AN INTRODUCTION TO: DIFFERENTIAL EQUATIONS AND THEIR NUMERICAL APPROXIMATION

Todd Arbogast

Department of Mathematics
and
Center for Subsurface Modeling,
Institute for Computational Engineering and Sciences (ICES)

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Outline

	Topic	Main application
1.	Ordinary differential equations (ODE)	Reaction dynamics
2.	Elliptic Partial differential equations (PDE)	Steady state single phase flow or diffusive equilibrium
3.	Parabolic Partial differential equations	Tracer diffusion
4.	Hyperbolic Partial differential equations	Tracer transport

III. Parabolic Partial differential equations

(for tracer diffusion and unsteady single phase flow)

The Heat Equation

Recall the general conservation equation

$$\xi_t + \nabla \cdot (\xi \mathbf{v}) = q,$$

and make the modeling assumption of Fickian diffusion, i.e., that

$$\mathbf{v} = -(D/\phi)\nabla c,$$

where

- $c(\mathbf{x}, t)$ is the concentration of an immiscible tracer fluid in a bulk fluid (mass/volume);
- $\mathbf{v}(\mathbf{x}, t)$ is the diffusive velocity of the tracer particles (length/time);
- $q(\mathbf{x}, t)$ is an external source or sink of fluid (mass/volume/time);
- $\phi(\mathbf{x}, t)$ is the porosity of the medium, so $\xi = \phi c$;
- $D(\mathbf{x})$ is the diffusion coefficient (area/time).

Then we have the heat equation, which also models the diffusion of tracer particles in a bulk fluid:

$$(\phi c)_t - \nabla \cdot (D \nabla c) = q.$$

We call this a second order parabolic partial differential equation.

Boundary and Initial Conditions

We need to specify boundary *and* initial conditions (BC's and IC's).
The problem is to find concentration c such that

$$\begin{cases} (\phi c)_t - \nabla \cdot (D \nabla c) = q(\mathbf{x}, t), & \text{in } \Omega,\ t > 0, \\ c(\mathbf{x}, t) = c_D(\mathbf{x}, t), & \text{on } \Gamma_D,\ t > 0, \\ -(D \nabla c) \cdot \nu = f(\mathbf{x}, t), & \text{on } \Gamma_N,\ t > 0, \\ c(\mathbf{x}, 0) = c_0(\mathbf{x}), & \text{on } \Omega. \end{cases}$$

Theorem. If $D \geq D_* > 0$ and $\phi \geq \phi_* > 0$ for some D_* and ϕ_*, then this initial-boundary value problem has a unique solution c for any (reasonable) domain Ω, Γ_D, and $\Gamma_N = \partial\Omega \setminus \Gamma_D$, diffusion coefficient $D(\mathbf{x})$, and for any reasonable data $q(\mathbf{x}, t)$, $c_D(\mathbf{x}, t)$, $f(\mathbf{x}, t)$, and $c_0(\mathbf{x})$.

Moreover, the solution depends continuously on the data. If we change the data q, c_D, f, and c_0 and also D and ϕ a little, then the solution changes only a little.

Steady State

Suppose that q, c_D, f, and ϕ depend only on space (i.e., they do not change with time). Then as time goes on, we should expect that the system settles down to a steady state.

Theorem. If q, c_D, and f depend only on space, then

$$c_t \longrightarrow 0 \quad \text{and} \quad \boxed{c(\mathbf{x},t) \longrightarrow c_\infty(\mathbf{x})} \quad \text{as} \quad t \longrightarrow \infty,$$

where

$$\begin{cases} -\nabla \cdot (D \nabla c_\infty) = q(\mathbf{x}), & \text{in } \Omega, \\ c_\infty(\mathbf{x}) = c_D(\mathbf{x}), & \text{on } \Gamma_D, \\ -(D \nabla c_\infty) \cdot \nu = f(\mathbf{x}), & \text{on } \Gamma_N, \end{cases}$$

provided that in the pure Neumann case, we satisfy the compatibility condition.

Remark. Note that we get the same steady state for any ϕ and c_0. In particular, the initial concentration does not matter.

Separation of Variables—1

- Assume that the domain Ω is rectangular. For simplicity, take $\Omega = (0, \ell) \subset \mathbb{R}^1$ (i.e., 1-D in space).
- Assume that D and ϕ are constant.

We solve by separation of variables the problem with homogeneous Dirichlet BC's but a nontrivial IC:

$$\begin{cases} \phi c_t - D c_{xx} = 0, & 0 < x < \ell, \ t > 0, \\ c(0,t) = c(\ell,t) = 0, & t > 0, \\ c(x,0) = c_0(x), & 0 < x < \ell. \end{cases}$$

Step 1, separate the variables. We look for solutions of the form

$$c(x,t) = X(x)T(t) \quad \Longrightarrow \quad \frac{\phi}{D}\frac{T'}{T} = \frac{X''}{X} = -\lambda^2$$

$$\Longrightarrow \quad X'' + \lambda^2 X = 0 \quad \text{and} \quad T' - \lambda^2 (D/\phi) T = 0.$$

Step 2, solve for X. Note that X has two homogeneous BC's:

$$X(0) = X(\ell) = 0 \quad \Longrightarrow \quad X(x) = \sin(\lambda_n), \quad \lambda_n = \frac{n\pi}{\ell}, \quad n = 1, 2, 3, \ldots.$$

Step 3, solve for T. $\quad T(t) = e^{-\lambda_n^2 D t/\phi}.$

Separation of Variables—2

Step 4, use superposition. We have derived infinitely many solutions, which we sum

$$c(x,t) = \sum_{n=1}^{\infty} c_n e^{-\lambda_n^2 Dt/\phi} \sin(\lambda_n x), \qquad \text{where} \qquad \lambda_n = \frac{n\pi}{\ell}.$$

Step 5, set the IC.

$$c_0(x) = \sum_{n=1}^{\infty} c_n \sin(\lambda_n x) \qquad \Longrightarrow \qquad c_n = \frac{2}{\ell}\int_0^{\ell} c_0(x)\, \sin(n\pi x/\ell)\, dx.$$

Remark. The highly oscillatory sine waves (large n) decay away quickly, leaving only the smoother components. For a given mode n, we have

- space scale $1/\lambda_n = \mathcal{O}(1/n)$ (to resolve space, we need $h = \mathcal{O}(1/n)$),
- time scale $\phi/\lambda_n^2 D = \mathcal{O}(1/n^2)$ (to resolve time, we need $\Delta t = \mathcal{O}(1/n^2)$).

