Simulation in Computer Graphics

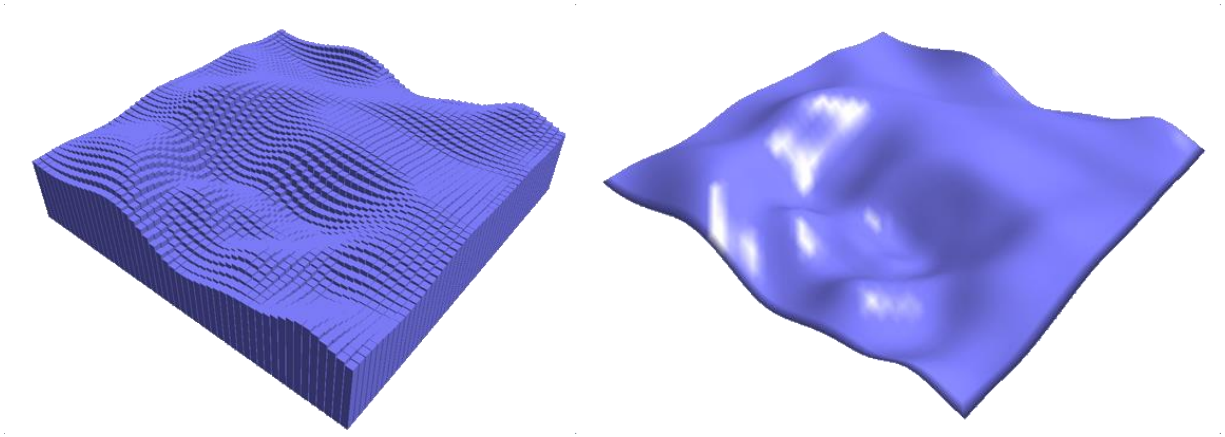
Partial Differential Equations

Matthias Teschner

Computer Science Department
University of Freiburg

Motivation

- various dynamic effects and physical processes are described by partial differential equations PDEs
  - e.g., wave propagation, advection, diffusion



- we consider PDEs that describe the time rate of change of a quantity at fixed positions

Motivation

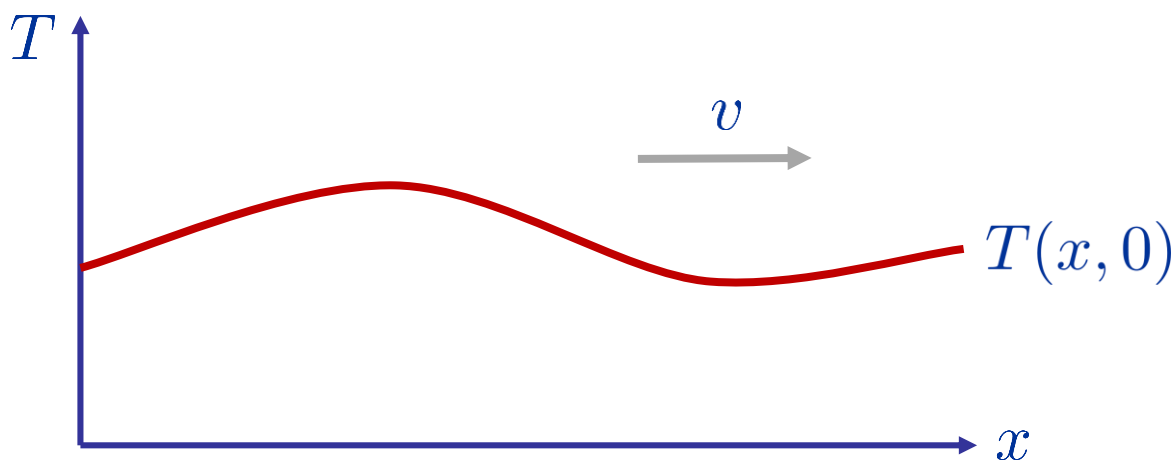
- this is a short overview of a large research field in mathematics and physics applied to the fields of animation and computer graphics
- goals:
  - you know what a PDE is
  - you know PDEs for specific effects
  - you know how to solve theses PDFs with finite differences

