Computational Physics

Partial Differential Equations

Lectures based on course notes by Pablo Laguna and Kostas Kokkotas

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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 $\partial_x \phi$

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

- 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.

Method of Lines

original advection equation $\partial_t \phi + v \partial_x \phi = 0$

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

MOL idea : replace spatial (boundary value) derivatives with algebraic approximations (FD)

$$\partial_x \phi = \frac{\phi^n_{i+1} - \phi^n_{i-1}}{2 \Delta x}$$

$$\approx \frac{\phi^n_i - \phi^n_{i-1}}{\Delta x}$$

NOW THERE IS ONLY ONE INDEPENDENT VARIABLE t

$$\frac{d\phi}{dt} = -v \left(\frac{\phi^n_i - \phi^n_{i-1}}{\Delta x} \right)$$

$\therefore$ ODE approximates our original PDE

WHY? Characteristics

$\phi(t-x)$

curves tangent to $\partial_t + v\partial_x$, $\phi(t,x)$ constant

$$\frac{d\phi}{dt} = \frac{\partial \phi}{\partial t} + \frac{dx}{dt} \frac{\partial \phi}{\partial x} = 0$$

Value of MOL?

Use RK4 to update $\frac{d\phi}{dt}$ + whatever we need for $\partial_x \phi$

↑

i.e. upwind ...

Psuedo Code

```
Set up parameters and grid
Set up initial data $\phi(t=0, x)$
LOOP OVER TIME
    LOOP OVER SPACE
        compute rhs
        apply boundary conditions
        update $u^{new}$ (euler, RK...)
        $u_i^{n+1} = u_i^n + \Delta t (rhs_i^n)$
            or
        k1 =  \
        k2 =   } all depend on rhs
        k3 =   }
        k4 =  /
        $u_i^{n+1} = u_i^n + (k1 + 2k2 + 2k3 + k4)/6$
    END
END
```

Euler $y' = f(x,y)$ $\qquad \frac{dy}{dx} = f(x,y)$; $\frac{d\phi}{dt} = f(t,\phi)$

$$y_{n+1} = y_n + f(x_n, y_n)h$$

RK2

$$k_1 = hf(x_n, y_n)$$
$$k_2 = hf(x_n + \frac{h}{2}, y_n + \frac{k_1}{2})$$
$$y_{n+1} = y_n + k_2 + O(h^3)$$

RK3

$$k_1 = hf(x_n, y_n)$$
$$k_2 = hf(x_n + \frac{h}{2}, y_n + \frac{k_1}{2})$$
$$k_3 = hf(x_n + \frac{h}{2}, y_n + \frac{k_2}{2})$$
$$k_4 = hf(x_n + h, y_n + k_3)$$
$$y_{n+1} = y_n + \frac{k_1}{6} + \frac{k_2}{3} + \frac{k_2}{3} + \frac{k_4}{6} + O(h^5)$$

$$\frac{d\phi}{dt} = -v\,\frac{\phi_i^n - \phi_{i-1}^n}{\Delta x}$$
$$= rhs(t, \phi)$$

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.

Burgers inviscid

$$\partial_t u + u\,\partial_x u = 0$$

B.C. $\frac{du}{dt} = 0$

$$u(0,x) = e^{-(x-x_0)^2/2\sigma^2}$$

$$\partial_t u = -u\,\partial_x u$$
$$= \text{adv}$$

$\frac{du}{dt} = \text{adv}(u,t)$ once I've specified FDA for $\partial_x u$

backward/upwind

$$\text{adv} = -u(i)\left[\frac{u(i)-u(i-1)}{\Delta x}\right]$$

Recall → FTBS (PDE_stability.pdf)

$$c = \frac{\Delta t\, u_i^n}{\Delta x}$$

$$u_i^{n+1} = u_i^n - c\,(u_i^n - u_{i-1}^n)$$

substitute $u_i^{n+1} = u_i^n + \Delta t\,\partial_t u_i^n + \frac{\Delta t^2}{2}\partial_t^2 u_i^n + \cdots$

$u_{i-1}^n = u_i^n - \Delta x\,\partial_x u_i^n + \frac{\Delta x^2}{2}\partial_x^2 u_i^n + \cdots$

$$u_i^n + \Delta t\,\partial_t u_i^n + \frac{\Delta t^2}{2}\partial_t^2 u_i^n = u_i^n - c\left[u_i^n - u_i^n + \Delta x\,\partial_x u_i^n - \frac{\Delta x^2}{2}\partial_x^2 u_i^n\right]$$

$$\Delta t\,\partial_t u_i^n + \frac{\Delta t^2}{2}\partial_t^2 u = -c\left[\Delta x\,\partial_x u - \frac{\Delta x^2}{2}\partial_x^2 u\right]$$

