

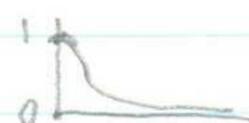
erf solution ...  $\infty$  propagation speed

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Important remark:

exact solution of diffusion problem with  $u_{init} = 0$ ,  $u_0 = 1$  is

$$u(x,t) = 1 - \operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right) \geq 0$$



So we start with  $u \equiv 0$  at  $t=0$ , and we raise bry value to  $u=1$ .

Instantaneously, for any  $t \neq 0$  we get  $u(x,t) \neq 0$  everywhere!!!

We say the diffusion equ propagates signals with infinite speed!

This is a fundamental property of solutions of parabolic PDEs, in sharp contrast to hyperbolic PDEs which propagate signals with finite speed.

Also note that the initial discontinuity (at  $x=0$ ) disappears instantly,

$$u(x,t) \in C^\infty \text{ for } t > 0.$$

Thus diffusion equ is infinitely smoothing! information is lost and cannot be recovered.

As a result, the backward (in time) <sup>diffusion</sup> problem is ill-posed, the past cannot be recovered! only the future can be determined

again in sharp contrast with hyperbolic equations.

The infinite propagation speed is clearly unphysical, so why is the heat equ still a good, enormously successful model ??? for 200 years

The unphysical behavior is more "theoretical" than "practical":

erf increases to 1 extremely rapidly:  $\operatorname{erf}(6) \approx 1 - 2 \cdot 10^{-17}$  !!!

so  $u = \operatorname{erfc}$  is detectably  $> 0$  only for  $x$  very close to 0,

(say  $x < 10\sqrt{Dt}$ ) the rest of the region is essentially zero

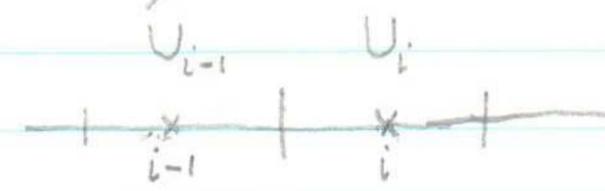
as far as any measurement can detect, in perfect agreement with experience!

$$\left. \begin{array}{l} \operatorname{erfc}(5) \approx 10^{-12} \\ \operatorname{erfc}(6) \approx 2 \cdot 10^{-17} \\ \operatorname{erfc}(7) \approx 4 \cdot 10^{-22} \\ \operatorname{erfc}(10) \approx 2 \cdot 10^{-42} \end{array} \right\}$$

## Explicit scheme - CFL condition for diffusion

Diffusion:  $F = -D u_x$  (Fick's Law, Fourier Law)

Approximation:  $F \approx F_{i-\frac{1}{2}} = -D_{i-\frac{1}{2}} \frac{U_i - U_{i-1}}{x_i - x_{i-1}}$



$= -D \frac{U_i - U_{i-1}}{\Delta x}$  for uniform mesh, const.  $D$   
 $i = 2:M$  (internal fluxes)

This is a major approximation, for expediency, simplicity:

we interpret mean values  $U_i$  as nodal values (at  $x_i$ )

Explicit FV scheme for  $u_t + F_x = 0$ :

$$U_i^{n+1} = U_i^n + \frac{\Delta t}{\Delta x} \left[ F_{i-\frac{1}{2}}^n - F_{i+\frac{1}{2}}^n \right] \quad \begin{array}{l} i=1:M \\ n=1:N_{\max} \end{array}$$

This is the simplest, most physical, and most accurate  $1^{\text{st}}$  order in time  
 $2^{\text{nd}}$  order in space  
 (discretization error =  $O(\Delta t + \Delta x^2)$ )

The penalty for such simplicity is that we must restrict  $\Delta t$  for stability.

