GORE: Modeling Filter Compression, Fluid Generation and Parallelizing the Potts Model

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GORE: Modeling the Movement of Gas and Fluid through a Diffusive Filter

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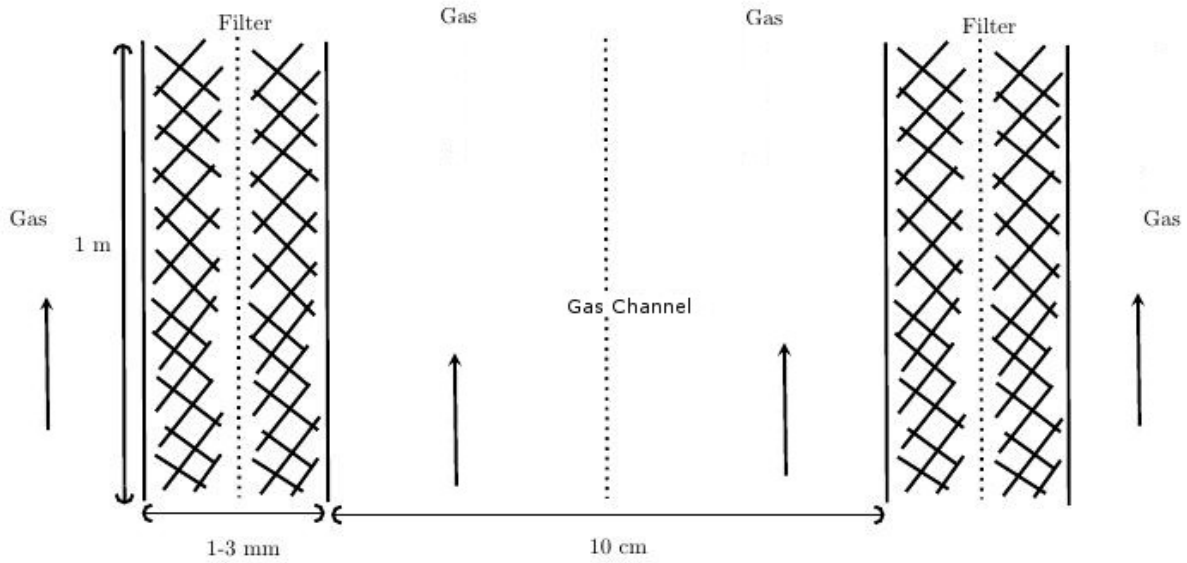
Our Problem

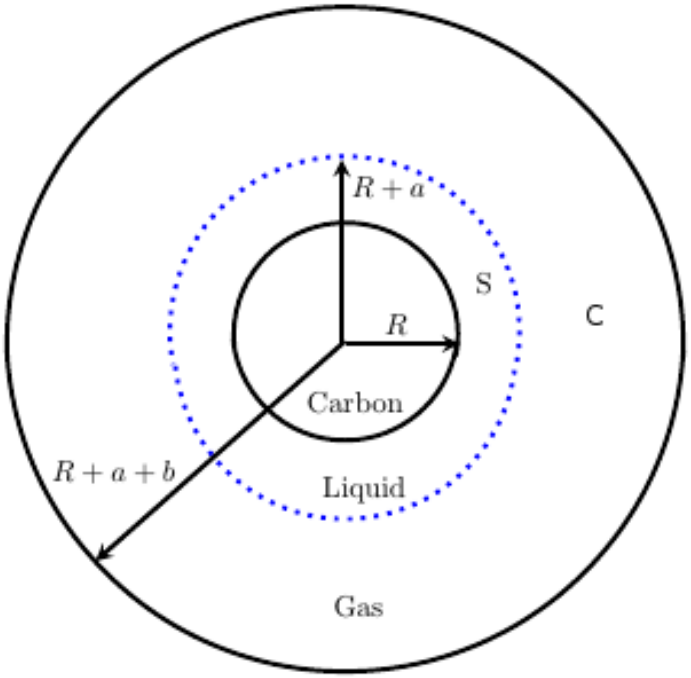
- Develop a mathematical model for characterizing fluid production and transport inside of a porous medium.
- Quantify the time scale and spatial profile of flooding of the pore space by the fluid.

A Coupled Multiscale Approach

- Small Scale - Analyze the formation of sulfuric acid on the surface of a single filter pellet.
- Large Scale - Analyze the transport of sulfur dioxide in the gas channel and filter.



Small Scale analysis



Gas diffuses into the filter from the gas channel. Sulfur Dioxide (bad) reacts with Oxygen and Water on the surface of the Activated Carbon to form Sulfuric Acid (good).

$$2SO_2 + O_2 + 2H_2O \rightarrow 2H_2SO_4$$

Outer Small Scale Problem

S_i is the concentration of SO_2 in layer i.
C_i is the concentration of O_2 in layer i.

$$\frac{\partial C_1}{\partial t} = D_1 \nabla^2 C_1, \quad \frac{\partial S_1}{\partial t} = d_1 \nabla^2 S_1, \quad \text{Outer Layer}$$

$$C_1 \to C^*, \quad S_1 \to S^*, \quad r \to \infty, \quad \text{Boundary Condition}$$

$$C_1 = k_1 C_2, \quad S_1 = k_2 S_2, \quad r = R + a \quad \text{Interface Condition}$$

Inner Small Scale Problem

$$\frac{\partial C_2}{\partial t} = D_2 \nabla^2 C_2, \quad \frac{\partial S_2}{\partial t} = d_2 \nabla^2 S_2, \quad \text{Inner Layer}$$

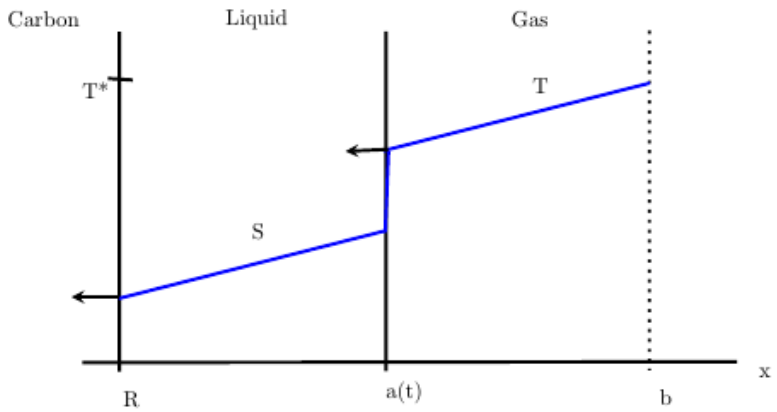
$$D_2 \frac{\partial C_2}{\partial r} = -\lambda S_2^2 C_2, \quad d_2 \frac{\partial S_2}{\partial r} = -2\lambda S_2^2 C_2, \quad r = R \quad \text{Boundary Condition}$$

$$D_1 \frac{\partial C_1}{\partial r} = D_2 \frac{\partial C_2}{\partial r}, \quad d_1 \frac{\partial S_1}{\partial r} = d_2 \frac{\partial S_2}{\partial r}, \quad r = R + a \quad \text{Interface Condition}$$

Area Increase Problem

$$\text{At} \quad r = R, \quad v = 2\delta\lambda S_2^2 C_2 \quad \text{and} \quad \nabla \cdot \mathbf{v} = \mathbf{0}$$

$$\text{At} \quad r = R + a, \quad v = a_t + u a_x \quad \text{and} \quad a_t = \frac{2\delta\lambda R^2 S_2^2 C_2}{(R+a)^2}$$



