

Computational Physics and Astrophysics

Partial Differential Equations

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Spring 2012

Introduction

- A differential equation involving more than one independent variable is called a **partial differential equation** (PDE)
- Many problems in applied science, physics and engineering are modeled mathematically with PDE.
- We will mostly focus on **finite-difference methods** to solve numerically PDEs.
- PDEs are classified as one of three types, with terminology borrowed from the **conic sections**.
- That is, for a 2nd-degree polynomial in x and y

$$Ax^2 + Bxy + Cy^2 + D = 0$$

the graph is a quadratic curve, and when

- $B^2 - 4AC < 0$ the curve is a **ellipse**,
- $B^2 - 4AC = 0$ the curve is a **parabola**
- $B^2 - 4AC > 0$ the curve is a **hyperbola**

Similarly, given

$$A \frac{\partial^2 \psi}{\partial x^2} + B \frac{\partial^2 \psi}{\partial x \partial y} + C \frac{\partial^2 \psi}{\partial y^2} + D \left(x, y, \psi, \frac{\partial \psi}{\partial x}, \frac{\partial \psi}{\partial y} \right) = 0$$

where A , B and C are constants. There are 3 types of equations:

- If $B^2 - 4AC < 0$, the equation is called **elliptic**,
- If $B^2 - 4AC = 0$, the equation is called **parabolic**
- If $B^2 - 4AC > 0$, the equation is called **hyperbolic**

The classification can be extended to PDEs in more than two dimensions.

Two classic examples of **elliptic** PDEs are the **Laplace** and **Poisson** equations:

$$\nabla^2 \phi = 0 \quad \text{and} \quad \nabla^2 \phi = \rho$$

where in 3D

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

$$\nabla^2 = \frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + \frac{1}{r^2 \sin \theta} \frac{\partial^2}{\partial \phi^2} + \frac{\partial^2}{\partial z^2}$$

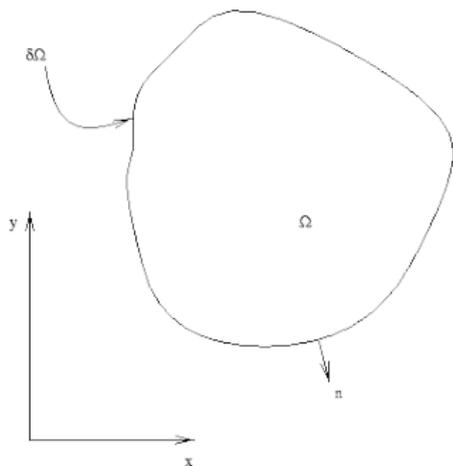
$$\nabla^2 = \frac{1}{r} \frac{\partial}{\partial r} r \frac{\partial}{\partial r} + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2}$$

Boundary-value Problem

$$\nabla^2 \phi = \rho \quad \text{in a domain } \Omega$$

Boundary Conditions

- **Dirichlet:** $\phi = b_1$ on $\partial\Omega$
- **Neumann:** $\frac{\partial\phi}{\partial n} = \hat{n} \cdot \nabla\phi = b_2$ on $\partial\Omega$
- **Robin:** $\frac{\partial\phi}{\partial n} + \alpha\phi = \hat{n} \cdot \nabla\phi = b_3$ on $\partial\Omega$



Classic examples of **hyperbolic** PDEs are:

$$-\frac{1}{c^2} \frac{\partial^2 \psi}{\partial t^2} + \nabla^2 \psi = 0 \quad \text{wave equation}$$

$$\frac{\partial \psi}{\partial t} + \vec{V} \cdot \nabla \psi = 0 \quad \text{advection equation}$$

Classic example of **parabolic** PDEs are

$$\frac{\partial \psi}{\partial t} - \nabla \cdot (D \nabla \psi) = 0 \quad \text{diffusion equation}$$

$$\frac{\partial \psi}{\partial t} - \alpha \nabla^2 \psi = 0 \quad \text{heat equation}$$

