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

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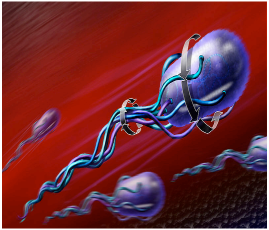
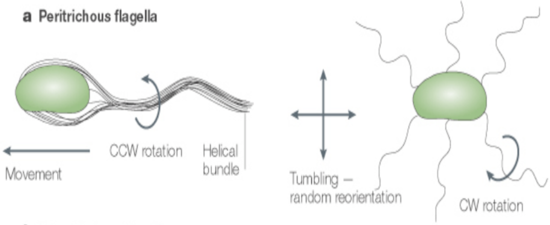
North Carolina (Jan. 2013)

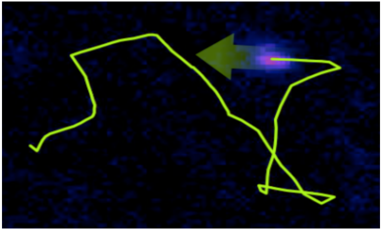
# Motion of bacteria






Alternatively[1]

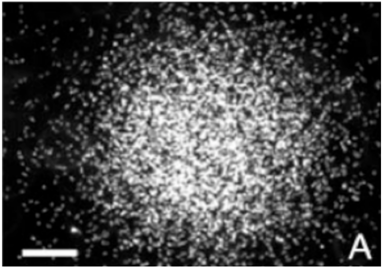
- Motion in straight line ($\simeq$ 1 sec.) : "run"
- Turning events ($\simeq 1/10$ sec.) : "tumble"

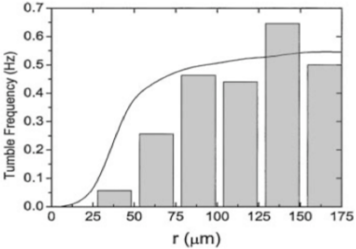


[1] N. Mittal *et al.*, Motility of E. coli cells in clusters formed by chemotactic aggregation, PNAS (2003).

# Influence of the chemical signal

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




Also : time dependence!

# Kinetic models

We are interested in run & tumble type models

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f = \frac{1}{\varepsilon}\mathcal{T}(f), \ \mathbf{x} \in \Omega_{\mathbf{x}} \subset \mathbb{R}^2, \ \mathbf{v} \in \mathbb{S}^1$$

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

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

- B. C.: *Maxwell's boundary condition*

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

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

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

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)

S. Tan and C.-W. Shu, *Inverse Lax-Wendroff procedure for numerical boundary conditions of conservation laws*, Journal of Computational Physics, 229 (2010), 8144–8166.

# Outline

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

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

The computational domain is covered by a uniform Cartesian mesh $\mathbf{X}_h \times \mathbf{V}_h$

$$\begin{cases} \mathbf{X}_h = \{x_{\min} = x_0 \leq \cdots \leq x_i \leq \cdots \leq x_{n_x} = x_{\max}\}, \\ \mathbf{V}_h = \left\{\mathbf{v}_j = j\,\Delta v, \quad j \in \mathbb{Z}, \quad |j| \leq n_v\right\}. \end{cases}$$

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 $\mathcal{R}[f(x_p, v_j)] = f(x_p, -v_j)$, $\mathcal{M}[f(x_p, v_j)] = \mu(x_p) f_w\left(v_j\right)$.

# ILW Procedure in 1D Case

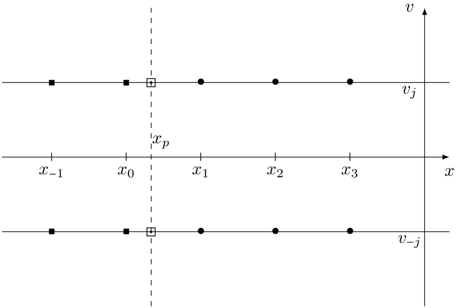
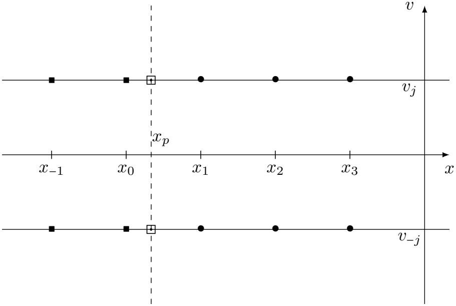



Figure: A portion of mesh in spatially one dimensional case. • is interior point, ▪ is ghost point $x_g$, ⊡ is the boundary $x_p$.

