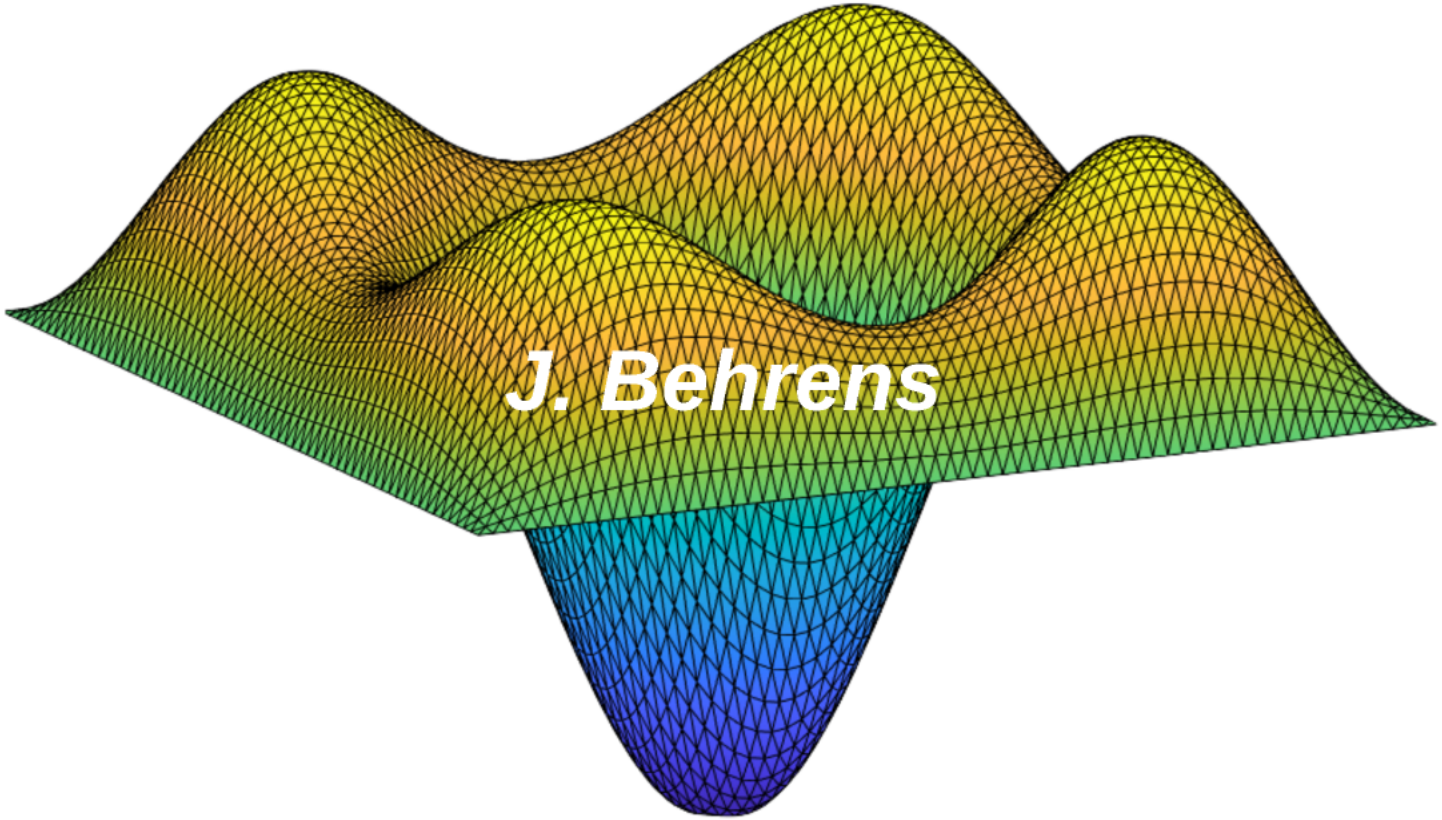
Numerical Approximation of Partial Differential Equations
Finite Difference and Finite Volume Methods



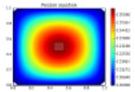
J. Behrens

Introduction

Motivation

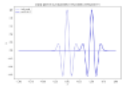
Geometry

We know how to solve Poisson's eq. in a square domain

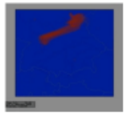


Dimensionality

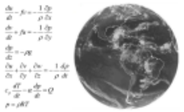
We may be able to solve a transport problem in 1D



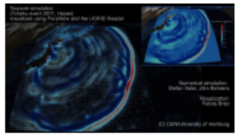
But already 2D may be difficult!