Notice from the diffusion equation that

$$\frac{\partial \psi}{\partial t} + \nabla \cdot \vec{J} = 0 \quad \text{continuity equation}$$

$$\vec{J} = -D \nabla \psi \quad \text{Fick's first law}$$

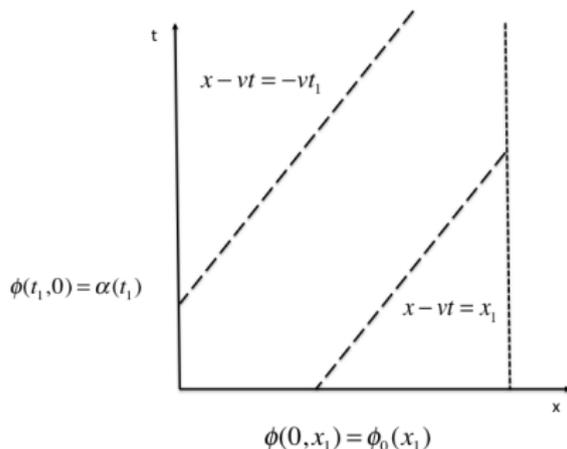
Advection or Convection Equation

- Let's consider the 1D case

$$\partial_t \phi + v \partial_x \phi = 0$$

with $v = \text{const} > 0$, $t \geq 0$ and $x \in [0, 1]$

- Initial data: $\phi(0, x) = \phi_0(x)$
- Boundary conditions:
 $\phi(t, 0) = \alpha(t)$ and
 $\phi(t, 1) = \beta(t)$
- Solutions to this equation have the form
 $\phi(t, x) = \phi(x - vt)$
- Therefore, the solution $\phi(t, x)$ is **constant** along the lines $x - vt = \text{const}$ called **characteristics**



Forward-Time Center-Space (FTCS) Discretization

- Let's consider the following discretization of the differential operators

$$\partial_t \phi_i^n = \frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} + O(\Delta t)$$

$$\partial_x \phi_i^n = \frac{\phi_{i+1}^n - \phi_{i-1}^n}{2 \Delta x} + O(\Delta x^2)$$

where we have used the notation $\phi_i^n \equiv \phi(t^n, x_i)$

- Therefore, the finite difference approximation to $\partial_t \phi + v \partial_x \phi = 0$ is

$$\frac{(\bar{\phi}_i^{n+1} - \bar{\phi}_i^n)}{\Delta t} + v \frac{(\bar{\phi}_{i+1}^n - \bar{\phi}_{i-1}^n)}{2 \Delta x} = 0$$

- Notice that we are making a distinction between the solution $\phi(t, x)$ to the **continuum** equation and $\bar{\phi}_i^n$ the solution to the **discrete** equation.

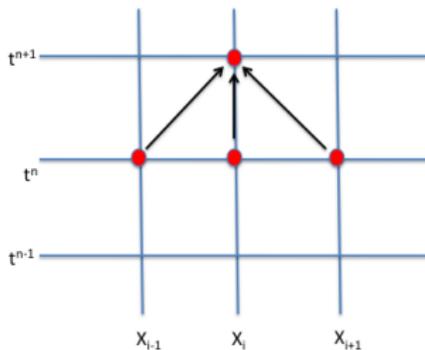
Solving

$$\frac{(\bar{\phi}_i^{n+1} - \bar{\phi}_i^n)}{\Delta t} + v \frac{(\bar{\phi}_{i+1}^n - \bar{\phi}_{i-1}^n)}{2 \Delta x} = 0$$

for $\bar{\phi}_i^{n+1}$, one gets the following relationship to **update** the solution

$$\bar{\phi}_i^{n+1} = \bar{\phi}_i^n - \frac{1}{2} C (\bar{\phi}_{i+1}^n - \bar{\phi}_{i-1}^n)$$

where $C \equiv \Delta t v / \Delta x$



- The tendency for any perturbation in the numerical solution to decay.
- That is, given a discretization scheme, we need to evaluate the degree to which errors introduced at any stage of the computation will grow or decay.
- We are then concerned with the behavior of the solution error

$$\epsilon_i^n = \phi_i^n - \bar{\phi}_i^n$$

- Substitution of $\bar{\phi}_i^n = \phi_i^n - \epsilon_i^n$ into

$$\bar{\phi}_i^{n+1} = \bar{\phi}_i^n - \frac{1}{2}C (\bar{\phi}_{i+1}^n - \bar{\phi}_{i-1}^n)$$

yields

$$\phi_i^{n+1} - \epsilon_i^{n+1} = \phi_i^n - \epsilon_i^n - \frac{1}{2}C (\phi_{i+1}^n - \epsilon_{i+1}^n - \phi_{i-1}^n + \epsilon_{i-1}^n)$$