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

# ILW Procedure in 1D Case

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Compute $f$ at ghost point $x_g$:

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

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

# ILW Procedure in 1D Case

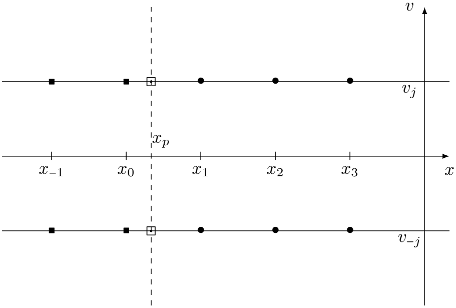



Figure: A portion of mesh in spatially one dimensional case. • is interior point, ▪ is ghost point $x_g$, ⊡ is the boundary $x_p$.

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
   - $\left.\frac{\partial f}{\partial x}\right|_{x=x_p} = \frac{1}{v_x}\left(-\frac{\partial f}{\partial t} + \frac{1}{\varepsilon}\mathcal{Q}(f)\right)_{x_p}$
     - ⋆ $\left.\frac{\partial f}{\partial t}\right|_{x=x_p} \approx \frac{f_{p,j}^n - f_{p,j}^{n-1}}{\Delta t}$ or by WENO type extrapolation
     - ⋆ compute $\mathcal{Q}(f)_{x=x_p}$ by using $f_{p,j},\ j \in \mathbf{V}_h$
   - $f_{g,j} \approx f_{p,j} + (x_g - x_p)\left.\frac{\partial f}{\partial x}\right|_{x=x_p}$

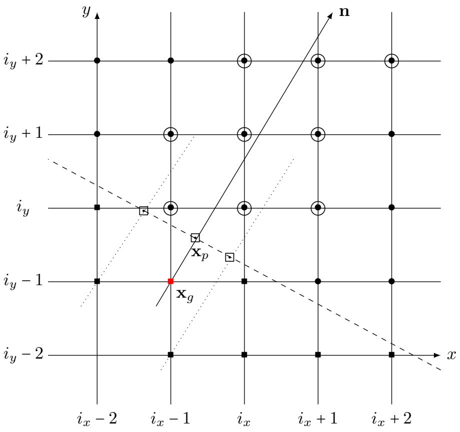



Figure: Spatially 2D Cartesian mesh. • is interior point, ▪ is ghost point, ⊡ is the point at the boundary, ◯ is the point for extrapolation, the dashed line is the boundary.

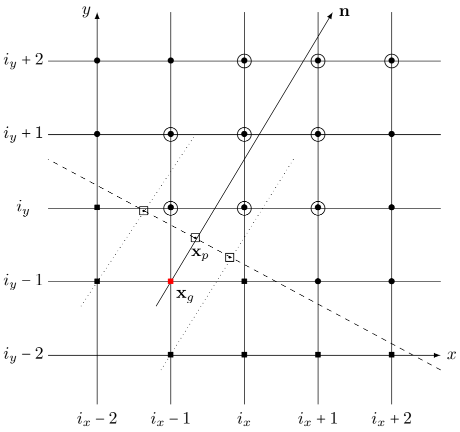
We consider 2D model

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

Compute $f$ at ghost point $x_g$:

1. Extrapolation of $f$ for the outflow
   - ⋆ compute $f(\mathbf{x}_p, \mathbf{v}\cdot\mathbf{n} < 0)$ and $f(\mathbf{x}_g, \mathbf{v}\cdot\mathbf{n} < 0)$ by WENO type extrapolation

# ILW Procedure in 2D Case

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

Compute $f$ at ghost point $x_g$:

1. Extrapolation of $f$ for the outflow
2. Compute B.C. at the boundary
   - ⋆ $\mathcal{R}[f(\mathbf{x}_p,\mathbf{v})] = f(\mathbf{x}_p, \mathbf{v} - 2(\mathbf{v}\cdot\mathbf{n})\mathbf{n}), \quad \mathbf{v}\cdot\mathbf{n} > 0$
   - ⋆ interpolate $f$ on $(\mathbf{x}_p, \mathbf{v} - 2(\mathbf{v}\cdot\mathbf{n})\mathbf{n})$
   - ⋆ $\mathcal{M}[f(\mathbf{x}_p,\mathbf{v})] = \mu(\mathbf{x}_p) f_w(v), \quad \mathbf{v}\cdot\mathbf{n} > 0$

# ILW Procedure in 2D Case

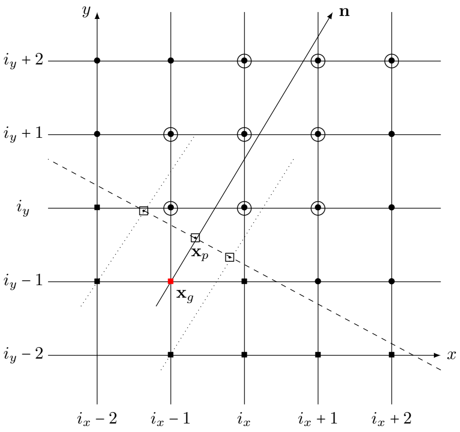



Figure: Spatially 2D Cartesian mesh. • is interior point, ▪ is ghost point, ⊡ is the point at the boundary, ◯ is the point for extrapolation, the dashed line is the boundary.

We consider 2D model

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

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 $\mathbf{x} \to \hat{\mathbf{x}}$
   - ⋆ $\frac{\partial \hat{f}}{\partial \hat{x}}(\hat{\mathbf{x}}_p, \mathbf{v}) = -\frac{1}{\hat{v}_x}\left(\frac{\partial \hat{f}}{\partial t} + \hat{v}_y \frac{\partial \hat{f}}{\partial \hat{y}} - \frac{1}{\varepsilon}\mathcal{Q}(\hat{f})\right)\Big|_{\hat{\mathbf{x}}=\hat{\mathbf{x}}_p}$
   - ⋆ $f(\mathbf{x}_g, \mathbf{v}) \approxeq \hat{f}(\hat{\mathbf{x}}_p, \mathbf{v}) + (\hat{x}_g - \hat{x}_p)\frac{\partial \hat{f}}{\partial \hat{x}}(\hat{\mathbf{x}}_p, \mathbf{v})$

We consider the run & tumble type equation

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f = \int_V T(\mathbf{v}, \mathbf{v}')\, f(t, \mathbf{x}, \mathbf{v}')\, d\mathbf{v}' - \int_V T(\mathbf{v}', \mathbf{v})\, f(t, \mathbf{x}, \mathbf{v})\, d\mathbf{v}', \quad (1)$$

with $T(\mathbf{v}, \mathbf{v}') = \lambda_S(\mathbf{v}')$ and

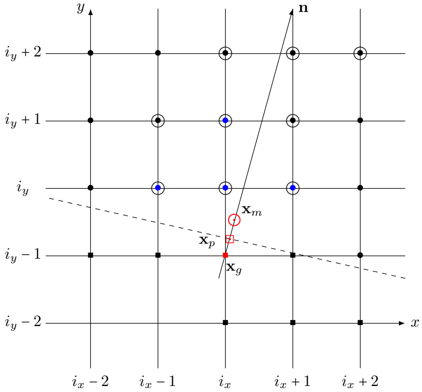
$$\lambda_S(\mathbf{v}') = \psi_S\left( \frac{D \log S}{Dt}\bigg|_{\mathbf{v}'} \right)$$

and

$$\frac{\partial S}{\partial t} - D_S \Delta S = -a S + b \int_V f(t, \mathbf{x}, \mathbf{v})\, d\mathbf{v}, \quad \mathbf{x} \in \Omega, \quad (2)$$

where $a$ and $b$ are degradation rate of the chemoattractant, production rate, whereas $D_S$ is the molecular diffusion coefficient.

