# Numerical PDEs

Fall 2024, A. Donev

## Advection-diffusion equations

as simple linear conservation laws

$u(x,t)$ in 1D

$u(\vec{r},t)$ in 2D/3D

is a scalar conserved quantity

(mass, energy, momentum)

$$\frac{\partial}{\partial t} u(x,t) + \frac{\partial}{\partial x}\Big[\underbrace{a(x,t)\, u(x,t)}_{\text{advective flux}}\Big] = \frac{\partial}{\partial x}\Big[\underbrace{d(x,t)\, u_x(x,t)}_{\text{(−) diffusive/dissipative flux}}\Big]$$

advection velocity (given!)

diffusion coefficient (given!)

(entropy law) $d \geq 0$

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## Parabolic $\xrightarrow{t\to\infty}$ Elliptic

Infinite speed of propagation

Smooth solutions $t>0$

BCs on the whole spatial boundary

Separation of variables (bounded domains) – modes

Green's functions

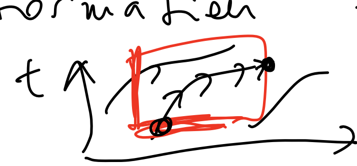
## Hyperbolic

Finite speed of propagation of information

Nonlinear eqs. generically develop shocks (weak formulation)

Discontinuities persist even in linear

Information propagates along characteristics




BC needed only where characteristic enter STD

# Numerics

## Parabolic

"Easy":

BCs easier than hyperbolic

Convergence easy to achieve (smoothness)

Hard:

Implicit

If explicit $\tau \sim \frac{h^2}{d}$

(often long time, refinement impossible)

## Hyperbolic

Easy:

Explicit schemes

$$\tau = \frac{h}{v_{prop}}$$

Hard:

Shocks: $\left\{ \begin{array}{l} \text{discontinuous} \\ \text{convergence not assured} \end{array} \right.$

## Example homework solution

$$u_t + a u_x = d u_{xx}$$

$$u(x,0) = (\sin(\pi x))^{100}$$

periodic

## Most accurate

Spectral ( pseudo for nonlinear

$(a(x)\, u)_x$

$(d(x)\, u_x)_x$

**Issues:** Temporal integration ?

(spectral collocation, exponential integrator)

BCs not easy

(esp. adv - dominated)

Non-smooth kills you

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## Finite-difference

$a > 0$

$$u_t + a u_x = d u_{xx}$$

$\boxed{\text{If } a=0 \quad \tau \sim h^2}$

$$\frac{u_j^{n+1} - u_j^n}{\tau} + a\,\frac{u_j^n - u_{j-1}^n}{h} = d\,\frac{u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1}}{h^2}$$

$\tau \leq h/a$

First order

$$\frac{\partial u(r,t)}{\partial t} + \nabla \cdot \underbrace{f(u,r)}_{} = 0$$

flux = advective + diffusive

In real world equations often non linear since advection velocity or diffusion coefficient depend on solution

$$u_t + (au)_x = (du_x)_x + f(u)$$

"reactions" sources/sinks

## Higher dimensions

My notation:

$$\nabla = (\partial_x, \partial_y, \partial_z)^T = \text{grad}$$

$$\nabla \cdot \; = \text{div}$$

$$\nabla^2 = \nabla \cdot \nabla = \partial_{xx} + \partial_{yy} + \partial_{zz}$$

$$u_t + \nabla\cdot(\vec{a}\, u) = \nabla\cdot(D\, u)$$

velocity vector field

$D \in \mathbb{R}^{d\times d}$ $\succcurlyeq 0$

diffusion tensor

Einstein notation

$$\nabla\cdot(\vec{a}u) = \sum_{\alpha=1}^{d} \partial_\alpha (a_\alpha u) =$$

$$= (\partial_\alpha a_\alpha) u + a_\alpha (\partial_\alpha u)$$

$$= (\nabla\cdot\vec{a}) u + \vec{a}\cdot\nabla u$$

If velocity field is incompressible

$\nabla\cdot\vec{a} = 0 \implies$

$$\nabla\cdot(\vec{a}u) = \vec{a}\cdot\nabla u$$

but do not assume this

and don't use chain rule

but rather keep advective flux $= \vec{a}\, u$

③

Why do we sometimes see advective derivative

$$D_t u = \partial_t u + a \cdot \nabla u$$

arise in fluid equations?

Either incompressible, or non-conservative / primitive form of equations (e.g., temperature instead of energy)

E.g. $c = \dfrac{u}{\rho}$ ← solute density / ← density

↑ concentration

$$u = \rho c \Rightarrow u_t = \rho c_t + c \rho_t$$

$$\boxed{\rho_t = -\nabla \cdot (\vec{a} \rho)}$$ (no diffusion of mass)

$$\rho_t = -a \cdot \nabla \rho - \rho (\nabla \cdot a)$$

$$\boxed{u_t + \nabla\cdot(\vec{a}u)} = \text{diffusive term}$$

$$u_t + \nabla\cdot(\rho c \vec{a}) =$$

$$\underbrace{\rho c_t - c\,\cancel{\nabla\cdot(\vec{a}\rho)}} + \overbrace{c\,\cancel{\nabla\cdot(\vec{a}\rho)} + \rho\vec{a}\cdot\nabla c}$$

$$= \rho\,(c_t + \vec{a}\cdot\nabla c) = \boxed{\rho D_t c}$$

$$\Rightarrow \quad \rho D_t c = \nabla\cdot(\text{diffusive flux})$$

$$= \nabla\cdot(\underbrace{\rho D \nabla c}_{\text{Fick's diffusion law}})$$

$$\cancel{\rho} D_t c = \nabla\cdot(\cancel{\rho} D \nabla c)$$

(not conservative unless $\rho = \text{const}$)