- Substitute the following Taylor expansions

$$\phi_i^{n+1} = \phi_i^n + \Delta t \partial_t \phi_i^n + O(\Delta t^2)$$

$$\phi_{i\pm 1}^n = \phi_i^n \pm \Delta x \partial_x \phi_i^n + O(\Delta x^2)$$

- Then

$$\begin{aligned} \phi_i^n + \Delta t \partial_t \phi_i^n - \epsilon_i^{n+1} &= \phi_i^n - \epsilon_i^n \\ -\frac{1}{2}C (\phi_i^n + \Delta x \partial_x \phi_i^n - \epsilon_{i+1}^n - \phi_i^n + \Delta x \partial_x \phi_i^n + \epsilon_{i-1}^n) \end{aligned}$$

or

$$\Delta t \partial_t \phi_i^n - \epsilon_i^{n+1} = -\epsilon_i^n - \frac{1}{2}C (2 \Delta x \partial_x \phi_i^n - \epsilon_{i+1}^n + \epsilon_{i-1}^n)$$

$$\epsilon_i^{n+1} = \epsilon_i^n - \frac{1}{2}C (\epsilon_{i+1}^n - \epsilon_{i-1}^n) + \Delta t \partial_t \phi_i^n - C \Delta x \partial_x \phi_i^n$$

$$\epsilon_i^{n+1} = \epsilon_i^n - \frac{1}{2}C (\epsilon_{i+1}^n - \epsilon_{i-1}^n) + \Delta t (\partial_t \phi_i^n - v \partial_x \phi_i^n)$$

$$\epsilon_i^{n+1} = \epsilon_i^n - \frac{1}{2}C (\epsilon_{i+1}^n - \epsilon_{i-1}^n)$$

- That is, the solution error satisfies also the discrete finite differences approximation

$$\epsilon_i^{n+1} = \epsilon_i^n - \frac{1}{2} C (\epsilon_{i+1}^n - \epsilon_{i-1}^n)$$

- **Von Neumann stability analysis:** Assume that the errors satisfy a “separation-of-variables” of the form

$$\epsilon_i^n = \xi^n e^{l x_j} = \xi^n e^{l k \Delta x_j}$$

where $l = \sqrt{-1}$, $k = 2\pi/\lambda$ and ξ is a complex amplitude. The n in ξ^n is understood to be a power.

- The condition of stability is $|\xi| \leq 1$ for all k .

Substitution of $\epsilon_i^n = \xi^n e^{lk \Delta x i}$ into the finite difference equation yields

$$\xi^{n+1} e^{lk \Delta x i} = \xi^n e^{lk \Delta x i} - \frac{1}{2} C \left(\xi^n e^{lk \Delta x (i+1)} - \xi^n e^{lk \Delta x (i-1)} \right)$$

$$\xi^{n+1} = \xi^n - \frac{1}{2} C \left(\xi^n e^{lk \Delta x} - \xi^n e^{-lk \Delta x} \right)$$

$$\xi = 1 - \frac{1}{2} C \left(e^{lk \Delta x} - e^{-lk \Delta x} \right)$$

$$\xi = 1 - \frac{1}{2} C 2l \sin(k \Delta x)$$

$$\xi = 1 - l C \sin(k \Delta x)$$

$$|\xi|^2 = 1 + C^2 \sin^2(k \Delta x)$$

Therefore FTCS discretization applied to the advection equation is **unstable**.

