Numerical methods for kinetic models describing collective phenomena : influence of the geometry

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Motion of bacteria

Alternatively

- Motion in straight line ($\approx 1$ sec.) : “run”
- Turning events ($\approx 1/10$ sec.) : “tumble”

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$^1$N. Mittal et al., Motility of E. coli cells in clusters formed by chemotactic aggregation, PNAS (2003).
Influence of the chemical signal

- Bacteria are sensitive to different chemical factors. Chemoattractants: some amino-acids (such as aspartate), glucose...
- Bacteria may produce themselves the chemical signal which attract them.
  loop: an accumulation of bacteria which is opposed to the natural dispersion.

Also: time dependence!
Kinetic models

We are interested in run & tumble type models

\[ \frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_x f = \frac{1}{\varepsilon} \mathcal{T}(f), \quad x \in \Omega_x \subset \mathbb{R}^2, \quad \mathbf{v} \in \mathbb{S}^1 \]

- collision operator \( \mathcal{T}(f) \) is the Othmer-Dunbar-Alt turning operator

\[ \mathcal{T}(f) = \int_{\mathbb{S}^1} \mathcal{T}[c](\mathbf{v}' \to \mathbf{v}) f(\mathbf{v}') d\mathbf{v}' - \int_{\mathbb{S}^1} \mathcal{T}[c](\mathbf{v} \to \mathbf{v}') d\mathbf{v}' f(\mathbf{v}), \]

- B. C.: Maxwell’s boundary condition

\[ f(t, x, \mathbf{v}) = (1 - \alpha) \mathcal{R}[f(t, x, \mathbf{v})] + \alpha \mathcal{M}[f(t, x, \mathbf{v})], \quad x \in \partial \Omega_x, \quad \mathbf{v} \cdot \mathbf{n}(x) \geq 0, \]

with \( \mathbf{n}(x) \) the unit inward normal, \( 0 \leq \alpha \leq 1 \) and

\[
\begin{aligned}
\mathcal{R}[f(t, x, \mathbf{v})] &= f(t, x, \mathbf{v} - 2(\mathbf{v} \cdot \mathbf{n}(x)) \mathbf{n}(x)), \\
\mathcal{M}[f(t, x, \mathbf{v})] &= \mu(t, x) f_w(\mathbf{v}).
\end{aligned}
\]

Difficulty in numerical resolution:

- High dimension property asks high computational consuming.
State of the art

*Solve numerically kinetic type equation on complex geometry.*

Some algorithms based on Cartesian meshes

- **Immersed boundary method (IBM)** of Peskin, Lai and etc
  - popular in fluid mechanics applications,
  - add a singular source term to fluid mechanics equations to take into account boundary effects
  - poor accuracy

- **Cartesian cut-cell method** (D. Ingram, D. Causon and C. Mingham)
  - reconstruct the domain around the boundary
  - apply a finite volume scheme on the new control volume

- **Inverse Lax-Wendroff (ILW)** procedure (finite difference method or whatever)

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I. Numerical method to Maxwell’s boundary conditions

II. Motility of E. Coli in clusters

III. Bacterial traveling pulses

IV. Conclusion
We start with 1D problem

\[
\frac{\partial f}{\partial t} + v_x \frac{\partial f}{\partial x} = \frac{1}{\varepsilon} Q(f), \quad (x, v) \in [x_l, x_r] \times \mathbb{R}.
\]

The computational domain is covered by a uniform Cartesian mesh \(X_h \times V_h\)

\[
\begin{align*}
X_h &= \{ x_{\min} = x_0 \leq \cdots \leq x_i \leq \cdots \leq x_{n_x} = x_{\max} \}, \\
V_h &= \{ v_j = j \Delta v, \quad j \in \mathbb{Z}, \quad |j| \leq n_v \}.
\end{align*}
\]

The discrete B.C. reads

\[
f(x_p, v_j) = (1 - \alpha) \mathcal{R}[f(x_p, v_j)] + \alpha \mathcal{M}[f(x_p, v_j)],
\]

where \(\mathcal{R}[f(x_p, v_j)] = f(x_p, -v_j), \quad \mathcal{M}[f(x_p, v_j)] = \mu(x_p) f_w(v_j).\)
Compute $f$ at ghost point $x_g$:

1. Extrapolation of $f$ for the outflow
   - compute $f_{g,-j}$, $f_{p,-j}$ by WENO type extrapolation

**Figure:** A portion of mesh in spatially one dimensional case. ● is interior point, ■ is ghost point $x_g$, □ is the boundary $x_p$. 
ILW Procedure in 1D Case