Outline

- introduction
  - 1D advection
- mathematical background
  - definition
  - types
  - boundary conditions
  - numerical solution methods
- examples
  - advection
  - diffusion
  - wave equation

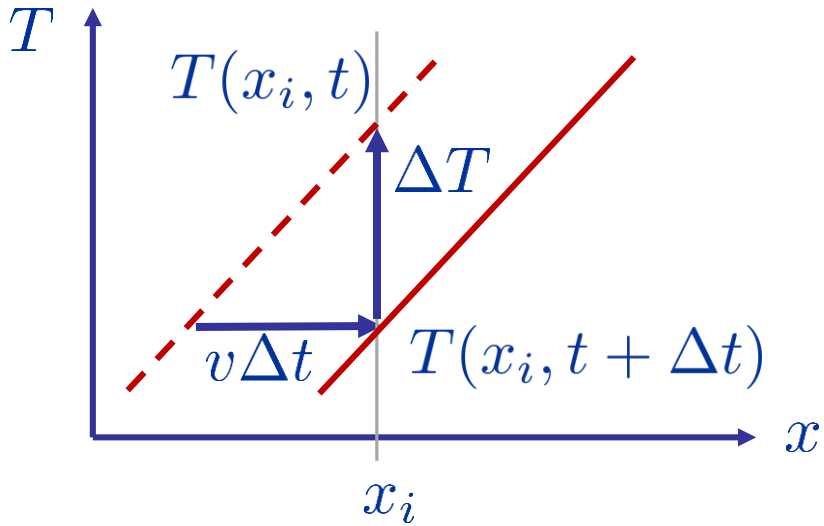
Advection

- simulation of temperate evolution
- consider temperature T at position x and time t
- start with known temperatures at time 0: $T(x, 0)$
- consider some wind speed v
- how to compute $T(x, t)$ at arbitrary position x and time t



Advection Equation in 1D

- consider temperature change within a small time step Δt at a fixed position x_i



$$\frac{\Delta T}{v\Delta t} \approx \frac{\partial T(x,t)}{\partial x} \quad \Delta t \to 0$$

$$\frac{T(x_i,t+\Delta t)-T(x_i,t)}{\Delta t} = \frac{-\Delta T}{\Delta t} \approx \frac{\partial T(x,t)}{\partial t}$$

$$\frac{\partial T(x,t)}{\partial t} = -v\frac{\partial T(x,t)}{\partial x}$$

T depends on two variables (space and time)
∂/ ∂t denotes the time derivative
∂/ ∂x denotes the space derivative

- temperature is only advected
- no additional effects

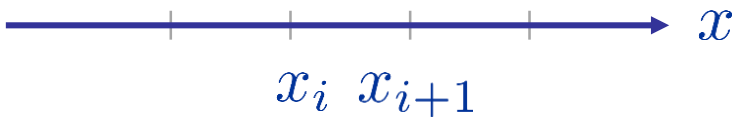
Analytical Solution

- define an initial condition $T(x, 0)$
  - temperature distribution at all positions x at time 0
- $T(x_i, t)$ at a position x_i and time t is obtained by shifting the temperature distribution at time 0 by the distance vt

  $T(x_i, t) = T(x_i - vt, 0)$

Numerical Solution with Finite Differences Discretization

- consider / sample the function $T(x,t)$ at discrete positions with distance h and discrete times with time step Δt



$$x_{i+1} - x_i = h$$
$$t_{j+1} - t_j = \Delta t$$

- approximate the partial derivatives with finite differences

$$\frac{\partial T(x,t)}{\partial t} \approx \frac{T(x_i,t_{j+1}) - T(x_i,t_j)}{\Delta t}$$

$$\frac{\partial T(x,t)}{\partial x} \approx \frac{T(x_{i+1},t_j) - T(x_i,t_j)}{h}$$

Numerical Solution with Finite Differences
Approximate Computation of T

- $\frac{\partial T(x,t)}{\partial t} = -v\frac{\partial T(x,t)}{\partial x} \rightarrow \frac{T(x_i,t_{j+1})-T(x_i,t_j)}{\Delta t} = -v\frac{T(x_{i+1},t_j)-T(x_i,t_j)}{h}$
- can be solved for $T(x_i, t_{j+1})$