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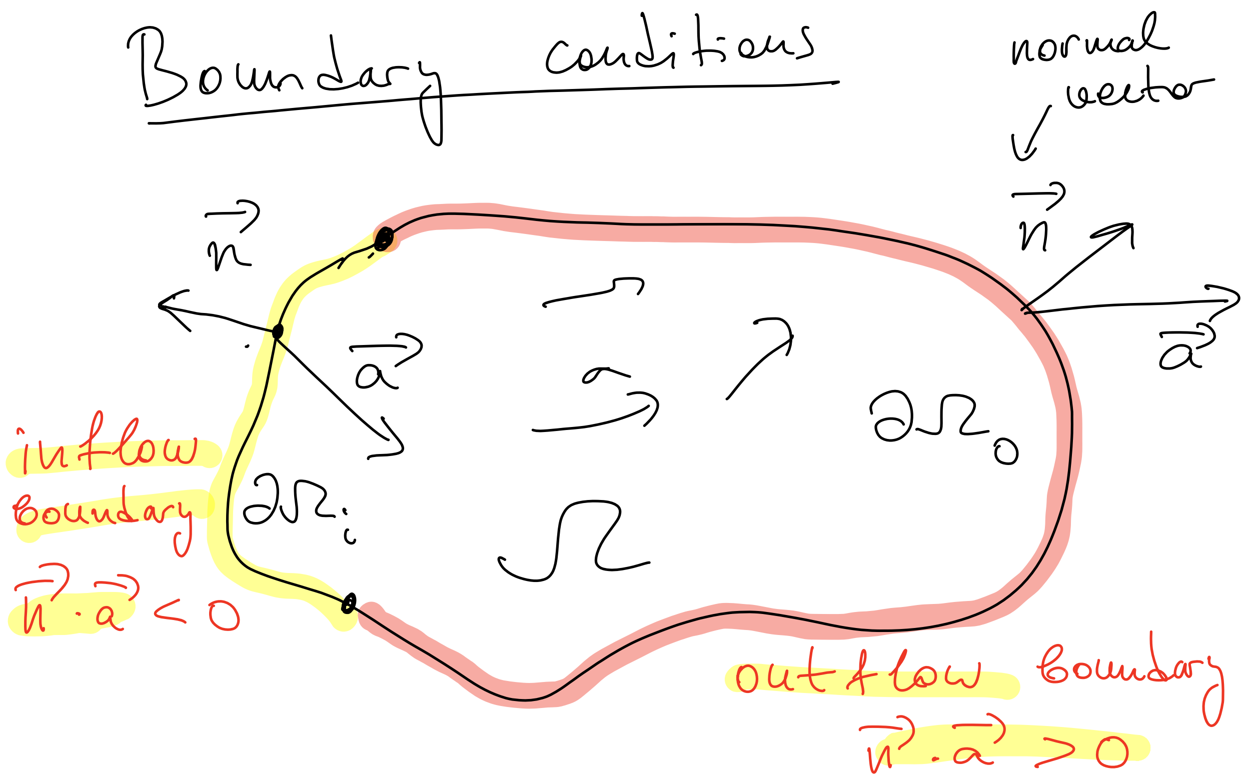
# Boundary conditions




Information comes into the domain at inflow boundary & flows outside of domain at outflow boundary.

For advection equation:

Dirichlet BC on $\partial\Omega_{inflow}$

No BC on $\partial\Omega_{outflow}$

For adv-diff equation, if
$D > 0$ everywhere
Need flux BC everywhere
on all of $\partial\Omega$

"Neumann" / Robin BC:

given $\vec{n} \cdot \vec{f} = \vec{n} \cdot (\vec{a} u - D \nabla u)$

OR

Dirichlet BC:

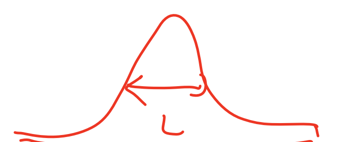
given $u$ itself
on pieces of $\partial\Omega$

We see that there is a change in character of PDE as diffusion becomes weaker compared to advection.

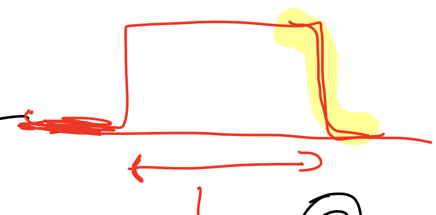
Before solving equation, we must know whether it is advection-dominated or diffusion-dominated

This is a property of the problem (the PDE + parameters)

If characteristic length scale of physic problem is $L$, and characteristic speed $\sim \|\vec{a}\|$ is $V$, and typical diffusion coefficient is $D$, then




$$\vec{a} \cdot \nabla u \sim V/L$$




$$\nabla \cdot (D \nabla u) \sim \frac{DU}{L^2}$$

Péchlet number

$$Pe = \frac{\text{advection}}{\text{diffusion}} = \frac{VL}{D}$$

If $Pe \gg 1$ problem is advection-dominated & we should use methods developed for advection equation (pure hyperbolic eqs.)

For numerical methods, the important length scale is the <u>grid size $h$</u>

$$\text{Cell } Pe = \frac{Vh}{D} \quad \text{(compare to 1)}$$

If grid is very fine, $h \ll L$ & problem is <u>resolved</u>.

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