That is, the space and time scales are interrelated, and we need

$$\Delta t = \mathcal{O}(h^2),$$

Question: What does this say about the stability of explicit numerical methods?

A Fundamental Solution

If D and ϕ are constant and $\Omega = \mathbb{R}^d$ is all of space, then a fundamental solution $\kappa(\mathbf{x}, t)$ for

$$\begin{cases} \phi c_t - D\Delta c = q(\mathbf{x}, t), \\ c(\mathbf{x}, 0) = c_0(\mathbf{x}), \end{cases} \quad \text{solves} \quad \begin{cases} \phi \kappa_t - D\Delta \kappa = 0, \\ \kappa(\mathbf{x}, 0) = \delta_0(\mathbf{x}). \end{cases}$$

The solution is the Gauss kernel

$$\boxed{\kappa(x, y, z, t) = \left(\frac{\phi}{4D\pi t}\right)^{d/2} e^{-(x^2+y^2+z^2)\phi/4Dt}}$$

(omit z in 2-D, y and z in 1-D).

The solution to the original problem is the sum of two convolutions

$$c(x, y, z, t) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} c_0(X, Y, Z)\, \kappa(x - X, y - Y, z - Z, t)\, dX\, dY\, dZ$$

$$+ \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_0^t q(X, Y, Z, s)\, \kappa(x - X, y - Y, z - Z, t - s)\, ds\, dX\, dY\, dZ.$$

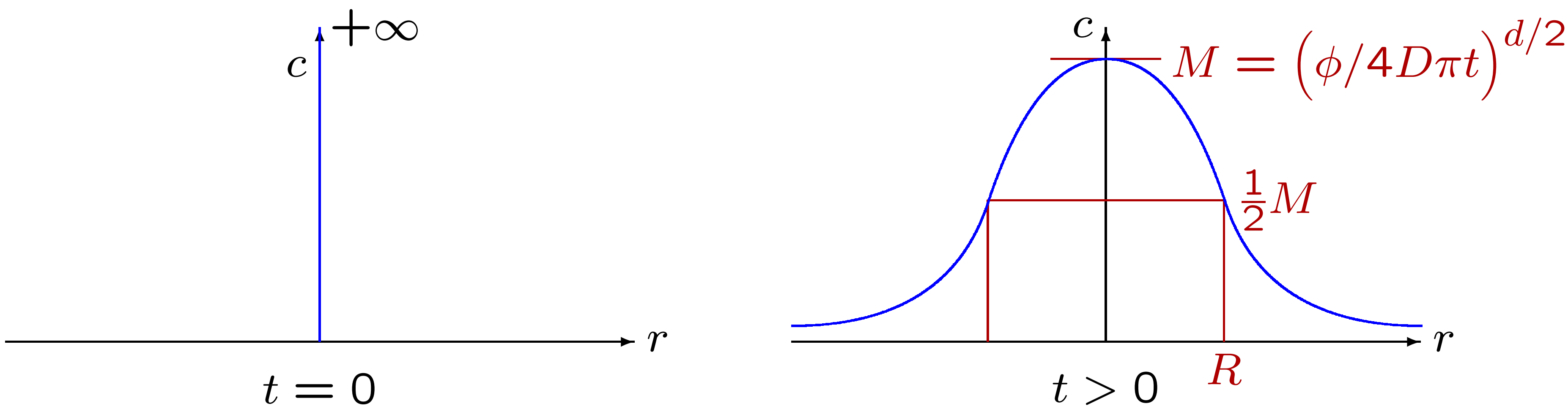
Question: Can you show that c indeed solves the problem?

Meaning of this Fundamental Solution

In spherical coordinates, $r^2 = x^2 + y^2 + z^2$ and

$$\kappa(r,t) = \left(\frac{\phi}{4D\pi t}\right)^{d/2} e^{-\phi r^2/4Dt},$$

which is the evolution of a unit mass at the origin $c_0 = \delta_0$.



- We see infinite speed of propagation, since the concentration is positive everywhere in space for $t > 0$. (Bad!)
- The spreading is $R(t)$:

$$Me^{-\phi R^2/4Dt} = \tfrac{1}{2}M \quad \Longrightarrow \quad R(t) = \sqrt{4\log 2Dt/\phi},$$

so the spreading in time is $\mathcal{O}\left(\sqrt{Dt/\phi}\right)$. This is a characteristic of the Fickian diffusion model. (Good or bad?)

The Green's Function

For general D, $\phi = \phi(x,y,z)$ only, and $\Omega \subset \mathbb{R}^d$, the Green's function for

$$\begin{cases} \phi c_t - \nabla \cdot D\nabla c = q(\mathbf{x},t), & \text{in } \Omega,\ t > 0, \\ c = 0, & \text{on } \partial\Omega,\ t > 0, \\ c(\mathbf{x},0) = c_0(\mathbf{x}), & \text{on } \Omega, \end{cases}$$

is $G(x,y,z,\ X,Y,Z,\ t)$, the response of the system at (x,y,z) to an initial unit mass at (X,Y,Z).