  $T(x_i, t_{j+1}) = T(x_i, t_j) - \Delta t \cdot v\frac{T(x_{i+1},t_j)-T(x_i,t_j)}{h}$
- from the initial condition, temperature $T(x_i, t_0)$ is known at all sample positions x_i at some time t_0
- i.e., for all positions x_i, we can compute

  $T(x_i, t_1) = T(x_i, t_0) - \Delta t \cdot v\frac{T(x_{i+1},t_0)-T(x_i,t_0)}{h}$
- if we have computed $T(x_i, t_1)$ for all positions x_i, we can compute

  $T(x_i, t_2) = T(x_i, t_1) - \Delta t \cdot v\frac{T(x_{i+1},t_1)-T(x_i,t_1)}{h}$
- and so on …

Numerical Solution with Finite Differences Boundary Conditions

- at time t_j, the temperature is known at n sample positions: $T(x_0, t_j), T(x_1, t_j), \ldots, T(x_{n-1}, t_j)$
- however, the computation of the temperature at x_{n-1} requires the temperature at x_n
- setting boundary conditions / define missing values
  - e.g., periodic boundaries
  - $T(x_n, t_j) = T(0, t_j)$
  - temperature leaving/entering the right-hand side of the simulation domain, enters/leaves the left-hand side of the domain

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Definition

- a partial differential equation PDE describes the behavior of an unknown multivariable function f using
  - partial derivatives of f , e.g. $\frac{\partial f}{\partial t}, \frac{\partial f}{\partial x}, \frac{\partial^2 f}{\partial t^2}, \frac{\partial^2 f}{\partial x \partial t}$
  - the function f and
  - the independent variables, e.g. x, t
- example: $\frac{\partial T(x,t)}{\partial t} = -v \frac{\partial T(x,t)}{\partial x}$
- notation $\frac{\partial T(x,t)}{\partial t} = T_t \quad \frac{\partial T(x,t)}{\partial x} = T_x \quad \frac{\partial^2 f}{\partial x \partial t} = f_{x,t}$

  $T_t = -v T_x$
- ordinary differential equations are a special case for functions that depend on one variable

PDEs in Physics

- independent variables are
  - static problems: x (1D), x, y (2D), x, y, z (3D)
  - dynamic problems: x, t (1D+1), x, y, t (2D+1), x, y, z, t (3D+1)

- unknown functions are
  - scalars, e.g. temperature T, density ρ
  - vectors, e.g. displacement $\mathbf{u}$, velocity $\mathbf{v}$

PDE Classification

- order
  - given by the highest order of a partial derivative
- linearity
  - the function and its partial derivatives only occur linearly
  - coefficients may be functions of independent variables
- e.g. second-order linear PDE of function $f(x, y)$ with two independent variables x, y
  - general form
    $$g_1(x,y)f_{xx} + g_2(x,y)f_{xy} + g_3(x,y)f_{yy} + g_4(x,y)f_x + g_5(x,y)f_y + g_6(x,y)f + g_7(x,y) = 0$$
- non-linear example
  $$f_{xx} \cdot f_{xy} = 0$$