Stability condition: plug in  $F_{i-\frac{1}{2}}$  to get updating formula for  $U_i$ :

$$U_i^{n+1} = U_i^n + \frac{D \Delta t}{\Delta x^2} \left[ U_{i-1}^n - 2U_i^n + U_{i+1}^n \right]$$

centered finite difference  $\approx U_{xx}$ ,  $2^{\text{nd}}$  order in  $\Delta x$

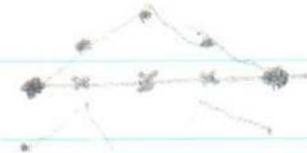
$$\Rightarrow U_i^{n+1} = \left[ 1 - 2 \frac{D \Delta t}{\Delta x^2} \right] U_i^n + \frac{D \Delta t}{\Delta x^2} \left[ U_{i-1}^n + U_{i+1}^n \right]$$

Set  $\mu = \frac{D \Delta t}{\Delta x^2}$  = CFL number, dimensionless (Courant-Friedrichs-Lewy)  $\sim 1927?$

$$\Rightarrow U_i^{n+1} = (1 - 2\mu) U_i^n + \mu U_{i-1}^n + \mu U_{i+1}^n$$

Choose  $\Delta x, \Delta t$  so that, say,  $\mu = 5$ :  $U_i^{n+1} = -9U_i^n + 5U_{i-1}^n + 5U_{i+1}^n$

	$i=0$	$i=1$	$i=2$	$i=3$	$i=4$
$n=0$	0	1	2	1	0
$n=1$	0	$-9+5 \cdot 2 = +1$	$-9 \cdot 2 + 5 \cdot 2 = -8$	$-9+10 = +1$	0
$n=2$	0	$-9-40 = -49$	$+72+10 = +82$	$= -49$	0
$n=3$	0	+851	-1220	+851	0



Clearly nonsense! why?

## CFL condition

Trouble arose

because  $1 - 2\mu < 0$  can produce negative values from positive ones,  
so can produce smaller (and larger) values than bry or initial values.

This violates the Maximum Principle, a fundamental property of heat equ:

The smallest and largest values of  $u(x,t)$   
must occur on the boundary or earlier (initially).

To prevent it, should respect the

Positive Coefficient Rule: in the update formula  $U_i^{n+1} = \dots$ ,  
all coefficients must be <sup>non-negative</sup> positive.

So, we must demand  $1 - 2\mu \geq 0$  i.e.  $\mu \leq \frac{1}{2}$ ; this is the famous

Courant-Friedrichs-Lewy (CFL) condition:  $0 < \mu = \frac{D \Delta t}{\Delta x^2} \leq \frac{1}{2}$

so must restrict the timestep:  $\Delta t \leq \frac{\Delta x^2}{2D} =: \Delta t_{\text{expl}}$

For safety against roundoff:  $\Delta t \leq \Delta t_{\text{expl}}$

or, better, choose  $\Delta t = \text{factor} \cdot \Delta t_{\text{expl}}$  and play with factor

0.99 or 0.95 or 0.90 ...

or 1 or 1.01 or 1.1 ...

## Derivation of Conservation law (balance)

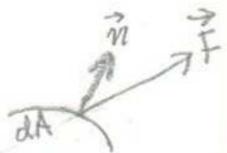
Consider a conserved quantity  $u(\vec{x}, t)$  in a fixed volume  $V$  in a region  $\Omega$  of fluid

basic balance (conservation): In any volume  $V$  in  $\Omega$ , for any time  
 change of quantity in  $V$  = amount crossing into  $V$  thru boundary  $\partial V$   
 amount gained + amount created within  $V$   
 per unit time (rates)

Let  $U(t)$  = total amount inside  $V$  at any time  $t$   
 $\mathcal{F}$  = net flow rate thru  $\partial V$  crossing into  $V$   
 $\Sigma$  = net amount created inside  $V$  per unit time

balance law:  $\frac{dU(t)}{dt} = \mathcal{F} + \Sigma$

$U(t) = \int_V u \cdot dV$ ,  $u$  = amount per unit volume, often written as  $\rho u$   
 $\rho u$  = amount per unit vol,  $\rho$  = density,  $u$  = amount/g



$\mathcal{F} = - \int_{\partial V} \vec{F} \cdot \vec{n} dA$ ,  $\vec{F}$  = flux = amount crossing unit area per unit time

$\vec{n}$  = outgoing unit normal to  $\partial V$

$\Sigma = \int_V \mathcal{S} dV$ ,  $\mathcal{S}$  = source = amount created inside  $V$  per unit vol; per unit time  
 or lost

⇒

Integral Form of Conservation law:

$$\frac{d}{dt} \int_V u dV = - \int_{\partial V} \vec{F} \cdot \vec{n} dA + \int_V \mathcal{S} dV$$

This is the most general expression of conservation, both physically and mathematically (only integrals need to exist, no smoothness required)  
 (averages)