Forward-Time Forward-Space (FTFS) Discretization

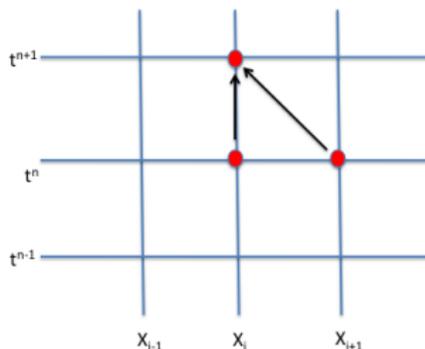
Approximate the advection equation as

$$\frac{(\bar{\phi}_i^{n+1} - \bar{\phi}_i^n)}{\Delta t} + v \frac{(\bar{\phi}_{i+1}^n - \bar{\phi}_i^n)}{\Delta x} = 0$$

thus

$$\bar{\phi}_i^{n+1} = \bar{\phi}_i^n - C (\bar{\phi}_{i+1}^n - \bar{\phi}_i^n)$$

where $C \equiv \Delta t v / \Delta x$



Substitute $\epsilon_j^n = \xi^n e^{jk \Delta x i}$ into

$$\epsilon_i^{n+1} = (1 + C)\epsilon_i^n - C\epsilon_{i+1}^n$$

$$\xi^{n+1} e^{jk \Delta x i} = (1 + C)\xi^n e^{jk \Delta x i} - C\xi^n e^{jk \Delta x (i+1)}$$

$$\xi^{n+1} = (1 + C)\xi^n - C\xi^n e^{jk \Delta x}$$

$$\xi = (1 + C) - C e^{jk \Delta x}$$

$$|\xi|^2 = \left[(1 + C) - C e^{jk \Delta x} \right] \left[(1 + C) - C e^{-jk \Delta x} \right]$$

$$|\xi|^2 = (1 + C)^2 + C^2 - (1 + C)C(e^{jk \Delta x} + e^{-jk \Delta x})$$

$$|\xi|^2 = (1 + C)^2 + C^2 - 2(1 + C)C \cos(k \Delta x)$$

$$|\xi|^2 = 1 + 2(1 + C)C [1 - \cos(k \Delta x)] \geq 1$$

the method is **unstable**

Forward-Time Backward-Space (FTFS) Discretization

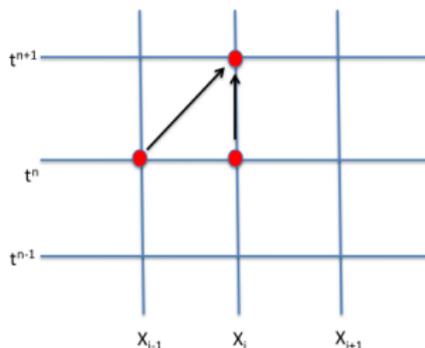
Approximate the advection equation as

$$\frac{(\bar{\phi}_i^{n+1} - \bar{\phi}_i^n)}{\Delta t} + v \frac{(\bar{\phi}_i^n - \bar{\phi}_{i-1}^n)}{\Delta x} = 0$$

thus

$$\bar{\phi}_i^{n+1} = \bar{\phi}_i^n - C (\bar{\phi}_i^n - \bar{\phi}_{i-1}^n)$$

where $C \equiv \Delta t v / \Delta x$



Substitute $\epsilon_i^n = \xi^n e^{lk \Delta x i}$ into

$$\epsilon_i^{n+1} = (1 - C)\epsilon_i^n + C\epsilon_{i-1}^n$$

$$\xi^{n+1} e^{lk \Delta x i} = (1 - C)\xi^n e^{lk \Delta x i} + C\xi^n e^{lk \Delta x (i-1)}$$

$$\xi^{n+1} = (1 - C)\xi^n + C\xi^n e^{-lk \Delta x}$$

$$\xi = (1 - C) + C e^{-lk \Delta x}$$

$$|\xi|^2 = \left[(1 - C) + C e^{-lk \Delta x} \right] \left[(1 - C) + C e^{lk \Delta x} \right]$$