With all space derivatives taken in (x,y,z), G solves

$$\begin{cases} \phi G_t - \nabla \cdot D\nabla G = 0, & \text{in } \Omega,\ t > 0, \\ G = 0, & \text{on } \partial\Omega,\ t > 0, \\ G(x,y,z,\ X,Y,Z,\ 0) = \delta_{X,Y,Z}(x,y,z), & \text{on } \Omega. \end{cases}$$

Then the solution is

$$c(x,y,z,t) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} c_0(X,Y,Z)\, G(x,y,z,\ X,Y,Z,\ t)\, dX\, dY\, dZ$$

$$+ \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_0^t q(X,Y,Z,s)\, G(x,y,z,\ X,Y,Z,\ t-s)\, ds\, dX\, dY\, dZ.$$

Numerical Approximation

Basic Strategy

Treat time and space separately.

- Use finite differences in time for the time derivative. Let

$$0 = t_0 < t_1 < t_2 < \cdots ,$$

  and, for simplicity, take uniform time steps $\Delta t = t_{n+1} - t_n > 0$.
- Use finite differences or finite elements in space for the space derivatives as for the elliptic problem. Let h be the maximal grid spacing.
- Approximate

$$c(x_i, y_j, z_k, t_n) \approx c^n_{i,j,k}.$$

For simplicity, we proceed using only 1 space dimension, a uniform grid, constant ϕ and D, and we solve

$$\begin{cases} \phi c_t - D c_{xx} = q, & 0 < x < \ell,\ t > 0, \\ c(x,0) = c_0(x), & 0 < x < \ell, \end{cases}$$

where we have ignored BC's, since they are handled at each time level as in the elliptic case described before.

Forward Euler

We use forward Euler in time and finite differences in space for simplicity. Then we have

$$\phi \frac{c_i^{n+1} - c_i^n}{\Delta t} - D \frac{c_{i+1}^n - 2c_i^n + c_{i-1}^n}{h^2} = q_i^n = q(x_i, t^n).$$

This is a simple explicit method,

$$c_i^{n+1} = \left(1 - 2\frac{D\Delta t}{\phi h^2}\right) c_i^n + \frac{D\Delta t}{\phi h^2}\left(c_{i+1}^n + c_{i-1}^n\right) + \frac{\Delta t}{\phi} q_i^n,$$

and the error is $\mathcal{O}(\Delta t + h^2)$.

Stability. Errors will grow unless we satisfy a stability constraint. We must require that

$$\frac{D\Delta t}{\phi h^2} \leq \frac{1}{2} \quad \Longleftrightarrow \quad \boxed{\Delta t \leq \frac{\phi h^2}{2D}.}$$

We saw earlier the constraint $\Delta t = \mathcal{O}(h^2)$ was needed to resolve space and time scales.

Remark. Since h is very small, Δt must be incredibly small! In practice, we almost always would need too many time steps to use this method efficiently. We thus consider only implicit methods.

Semidiscrete Backward Euler

It is convenient to discuss discretization in time first, and then discretization in space. An equation approximated in time, but not in space, is said to be semidiscrete.

Backward Euler. We approximate the time derivative as

$$\phi \frac{c^n - c^{n-1}}{\Delta t} - D c^n_{xx} = q^n.$$

Rearranging, we see that

$$\phi c^n - \Delta t D c^n_{xx} = \phi c^{n-1} + \Delta t q^n.$$

To solve, we march along in time, so we have computed c^{n-1} at this stage, and it remains to compute c^n. Note that c^n is the solution to an elliptic equation (with an extra term on the right involving no derivatives).

We can apply any available technique for approximating this elliptic equation, such as finite differences or finite elements.

Fully Discrete Backward Euler

Backward Euler and Vertex Finite Differences.

$$\phi \frac{c_i^n - c_i^{n-1}}{\Delta t} - D \frac{c_{i+1}^n - 2c_i^n + c_{i-1}^n}{h^2} = q_i^n.$$

Backward Euler and Cell Centered Finite Differences.

$$Z_{i+1/2}^n = -D \frac{c_{i+1}^n - c_i^n}{h},$$

$$\phi \frac{c_i^n - c_i^{n-1}}{\Delta t} + \frac{Z_{i+1/2}^n - Z_{i-1/2}^n}{h} = q_i^n.$$

Backward Euler and Finite Elements.

$$c^n(x) = \sum_j \alpha_j^n \varphi_j(x),$$

$$\int_0^\ell \phi \frac{c^n(x) - c^{n-1}(x)}{\Delta t} \varphi_i(x)\, dx + \int_0^\ell D \frac{dc^n(x)}{dx} \frac{d\varphi_i(x)}{dx}\, dx$$

$$= \int_0^\ell q^n(x)\, \varphi_i(x)\, dx.$$

Theorem. These methods reduce to solving a linear system, and they are unconditionally stable and accurate to $\mathcal{O}(\Delta t + h^2)$.

The Theta Method—1

We have the single semidiscrete expression

$$\phi \frac{c^{n+1} - c^n}{\Delta t} - D c_{xx}^{n+\theta} = q^{n+\theta}.$$

- If $\theta = 0$, we have the explicit method Forward Euler.
- If $\theta = 1$, we have the implicit method Backward Euler.

Idea. Interpret θ as a parameter, $0 \le \theta \le 1$, which represents the time

$$t_{n+\theta} = \theta\, t_{n+1} + (1 - \theta)\, t_n$$

at which diffusion and q are evaluated.

We do not have c at this time, but Taylor's theorem gives that

$$\begin{aligned} c(t^n) \quad &= c(t^{n+\theta}) - c'(t^{n+\theta})\, \theta \Delta t \qquad\qquad + \mathcal{O}(\Delta t^2), \\ c(t^{n+1}) &= c(t^{n+\theta}) + c'(t^{n+\theta})\, (1 - \theta) \Delta t + \mathcal{O}(\Delta t^2), \end{aligned}$$

so

$$c^{n+\theta} = \theta c^n + (1 - \theta) c^{n-1} + c'(t^{n+\theta})\, [(1 - \theta)^2 - \theta^2]\, \Delta t + \mathcal{O}(\Delta t^2).$$

This is $\mathcal{O}(\Delta t)$ accurate, unless $[(1 - \theta)^2 - \theta^2] = 0$, i.e., $\theta = 1/2$, which is $\mathcal{O}(\Delta t^2)$ accurate.