Complexity



Applicability



Tsunami-Simulation

Knowledge Gain

Geometry

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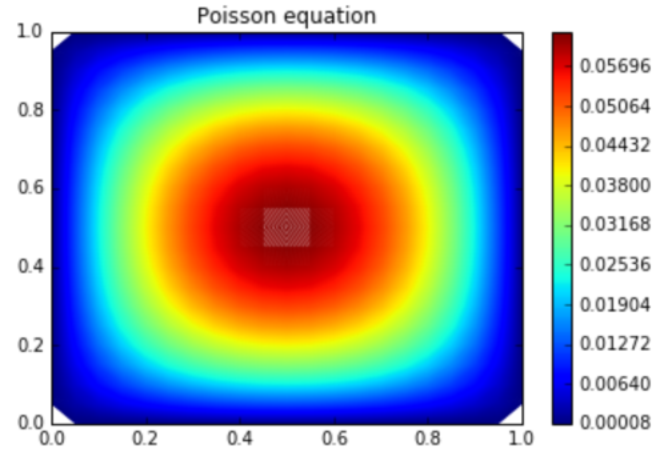
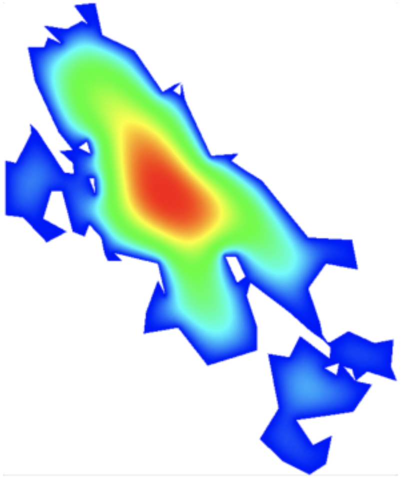


But what about this domain?



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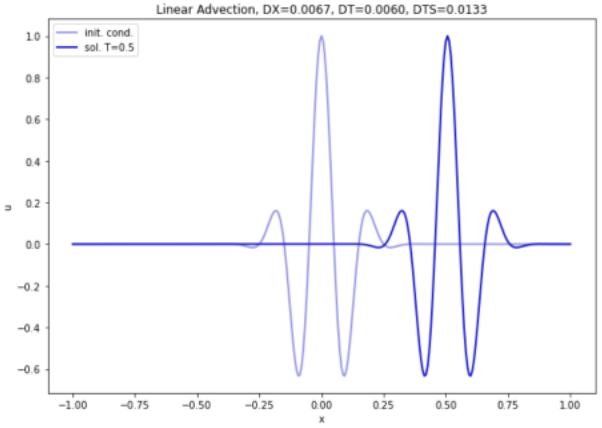

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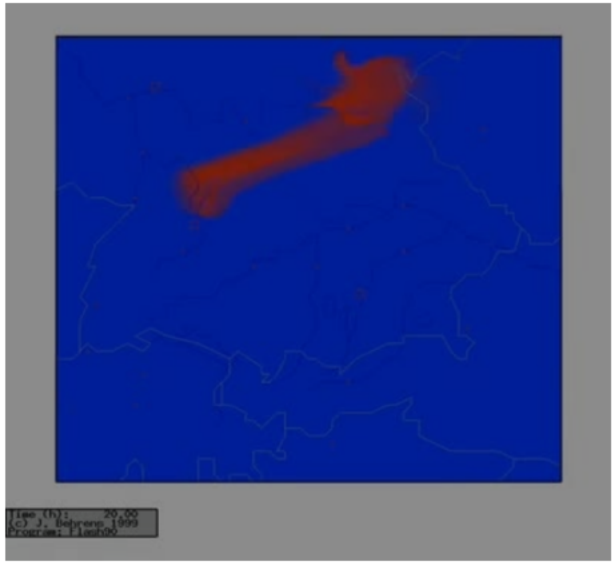