Reduced Micro Scale Model

The nondimensionalized reduced model is

$$S_t = DS_{xx}, \quad T_t = T_{xx}, \tag{1}$$

with boundary conditions

$$DS_x = 2\lambda S^2|_{x=0}, \quad T = T^*|_{x=b}, \tag{2}$$

and interface conditions

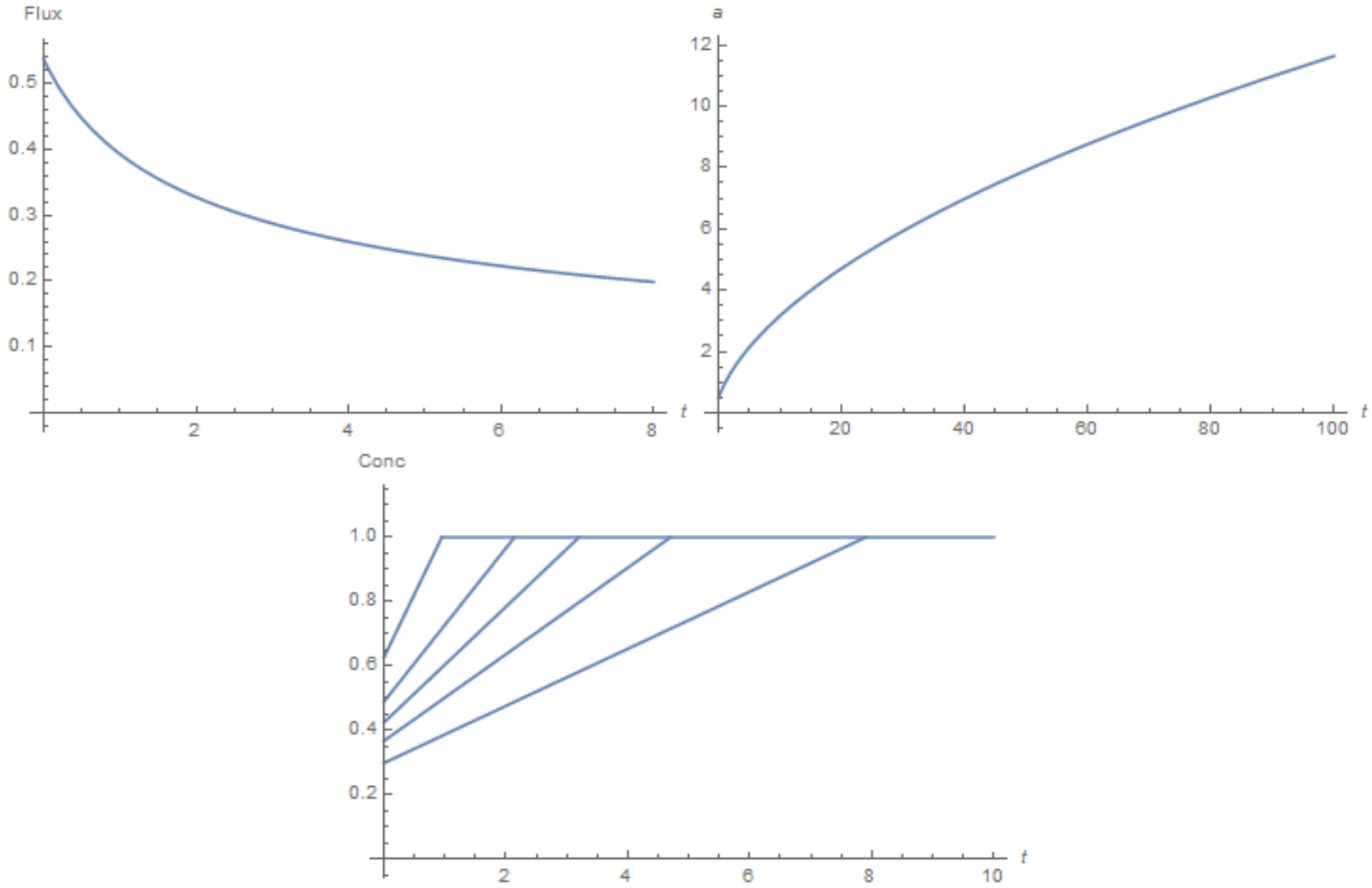
$$T = \chi S|_{x=a}, \quad DS_x = T_x|_{x=a}. \tag{3}$$

Here $S = S_2$, $T = S_1$.

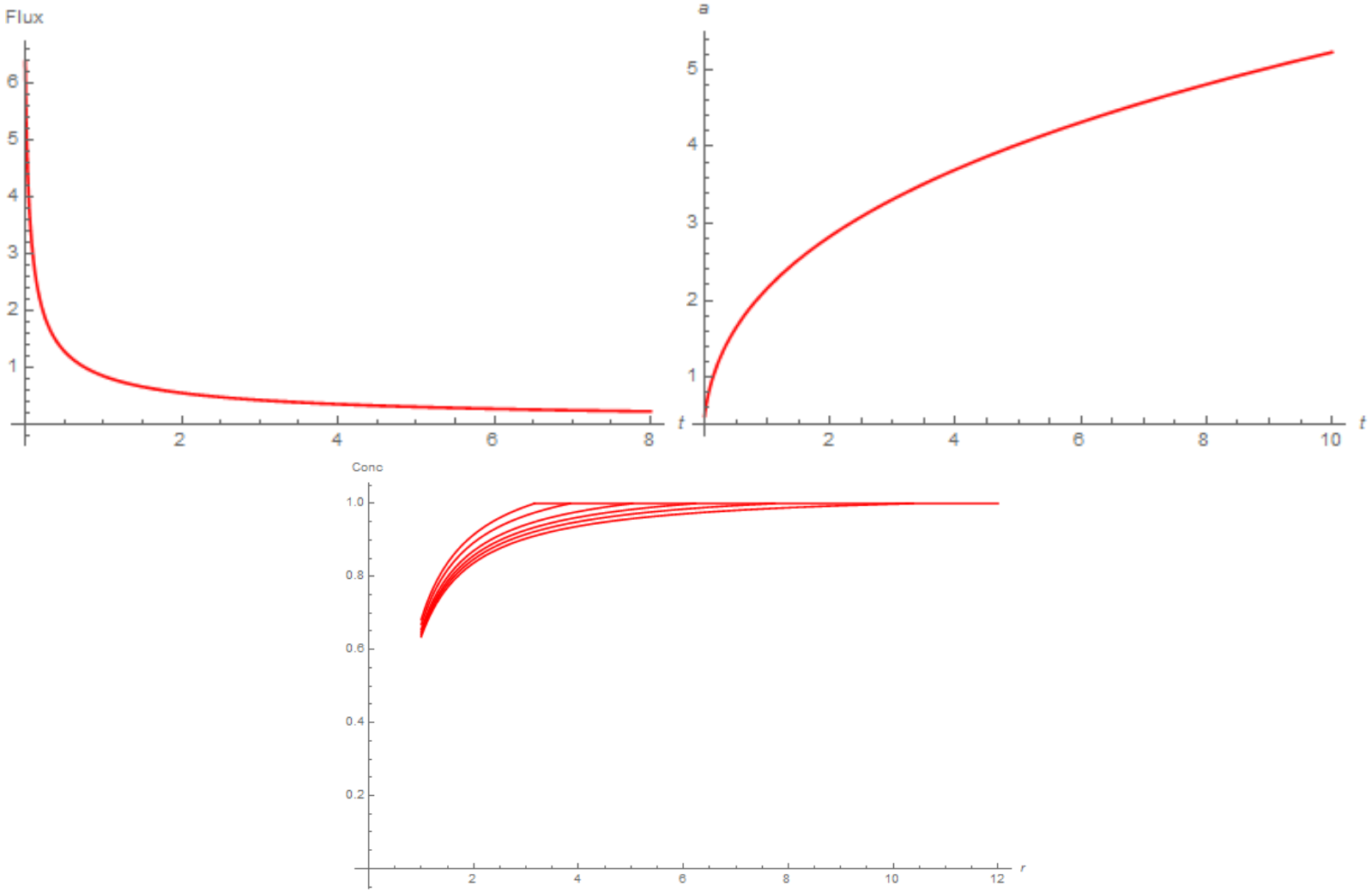
- Time scale: The flux in each layer is approximately constant.
- Quasi-Steady Diffusion: Diffusion is much faster than liquid layer growth. Solutions take the form

$$S = \bar{S} + S', \quad T = \bar{T} + T'.$$

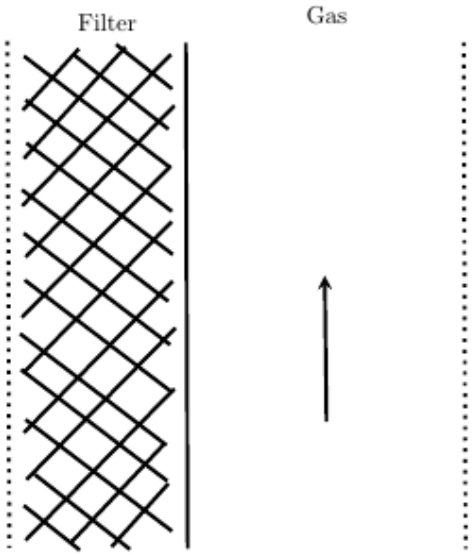
Graphs (1D cartesian)

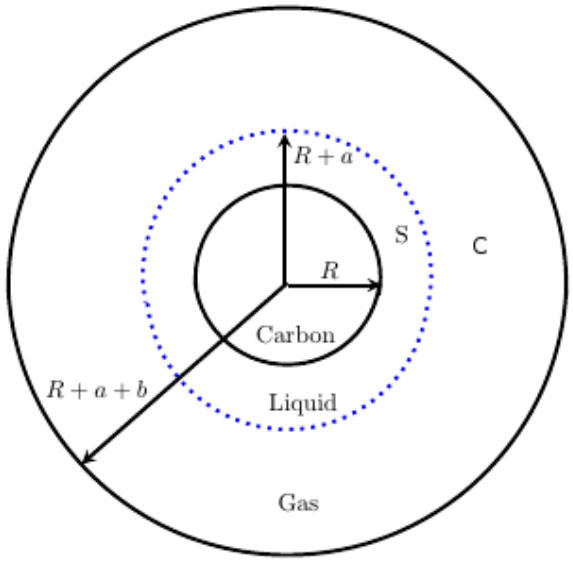


Graphs (1D spherical symmetric)



Zooming Out





Macroscale Model

W is the concentration of a particular gas species in the channel.
T is the concentration of a particular gas species in the filter.