The Theta Method—2

The semidiscrete theta method. For $0 \le \theta \le 1$,

$$\phi \frac{c^{n+1} - c^n}{\Delta t} - D\Big[\theta c_{xx}^{n+1} + (1-\theta) c_{xx}^n\Big] = q^{n+\theta}.$$

We can then apply finite differences or finite elements to the space derivatives.

Theorem. The fully discrete theta method has accuracy $\mathcal{O}(\Delta t + h^2)$ for $\theta \ne 1/2$, but acuracy $\mathcal{O}(\Delta t^2 + h^2)$ for $\theta = 1/2$. Moreover, the method is unconditionally stable if $\theta \ge 1/2$, but for $\theta < 1/2$, stability requires

$$\Delta t \le \frac{\phi h^2}{2(1-2\theta)D}.$$

The optimal choice appears to be $\theta = 1/2$, which we call the Crank-Nicolson method.

Caution. Crank-Nicolson is accurate and stable for linear problems, but only critically so, since $\theta = 1/2$ divides $\mathcal{O}(\Delta t^2)$ from $\mathcal{O}(\Delta t)$ accuracy, and stable from unstable. Thus, it is not so effective for nonlinear problems.

Crank-Nicolson and Vertex Finite Differences.

$$\phi\frac{c_i^{n+1}-c_i^n}{\Delta t}-D\left[\theta\frac{c_{i+1}^{n+1}-2c_i^{n+1}+c_{i-1}^{n+1}}{h^2}+(1-\theta)\frac{c_{i+1}^n-2c_i^n+c_{i-1}^n}{h^2}\right]=q_i^{n+\theta}.$$

Crank-Nicolson and Cell Centered Finite Differences.

$$Z_{i+1/2}^{n+1}=-D\frac{c_{i+1}^{n+1}-c_i^{n+1}}{h}\quad\text{and}\quad Z_{i+1/2}^{n}=-D\frac{c_{i+1}^{n}-c_i^{n}}{h},$$

$$\phi\frac{c_i^{n+1}-c_i^n}{\Delta t}+\theta\frac{Z_{i+1/2}^{n+1}-Z_{i-1/2}^{n+1}}{h}+(1-\theta)\frac{Z_{i+1/2}^{n}-Z_{i-1/2}^{n}}{h}=q_i^{n+\theta}.$$

Crank-Nicolson and Finite Elements.

$$c^{n+1}(x)=\sum_j\alpha_j^{n+1}\varphi_j(x)\quad\text{and}\quad c^n(x)=\sum_j\alpha_j^n\varphi_j(x),$$

$$\int_0^\ell\phi\frac{c^{n+1}(x)-c^n(x)}{\Delta t}\,\varphi_i(x)\,dx+\theta\int_0^\ell D\frac{dc^{n+1}(x)}{dx}\,\frac{d\varphi_i(x)}{dx}\,dx$$
$$+(1-\theta)\int_0^\ell D\frac{dc^n(x)}{dx}\,\frac{d\varphi_i(x)}{dx}\,dx=\int_0^\ell q^{n+\theta}(x)\,\varphi_i(x)\,dx.$$

IV. Hyperbolic Partial differential equations (for tracer transport)

The Conservation Law

Recall the general conservation equation

$$\boxed{\xi_t + \nabla \cdot (\xi \mathbf{v}) = q,}$$

where

$C(\mathbf{x}, t)$ is the concentration of a conservative tracer (mass/volume);
$\phi(\mathbf{x}, t)$ is the porosity of the medium, so $c = \xi = \phi C$;
$\mathbf{v}(\mathbf{x}, t)$ is the velocity of the tracer particles (length/time);
$q(\mathbf{x}, t)$ is an external source or sink of fluid (mass/volume/time).

In the absence of sources and sinks, we have the conservation Law for the transport of tracer particles

$$\boxed{c_t + \nabla \cdot (c \mathbf{v}) = 0.}$$

We call this a first order hyperbolic partial differential equation for $c.$, given $\mathbf{v}$. This is a complex equation, so we consider only 1-D in space:

$$\boxed{c_t + (cv)_x = 0.}$$

The Case of Constant Velocity

If v is constant, with an IC, we have

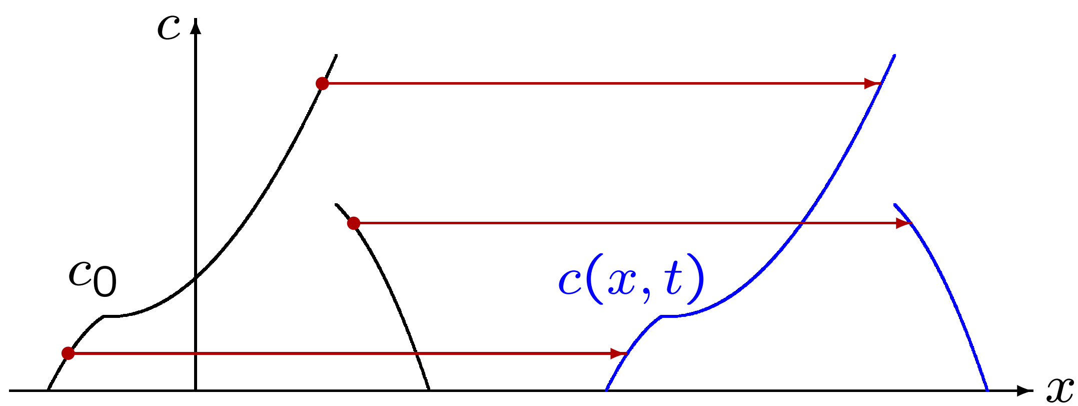
$$\begin{aligned} &c_t + v c_x = 0, \quad -\infty < x < \infty,\ t > 0, \\ &c(x,0) = c_0(x), \end{aligned}$$

which is solved by

$$\boxed{c(x,t) = c_0(x - vt).}$$

Question: Can you show this using the chain rule?

