Computational Cardiology Lecture 5

Finite-volume advection and diffusion

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The represented concentration

$$\bar{c}_i = \frac{1}{\Delta x} \int_{x_{i-1/2}}^{x_{i+1/2}} c(x,t)\,\mathrm{d}x.$$

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The unknown is a cell average, not a value at an arbitrary point.

Integrate the conservation law

$$c_t + J_x = 0 \quad \Longrightarrow \quad \Delta x \, \dot{\bar{c}}_i = J_{i-1/2} - J_{i+1/2}.$$

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The same face flux enters adjacent cells with opposite signs.

The global boundary budget

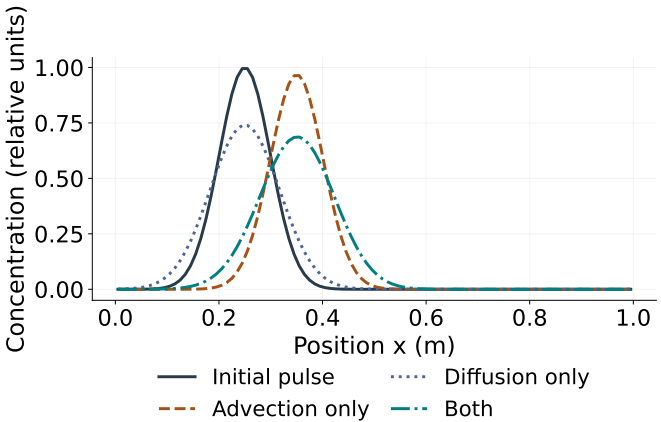
$$M = \Delta x \sum_i c_i, \qquad M^{n+1} - M^n = \Delta t (J_{1/2} - J_{N+1/2}).$$

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Periodic endpoints have identical fluxes.

Transport redistributes a conserved amount



Constitutive transport flux

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$$c_t = -ac_x + Dc_{xx}.$$

Upwind advection

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$$J^{\text{adv}}_{i+1/2} = a^+ c_i + a^- c_{i+1}.$$

The upstream cell changes when the velocity changes sign.

Centered diffusion

$$J^{\text{diff}}_{i+1/2} = -D\frac{c_{i+1} - c_i}{\Delta x}.$$

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$$J_{i+1/2}^{\text{diff}} = -D\frac{c_{i+1} - c_i}{\Delta x}.$$

A concentration increasing to the right produces a diffusive flux to the left.

The positive-velocity update

$$c_i^{n+1} = (\nu + \mu)c_{i-1}^n + (1 - \nu - 2\mu)c_i^n + \mu c_{i+1}^n.$$

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$$c_i^{n+1} = (\nu + \mu)c_{i-1}^n + (1 - \nu - 2\mu)c_i^n + \mu c_{i+1}^n.$$

$$\nu = \frac{a\Delta t}{\Delta x}, \qquad \mu = \frac{D\Delta t}{\Delta x^2}.$$

A discrete maximum principle

If $\nu + 2\mu \leq 1$, all three coefficients are nonnegative and sum to one.

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$$\min_j c_j^n \leq c_i^{n+1} \leq \max_j c_j^n.$$

A time-step restriction for either direction

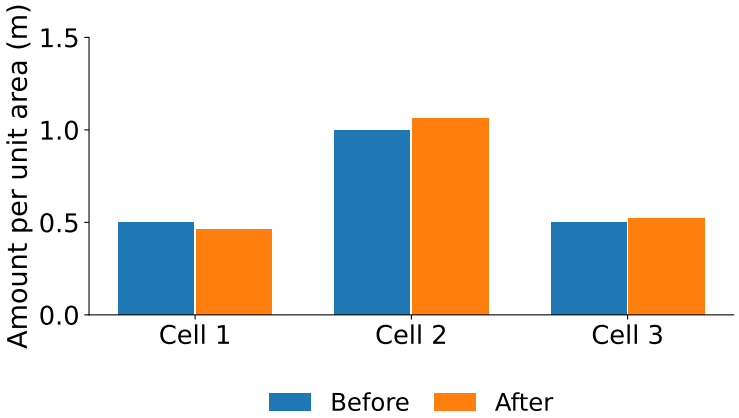
$$\Delta t \left(\frac{|a|}{\Delta x} + \frac{2D}{\Delta x^2} \right) \leq 1.$$

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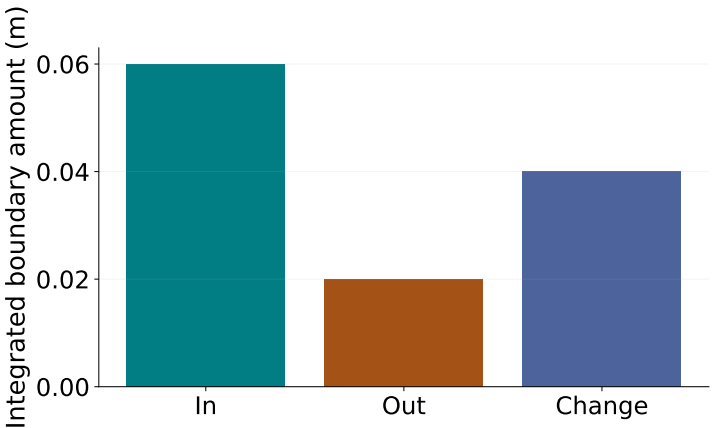
$$\Delta t \left(\frac{|a|}{\Delta x} + \frac{2D}{\Delta x^2} \right) \leq 1.$$

Halving Δx doubles the advective rate and quadruples the diffusive rate.

Internal transfers cancel



Boundary flux sets the change



An open-boundary step

$$c^n = (1, 2, 1), \quad \Delta x = .5, \quad \Delta t = .2.$$

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Four prescribed face fluxes $(.3, .5, .2, .1)$ give $c^{n+1} = (.92, 2.12, 1.04)$.

The amount balance

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$$\Delta M = .2(.3 - .1) = .04.$$

Internal faces redistribute amount without changing this total.

An exact shift of the cell vector

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$$c_i^{n+1} = c_{i-1}^n.$$

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Negative velocity reverses the shift. This identity fixes the indexing convention.

Constant and stationary states

If $c_i = c_0$, every flux difference is zero.

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Numerical diffusion

For smooth pure advection with $a > 0$, the leading modified equation is

$$c_t + ac_x = \frac{a\Delta x}{2}(1-\nu)c_{xx} + \cdots .$$

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Upwind smoothing can occur even when the physical D is zero.

Transport mechanisms and model interpretation

A tracer requires a justified velocity field and inlet conditions. An activation model requires reaction kinetics.

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