# Computation of $S(t, x)$




Boundary conditions for $S$ are:

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

The finite difference scheme are used. For example:

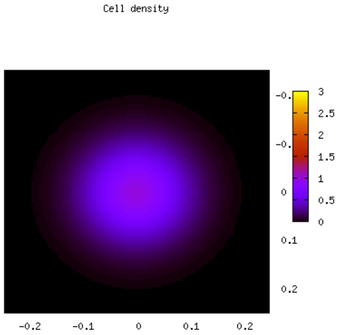
$$\Delta S_{i,j} \approx \frac{S_{i+1,j} - 2S_{i,j} + S_{i-1,j}}{\Delta x^2} + \frac{S_{i,j+1} - 2S_{i,j} + S_{i,j-1}}{\Delta y^2}.$$

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

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

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

# Numerical results 2D



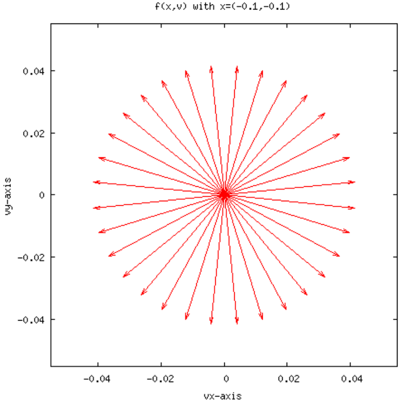
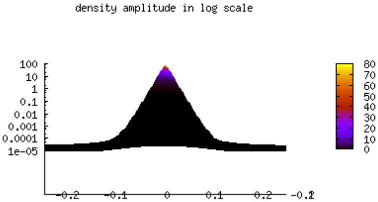
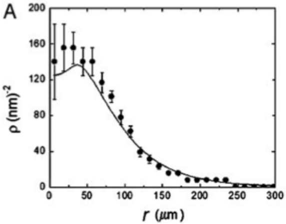



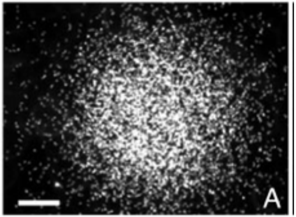

Figure: (a) Time evolution of the bacteria's density (b) time evolution of the velocity distribution at $(x, y) = (-0.1, -0.1)$

# Numerical results 2D




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




N. Mittal, E. O. Budrene, M.P. Brenner, and A. van Oudenaarden, PNAS (2003)

We consider the run & tumble type equation

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

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

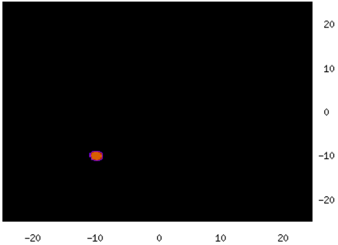
$$\begin{aligned} \lambda(\mathbf{v}') &= \frac{1}{2}\left(\lambda_N(\mathbf{v}') + \lambda_S(\mathbf{v}')\right) \\ &= \frac{1}{2}\left(\psi_N\left(\frac{D\log N}{Dt}\Big|_{\mathbf{v}'}\right) + \psi_S\left(\frac{D\log S}{Dt}\Big|_{\mathbf{v}'}\right)\right) \end{aligned}$$

and

$$\begin{cases} \dfrac{\partial S}{\partial t} - D_S\,\Delta S = -a\,S + b\displaystyle\int_V f(t,\mathbf{x},\mathbf{v})\, d\mathbf{v}, & \mathbf{x}\in\Omega, \\ \dfrac{\partial N}{\partial t} - D_N\,\Delta N = -c\,N\displaystyle\int_V f(t,\mathbf{x},\mathbf{v})\, d\mathbf{v}, & \mathbf{x}\in\Omega \end{cases} \quad (4)$$

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



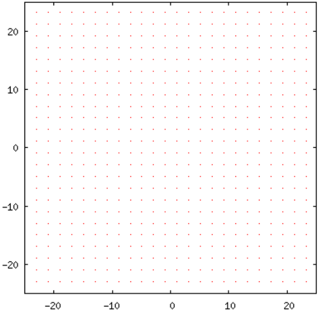




Figure: (a) Time evolution of the bacteria's density (b) time evolution of the mean velocity

# Numerical results 2D

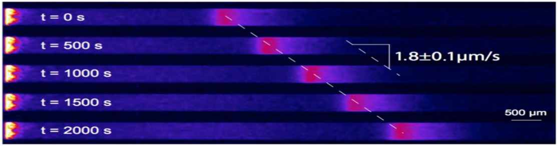



Figure: Experimental evidence for pulses of E. coli traveling across a channel.