$$|\xi|^2 = (1 - C)^2 + C^2 + (1 - C)C(e^{lk \Delta x} + e^{-lk \Delta x})$$

$$|\xi|^2 = (1 - C)^2 + C^2 + 2(1 - C)C \cos(k \Delta x)$$

$$|\xi|^2 = 1 - 2(1 - C)C [1 - \cos(k \Delta x)]$$

Given

$$|\xi|^2 = 1 - 2(1 - C)C [1 - \cos(k \Delta x)]$$

in order to have $|\xi|^2 \leq 1$

$$-1 \leq 1 - 2(1 - C)C [1 - \cos(k \Delta x)] \leq 1$$

$$-2 \leq -2(1 - C)C [1 - \cos(k \Delta x)] \leq 0$$

$$1 \geq (1 - C)C [1 - \cos(k \Delta x)] \geq 0$$

thus

$$1 - C \geq 0$$

$$C \leq 1$$

$$\frac{v \Delta t}{\Delta x} \leq 1$$

Thus for **stability** we need to pick a time-step

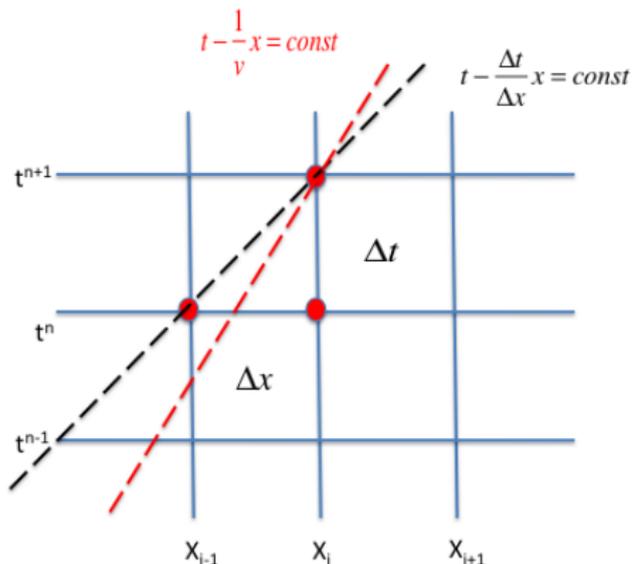
$$\Delta t \leq \frac{\Delta x}{v}$$

The **stability** condition

$$\Delta t \leq \frac{\Delta x}{v}$$

implies that the **numerical** characteristics are contained within the **physical** characteristics since

$$\frac{\Delta t}{\Delta x} \leq \frac{1}{v}$$



How does FTBS prevent the onset of instabilities?

Recall

$$\phi_i^{n+1} = \phi_i^n - C (\phi_i^n - \phi_{i-1}^n)$$

where $C \equiv \Delta t v / \Delta x$. Substitute

$$\phi_i^{n+1} = \phi_i^n + \Delta t \partial_t \phi_i^n + \frac{\Delta t^2}{2} \partial_t^2 \phi_i^n + O(\Delta t^3)$$

$$\phi_{i-1}^n = \phi_i^n - \Delta x \partial_x \phi_i^n + \frac{\Delta x^2}{2} \partial_x^2 \phi_i^n + O(\Delta x^3)$$

then

$$\begin{aligned} \phi_i^n + \Delta t \partial_t \phi_i^n + \frac{\Delta t^2}{2} \partial_t^2 \phi_i^n &= \phi_i^n \\ -C \left[\phi_i^n - \phi_i^n + \Delta x \partial_x \phi_i^n - \frac{\Delta x^2}{2} \partial_x^2 \phi_i^n \right] & \end{aligned}$$

Then

$$\Delta t \partial_t \phi + \frac{\Delta t^2}{2} \partial_t^2 \phi = -v \frac{\Delta t}{\Delta x} \left[\Delta x \partial_x \phi - \frac{\Delta x^2}{2} \partial_x^2 \phi \right]$$

$$\partial_t \phi + \frac{\Delta t}{2} \partial_t^2 \phi = -v \left[\partial_x \phi - \frac{\Delta x}{2} \partial_x^2 \phi \right]$$

$$\partial_t \phi + v \partial_x \phi + \frac{\Delta t}{2} \partial_t^2 \phi - v \frac{\Delta x}{2} \partial_x^2 \phi = 0$$

but from $\partial_t \phi = -v \partial_x \phi$ we have that

$$\partial_t^2 \phi = -v \partial_t \partial_x \phi = -v \partial_x \partial_t \phi = v^2 \partial_x^2 \phi$$

thus

$$\partial_t \phi + v \partial_x \phi + v^2 \frac{\Delta t}{2} \partial_x^2 \phi - v \frac{\Delta x}{2} \partial_x^2 \phi = 0$$