PDE Classification

- second-order PDEs

$$A(x,y)f_{xx} + B(x,y)f_{xy} + C(x,y)f_{yy} + \ldots + F(x,y,f,f_x,f_y) = 0$$

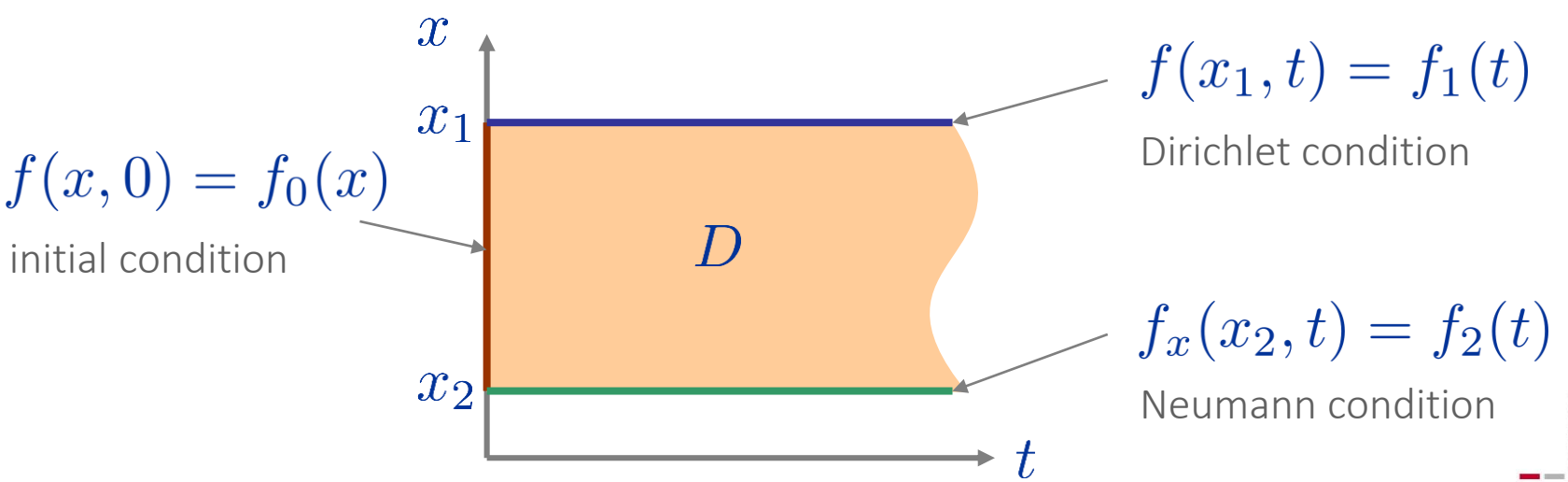
- can be classified into
  - hyperbolic $B^2 - A \cdot C > 0$
  - parabolic $B^2 - A \cdot C = 0$
  - elliptic $B^2 - A \cdot C < 0$
- classification
  - is geometrically motivated
  - is characterized by different mathematical and physical behavior
  - determines type of required boundary conditions

PDE Classification

- hyperbolic
  - time-dependent processes
  - reversible, not evolving to a steady state
  - undiminished propagation
  - e.g., wave motion
- parabolic
  - time-dependent processes
  - irreversible, evolving to a steady state
  - dissipative
  - e.g., heat diffusion
- elliptic
  - time-independent
  - already in a steady state

Boundary Conditions

- generally, many functions f solve a PDE
- physical applications expect one solution
- f is typically defined in a simulation domain D
- the physical solution is required to satisfy certain conditions on the boundary of D



Numerical Solution - Overview

Governing Equations IC / BC → Discretization → System of Algebraic Equations → Equation (Matrix) Solver → Approx. Solution

continuous form

Finite Difference
Finite Volume
Finite Element
Spectral
Boundary Element

Discrete Nodal Values

e.g., CG

Discretization

- time derivatives
  - finite differences
- spatial derivatives
  - finite differences FDM, finite elements FEM, finite volumes FVM
- example
  - 1D advection
  - continuous form
  - discretizing the time derivative with FD
  - discretizing the spatial derivative with FD
  - algebraic equation

$$\frac{\partial T(x,t)}{\partial t} = -v\frac{\partial T(x,t)}{\partial x}$$

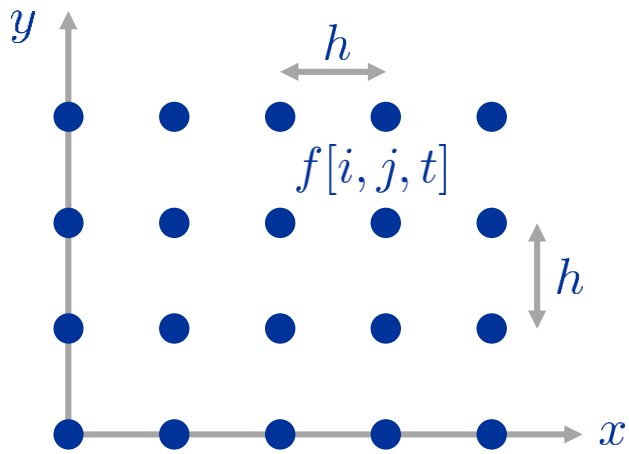
$$\frac{\partial T(x,t)}{\partial t} \approx \frac{T(x_i,t_{j+1})-T(x_i,t_j)}{\Delta t}$$