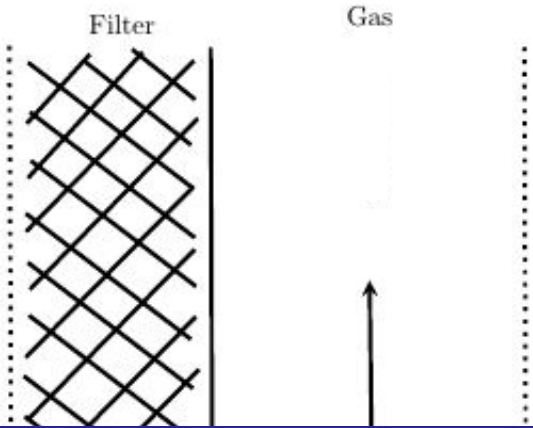
$$\text{Outer} \quad U\frac{h}{2}W_z = d_1 T_y|_{y=0}, \quad 0 < z < L \tag{4}$$

$$W(0,t) = W_{\text{in}}$$

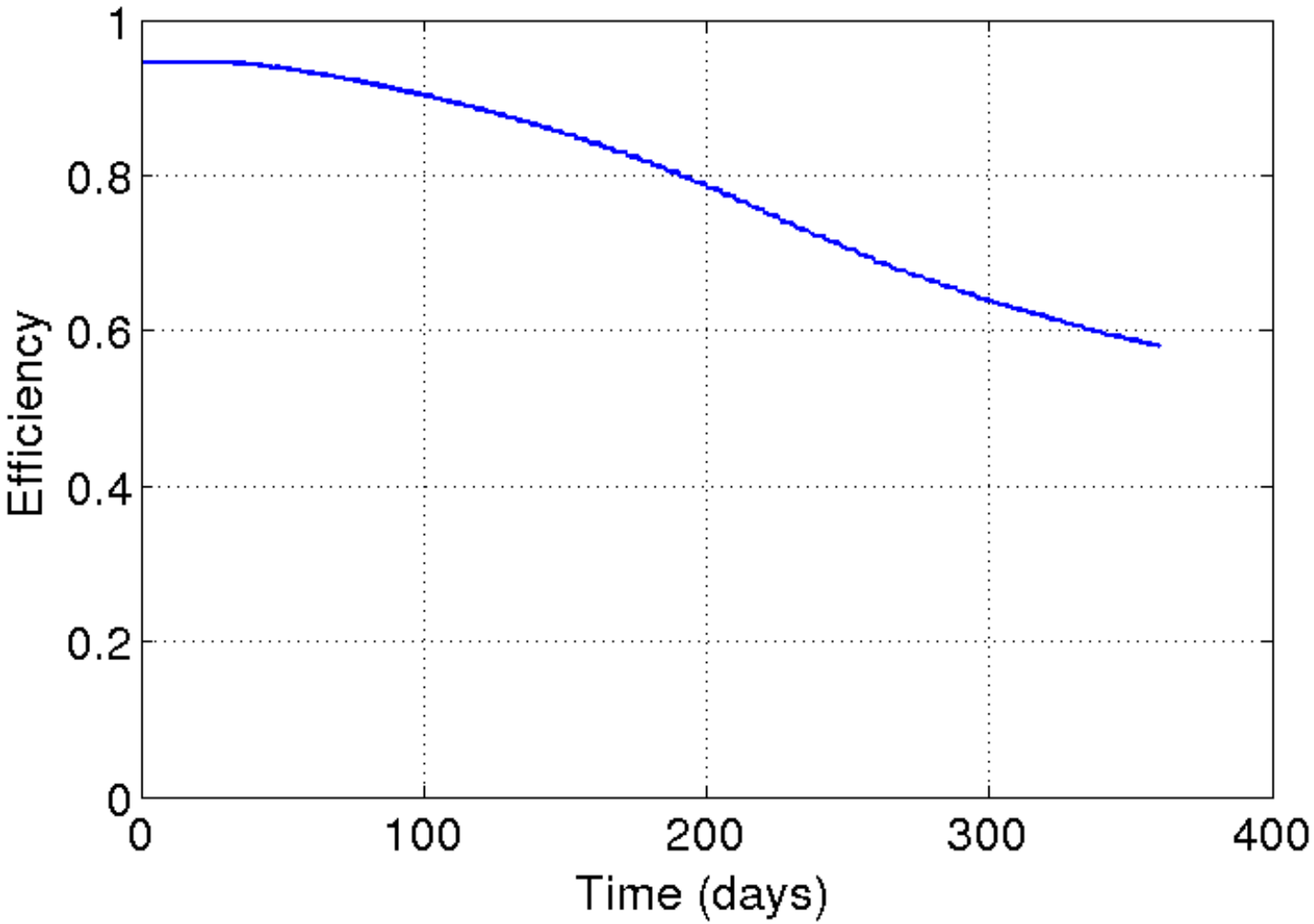
$$\text{Inner} \quad d_1 T_{yy} = \frac{3}{R\phi}F(a,T), \quad 0 < y < H/2, \quad 0 < z < L \tag{5}$$

$$a_t = \delta F(a,T), \quad t > 0. \tag{6}$$

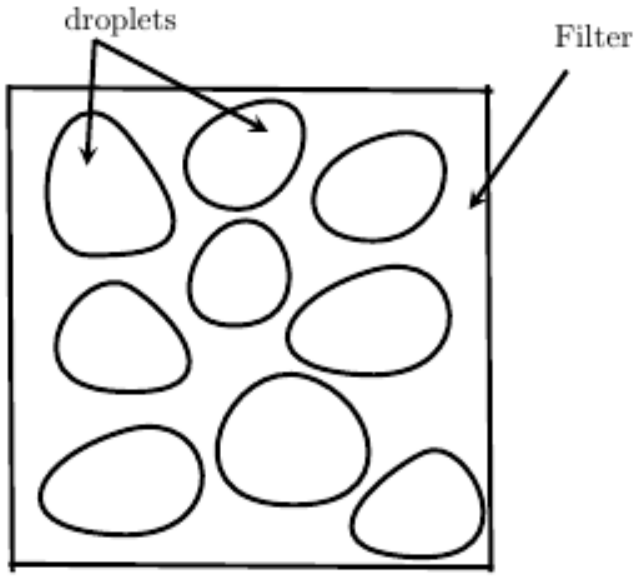
$$T_y|_{y=H/2} = 0, \quad T|_{y=0} = W, \quad a|_{t=0} = 0.$$

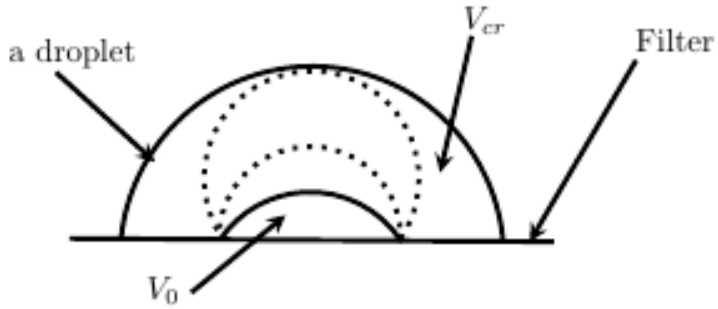


Breakthrough Curve



Critical Time Estimate for Surface Clogging





- Chemical reaction at droplet perimeter: $q_1 \sim 2\pi r$
- Imbibing liquid from pores: $q_2 \sim \int_A c(x, y, t)dxdy$
- Absorbing H_2O (hygroscopicity): $q_3 \sim S$
- Droplet coalescence: $dA \sim fp$ Use this formation to determine critical time for filter surface clogging.

Progress

- Determined that the concentration profile around the filter particles is governed by Laplace's equation.
- Physical chemistry results in ODE nonlinearity (messy but solvable) that can be easily translated to fluid formation in the fluid.
- Generated reasonable breakthrough curve with our model.
- Estimated surface clog time as a function of the area of the absorbing wall covered by a droplet.