If $v > 0$, we have a wave traveling to the right, of fixed shape.



Particles simply translate to the right with velocity v. We could have a jump in the IC, which propagates as a contact discontinuity.

Inflow Boundary Conditions

On a domain $0 < x < \ell$, we have only one BC. If $v > 0$ is constant, we need to specify c on the inflow side $x = 0$, but not on the outflow side $x = \ell$. That is,

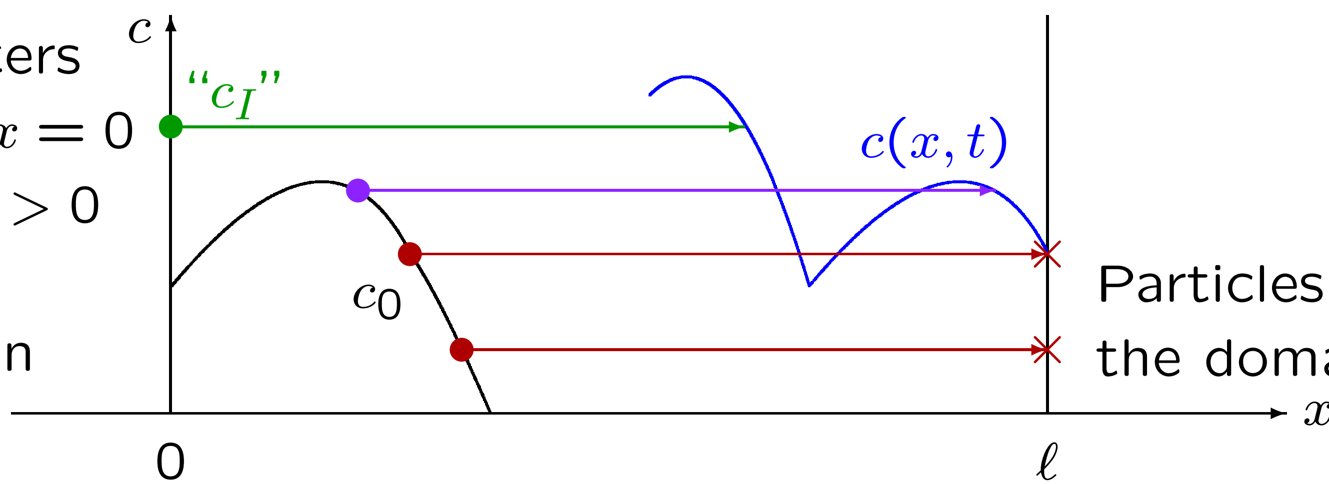
$$\begin{aligned} &c_t + v c_x = 0, \quad 0 < x < \ell,\ t > 0, \\ &c(0,t) = c_I(t), \\ &c(x,0) = c_0(x), \end{aligned}$$

which is solved by

$$c(x,t) = \begin{cases} c_0(x - vt), & x - vt \geq 0, \\ c_I(t - x/v), & x - vt < 0. \end{cases}$$

Question: Can you show this?

Particle enters domain at $x = 0$ and some $t > 0$ and then transports in time.

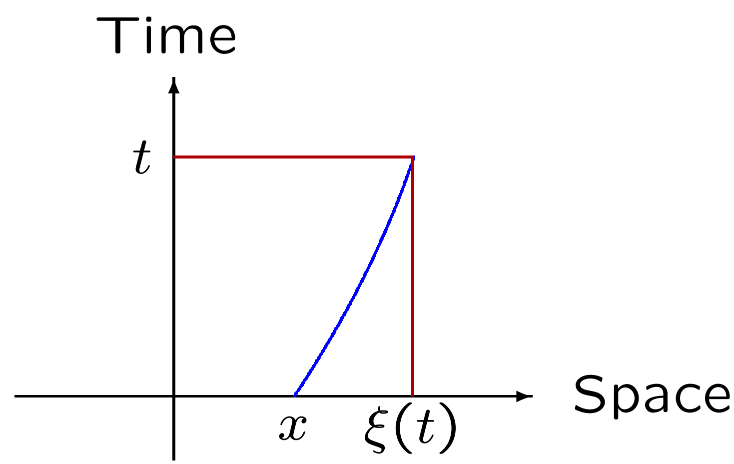


Particles leave the domain.

Characteristics

In a perfect world, tracer particles would simply travel along paths called the characteristics of the equation. Given a starting position x, the path would be $(\xi(t), t)$, where

$$\frac{d\xi}{dt} = v(\xi(t), t), \quad t > 0,$$
$$\xi(0) = x.$$



If there are no sources and sinks (i.e., $\nabla \cdot \mathbf{v} = 0$ or $v_x = 0$ in 1-D), then the concentration is constant along these space-time paths, since

$$\frac{dc(\xi(t), t)}{dt} = c_t + c_x \xi_t = c_t + v c_x = c_t + (vc)_x = 0.$$

If we know where the particle starts, we can simply follow it in time along the characteristics.

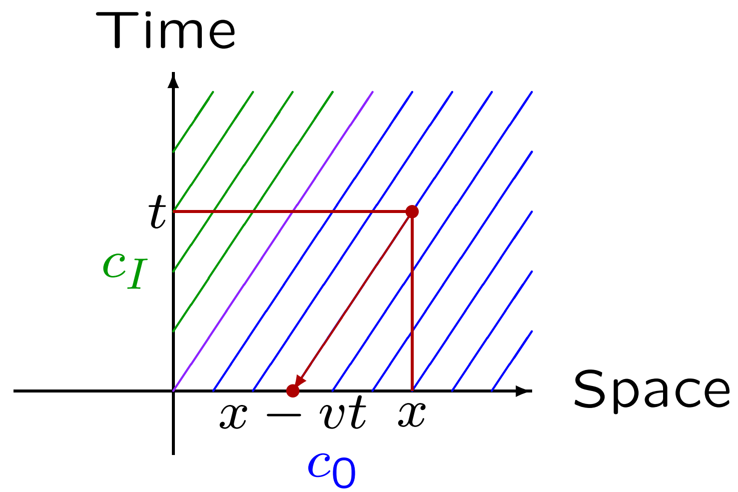
Question: Is this correct? Could anything go wrong?