Compute $f$ at ghost point $x_g$:

1. Extrapolation of $f$ for the outflow
2. Compute B.C. at the boundary

   - compute $f(x_p, v_j)$
     - $\mathcal{R}[f_{p,j}] = f_{p,-j}$
     - $\mathcal{M}[f_{p,j}] = \mu_p f_w(v_j)$

**Figure:** A portion of mesh in spatially one dimensional case. ● is interior point, ● is ghost point $x_g$, □ is the boundary $x_p$. 
ILW Procedure in 1D Case

Compute $f$ at ghost point $x_g$:

1. Extrapolation of $f$ for the outflow

2. Compute B.C. at the boundary

3. Approximation of $f$ for inflow

$$\frac{\partial f}{\partial x}\bigg|_{x=x_p} = \frac{1}{v_x} \left( -\frac{\partial f}{\partial t} + \frac{1}{\varepsilon} Q(f) \right)_{x_p}$$

or by WENO type extrapolation

* compute $Q(f)_{x=x_p}$ by using $f_{p,j}$, $j \in V_h$

$$f_{g,j} \approx f_{p,j} + (x_g - x_p) \frac{\partial f}{\partial x}\bigg|_{x=x_p}$$

Figure: A portion of mesh in spatially one dimensional case. ● is interior point, ■ is ghost point $x_g$, □ is the boundary $x_p$. 
ILW Procedure in 2D Case

We consider 2D model

$$\frac{\partial f}{\partial t} + v_x \frac{\partial f}{\partial x} + v_y \frac{\partial f}{\partial y} = \frac{1}{\varepsilon} Q(f),$$

Compute $f$ at ghost point $x_g$:

1. Extrapolation of $f$ for the outflow

   * compute $f(x_p, \mathbf{v} \cdot \mathbf{n} < 0)$ and $f(x_g, \mathbf{v} \cdot \mathbf{n} < 0)$ by WENO type extrapolation

Figure: Spatially 2D Cartesian mesh.
- is interior point, ■ is ghost point, □ is the point at the boundary, ○ is the point for extrapolation, the dashed line is the boundary.
ILW Procedure in 2D Case

We consider 2D model

$$\frac{\partial f}{\partial t} + v_x \frac{\partial f}{\partial x} + v_y \frac{\partial f}{\partial y} = \frac{1}{\varepsilon} Q(f),$$

Compute $f$ at ghost point $x_g$:

1. Extrapolation of $f$ for the outflow
2. Compute B.C. at the boundary

- $R[f(x_p, v)] = f(x_p, v - 2(v \cdot n)n), \quad v \cdot n > 0$
- Interpolate $f$ on $(x_p, v - 2(v \cdot n)n)$
- $M[f(x_p, v)] = \mu(x_p)f_w(v), \quad v \cdot n > 0$

Figure: Spatially 2D Cartesian mesh.
- $\bullet$ is interior point, $\square$ is ghost point, $\Box$ is the point at the boundary, $\bigcirc$ is the point for extrapolation, the dashed line is the boundary.
ILW Procedure in 2D Case

We consider 2D model
\[
\frac{\partial f}{\partial t} + v_x \frac{\partial f}{\partial x} + v_y \frac{\partial f}{\partial y} = \frac{1}{\varepsilon} Q(f),
\]

Compute \( f \) at ghost point \( x_g \):
1. Extrapolation of \( f \) for the outflow
2. Compute B.C. at the boundary
3. Approximation of \( f \) for inflow
   * local coordinate system
     \( \mathbf{x} \rightarrow \hat{\mathbf{x}} \)
     \[
     \frac{\partial \hat{f}}{\partial \hat{x}} (\hat{x}_p, \mathbf{v}) = \\
     - \frac{1}{\hat{v}_x} \left( \frac{\partial \hat{f}}{\partial t} + \hat{v}_y \frac{\partial \hat{f}}{\partial \hat{y}} - \frac{1}{\varepsilon} Q(\hat{f}) \right) \bigg|_{\hat{x} = \hat{x}_p}
     \]
   * \( f(x_g, \mathbf{v}) \approx \)
     \[
     \hat{f}(\hat{x}_p, \mathbf{v}) + (\hat{x}_g - \hat{x}_p) \frac{\partial \hat{f}}{\partial \hat{x}} (\hat{x}_p, \mathbf{v})
     \]

Figure: Spatially 2D Cartesian mesh.
● is interior point, ■ is ghost point, □ is the point at the boundary, ○ is the point for extrapolation, the dashed line is the boundary.
Collective behavior of cells with chemoattractant

