Plan

Chapter 7: Time-Dependent Problems

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Mathematical Models, Analysis and Simulation, Part I

- Conservation laws
- Flux vector Φ
- Fourier's law $\Phi = -k\nabla T$
- The 1D heat equation by separation of variables
- Transport equation, characteristics
- Second order wave equation in 1D; d'Alembert's solution
- The wave equation and Newton's law; spring-mass oscillator

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Conservation Laws

• Consider the flow of a fluid with velocity field

$$\mathbf{u}(x,y,t) = \begin{pmatrix} u(x,y,t) \\ v(x,y,t) \end{pmatrix}$$

- Let c(x,y,t) denote the concentration of a species (e.g., number of molecules per m² in 2D)
- **Q**: How many molecules pass in time ∆*t* across a line of length *l* with normal **n**?

Conservation Laws (Cont)



- $A = \text{area of parallelogram} = l |\mathbf{u}| \Delta t \cos \phi$
- number of molecules: *cA*
- At every instant (number of molecules per second and meter):

 $c|\mathbf{u}|\cos\phi = c\mathbf{u}\cdot\mathbf{n}$

Definition. The flux vector is Φ if the number of molecules per length and time unit is $\Phi \cdot \mathbf{n}$.

In case of (passive) advection in velocity field \boldsymbol{u}



Conservation Laws (Cont)

- Consider the number *c* of molecules in a fixed *control volume* Ω.
- c can only change if molecules are going through (in/out) of the boundary ∂Ω:

$$\frac{d}{dt} \int_{\Omega} c d\Omega = - \int_{\partial \Omega} \mathbf{\Phi} \cdot \mathbf{n} d\Gamma.$$

• Divergence theorem provides:

$$\int_{\Omega} \frac{\partial}{\partial t} c d\Omega = -\int_{\Omega} \operatorname{div} \Phi d\Omega$$

This equation holds for any control volume.

• Conservation law (continuity equation)

$$\frac{\partial}{\partial t}c + \operatorname{div} \Phi = 0$$

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The Heat Equation

- Consider heat conduction: temperature T.
- Conserved quantity is energy:

 $\Delta H = \rho c_p \Delta T$

(change in energy per volume).

• Fourier's law:

$$\Phi = -k\nabla T$$

• Conservation of energy:

$$\frac{\partial}{\partial t}(\rho c_p T) - \operatorname{div}(k\nabla T) = 0$$

• For constant ρ, c_p, k:

$$\frac{\partial T}{\partial t} - \alpha \Delta T = 0$$

with $\Delta \equiv \operatorname{div} \nabla$ is the Laplacian operator. This is the celebrated *heat equation*.

- $\frac{\partial}{\partial t}c + \operatorname{div} \Phi = 0$
- In integral form:

• Continuity equation:

$$\int_{\Omega} \frac{\partial}{\partial t} c d\Omega + \int_{\partial \Omega} \boldsymbol{\Phi} \cdot \mathbf{n} d\Gamma = 0$$

• In our case:

$$\frac{\partial}{\partial t}c + \operatorname{div}(c\mathbf{u}) = 0.$$

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The 1D Heat Equation

- Let $\Omega = (0, 1)$:
- $u_t = \alpha u_{xx}, x \in (0,1).$
- Boundary conditions:
 prescribed temperature: Dirichlet condition (e.g.,
 - u(0) = 0) - isolated boundary: Neumann condition (no flux, e.g., $\partial u/\partial \mathbf{n} = 0$)
 - partly isolated boundary: Robin condition
- Initial condition: $u(x,0) = u_0(x)$ for $x \in (0,1)$.