$$\frac{\partial T(x,t)}{\partial x} \approx \frac{T(x_{i+1},t_j)-T(x_i,t_j)}{h}$$

$$\frac{T(x_i,t_{j+1})-T(x_i,t_j)}{\Delta t} = -v\frac{T(x_{i+1},t_j)-T(x_i,t_j)}{h}$$

2D Sampling

- function f is reconstructed at fixed sample positions at fixed time points
- simplest case: sampling of f on a regular grid
  - e.g., 2D+1 dimensions
  - $f[i,j,t] = f(x_i, y_j, t_t) = f(x_0 + i \cdot h, y_0 + j \cdot h, t_0 + t \cdot \Delta t)$
  - $i \in (0, \ldots, n-1), j \in (0, \ldots, m-1), t \in (0, 1, 2, \ldots)$
  - grid spacing h and time step Δt



2D Finite Difference Approximations

- time derivative
  - $f_t[i,j,t] = \frac{f[i,j,t+1]-f[i,j,t]}{\Delta t} + O(\Delta t)$ time marching
- spatial derivatives
  - $f_x[i,j,t] = \frac{f[i+1,j,t]-f[i,j,t]}{h} + O(h)$ forward scheme
  - $f_x[i,j,t] = \frac{f[i,j,t]-f[i-1,j,t]}{h} + O(h)$ backward scheme
  - $f_x[i,j,t] = \frac{f[i+1,j,t]-f[i-1,j,t]}{2h} + O(h^2)$ central scheme
  - if information moves from left to right, backward is upwind, otherwise forward is upwind
  - upwind is typically preferred

2D Finite Difference Approximations

- higher-order derivatives, e.g.
  - $f_{xx}[i,j,t] = \frac{f_x[i,j,t]-f_x[i-1,j,t]}{h} = \frac{f[i+1,j,t]-2f[i,j,t]+f[i-1,j,t]}{h^2} + O(h^2)$
- higher-order approximations, e.g.
  - $f_x[i,j,t] = \frac{f[i-2,j,t]-8f[i-1,j,t]+8f[i+1,j,t]-f[i+2,j,t]}{12h} + O(h^4)$
  - $f_{xx}[i,j,t] =$

$$\frac{-f[i-2,j,t]+16f[i-1,j,t]-30f[i,j,t]+16f[i+1,j,t]-f[i+2,j,t]}{12h^2} + O(h^4)$$

Explicit Solution Schemes - 1D Advection

- advection equation $\frac{\partial f(x,t)}{\partial t} = -v \frac{\partial f(x,t)}{\partial x}$
- upwind $(v > 0)$

$$\frac{f[i,t+1]-f[i,t]}{\Delta t} + v \frac{f[i,t]-f[i-1,t]}{h} = 0$$ discretization

$$f[i,t+1] = f[i,t] - v \frac{\Delta t}{h} \left(f[i,t] - f[i-1,t] \right)$$ solver (solution scheme)

- simple stability rule
  - information must not travel more than one grid cell per time step
  - $v\Delta t < h \;\rightarrow\; \Delta t < \frac{h}{v}$
  - $v\Delta t < h \;\rightarrow\; \frac{v\Delta t}{h} = \sigma < 1$ CFL number
  - time step should be sufficiently small to result in $\sigma < 1$