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

$$\underbrace{\partial_t u + u\,\partial_x u}_{=0} + \frac{\Delta t}{2}\partial_t^2 u - u\,\frac{\Delta x}{2}\partial_x^2 u = 0$$

$$\partial_t^2 u = -u\,\partial_t\partial_x u = -u\,\partial_x\partial_t u = u^2\partial_x^2 u$$

$$\therefore\ \partial_t u + u\,\partial_x \phi - (1-\alpha\partial_x^2 u = 0$$

$\longrightarrow$ diffusion acts like viscosity

$$\alpha = u\,\frac{\Delta x}{2}\left(1 - u\,\frac{\Delta t}{\Delta x}\right)$$

Looks like $\partial_t u + u \partial_x u = \underbrace{\nu \partial^2 u}_{\text{viscosity term}}$

you will find that $\partial_t u + v \partial_x u = 0$ requires UPWIND

but

$\nu \partial^2 u$ does not!

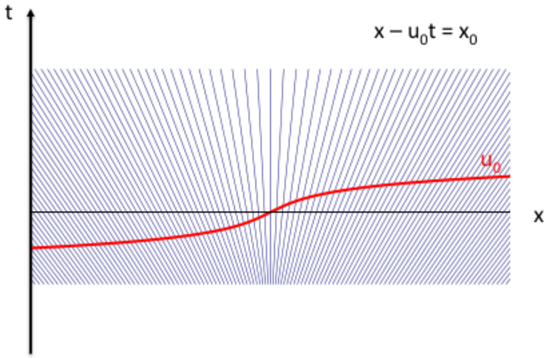
- Consider the inviscid Burger's equation $\partial_t u + u\,\partial_x u = 0$ with initial data $u(t=0,x) = u_0(x)$
- Method of Characteristics: Find the curves $x(t)$ tangent to the vector $\partial_t + u\,\partial_x$, such that $u(t,x(t))$ is constant.
- That is,

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

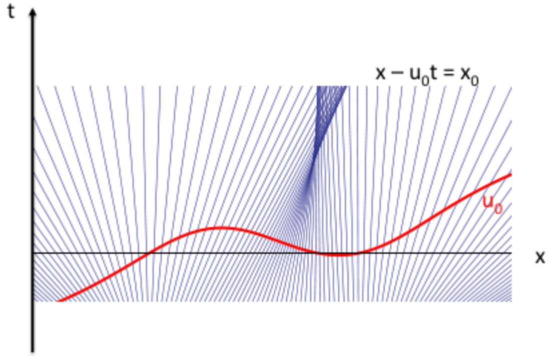
- The solutions are

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

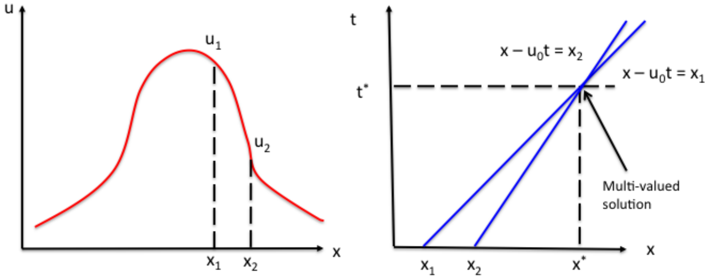
- Therefore, the solution to the Burger's equation reads $u(t,x) = u_0(x - t\, u_0(x_0))$
- Thus, the solution is constant along the characteristics $x_0 = x - t\, u_0(x_0)$.
- The characteristics are straight lines with slope $1/u_0(x_0)$ in the $t - x$ plain.
- For each characteristic, the value of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



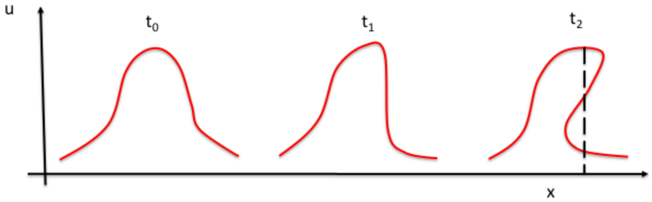
t
$x - u_0 t = x_0$
u_0
x


t
$x - u_0 t = x_0$
u_0
x

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.

