Modeling Chemotaxis with Fractional Step Approaches

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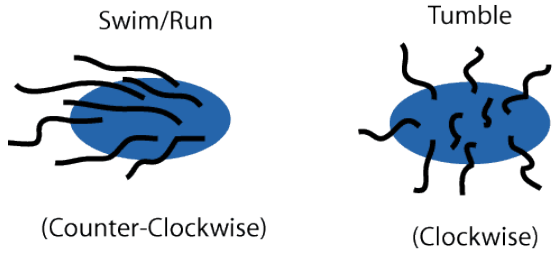
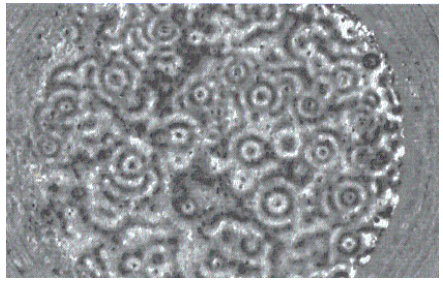
Outline

Chemotaxis

- Bacteria exhibits a random walk in nature.



- In the presence of a chemical stimulus, they exhibit a motion called chemotaxis which leads to the formation of special patterns.



The Advection-Diffusion-Reaction Equation

- *E.coli* and *S.typhimurium* form these complex patterns after feeding on succinate. In response to succinate, the bacteria secretes aspartate which is the chemoattractant. The equations relating the bacteria, aspartate and the succinate are shown below.
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$$\frac{\partial n}{\partial t} = D_n \nabla^2 n - \alpha \nabla \left[\frac{n}{(1+c)^2} \nabla c \right] + \rho n \left(\delta \frac{s}{1+s^2} - n \right)$$

$$\frac{\partial c}{\partial t} = D_c \nabla^2 c + \beta s \frac{n}{\gamma + n^2} - nc$$

$$\frac{\partial s}{\partial t} = D_s \nabla^2 s - \kappa n \frac{s^2}{1+s^2}$$

Outline

The Advection step

- The advection arises in response to the chemical stimulus.
- The cell density n is modeled by

$$n_t + [un]_x = 0$$

where

$$u = \frac{\alpha}{(1+c)^2} \frac{\partial c}{\partial x}$$

- As a result, we have velocities that depend on the concentration gradient and thus, variable coefficients in our advection equation.

Variable Coefficients

- For $x < x_{i-1/2}$,

$$q_t + u_{i-1} q_x = 0$$

  For $x > x_{i-1/2}$,

$$q_t + u_i q_x = 0$$

- So, this cannot be modeled by the regular wave speed traveling with the strength $Q_i - Q_{i-1}$. We try balancing the flux at the interface

$$u_{i-1} Q_{i-1} = u_i Q^*_{i-1/2}$$

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$$A^+ \Delta Q_{i-1/2} = u_i Q_i - u_{i-1} Q_{i-1}$$

The Advection Scheme

- We use something similar

$$A^{+}\Delta Q = F_{i-1/2} - u_{i-1}n_{i-1}$$

$$A^{-}\Delta Q = u_i n_i - F_{i-1/2}$$

where

$$u_i = max(u_{i-1/2}, 0) + min(u_{i+s1/2}, 0)$$

and

$$F_{i-1/2} = \begin{cases} u_{i-1/2}n_{i-1} & u_{i-1/2} \geq 0 \\ u_{i-1/2}n_i & u_{i-1/2} < 0 \end{cases}$$

The Diffusion and Reaction Schemes

- For Diffusion, we use the implicit CN scheme and solve it using the tridiag solver from LAPACK.s
- For the reaction step, the authors determine that the scheme hardly matters as fourth order explicit Runge-Kutta has the same results as the first order implicit backward Euler scheme. We use the regular forward Euler scheme.