Explicit Solution Schemes - 1D Advection

- downwind $(v < 0)$

$$\frac{f[i,t+1]-f[i,t]}{\Delta t} + v\frac{f[i+1,t]-f[i,t]}{h} = 0$$

$$f[i,t+1] = f[i,t] - v\frac{\Delta t}{h}\left(f[i+1,t] - f[i,t]\right)$$

- centered, FTCS (forward time centered space)

$$\frac{f[i,t+1]-f[i,t]}{\Delta t} + v\frac{f[i+1,t]-f[i-1,t]}{2h} = 0$$

$$f[i,t+1] = f[i,t] - v\frac{\Delta t}{2h}\left(f[i+1,t] - f[i-1,t]\right)$$

- Leap-frog

$$\frac{f[i,t+1]-f[i,t-1]}{2\Delta t} + v\frac{f[i+1,t]-f[i-1,t]}{2h} = 0$$

$$f[i,t+1] = f[i,t-1] - v\frac{\Delta t}{h}\left(f[i+1,t] - f[i-1,t]\right)$$

Explicit Solution Schemes - 1D Advection

- Lax-Wendroff

$$f[i,t+1] =$$

$$f[i,t] - v\frac{\Delta t}{2h}\left(f[i+1,t] - f[i-1,t]\right) + \frac{1}{2}\left(v\frac{\Delta t}{h}\right)^2\left(f[i+1,t] - 2f[i,t] + f[i-1,t]\right)$$

- Beam-Warming $(v > 0)$

$$f[i,t+1] =$$

$$f[i,t] - v\frac{\Delta t}{2h}\left(3f[i,t] - 4f[i-1,t] + f[i-2,t]\right) + \frac{1}{2}\left(v\frac{\Delta t}{h}\right)^2\left(f[i,t] - 2f[i-1,t] + f[i-2,t]\right)$$

- Lax-Friedrich

$$f[i,t+1] =$$

$$\frac{1}{2}\left(f[i+1,t] - f[i-1,t]\right) - v\frac{\Delta t}{2h}\left(f[i+1,t] - f[i-1,t]\right)$$

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  - wave equation

Advection in 2D and 3D

- 1D advection $f_t = -v f_x$
- generally, the velocity is a vector $\mathbf{v}$ with direction $\mathbf{n}_v$ and length v
- spatial derivative of f in direction $\mathbf{n}_v$

$$\frac{\partial f}{\partial \mathbf{n}_v} = \mathbf{n}_v \cdot \nabla f \qquad \nabla f \underset{\text{2D}}{=} \begin{pmatrix} f_x \\ f_y \end{pmatrix} \qquad \nabla f \underset{\text{3D}}{=} \begin{pmatrix} f_x \\ f_y \\ f_z \end{pmatrix}$$

- therefore, $f_t = -v\,(\mathbf{n}_v \cdot \nabla f) = -\mathbf{v} \cdot \nabla f$

2D Finite Difference Solution Scheme

- advection equation

$$f_t + \mathbf{v} \cdot \nabla f = f_t + v_x \cdot f_x + v_y \cdot f_y = 0$$

- discretization

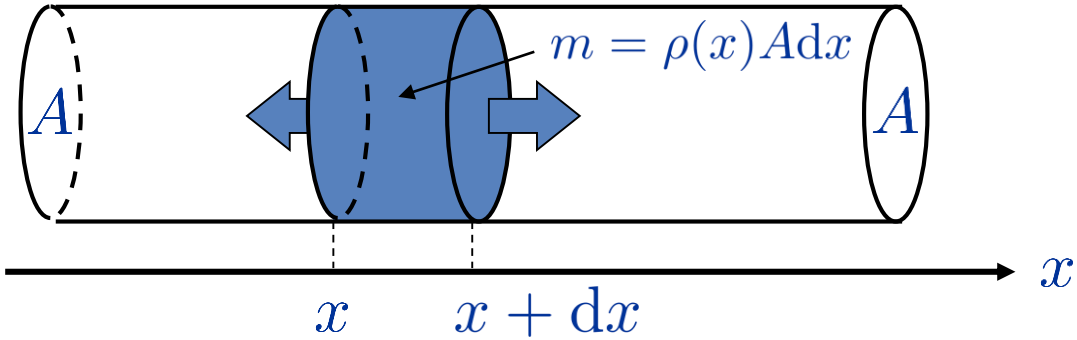
$$\frac{f[i,j,t+1]-f[i,j,t]}{\Delta t} + v_x \frac{f[i,j,t]-f[i-1,j,t]}{h} + v_y \frac{f[i,j,t]-f[i,j-1,t]}{h} = 0$$