Models for Filter Membrane Compression

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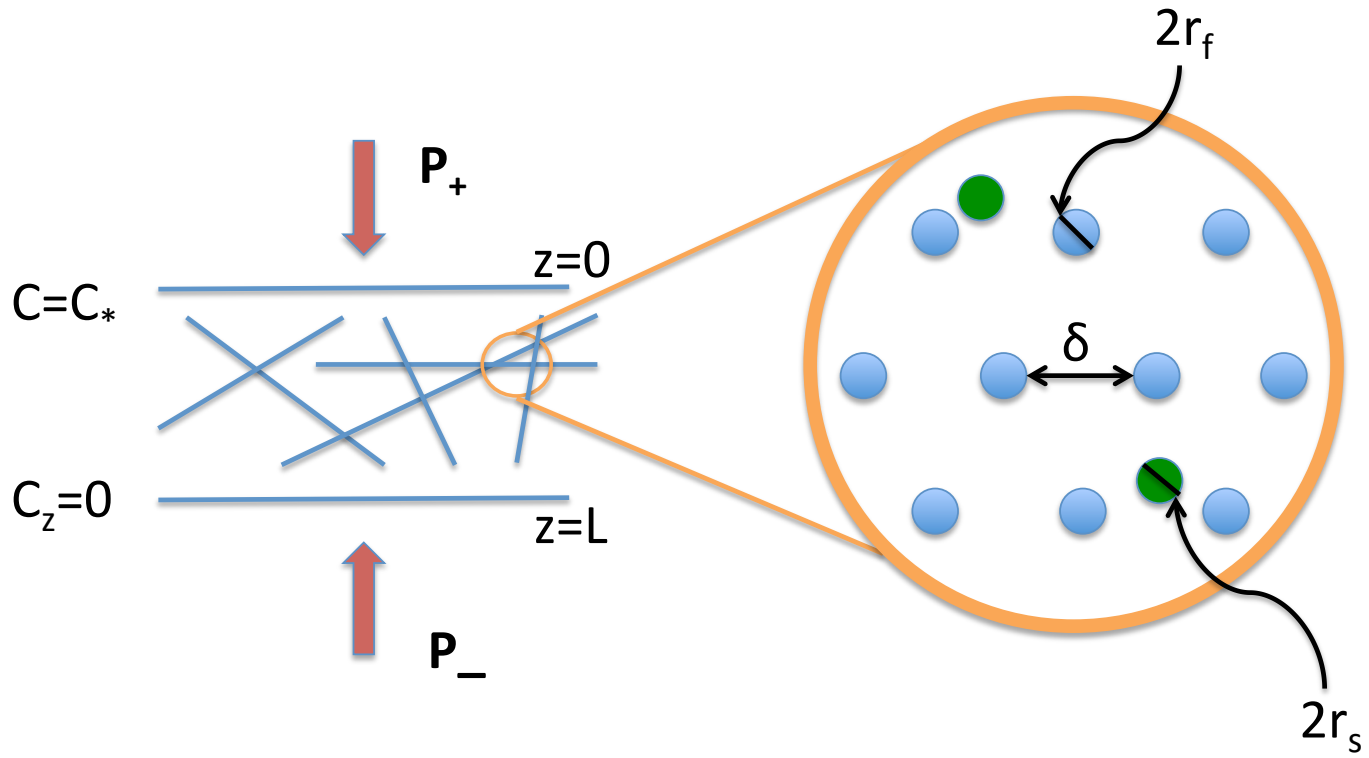
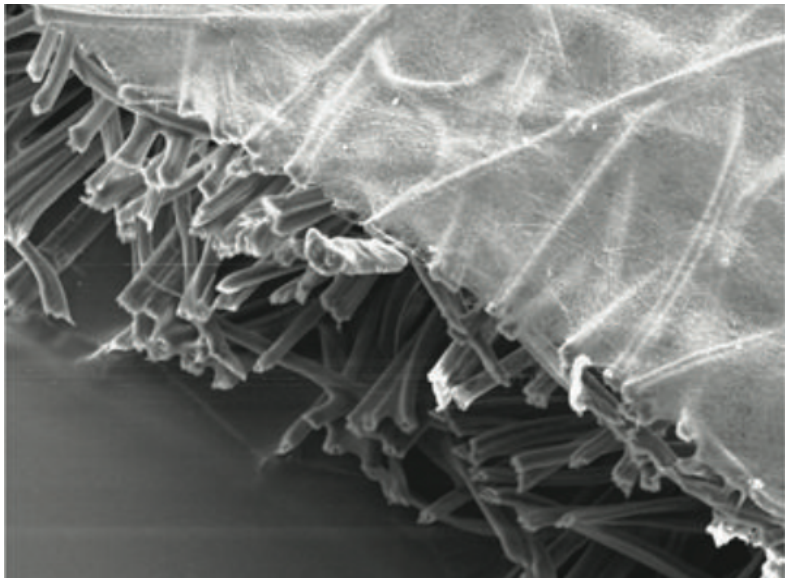
A Membrane under Compression and Flow



Gore Mission Statement

Goal:

- Mathematically characterize an idealized fibrous structure
- Use fiber matrix structure for transport parameters
  - Darcy permeability
  - void fraction
  - species fraction
  - effective tracer diffusivity
  - retardation coefficient
- Examine how changes in filter compression affect parameters



[1] M. Faccini 2012. doi:10.1155/2012/892894, [2] www.gore.com

Model

Darcy's Law

$$\overrightarrow{u} = \frac{-K_{p_{\text{eff}}}}{\mu} \nabla p \tag{7}$$

Continuity Equation

$$\nabla \cdot \overrightarrow{u} = 0 \tag{8}$$

This gives

$$\nabla \cdot \left(\frac{-K_{p_{\text{eff}}}}{\mu} \nabla p \right) = 0 \,. \tag{9}$$

Advection-Diffusion

$$\frac{\partial c}{\partial t} + \frac{1}{\gamma} \nabla \cdot (f c \overrightarrow{u}) = D_{\text{eff}} \nabla^2 c \tag{10}$$

- c - concentration of solute
- p - pressure
- u - velocity

Note: $K_{p_{\text{eff}}}, \mu, \gamma, f, D_{\text{eff}}$ are functions of void fraction (ϵ).

1D Model

For uniform ϵ:

$$\begin{aligned} p_{zz} &= 0 \\ c_t + \frac{f}{\gamma} c_z u &= D_{\text{eff}} c_{zz} \end{aligned} \tag{11}$$