Complexity

$$\frac{du}{dt} - fv = -\frac{1}{\rho}\frac{\partial p}{\partial x}$$

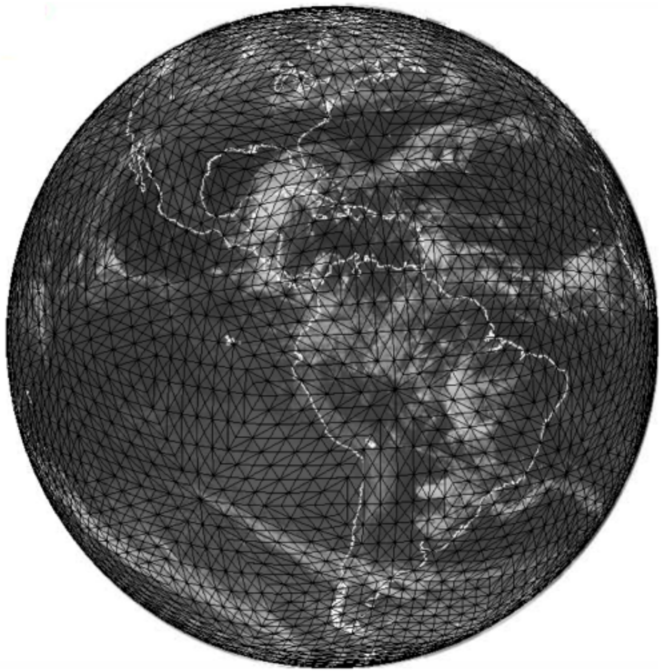
$$\frac{dv}{dt} + fu = -\frac{1}{\rho}\frac{\partial p}{\partial y}$$

$$\frac{dp}{dz} = -\rho g$$

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = -\frac{1}{\rho}\frac{d\rho}{dt}$$

$$c_p \frac{dT}{dt} - \alpha \frac{dp}{dt} = Q$$

$$p = \rho R T$$



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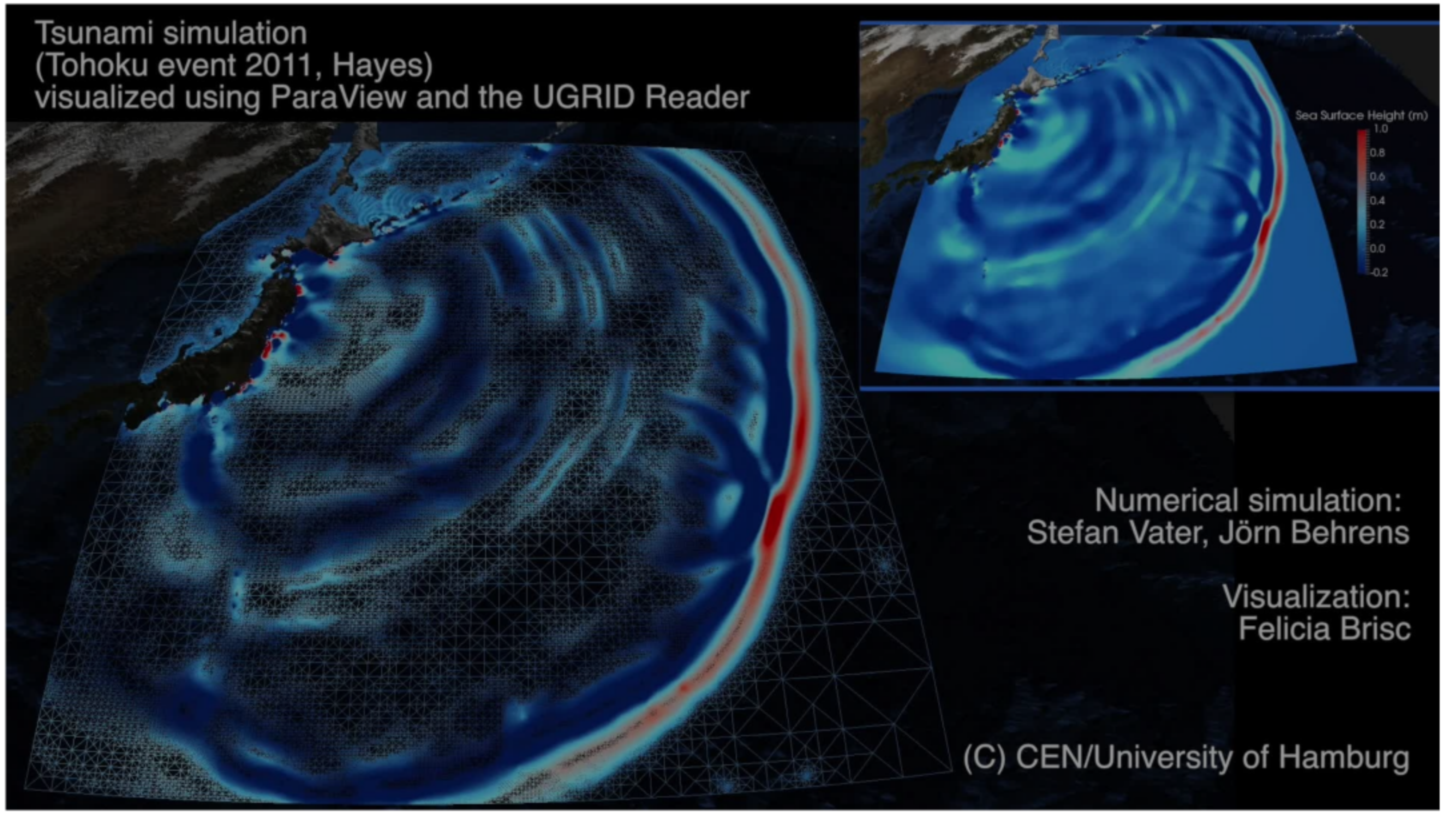