- solution scheme

$$f[i,j,t+1] = f[i,j,t] - \Delta t \left(v_x \frac{f[i,j,t]-f[i-1,j,t]}{h} + v_y \frac{f[i,j,t]-f[i,j-1,t]}{h} \right)$$

- variant
  - velocity can vary with the location
  - PDE still first order and linear
  - $f_t + \mathbf{v}(x,y) \cdot \nabla f = 0$

Diffusion in 1D



- density $\rho(x)$ describes the concentration of a substance in a tube with cross section A
- conduction law: the mass flow through an area A (flux) is prop. to the neg. gradient of the density normal to A

$$\frac{\mathrm{d}m}{\mathrm{d}tA} = \frac{\mathrm{d}\rho(x)A\mathrm{d}x}{\mathrm{d}tA} = k\rho_x(x + \mathrm{d}x) - k\rho_x(x)$$

$$\rho_t = k\frac{\rho_x(x+\mathrm{d}x) - \rho_x(x)}{\mathrm{d}x} = k\rho_{xx}$$

$$\rho_t = k\rho_{xx}$$ k - conductivity

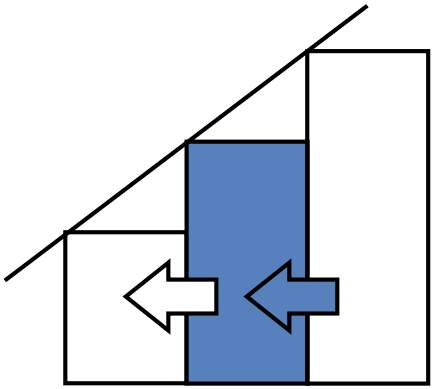
Diffusion in 2D and 3D

- equation

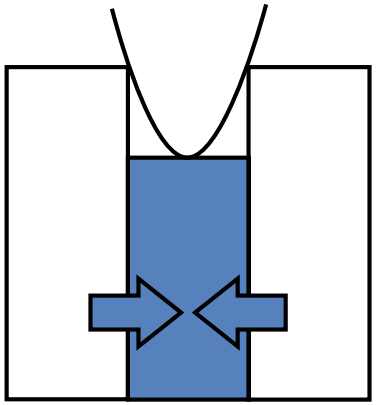
$$f_t = k\nabla^2 f = k\Delta f = k\left(f_{xx} + f_{yy}\right) \qquad f_t = k\left(f_{xx} + f_{yy} + f_{zz}\right)$$

Laplace operator — 2D — 3D

- intuition for second spatial derivative
- constant gradient, i.e. $f(x) = a + bx$, has no effect