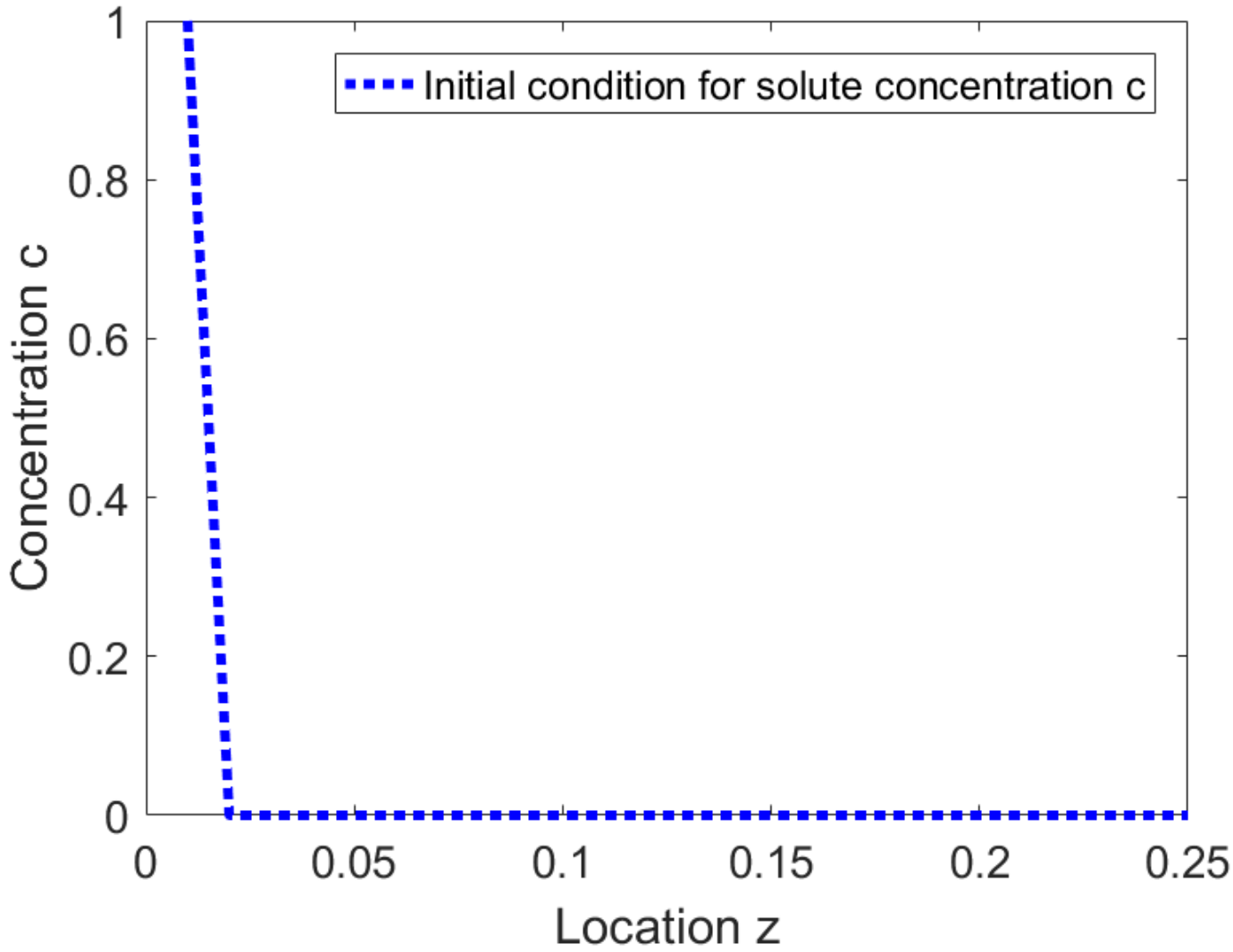
Nondimensionalize

$$\begin{aligned} p_{zz} &= 0 \\ c_t + \tilde{b} c_z p_z &= Pe^{-1} c_{zz} \end{aligned} \tag{12}$$

where

$$\tilde{b} = \frac{f K_p}{\gamma \mu} \,. \tag{13}$$

Concentration Profile



1D Model with Compression

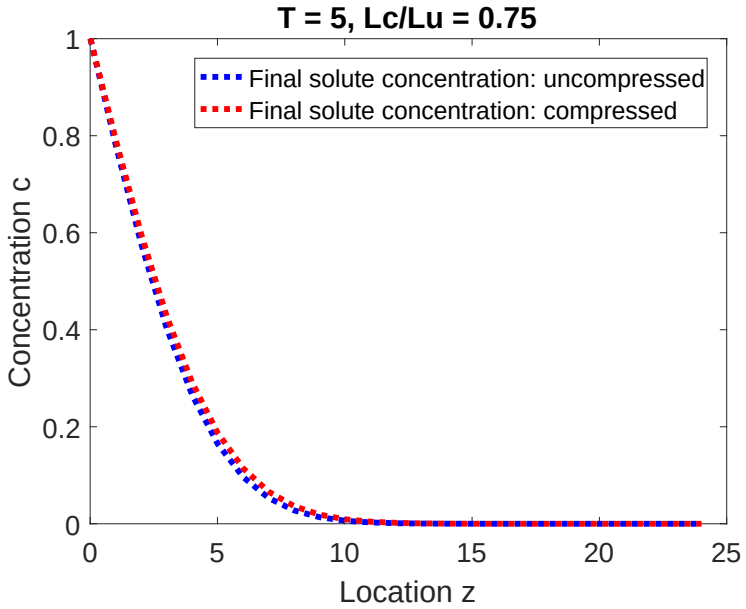
Compression reduces ϵ (void fraction).

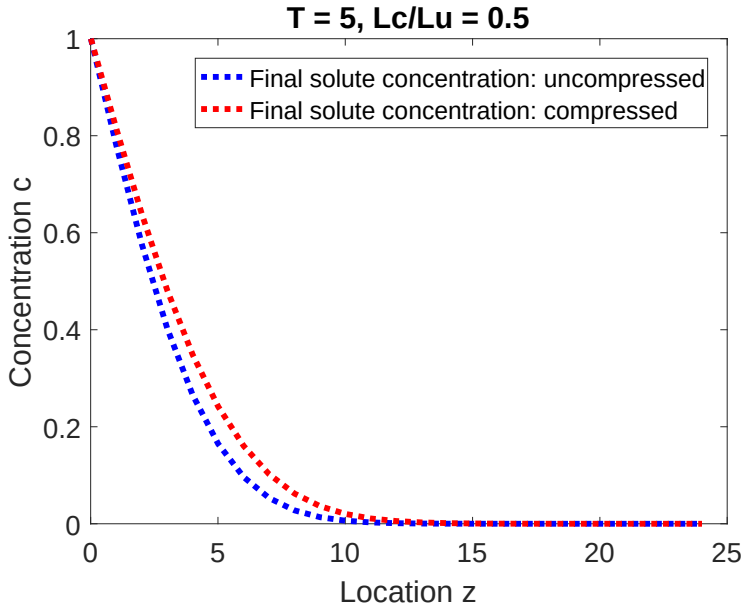
Conservation of solid mass:

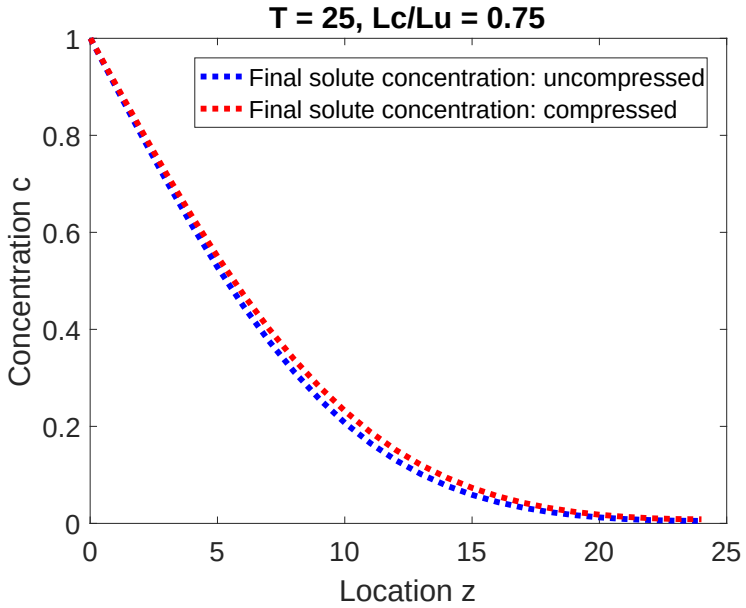
$$AL_u(1-\epsilon_u) = AL_c(1-\epsilon_c) \tag{14}$$

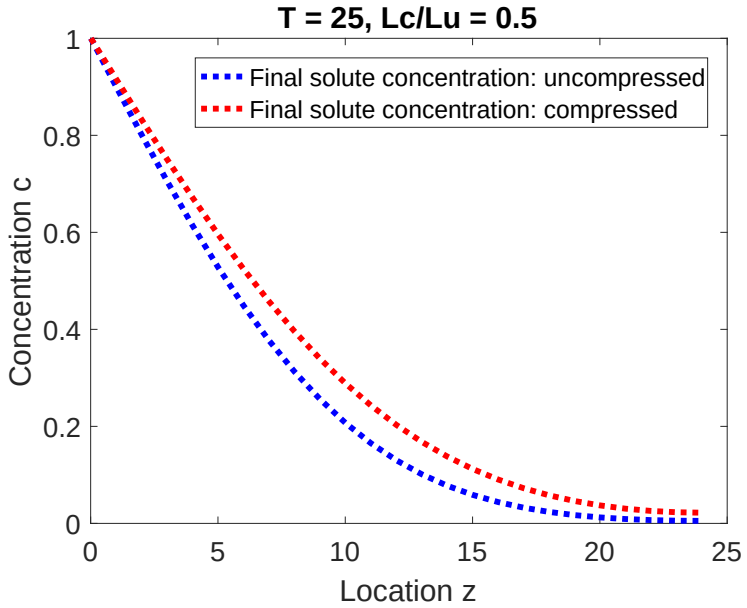
Change in $\frac{L_c}{L_u} \implies$ change in $c(z,t)$.

Results of Compression









Mechanical Model for Compressed Fiber Structure

Goal: Simulate fiber deformation due to compression

Method: Stiffness method

- Solve

$$[k]d = f$$

  - $[k]$ - stiffness matrix
  - d - vector of deformation of nodes (Cartesian coordinates)
  - f - force due to compression

- Treat fibers as springs

  1. Truss: angle varies; fibers straight
     - simple geometry case $\rightarrow$ collapse under shear force
  2. Frame: angle constant; fibers can bend

Results: See Videos

- Compression of fiber bundle in cube
- More complex geometry

Next Steps

1D Compression Model

- Prescribe $u(z = 0)$ instead of $p(z = 0)$
- Introduce clogging:

$$\frac{d\xi}{dt} = kc$$

  where ξ is bound solute.