$$\partial_t \phi + v \partial_x \phi + \left(v^2 \frac{\Delta t}{2} - v \frac{\Delta x}{2} \right) \partial_x^2 \phi = 0$$

$$\partial_t \phi + v \partial_x \phi + \left(v^2 \frac{\Delta t}{2} - v \frac{\Delta x}{2} \right) \partial_x^2 \phi = 0$$

$$\partial_t \phi + v \partial_x \phi - v \frac{\Delta x}{2} \left(1 - v \frac{\Delta t}{\Delta x} \right) \partial_x^2 \phi = 0$$

$$\partial_t \phi + v \partial_x \phi - v \frac{\Delta x}{2} (1 - C) \partial_x^2 \phi = 0$$

This equation has the form

$$\partial_t \phi + v \partial_x \phi - \alpha \partial_x^2 \phi = 0$$

advection-diffusion equation with

$$\alpha \equiv v \frac{\Delta x}{2} (1 - C)$$

Recall that for stability $C \leq 1$, thus $\alpha \geq 0$.

Given

$$\phi(t, x) = \phi_0 e^{-pt} e^{-ik(x-qt)}$$

Substitution into

$$\partial_t \phi + v \partial_x \phi = 0 \Rightarrow p = 0 \quad q = v$$

$$\partial_t \phi + v \partial_x \phi - \alpha \partial_x^2 \phi = 0 \Rightarrow p = \alpha k^2 \quad q = v \quad \text{dissipation}$$

$$\partial_t \phi + v \partial_x \phi - \beta \partial_x^3 \phi = 0 \Rightarrow p = 0 \quad q = v - \beta k^2 \quad \text{dispersion}$$

- That is, the FTBS discretization introduces **artificial numerical dissipation** to prevent the growth of instabilities.
- Notice that the dissipation coefficient $\alpha \propto \Delta t$.
- Therefore, in the continuum limit $\lim_{\Delta x \rightarrow 0} \alpha = 0$

Method of Lines

- The **method of lines** (MOL) is a numerical technique for solving PDEs by discretizing all the spatial derivatives.
- The net effect is translating the problem into an initial-value-problem with only **one independent variable**, time.
- The resulting system of ODEs (semi-discrete problem) is solved using sophisticated general purpose methods and software that have been developed for numerically integrating ODEs.

As an example, let's consider the advection equation

$$\partial_t \phi = -v \partial_x \phi$$

with $t \leq 0$, $v > 0$, and $x \in [0, 1]$. The initial data is $\phi(t = 0, x) = f(x)$ and the boundary condition $\phi(t, x = 0) = g(t)$.

- We first discretize the spatial derivative $\partial_x \phi$

$$\partial_x \phi|_i = \frac{\phi_{i+1} - \phi_{i-1}}{2 \Delta x}$$

- Thus, the semi-discrete problem is

$$\frac{d\phi_i}{dt} = -v \frac{(\phi_{i+1} - \phi_{i-1})}{2 \Delta x}$$

- Notice that we now have a coupled system of ODEs of the form

$$\frac{d\phi_i}{dt} = \rho(t, \phi_j)$$

for which we can apply the methods we discussed before, in particular Runge-Kutta methods.

- Given that we are using **center-space** discretization, applying an Euler step (i.e. forward-time) will be unstable.

Burger's Equation

- Recall the advection equation $\partial_t \phi + u \partial_x \phi = 0$ in which the quantity ϕ is **advected or convected** with a velocity u .
- Consider instead $\partial_t u + u \partial_x u = 0$. That is, the velocity at which the quantity is advected depends on the quantity itself.
- This equation is called the **inviscid Burger's equation**.
- This equation is widely used as a model to investigate **non-linearities** in fluid dynamics traffic control, etc..
- The general form of the Burger's equation is

$$\partial_t u + u \partial_x u = \nu \partial^2 u$$

with ν a **viscosity** coefficient.