Characteristics for Constant Velocity

If v is constant, then

$$\begin{cases} \dfrac{d\xi}{dt} = v, & t > 0, \\ \xi(0) = x. \end{cases} \quad \Longrightarrow \quad \xi = x + vt,$$

which are straight lines.



Conclusion. If you know c_0 and c_I, you know the solution for all time. We saw that in fact

$$c(x,t) = \begin{cases} c_0(x - vt), & x - vt \geq 0, \\ c_I(t - x/v), & x - vt < 0. \end{cases}$$

Remark. Similar results hold in 3-D for $\mathbf{v}(x,t)$ (with $\nabla \cdot \mathbf{v} = 0$), though the characteristic ξ may need to be approximated numerically.

The Nonlinear Burgers' Equation

In practice, often v depends on c. For example, we have the Burgers' equation

$$c_t + c\,c_x = 0 \qquad \Longleftrightarrow \qquad c_t + (f(c))_x = 0, \quad \text{where } f(c) = \frac{1}{2}c^2.$$

Note that the velocity $v(c) = c/2$ increases as c increases.

We consider the Riemann Problem

$$c_t + (f(c))_x = 0$$
$$c(x,0) = \begin{cases} c_L, & x < 0, \\ c_R, & x > 0, \end{cases}$$

for which the IC has just two values or states.

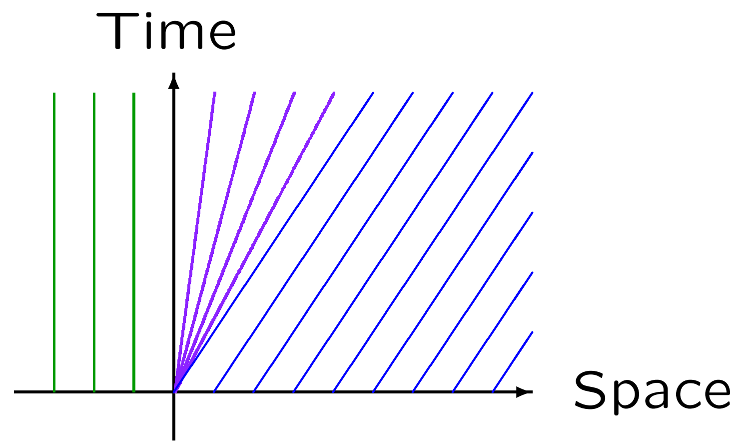
Burgers' Equation. Since $v = c/2$, we have the characteristics

$$\xi(t) = \begin{cases} x + c_L t/2, & x < 0, \\ x + c_R t/2, & x > 0. \end{cases}$$

Rarefactions

Consider $u_L = 0$ and $u_R = 1$. Then the characteristics are

$$\xi(t) = \begin{cases} x, & x < 0, \\ x + t/2, & x > 0. \end{cases}$$

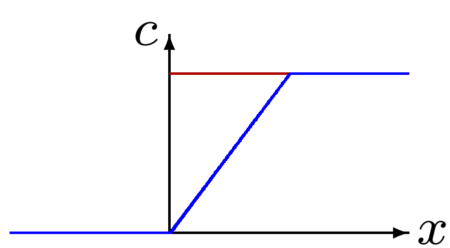


Question: What happens between the two sets of characteristics? Does a vaccuum open up?

The solution will form a rarefaction wave, i.e., a spreading of the solution to smooth out the mass distribution. It has the form

$$c(x,t) = \begin{cases} c_L, & x < f'(c_L)\,t, \\ \gamma(x/t), & f'(c_L)\,t < x < f'(c_R)\,t, \\ c_R, & f'(c_R)\,t < x, \end{cases}$$

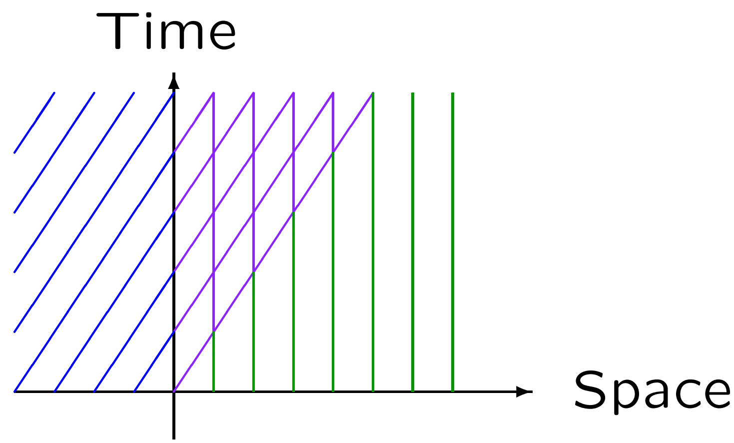
where $f'(\gamma(s)) = s$. For Burgers' equation, $f'(s) = s$, so $\gamma(x/t) = x/t$.



Shocks and the Rankin-Hugoniot Speed

Consider $u_L = 1$ and $u_R = 0$. Then the characteristics are

$$\xi(t) = \begin{cases} x + t/2, & x < 0, \\ x, & x > 0. \end{cases}$$

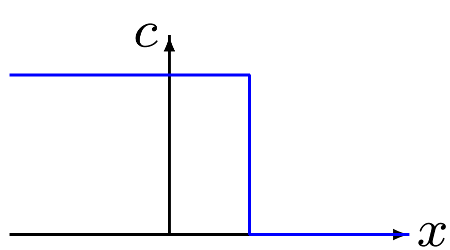


Question: Does mass build up where the two sets of characteristics collide?

