(\zeta), & b_{\min}(\xi) \leq \zeta \leq b_{\max}(\xi), \\
0, & \text{otherwise} 
\end{cases} \]

\[
\int_{\xi_{\min}}^{\xi_{\max}} k(\xi, \zeta) \delta(\zeta) F(\zeta) \, d\zeta = \phi(\xi) \cdot (\Psi(b_{\max}(\xi)) - \Psi(b_{\min}(\xi))),
\]

where \( \Psi(\xi) = \int_{\xi_{\min}}^{\xi} \psi(\zeta) \delta(\zeta) F(\zeta) \, d\zeta \).

General 1d kernels: \( \Psi \) is defined by panel clustering for a smooth extension.

High-dim. problems: Special but important cases. Efficient if \( k \) is non-smooth on hypersurfaces.
Crystal growth \((KNO_3 + \text{water})\)

Moment \(k_V L^3 F(L)\) (volume fraction distribution)

\[
\begin{array}{ccccccc}
0.1027 & 0.2023 & 0.3019 & 0.4015 & 0.5011 & 0.6008 & 0.7004 \\
3.050e-03 & 0.1027 & 0.2023 & 0.3019 & 0.4015 & 0.5011 & 0.6008 \\
0 & 4.230e-2 & 6.346e-2 & 8.461e-2 & \hline
\end{array}
\]

\(t = 200\)

(Explicit 2nd order finite volume scheme, 1201 grid points.)
2d Flow + Crystal Growth ($KN{O_3}$)

<table>
<thead>
<tr>
<th>Time 300 (no. 300)</th>
<th>Flow+T+Population</th>
<th>51 properties</th>
</tr>
</thead>
</table>

- **Velocity** (max 0.0062455049695729)
- **Dissolved** (max 0.075000256801496)
- **Temperature** (max 40.000147802082)
- **Small** (max 0.013462930211565)
- **Medium** (max 0.022235224781352)
- **Big** (max 0.020361423175047)

4000–12500 spatial grid nodes (adaptive refinement), Δ$t$ = 1 s, $UG$, parallel computation.
### 3d Flow + Crystal Growth ($KNO_3$)

<table>
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<tr>
<th>Time 200 (step no. 800)</th>
<th>Simulation Flow+T+Population</th>
<th>Properties: 51</th>
</tr>
</thead>
<tbody>
<tr>
<td>Velocity</td>
<td>Dissolved</td>
<td>Temperature</td>
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<tr>
<td></td>
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<td></td>
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<tr>
<td>(max 0.053812840534878)</td>
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<td>(max 34.517076741482)</td>
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<tr>
<td>Small</td>
<td>Medium</td>
<td>Big</td>
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<tr>
<td>(max 0.0031694152577533)</td>
<td>(max 0.017952966814043)</td>
<td>(max 0.00078685342299655)</td>
</tr>
</tbody>
</table>

∼ 3000 spatial grid nodes, $\Delta t = 0.25$ s, $UG$, parallel computation.
Bacteria Growth (2D Model)

Cellular density at times 0, 0.25 and 25 for a 2d cell growth model

(Explicit 2nd order finite volume scheme, 16641 grid nodes.)
Conclusions

Done:

- Simulation of 1- and 2d population models
- Coupling of 1d population models with the flow in a stirred tank

Plans, perspectives:

- Coupling of the flow with high-dim. population models discretized on the sparse grids (combination technique)
- More complicated flows: turbulence and sedimentation
- Attractors of population models (without the flow)
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