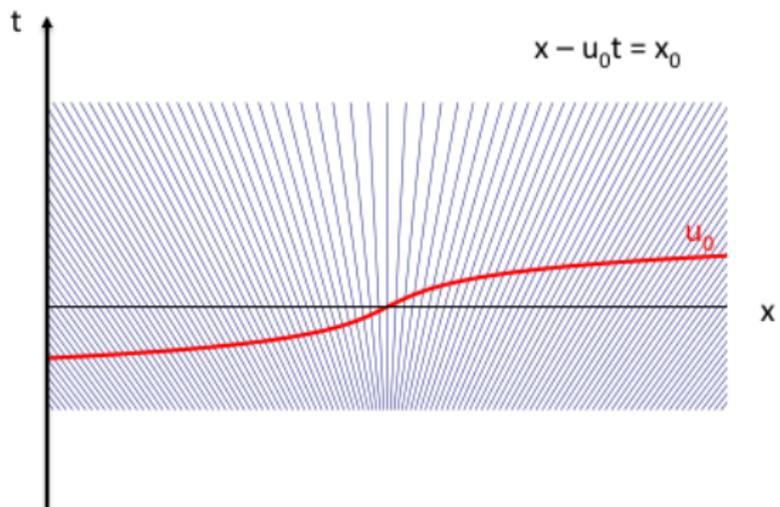
- Consider the inviscid Burger's equation $\partial_t u + u \partial_x u = 0$ with initial data $u(t = 0, x) = u_0(x)$
- **Method of Characteristics:** Find the curves $x(t)$ tangent to the vector $\partial_t + u \partial_x$, such that $u(t, x(t))$ is constant.
- That is,

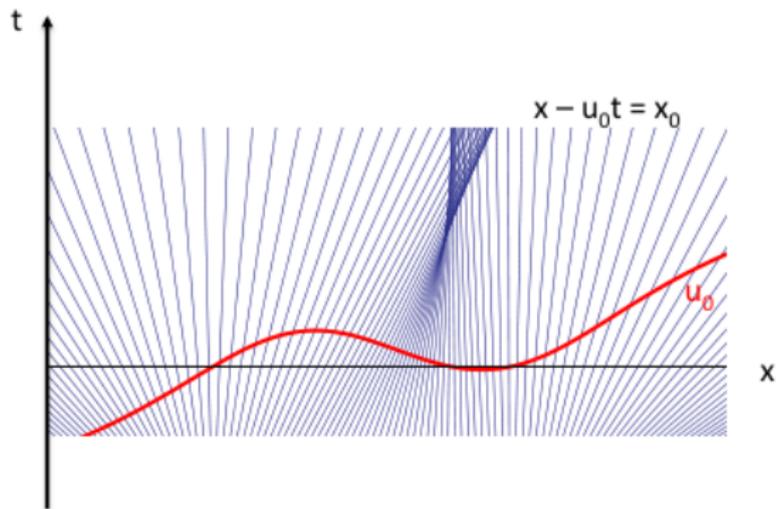
$$\begin{aligned} \frac{dx(t)}{dt} &= u(t, x(t)) \\ \frac{du(t, x(t))}{dt} &= \frac{\partial u}{\partial t} + \frac{dx}{dt} \frac{\partial u}{\partial x} \\ &= \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = 0 \end{aligned}$$

- The solutions are

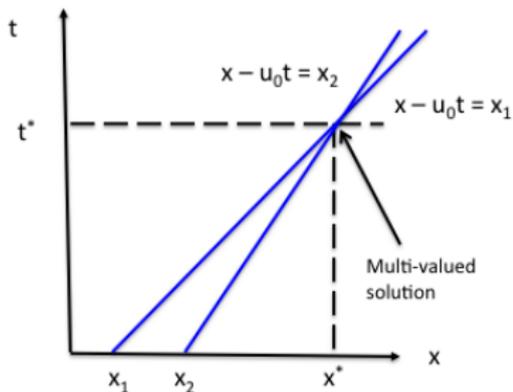
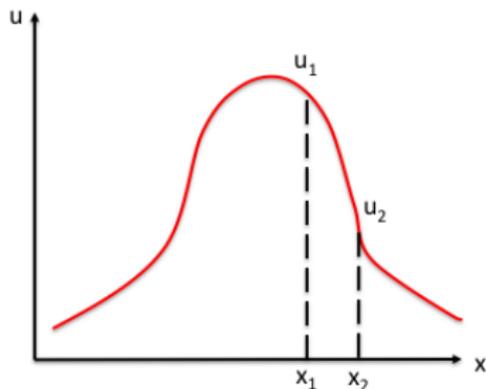
$$\begin{aligned} u(t, x(t)) &= u(0, x(0)) = u_0(x_0) \\ x(t) &= x_0 + t u(0, x(0)) = x_0 + t u_0(x_0) \end{aligned}$$