The solution develops a shock wave, i.e., a discontinuity to maintain mass conservation. The shock travels at the Rankin-Hugoniot speed σ:

$$\sigma = \frac{f(c_L) - f(c_R)}{c_L - c_R} \quad \text{and} \quad c(x,t) = \begin{cases} c_L, & x < s\,t, \\ c_R, & s\,t < x. \end{cases}$$

For Burgers' equation, $\sigma = 1/2$.



Summary

Conservation laws (without diffusion) exhibit:

- Transport along the flow characteristic curves;
- Smooth spreading or rarefaction waves where characteristics diverge;
- Discontinuities that
  - simply transport with the flow (a contact discontinuity),
  - or form as shocks where characteristics collide.

Remark. If diffusion is present, discontinuities cannot form, but the solution can be nearly discontinuous (i.e., they have steep or sharp fronts).

Changes to the Concentration Variable—1

Burgers' equation is

$$c_t + \left(\tfrac{1}{2}\,c^2\right)_x = 0,$$

Multiply through by $2c$ and set $\xi = c^2$, to obtain that

$$2cc_t + 2\,c\left(\tfrac{1}{2}\,c^2\right)_x = 0 \quad \Longrightarrow \quad \left(c^2\right)_t + \left(\tfrac{2}{3}\,c^3\right)_x = 0$$

$$\Longrightarrow \quad \boxed{\xi_t + \left(\tfrac{2}{3}\,\xi^{3/2}\right)_x = 0.}$$

This is a conservation law for ξ.

Question: Are these two equations essentially the same?

Changes to the Concentration Variable—2

Suppose a shock forms. With what speed does it travel?

$$\sigma_c = \frac{\frac{1}{2}c_L^2 - \frac{1}{2}c_R^2}{c_L - c_R} = \frac{1}{2}(c_L + c_R) \qquad \text{and} \qquad \sigma_\xi = \frac{\frac{2}{3}\xi_L^3 - \frac{2}{3}\xi_R^3}{\xi_L - \xi_R} = \frac{2}{3}(\xi_L^2 + \xi_L\,\xi_R + \xi_R^2) = \frac{2}{3}(c_L^4 + c_L^2\,c_R^2 + c_R^4).$$

We are conserving the wrong quantity, so it travels at the wrong speed!

Theorem. There are infinetly many solutions to a hyperbolic conservation law. The physically relevant solution is the entropy solution, which is

$$c = \lim_{\epsilon \to 0} c_\epsilon \quad \text{where} \quad c_{\epsilon,t} + (f c_\epsilon)_x \underbrace{- \epsilon c_{xx}}_{\text{diffusion}} = 0.$$

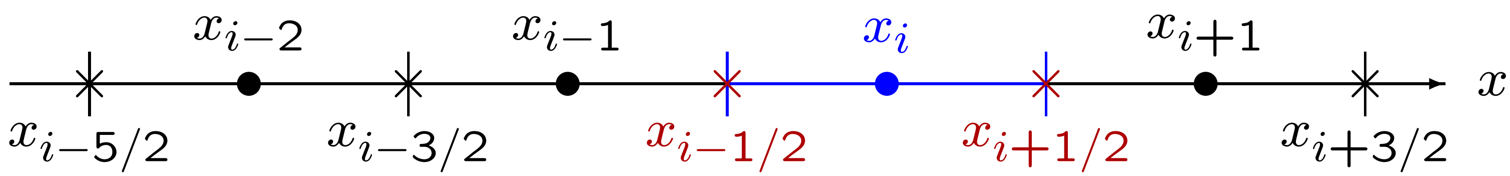
That is, the entropy solution is the one that is stable with respect to random diffusive processes.

Remark. We always have some physical diffusion. However, it may be very small and unresolved by a numerical method. Thus, the numerical method must respect the complexity of the nearly hyperbolic equation.

Numerical Methods

Conservative Methods

We generally use a cell centered grid



A locally conservative method for

$$c_t + (f(c))_x = 0$$

is a method such that

$$\frac{c_i^{n+1} - c_i^n}{\Delta t} + \frac{F_{i+1/2} - F_{i-1/2}}{h} = 0,$$

where the numerical flux $F_{i\pm1/2} \approx f(c)$ at $x_{i\pm1/2}$ needs to be defined.

A simple choice. The following implicit method is unstable!

$$\frac{c_i^{n+1} - c_i^n}{\Delta t} + \frac{f\left(\frac{1}{2}(c_{i+1}^{n+1} + c_i^{n+1})\right) - f\left(\frac{1}{2}(c_i^{n+1} + c_{i-1}^{n+1})\right)}{h} = 0.$$

Question: If $v = f'(c) > 0$, which direction is the fluid going? Across the point $x_{i+1/2}$, what is the usual value of c?

Upstream Weighted Finite Differences

A simple stable and implicit finite difference approximation to

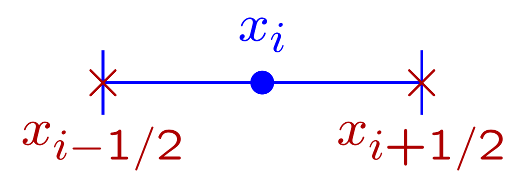
$$c_t + (f(c))_x = c_t + f'(c)c_x = 0$$

is

$$\boxed{\frac{c_i^{n+1} - c_i^n}{\Delta t} + \frac{f\left(c_{\text{up},i+1/2}^{n+1}\right) - f\left(c_{\text{up},i-1/2}^{n+1}\right)}{h} = 0,}$$

wherein the concentration is upstream weighted, meaning that

$$c_{\text{up},i+1/2} = \begin{cases} c_i & \text{if } v_{i+1/2} = f' > 0, \\ c_{i+1} & \text{if } v_{i+1/2} = f' < 0. \end{cases}$$



This is well defined unless f' is particularly nasty.

Theorem. The method is $\mathcal{O}(\Delta t + h)$ accurate.