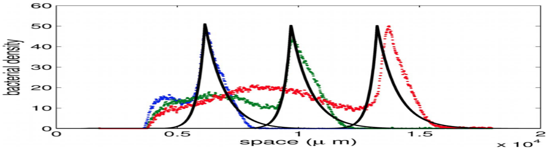
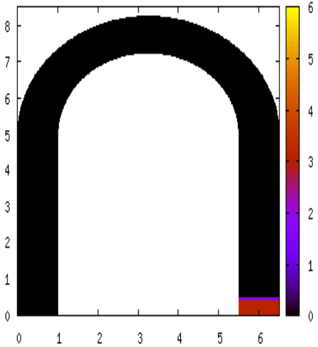
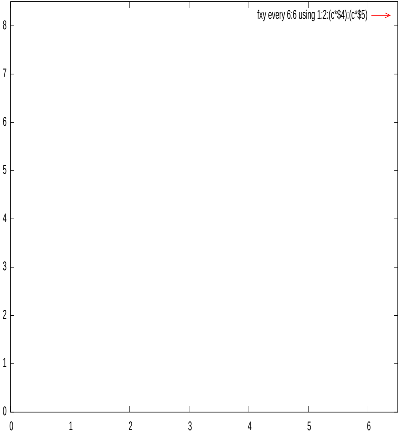



Figure: Comparison between experimental data and numerical results

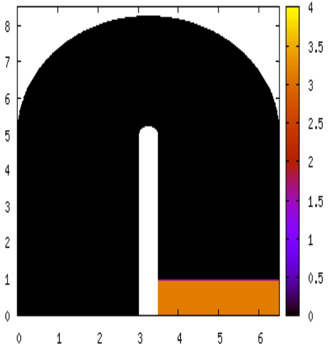

J. SARAGOSTI, V. CALVEZ, N. BOURNAVEAS, A. BUGUIN, P. SILBERZAN, BENOÎT PERTHAME, Mathematical Description of Bacterial Traveling Pulses PLos (2010)

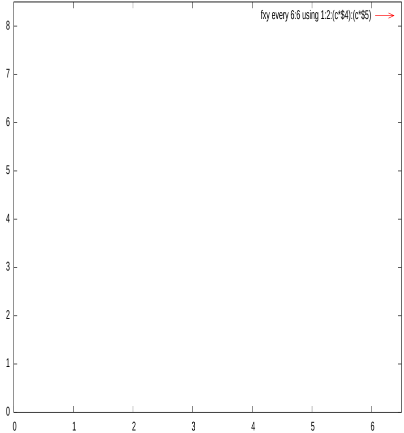
# Numerical results 2D

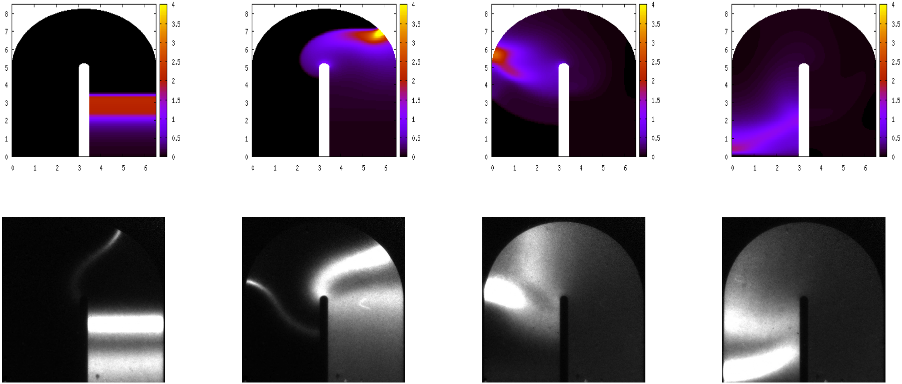


# Numerical results 2D




0 1 2 3 4 5 6 7 8
0 1 2 3 4 5 6
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# Conclusion and perspectives

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.