- Therefore, the solution to the Burger's equation reads
 $u(t, x) = u_0(x - t u_0(x_0))$
- Thus, the solution is constant along the **characteristics**
 $x_0 = x - t u_0(x_0)$.
- The characteristics are straight lines with slope $1/u_0(x_0)$ in the $t - x$ plain.
- For each characteristic, the value of the slope is fixed by the initial data $u_0(x)$ at $x = x_0$

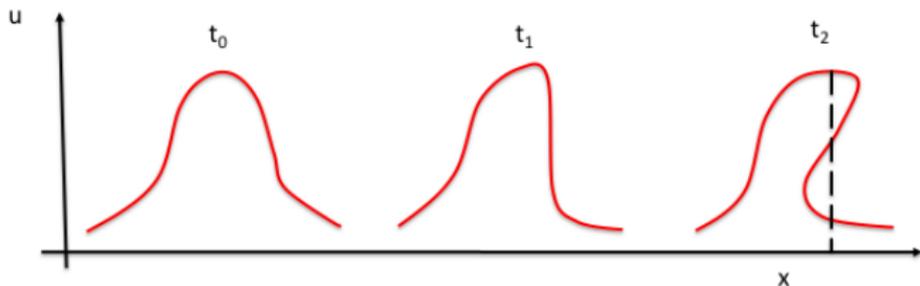




Consider initial data of the form



The pulse evolves as



Notice that the larger the value of u the more advected that portion of the solutions gets.

Let $S \equiv \partial_x u$, then

$$\begin{aligned}\frac{dS}{dt} &= \partial_t S + \frac{dx}{dt} \partial_x S = \partial_t S + u \partial_x S \\ &= \partial_t \partial_x u + u \partial_x^2 u = \partial_x (\partial_t u + u \partial_x u) - (\partial_x u)^2 \\ &= -S^2\end{aligned}$$

The solution to this equation is

$$S = \frac{S_0}{t S_0 + 1} \quad \text{or} \quad \partial_x u = \frac{\partial_x u_0}{t \partial_x u_0 + 1}$$

Therefore, as $t \rightarrow -1/\partial_x u_0$ the slope of the solution **diverges**, that is, $\partial_x u \rightarrow \infty$. In other words, the solution develops a **shock** discontinuity.

In the case of the general viscous Burger's equation ($\nu \neq 0$), the shock profile gets smoothed out due to the dissipation.

Shock Boundary

- Consider initial data such that $\partial_x^2 u_0(x) = 0$ everywhere and $\partial_x u_0(x) = \text{const} < 0$ if $x \in [x_1, x_2]$.
- Recall that the characteristics are given by the straight lines $x = \bar{x} + u_0(\bar{x}) t$ where \bar{x} is the value of x at $t = 0$.
- Recall also that the shock will develop when $t^* = -1/\partial_x u_0(\bar{x})$.
- Therefore, the location where the shock develops is $x = \bar{x} + u_0(\bar{x}) t^*$
- Consider to points x_a, x_b such that $x_1 \leq x_a, x_b \leq x_2$
- Then

$$\begin{aligned}x_a + u_0(x_a) t^* &= x_b + (x_a - x_b) + [u_0(x_b) + (x_a - x_b) \partial_x u_0(x_b)] t^* \\&= x_b + (x_a - x_b) + u_0(x_b) t^* - (x_a - x_b) \frac{\partial_x u_0(x_b)}{\partial_x u_0(x_b)} \\&= x_b + u_0(x_b) t^*\end{aligned}$$

- Therefore, all the characteristics starting within the interval $[x_1, x_2]$ cross at the same point given by $x = \bar{x} - u_0(\bar{x})/\partial_x u_0(\bar{x})$

- Location of the shock boundary point $x = \bar{x} - u_0(\bar{x})/\partial_x u_0(\bar{x})$
- Notice that the characteristics have different slopes but the same shock developing time.
- Thus, the shape of the boundary shock depends on the “shape” of the initial data.