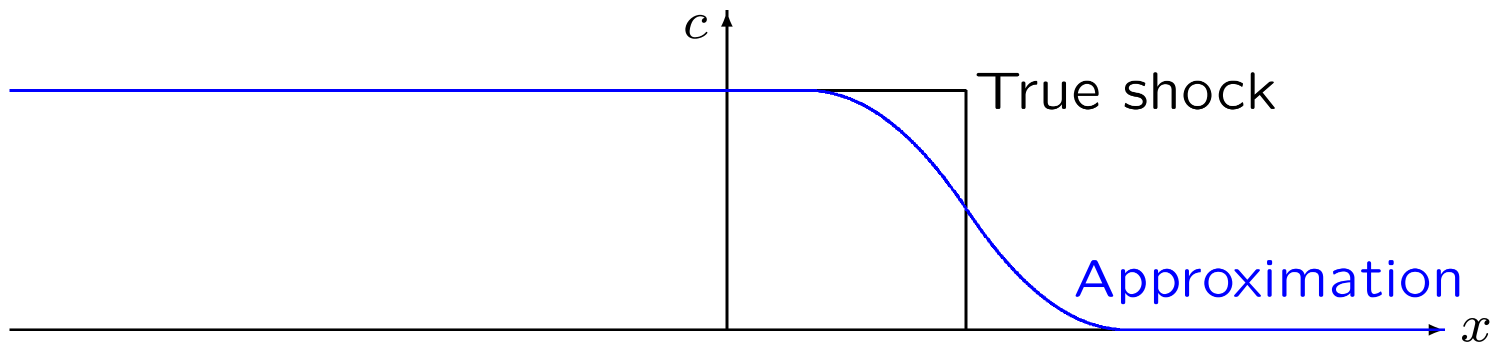
This is not a very accurate method, and we need to use small Δt and h.

Question: Should we simply use explicit methods, then?

Numerical Diffusion

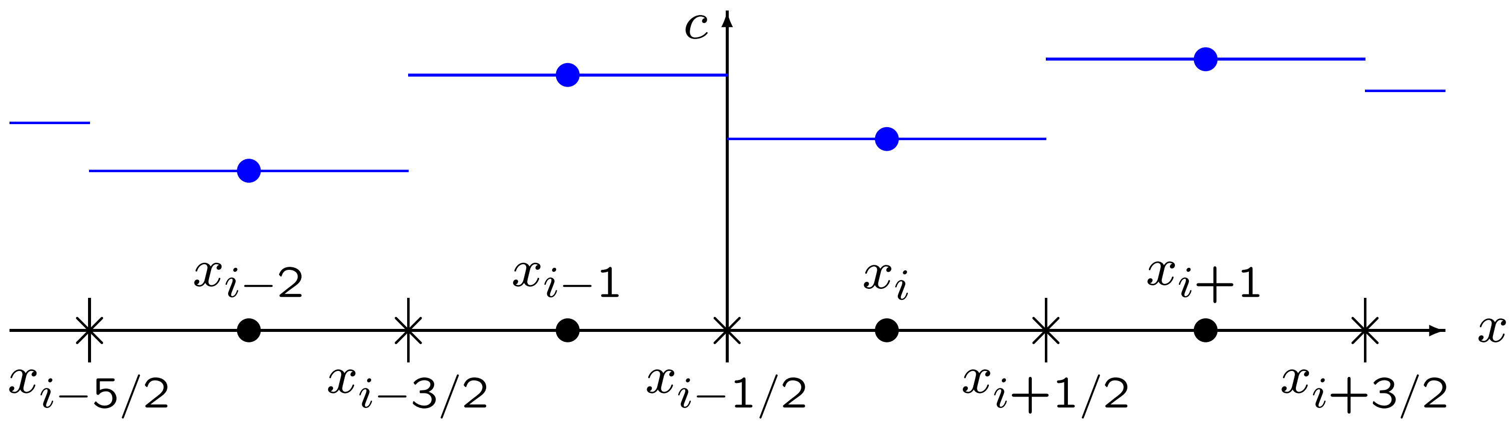
The upstream weighted finite difference method suffers from excessive numerical diffusion. That is, it is stable because it smears sharp features in the solution, so it does not achieve high resolution.

Example. A shock will be approximated like



Godunov's Method

Approximate c as a piecewise constant



Godunov's method is explicit. One advances the solution by solving the Riemann problem for left and right states at each grid line $x_{i+1/2}$.

CFL stability constraint. We do not allow the characteristics from two grid lines to interact, so we must limit the time step size. This limitation is the Courant-Friedrichs-Lewy (CFL) constraint:

$$\Delta t \leq \frac{h}{\max |v|}.$$

Theorem. If the CFL constraint is satisfied, then Godunov's method is well defined, stable, and has error $\mathcal{O}(\Delta t + h)$. Moreover, it has minimal numerical diffusion (it is the best of the locally conservative explicit methods).

A Final Remark

Complex PDE's are combinations of the Simple PDE's

Convection-diffusion equation.

$$\underbrace{(\phi c)_t}_{\text{Accumulation}} \underbrace{+\nabla \cdot (c\mathbf{u})}_{\text{Transport}} \underbrace{-\nabla \cdot D\nabla c)}_{\text{Diffusion}} = q.$$

- This equation is technically parabolic (accumulation plus diffusion).
- Normally $D \approx 0$, so this equation is *almost* hyperbolic (accumulation plus transport).

Richards' equation.

$$\underbrace{\theta(\psi)_t}_{\text{Accumulation}} \underbrace{-\nabla \cdot K(\psi)\nabla\psi)}_{\text{Diffusion}} \underbrace{+K(\psi)_z}_{\text{Gravitational ``transport''}} = q.$$

- This equation is parabolic when $\theta' > 0$ (unsaturated vadose zone).
- This equation is elliptic when $\theta' = 0$ (saturated zone).
- We say that this equation changes type from elliptic to parabolic at the water table (interface between vadose and saturated zones).
- It happens that $K(\psi) = 0$ at the top of the vadose zone, where the soil dries out completely, so we have degenerate diffusion.