Stiffness Method-Simulated Model

- Randomly distribute fibers versus using mesh structure
- Consider how to derive porosity, etc. from results
- Remove rigidity imposed by boundary conditions

Cellular Potts Model

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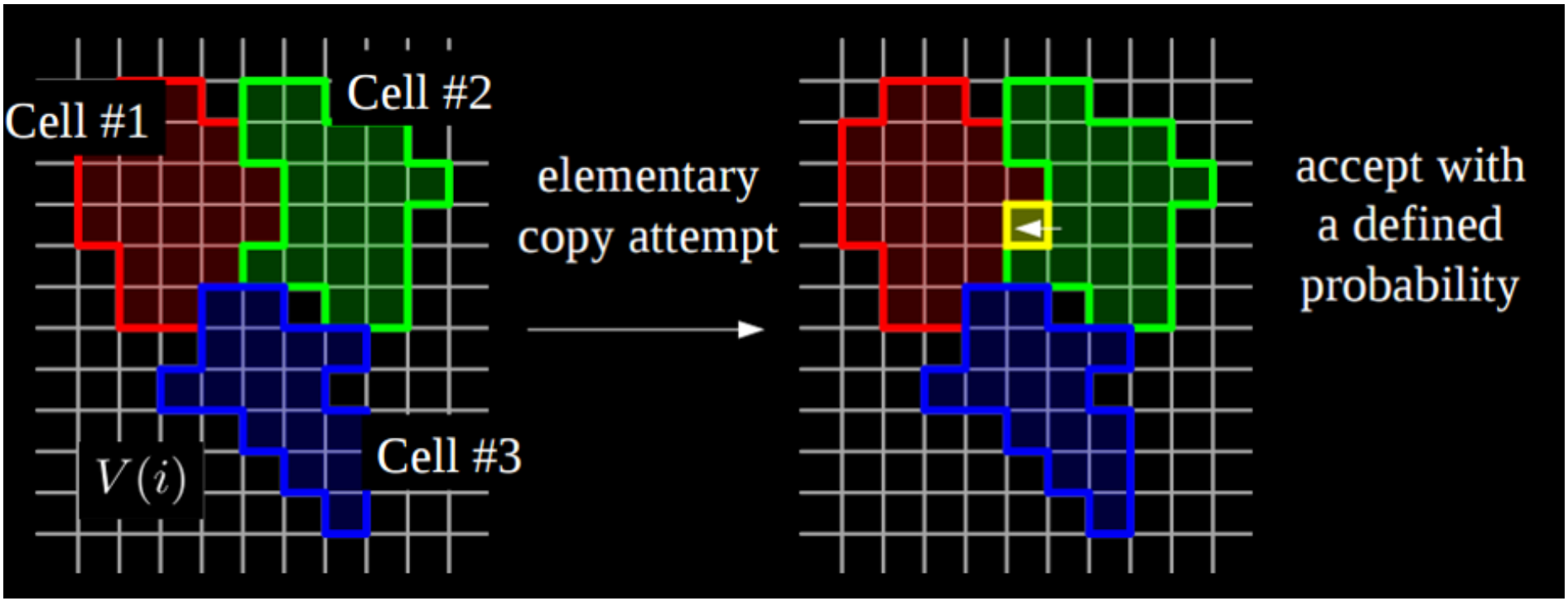
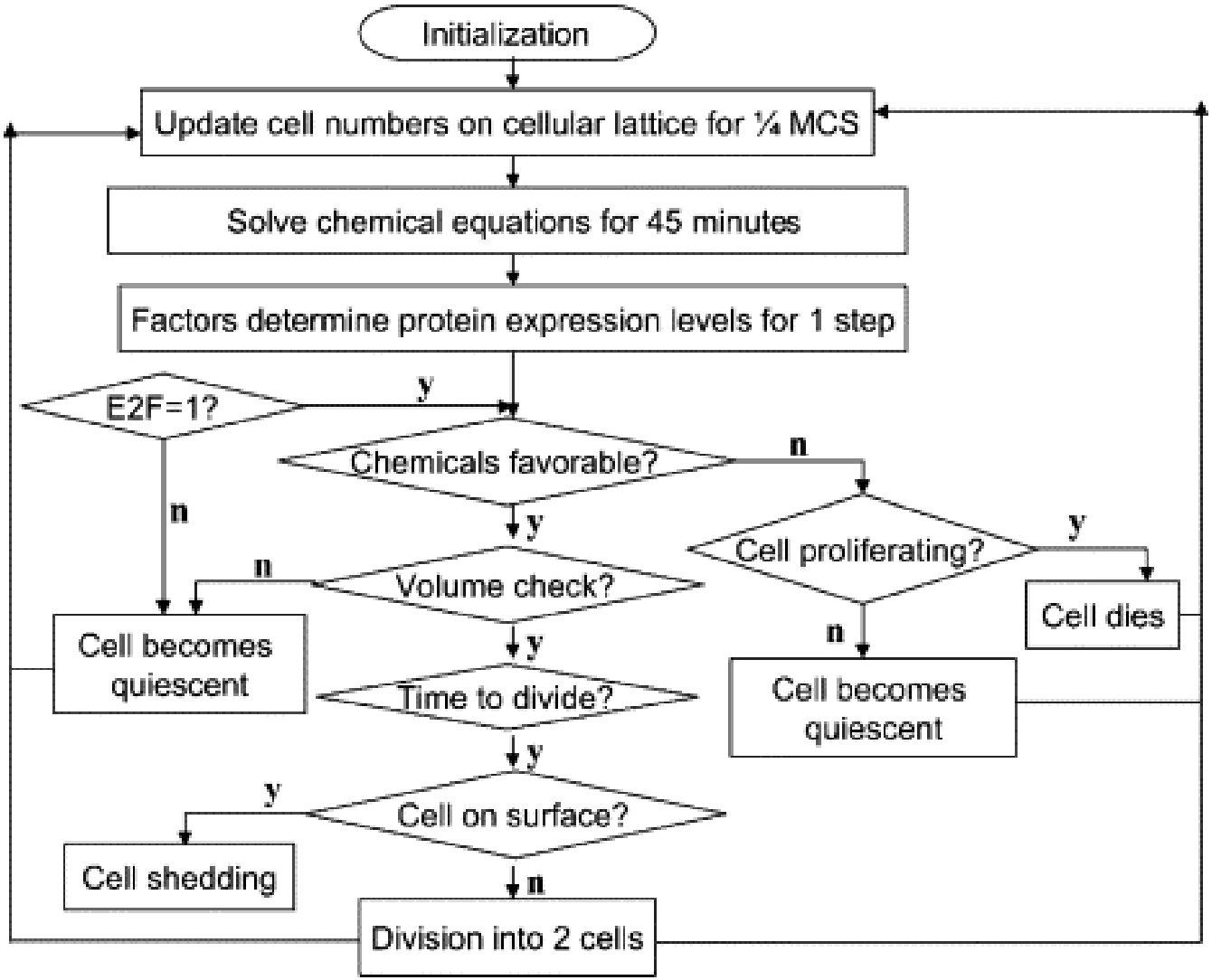
Problem Introduction: Cellular Potts Model

- Lattice model with cells
  - Extensively used in solid-state physics
  - Recently used in biology
  - Avascular tumor growth
- Build parallel simulation framework
- Studying growth of cells and influence of nutrient transport



Goal: Monte Carlo simulation in parallel

- Model algorithm development based on paper
- Implement portions of the algorithm using MPI



Chemical Reaction-Diffusion of Oxygen and Nutrients

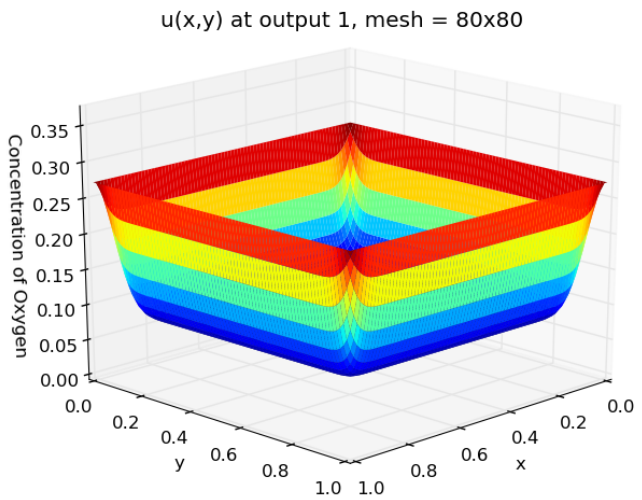
$$
\begin{aligned}
\frac{\partial u_{\mathrm{O}_2}}{\partial t} &= D_{\mathrm{O}_2}\nabla^2 u_{\mathrm{O}_2} + a_0 \frac{u_{\mathrm{O}_2} - u_{\mathrm{O}_2}^{\mathrm{T}}}{u_{\mathrm{O}_2}^{\mathcal{O}} - u_{\mathrm{O}_2}^{\mathrm{T}}} \\
\frac{\partial u_{\mathrm{n}}}{\partial t} &= D_{\mathrm{n}}\nabla^2 u_{\mathrm{n}} + b_0 \frac{u_{\mathrm{n}} - u_{\mathrm{n}}^{\mathrm{T}}}{u_{\mathrm{n}}^{\mathcal{O}} - u_{\mathrm{n}}^{\mathrm{T}}} \\
u_{\mathrm{O}_2}|_{\partial\Omega} &= c_{\mathrm{O}_2} \\
u_n|_{\partial\Omega} &= c_n
\end{aligned}
$$