4

7

Solution by Separation of Variables

- To be specific assume u(0,t) = u(1,t) = 0.
- Ansatz: Find solutions of the form u(x,t) = T(t)X(x).
- $T'X \alpha TX'' = 0$ yields

 $\frac{T'}{T} = \alpha \frac{X''}{X}$

 Since this identity must be fulfilled for all (x,t), the quotient must be constant. Denote this constant by λ:

$$T' = \lambda T, \quad X'' - \frac{\lambda}{\alpha}X = 0.$$

• Solutions

$$T(t) = ce^{\lambda t}, \quad X(x) = Ae^{\mu x} + Be^{-\mu x} \quad (\mu = \sqrt{\lambda/\alpha})$$

• We must have X(0) = X(1) = 0, hence A and B must fulfil

$$\begin{pmatrix} 1 & 1 \\ e^{\mu} & e^{-\mu} \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

In order to obtain nontrivial solutions, the system matrix must be singular.

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Separation of Variables (Cont)

• This leads to the (imaginary!!) values $\mu = n \cdot 2\pi i$,

$$\lambda = -n^2 \pi^2 \alpha, n = \pm 1, \pm 2, \dots$$

• Solutions to the odes:

$$T_n(t) = c_n e^{-\alpha n^2 \pi^2 t}, \quad X_n(x) = \sin n\pi x.$$

• Superposition principle:

$$u(x,t) = \sum_{n=1}^{\infty} c_n e^{-\alpha n^2 \pi^2 t} \sin n\pi x$$

- Theorem: If *u*₀ permits a convergent Fourier series, then this representation is the solution of the heat equation.
- The coefficients c_n can be determined from u_0 .

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The Heat Equation: Comments

- small n: low frequency components
 large n: high frequency components
- High frequency components decay very rapidly: like $\exp(-\alpha n^2 \pi^2)$.
- After some time, only the component for n = 1 is left.
- The smoothing property is expected from intuition about heat conduction.
- The strong smoothing property makes solving the heat equation *backwards* very difficult.
 The initial value problem u_t = -u_{xx} is *ill-posed*, i.e., perturbations of the initial state grow exponentially fast.
- Heat conduction has a wide range of time scales $\exp(-\alpha^2 \pi^2)$. Even on a grid (which limits *n* to a finite number) it requires *small* time steps to follow the fastest variations whereas the solution changes globally only like $\exp(-\alpha \pi^2 t)$. (A very stiff problem!)

The Transport Equation

- Consider (in 2D)
 - $c_t + \operatorname{div}(c\mathbf{u}) = 0.$
- Assume that *c* is given on a curve Γ in the (x, y)-plane.



Q: Can we determine c(x,y,t) in some region in (x,y,t) from this? **A**: In general, *yes*!

8

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The Material Derivative

The transport equation can be written as

$$c_t + uc_x + vc_y = -c \operatorname{div} \mathbf{u}.$$

Definition. The expression

$$\frac{Dc}{Dt} = c_t + uc_x + vc_y$$

is the material derivative of c.

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The material derivative is the time rate of change of a fluid particle which moves with the stream.

There is a nice discussion of the material derivative in Strang!

The Transport Equation: Characteristics

Read: Strang, p 472–474

• Taylor expansion:

 $c(x+\Delta x, y+\Delta y, t+\Delta t) = c(x, y, t) + c_t \Delta t + c_x \Delta x + c_y \Delta y + h.$ o. t..

Let (x(t), y(t)) be the trajectory of a particle following the stream:

$$\frac{dt}{dt} = u(x, y, t), \quad \frac{dy}{dt} = v(x, y, t)$$

This curve is called a *characteristic*.

• In differentials: $\Delta x = u\Delta t, \Delta y = v\Delta t$.

• Thus, on a characteristic it holds

$$\Delta c = \underbrace{\Delta t(c_t + uc_x + vc_y)}_{-\text{ediv } \mathbf{n}} + \text{higher order terms}$$

Going to the limit:

$$\frac{dx}{dt} = u, \quad \frac{dy}{dt} = v$$
$$\frac{Dc}{Dt} = -c \text{div } \mathbf{u}$$

This is a system of ordinary differential equations (on the characteristic!)