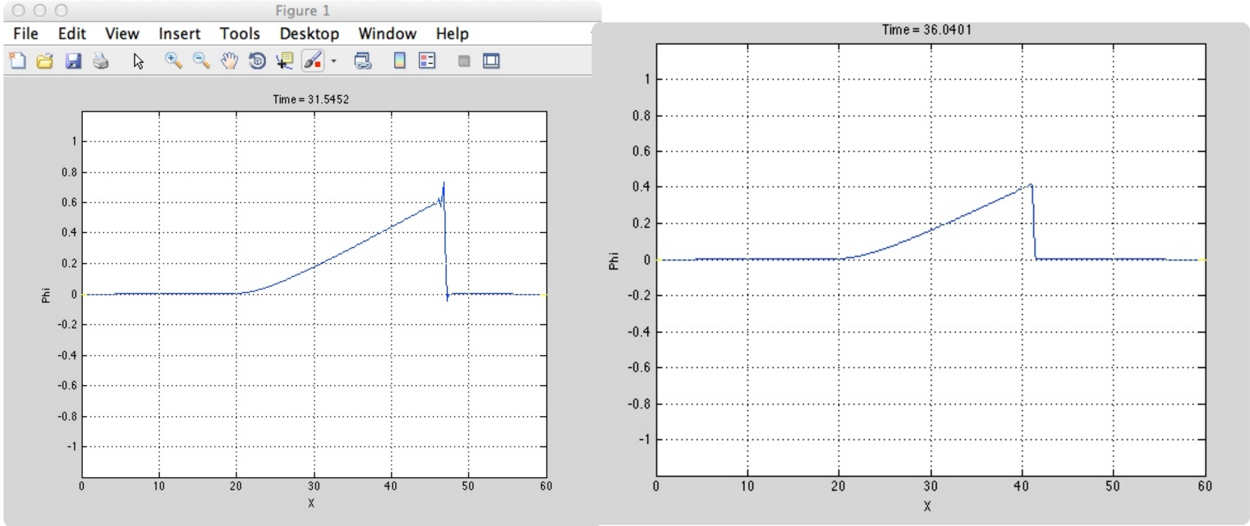
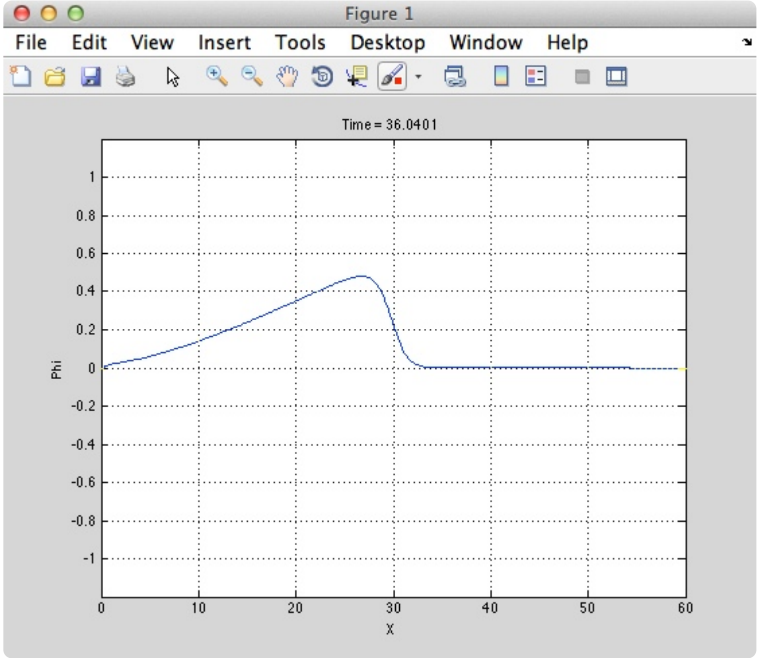


Figure 1
File Edit View Insert Tools Desktop Window Help
Time = 31.5452
Phi
X
1
0.8
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
-1
0
10
20
30
40
50
60
Time = 36.0401
Phi
X
1
0.8
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
-1
0
10
20
30
40
50
60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-0.8
-1
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10
20
30
40
50
60

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 $t \to -1/\partial_x u_0$ the slope of the solution diverges, that is, $\partial_x u \to \infty$. 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.