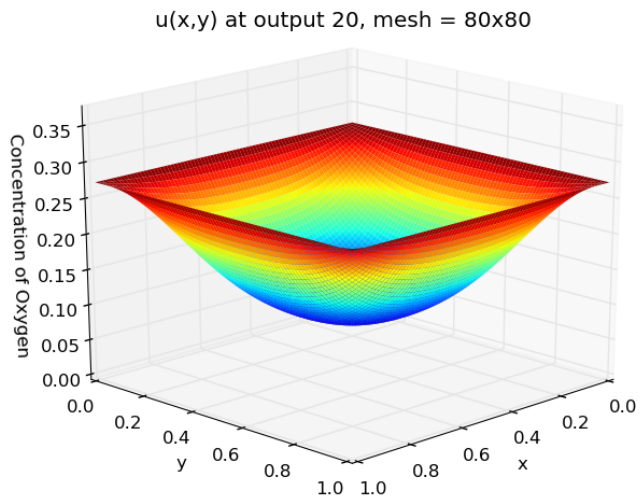
Hamiltonian

$$
H = \sum_{\text{lattice sites}} J_{\tau(S_1)\tau(S_2)} \left[1 - \delta\left(S_1, S_2\right)\right] + \sum_{\text{cells}} \gamma \left(v - V^{\mathrm{T}}\right)^2
$$

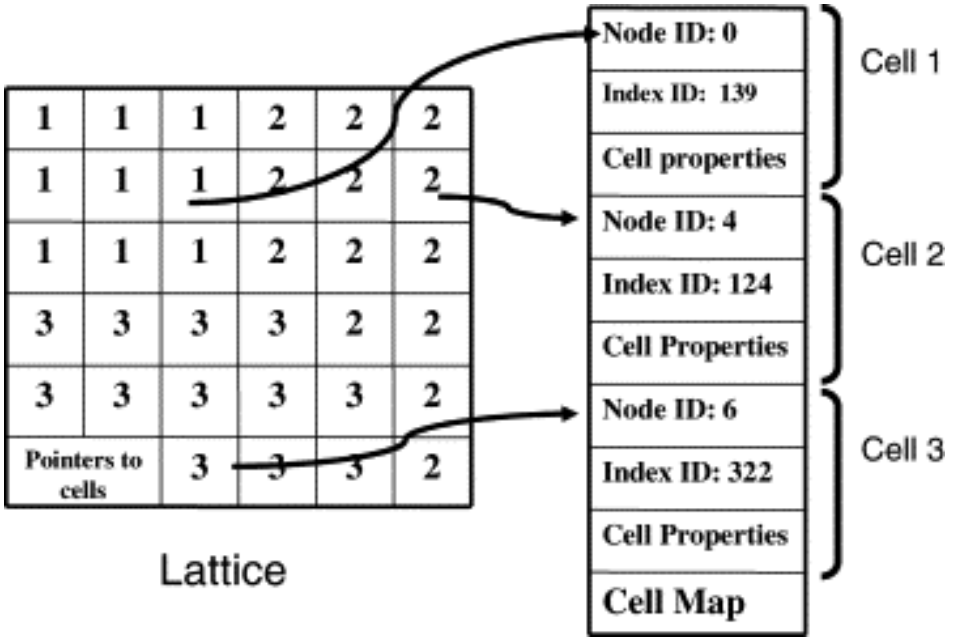
$$
P_{Acc} = \begin{cases} 1 & \triangle H < 0 \\ e^{-\frac{\triangle H}{k_b^{\mathrm{T}}}} & \triangle H \geq 0 \end{cases}
$$

Preliminary Numerical Results





Data Structure for Parallel Description



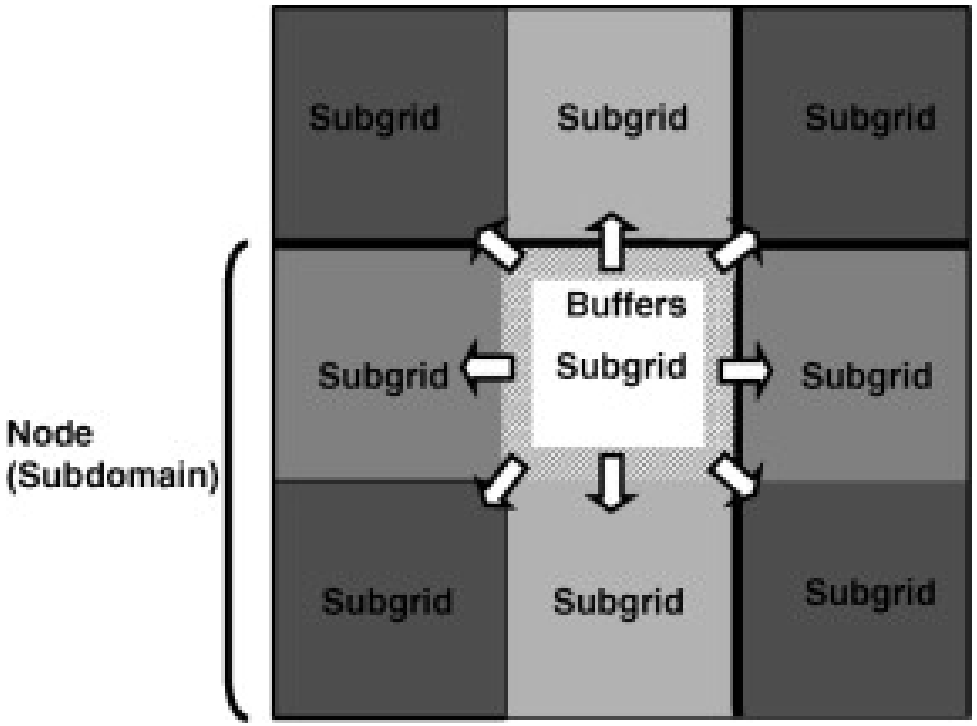
Lattice

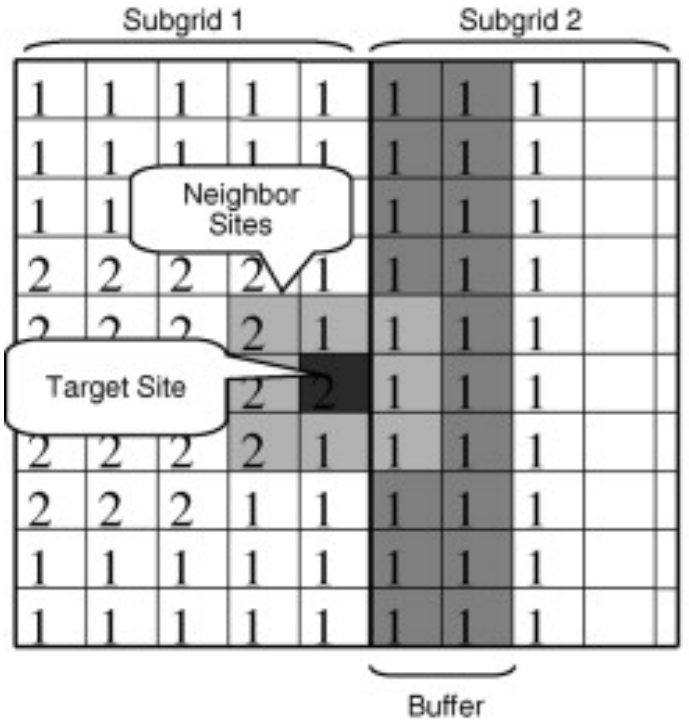
- Cell index S_i
- Cell type $\tau(S_i)$
- Neighbor list
- Oxygen: u_{O_2}
- Nutrition: u_{n}

Cell

- Cell Type: Proliferating, Quiescent, Necrotic
- Occupying lattice points list
- Average Oxygen: mean $\left(u_{\mathrm{O}_2}\right)$
- Average Nutrition: mean $\left(u_{\mathrm{n}}\right)$