Flux, no change



Flux, positive change

2D Finite Difference Solution Scheme

- diffusion equation

$$f_t - k\left(f_{xx} + f_{yy}\right) = 0$$

- discretization

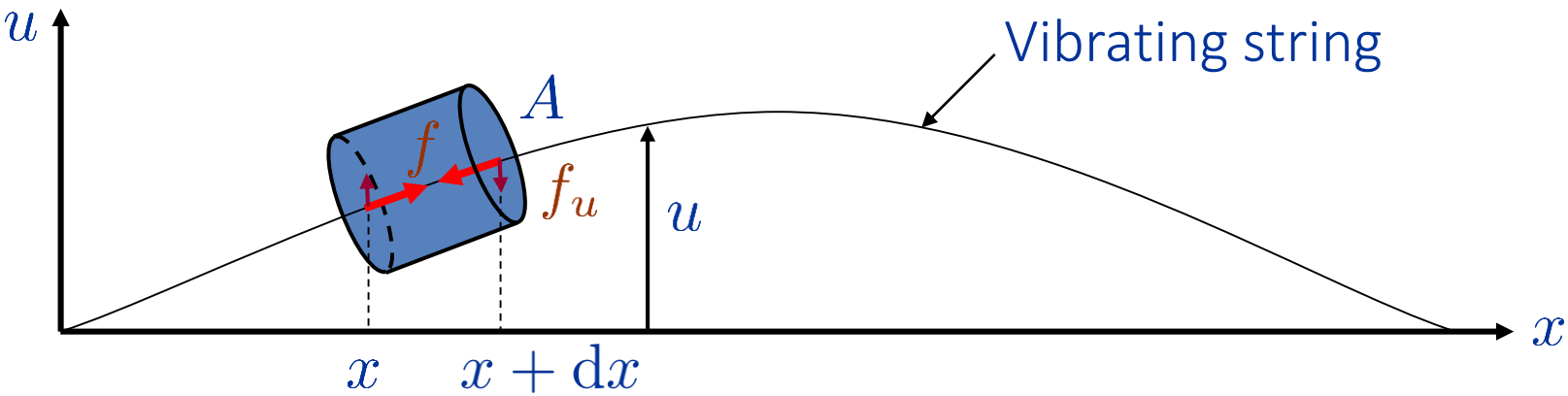
$$\frac{f[i,j,t+1]-f[i,j,t]}{\Delta t} - k\left(\frac{f[i+1,j,t]-2f[i,j,t]+f[i-1,j,t]}{h^2} + \frac{f[i,j+1,t]-2f[i,j,t]+f[i,j-1,t]}{h^2}\right) = 0$$

- solution scheme

$$f[i,j,t+1] = f[i,j,t] + \Delta t k \frac{f[i+1,j,t]+f[i-1,j,t]+f[i,j+1,t]+f[i,j-1,t]-4f[i,j,t]}{h^2}$$

- intuition
  - if the average value of the neighboring cells is larger than the cell value, the value increases and vice versa

Wave Equation in 1D



- function $u(x)$ is the displacement of the string normal to x
- assuming small displacement and constant stress σ
- force acting normal to cross section A is $f = \sigma A$
- component in u-direction $f_u \approx \sigma A u_x$
- Newton's Second Law for an infinitesimal segment

$$(\rho A \mathrm{d}x)\, u_{tt} = \sigma A u_x(x + \mathrm{d}x) - \sigma A u_x(x)$$

$$\rho_{tt} = \sigma u_{xx}$$

Wave Equation in 2D and 3D

- 1D wave equation $f_{tt} = -c^2 f_{xx}$ c – speed of wave propagation
- 2D: $f_{tt} = c^2 \nabla^2 f = c^2 \Delta f = c^2 \left(f_{xx} + f_{yy} \right)$
- 3D: $f_{tt} = c^2 \left(f_{xx} + f_{yy} + f_{zz} \right)$
- 2D finite difference solution scheme

$$v[i,j,t+1] = v[i,j,t] + \Delta t c^2 \frac{f[i+1,j,t]+f[i-1,j,t]+f[i,j+1,t]+f[i,j-1,t]-4f[i,j,t]}{h^2}$$

$$f[i,j,t+1] = f[i,j,t] + \Delta t v[i,j,t+1]$$

Demo

- combination of wave equation, advection, and diffusion

$$f_{tt} = c^2 \nabla^2 f$$ wave equation

$$f_t = -\mathbf{v}_{adv} \cdot \nabla f$$ advection equation

$$f_t = k \nabla^2 f$$ diffusion equation

- update rule (spatial derivatives not discretized)

$$v[i,j,t+1] = v[i,j,t] + \Delta t c^2 \nabla^2 f[i,j,t]$$

$$u[i,j,t+1] = u[i,j,t] + \Delta t \left(v[i,j,t+1] + k \nabla^2 f[i,j,t] - \mathbf{v}_{adv} \cdot \nabla f[i,j,t] \right)$$

Literature

- Alan Jeffrey, “Applied Partial Differential Equations – An Introduction,” Academic Press, Amsterdam, ISBN 0-12-382252-1
- John D. Anderson, “Computational Fluid Dynamics – The Basics with Applications,” McGraw-Hill Inc., New York, ISBN 0-07-001685-2