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13

Characteristics: Consequences

- If we know c at (x₀,y₀) ∈ Γ, the values of c(x,y,t) can be determined on the characteristic.
- If Γ is *not* a characteristic, the solution is determined in a region of (*x*, *y*, *t*)-space.
- Incompressible flow means div u = 0.
 For an incompressible flow, c is constant along characteristics.
- If there are sources and sinks *Q*(*x*, *y*, *t*), the transport equation reads

$$\frac{Dc}{Dt} = -c \operatorname{div} \mathbf{u} + Q.$$

c will be smooth along trajectories, but can be discontinuous *across*.
 Such a solution does not satisfy the differential equation, but of course the integral form,

$$\frac{d}{dt}\int_{\Omega} cd\Omega + \int_{\partial\Omega} c\mathbf{u} \cdot \mathbf{n} d\Gamma = Q.$$

Method of Characteristics: Example

• Burger's equation:

$$u_t + uu_x = 1$$
 for $t \ge 0$,
 $u(x,0) = x$ for $x \in \mathbb{R}$.



• Here, we have c = u. Hence, $\frac{Du}{Dt} = u_t + uu_x$ such that the system becomes

$$\frac{dx}{dt} = u, \frac{Du}{Dt} = 1.$$

• Solutions (note: $u(x_0, 0) = x_0$):

$$u = x_0 + t, x = x_0 + x_0 t + \frac{1}{2}t^2.$$

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Example (Cont)

 Material derivative = moving with the particle. Hence, we must go back in time to find the initial point on the characteristics:

$$x_0 = \frac{x - t^2/2}{1 + t}.$$

• Insert this into the expression for *u*:

$$u(x,t) = t + \frac{x - t^2/2}{1 + t}$$

Exercise: Verify this!

• Note: This is a pure initial-value problem, or *Cauchy problem*.

A Vibrating Bar: The Wave Equation

Read: Strang, p 546-548

- Consider longitudinal vibrations of a bar. The displacement is *u*, assumed to be small.
- Let S denote the tension in the bar. Consider a small element of length dx.
 Force over that element: dS
- Newton's law: mass times acceleration equals force:

$$\rho dx \cdot \frac{\partial^2 u}{\partial t^2} = dS$$

Going to differentials: $\rho u_{tt} = S_x$.

• Hooke's law (modulus of elasticity E):

 $S = E \frac{\partial u}{\partial x}.$

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16

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17

The Vibrating Bar (Cont)

• Putting everything together,

 $u_{tt} = c^2 u_{xx}$

where $c^2 = E/\rho$.

• This is the *wave equation*. Since it is *second* order in time, we need two initial conditions,

$$u(x,0) = u_0(x), \quad \frac{\partial u}{\partial t}(x,0) = v_0(x).$$

Solution of The 1D Wave Equation

Read: Strang, p 485-486

- The standard way to solve the wave equation would be to use the separation of variables approach.
- Here, we observe

$$u_{tt} - c^2 u_{xx} = \left(\frac{\partial}{\partial t} - c\frac{\partial}{\partial x}\right) \left(\frac{\partial}{\partial t} + c\frac{\partial}{\partial x}\right) u$$

The equation $u_t \pm cu_x = 0$ can be solved by the method of characteristics which provides $F(x \mp ct)$.

• This motivates the change of variables

$$\xi = x + ct, \eta = x - ct.$$

Exercise: Show that the wave equations is $\frac{\partial^2 u}{\partial \xi \partial \eta} = 0!$ The general solution is (called *d'Alembert's solution*)

$$u = F_1(\xi) + F_2(\eta) = F_1(x + ct) + F_2(x - ct)$$

Consequences of d'Alembert's Solution

- The solution consists of one wave traveling *right* $F_2(x-ct)$ and one wave travelling *left* $F_1(x+ct)$.
- *F*₁ is the general solution of *u*_t *cu*_x = 0, while *F*₂ is the general solution of *u*_t + *cu*_x = 0.
- The wave equation (scalar of second order) has *two* sets of characteristics,

$$\frac{dx}{dt} = +c \text{ and } \frac{dx}{dt} = -c.$$

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