We consider the run & tumble type equation
\[
\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_x f = \int_V T(\mathbf{v}, \mathbf{v}') f(t, \mathbf{x}, \mathbf{v}) \, d\mathbf{v}' - \int_V T(\mathbf{v}', \mathbf{v}) f(t, \mathbf{x}, \mathbf{v}) \, d\mathbf{v}',
\]
(1)
with \( T(\mathbf{v}, \mathbf{v}') = \lambda_S(\mathbf{v}') \) and
\[
\lambda_S(\mathbf{v}') = \psi_S \left( \frac{D \log S}{Dt} \vbar_{\mathbf{v}'} \right)
\]
and
\[
\frac{\partial S}{\partial t} - D_S \Delta S = -a S + b \int_V f(t, \mathbf{x}, \mathbf{v}) \, d\mathbf{v}, \quad \mathbf{x} \in \Omega,
\]
(2)
where \( a \) and \( b \) are degradation rate of the chemoattractant, production rate, whereas \( D_S \) is the molecular diffusion coefficient.
Computation of $S(t, x)$

The finite difference scheme are used. For example:

$$\Delta S_{i,j} \approx \frac{S_{i+1,j} - 2S_{i,j} + S_{i-1,j}}{\Delta x^2} + \frac{S_{i,j+1} - 2S_{i,j} + S_{i,j-1}}{\Delta y^2}.$$  

$S_{i,j-1}$ is approximated by extrapolation

$$S_{i,j-1} = S(x_m) \approx \sum_{k=1}^{9} c_k S(x_k).$$

Boundary conditions for $S$ are:

$$\nabla S \cdot \vec{n} = 0.$$  

Note that $S_{i,j-1}$ is linear combination of $S(x_k), k = 1, \ldots, 9.$
Numerical results 2D

Figure: (a) Time evolution of the bacteria’s density (b) time evolution of the velocity distribution at \((x, y) = (-0.1, -0.1)\)
Numerical results 2D

- steady state of the density $n$ has an exponential decay rate with respect to $|x|$;
- good agreement with Mittal et al.

Bacterial traveling pulses

We consider the run & tumble type equation

\[
\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_x f = \int_V T(\mathbf{v}, \mathbf{v}') f(t, \mathbf{x}, \mathbf{v}') \, d\mathbf{v}' - \int_V T(\mathbf{v}', \mathbf{v}) f(t, \mathbf{x}, \mathbf{v}) \, d\mathbf{v}', \quad (3)
\]

with \( T(\mathbf{v}, \mathbf{v}') = \lambda(\mathbf{v}') K(\mathbf{v}, \mathbf{v}') \) and

\[
\lambda(\mathbf{v}') = \frac{1}{2} \left( \lambda_N(\mathbf{v}') + \lambda_S(\mathbf{v}') \right)
\]

\[
= \frac{1}{2} \left( \psi_N \left( \frac{D \log N}{D t} \right|_{\mathbf{v}'} \right) + \psi_S \left( \frac{D \log S}{D t} \right|_{\mathbf{v}'} \right)
\]

and

\[
\begin{aligned}
\frac{\partial S}{\partial t} - D_S \Delta S &= - a S + b \int_V f(t, \mathbf{x}, \mathbf{v}) \, d\mathbf{v}, \quad \mathbf{x} \in \Omega, \\
\frac{\partial N}{\partial t} - D_N \Delta N &= - c N \int_V f(t, \mathbf{x}, \mathbf{v}) \, d\mathbf{v}, \quad \mathbf{x} \in \Omega
\end{aligned}
\]

(4)

where \( a, b \) and \( c \) are degradation rate of the chemoattractant, production rate and the consumption rate of the nutrient by the bacteria, whereas \( D_S \) and \( D_N \) are the molecular diffusion coefficients.
Numerical results 2D

Figure: (a) Time evolution of the bacteria’s density (b) time evolution of the mean velocity
Numerical results 2D

Figure: Experimental evidence for pulses of E. coli traveling across a channel.

Figure: Comparison between experimental data and numerical results

Numerical results 2D
Numerical results 2D
Conclusion

- We solve a run & tumble type model
  - based on finite difference method
  - the ghost point values approximated by ILW procedure
  - collision operator solved explicitly

- ILW procedure
  - second-order accurate in $L^1$ norm
  - reproduces similar numerical results in literature

Perspectives

- Use a more precise tumble operator (depending on internal energy? memory effects?)
- Use different geometry for traveling pulses
- Design a hybrid method based on a domain decomposition method coupling kinetic and fluid models.