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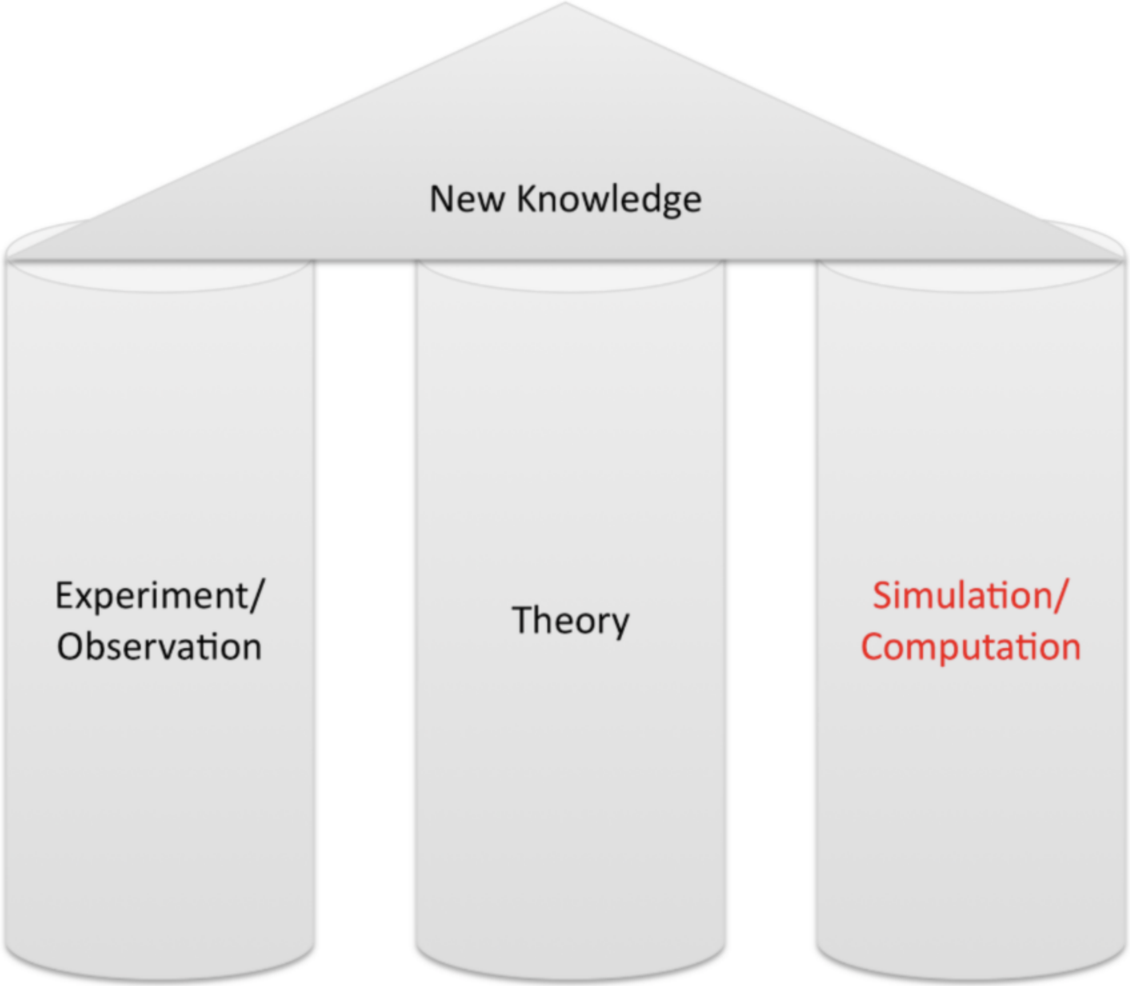