1st Order (Godunov) Splitting

- Consider the linear system, $q_t = Aq$, where A is a discrete differential operator typically formed from some sort of differencing scheme.
- The general solution is $q(t_{n+1}) = e^{\Delta t A} q(t_n)$ assuming homogeneous or periodic BCs.
- Often the operator A may be split up into $A = A_1 + A_2 + ... + A_n$, which in this case corresponds to the RHS of the system representing multiple source terms in a system of non-homogeneous hyperbolic PDEs.
- Then a set of sub-problems, $q_t = A_1 q$, $q_t = A_2 q$, ... ,$q_t = A_n q$, can be solved and their solutions combined to approximate the exact solution as $q(t_{n+1}) = e^{\Delta t A_1} e^{\Delta t A_2} \dots e^{\Delta t A_n} q(t_n)$.

2nd Order (Strang) Splitting

- Instead of taking whole time steps as with Godunov splitting, Strang splitting takes two half steps, reversing the order of the operators for the advection, diffusion, and reaction solutions.
- $q(t_{n+1}) =$
$$\left(e^{A_1 \Delta t/2} e^{A_2 \Delta t/2} \dots e^{A_n \Delta t/2}\right)\left(e^{A_n \Delta t/2} \dots e^{A_2 \Delta t/2} e^{A_1 \Delta t/2}\right) q(t_n) =$$
$$\left(e^{A_1 \Delta t/2} e^{A_2 \Delta t} \dots e^{A_n \Delta t} \dots e^{A_2 \Delta t} e^{A_1 \Delta t/2}\right) q(t_n)$$

- The chemotaxis problem presents a set of three operators; however, each is non-linear and the matrix multiplication solutions presented above no longer are applicable
- $q_t = \mathscr{A}(q) + \mathscr{D}(q) + \mathscr{R}(q)$
- $\mathscr{A}(q) = \begin{Bmatrix} -\alpha\nabla\left(\frac{n}{(1+c)^2}\nabla c\right) \\ 0 \\ 0 \end{Bmatrix}$
- $\mathscr{D}(q) = \begin{Bmatrix} D_n\nabla^2 n \\ D_c\nabla^2 c \\ D_s\nabla^2 s \end{Bmatrix}, \qquad \mathscr{R}(q) = \begin{Bmatrix} \rho n\left(\frac{\delta s^2}{1+s^2} - n\right) \\ \frac{\beta s n^2}{\gamma+n^2} - nc \\ -\frac{\kappa n s^2}{1+s^2} \end{Bmatrix}$

Non-linear Godunov Splitting

For 1st Order splitting applied to the chemotaxis problem

- solve $q_t = \mathscr{A}(q)$ using the IC q^n over the interval $t_n \leq t \leq t_{n+1}$ to find q^*
- solve $q_t = \mathscr{D}(q)$ using the IC q^* over the interval $t_n \leq t \leq t_{n+1}$ to find q^{**}
- solve $q_t = \mathscr{R}(q)$ using the IC q^{**} over the interval $t_n \leq t \leq t_{n+1}$ to find q_{n+1}

Non-linear Strang Splitting

For 2nd Order splitting applied to the chemotaxis problem

- solve $q_t = \mathscr{A}(q)$ using the IC q^n over the interval $t_n \leq t \leq t_{n+1/2}$ to find q^*
- solve $q_t = \mathscr{D}(q)$ using the IC q^* over the interval $t_n \leq t \leq t_{n+1/2}$ to find q^{**}
- solve $q_t = \mathscr{R}(q)$ using the IC q^{**} over the interval $t_n \leq t \leq t_{n+1}$ to find q^{***}
- solve $q_t = \mathscr{D}(q)$ using the IC q^{***} over the interval $t_n \leq t \leq t_{n+1/2}$ to find q^{****}
- solve $q_t = \mathscr{A}(q)$ using the IC q^{****} over the interval $t_n \leq t \leq t_{n+1/2}$ to find q_{n+1}

Outline

Advection without second order corrections

Pure advection

Advection with a different chemoattractant profile

The Advection-Diffusion-Reaction Equation : Case 1

The Advection-Diffusion-Reaction Equation : Case 2

Outline

Thanks

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