Parallel Domain Decomposition for PDE and H





Equilibrium Gibbs Measure

$$\langle \rho_{ij}^{\kappa} \rangle = \frac{1}{Z} \sum_{\tau=\{\tau_{mn}\}}^{\text{types}} \sum_{S=part(\{\tau\})}^{\text{cell IDs}} \underbrace{\delta_{(\tau_{ij}=\kappa)}}_{\rho_{ij}^{\kappa}} \delta_{(\text{enough } O_2)} e^{-\beta H(\tau,S))}$$

$\tau \in$ cite types $=\{A, Q, D, M\}$ (active, quiescent, dead, medium).
$S = part(\{\tau\})$: split A, Q cites into cells with distinct IDs ('coloring') .
H penalizes for cell volume not optimal, or long particle boundary.
Number of colorings of n cites grow quickly:

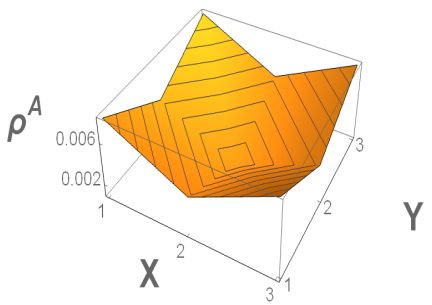
$part[2] = \{\{(1,2)\},\{(1),(2)\}\})$ $\quad \# = 2$

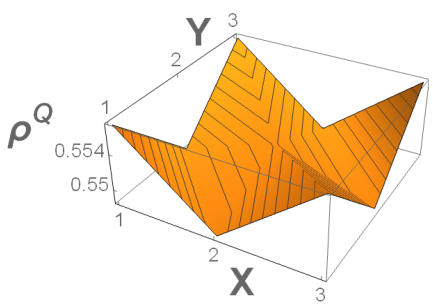
$part[3] = \{\{(1,2,3)\},\{(1),(2,3)\},\{(1,2),(3)\},\{(1,3),(2)\},\{(1),(2),(3)\}$ $\quad \# = 5$

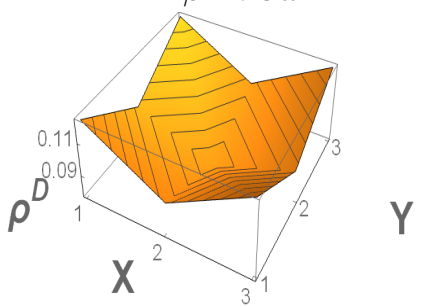
$\mid part[4] \mid = 15;$ $\quad \mid part[5] \mid = 52;$ $\quad \ldots \mid part[9] \mid = 21147 \ldots$

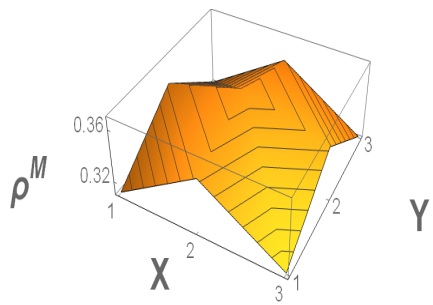
Q:• Ensuring that cells are simply connected

- 'Thermodynamic'/large lattice limit ? $F = -\frac{1}{\beta Area} \lim_{Area\to\infty} \log Z$ =???









Conclusions & Future Work

- Consider more complicated reaction and energy terms
- Parallelize other cell dynamics
- Construct Monte Carlo simulation

Many thanks go to...

- NSF
- Duke University
- RPI
- MPI
- Our industrial sponsors:
  Dr. Vasu Venkateshwaran and Dr. Zhenyu He
- Our patient faculty mentors

Reduction to Macroscale Model

Begin with

$$W_t + UW_z = d_1(W_{y'y'} + W_{zz})$$

Average over y' measured from center of channel to filter surface by integrating to get

$$\frac{h}{2}(\hat{W}_t + U\hat{W}_z) = d_1 W_{y'}|_{y'=h/2}$$

Assume change in time is negligible, then we see

$$\frac{h}{2}U\hat{W}_z = d_1 T_y|_{y=0}$$

1D Problem Method

- Solve using Crank-Nicholson in time
- Because of nonlinearity, set up as a Newton's Method problem:

$$F(\overrightarrow{x}^{n+1}) = G(\overrightarrow{x}^{n})$$

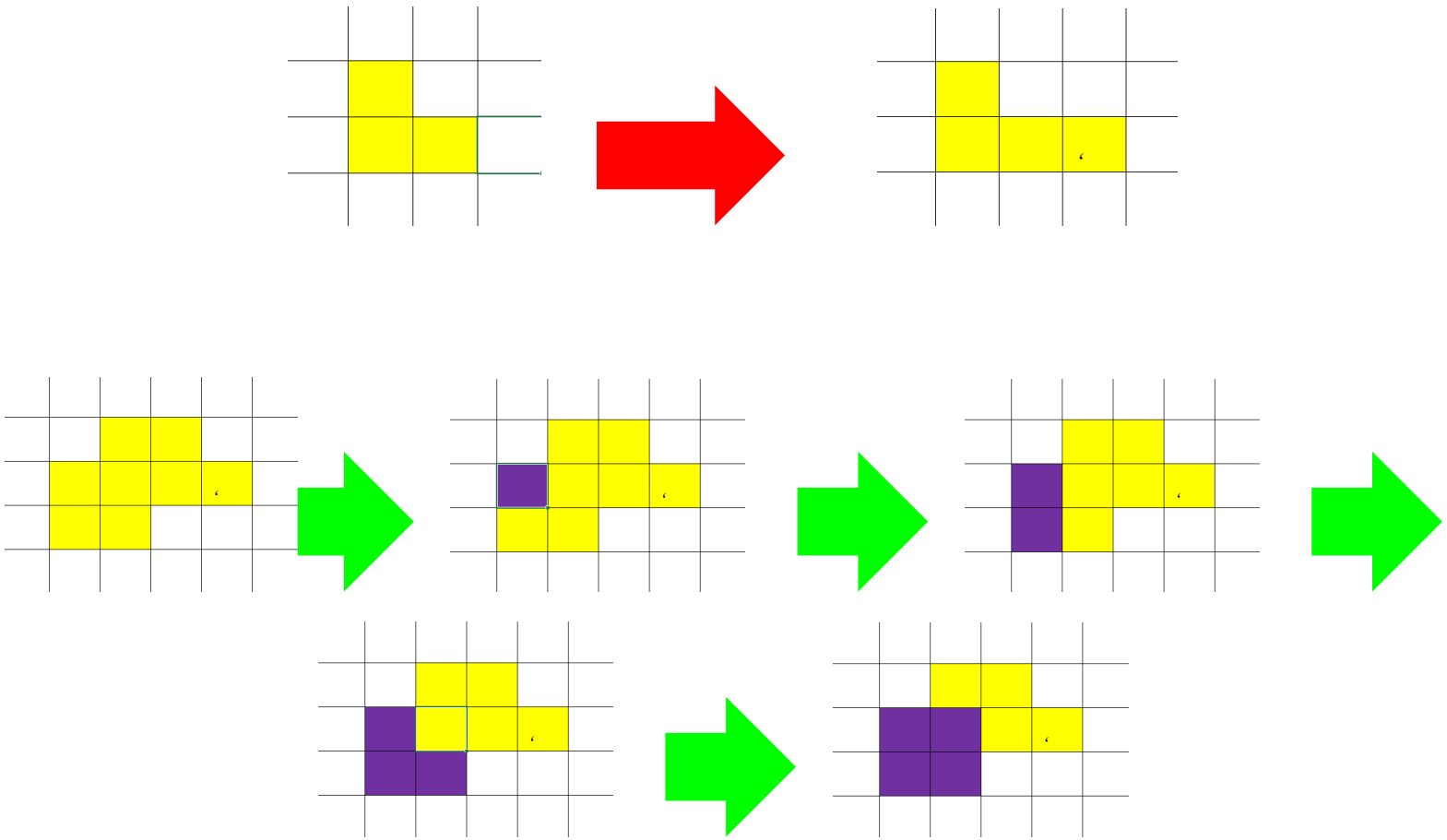
Solve for $\overrightarrow{x}^{n+1}$, where

$$\overrightarrow{x}^{n} = \begin{pmatrix} c_1^n \\ \vdots \\ c_{N+1}^n \\ p_1^n \\ \vdots \\ p_N^n \end{pmatrix}$$

Parameters and Variables

- c - concentration of solute inside filter
- p - pressure
- u - velocity
- $K_{p_{\text{eff}}}$ - Darcy coefficient/permeability
- μ - viscosity
- f - sieving coefficient
- γ partition coefficient/species volume fraction
- ϵ - void fraction
- r_f - fiber radius
- r_s - solute particle radius
- δ - distance between fiber bundles
- A - surface area
- L_u = uncompressed membrane thickness
- L_c = compressed filter thickness

Further cell dynamics: Cell growth and division



Potts Model Reference Slide: breadth first search (BFS)