Recap: Numerical Methods

Solution of Linear Systems

Idea of LU Factorization:

We have to solve:

$$\boxed{Ax = b}$$

If we could find a decomposition

$$A = L \cdot U \qquad L : \quad U :$$

Then it would be easy to solve by Forward/Backward substitution:

$$Ly = b,$$
$$Ux = y.$$

Interpolation and Quadrature

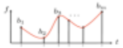
Given: $i = 1 : m \quad (t_i, b_i)$

Think of t_i times and b_i states (values)

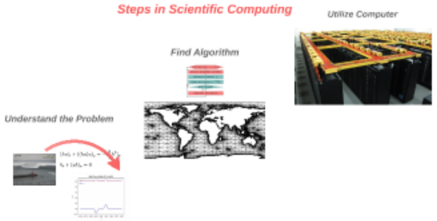
Suppose: b_i exact

Find: $f(x)$ such that $f(t_i) = b_i$

Interpolation Problem



Condition and Stability



Mantra of Numerical Analysis

1. Is there a solution?
2. Is the solution unique?
3. Is there an algorithm?
4. Is the algorithm efficient?
5. Is the solution accurate?

Solution of Linear Systems

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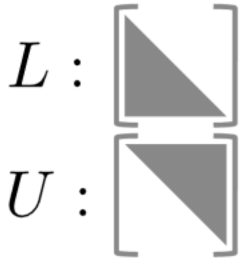

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Idea of Classical Iteration Methods

We have to solve $\quad Ax = b$

Split Matrix: $\quad A = M - N \qquad M^{-1}$ simple

Then solve $\quad Ax = \underset{\substack{\uparrow \\ \text{new}}}{Mx} - \underset{\substack{\uparrow \\ \text{old}}}{Nx} = b$

Iteration: $\quad Mx^{k+1} = Nx^k + b$

$$\Leftrightarrow x^{k+1} = \underbrace{M^{-1}N}_{C} x^k + \underbrace{M^{-1}b}_{d}$$

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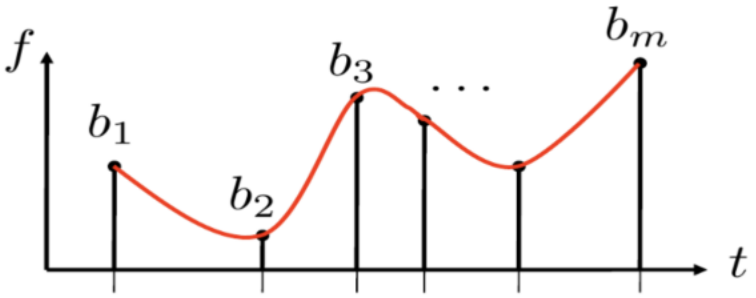


Generic Quadrature Formulation

Observation

Elementary positive linear forms are *evaluation functionals*:

$$[x] : f \mapsto f(x), \quad x \in [a, b]$$

for $a \leq x_0 < x_1 < \cdots < x_n \leq b$ we use the ansatz:

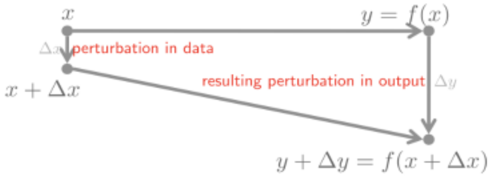
$$\boxed{\hat{I}_n(f) = (b-a) \cdot \sum_{k=0}^{n} \lambda_k f(x_k)}$$

weight node

Condition and Stability

Error Analysis

Sensitivity



Perturbation with small value Δx

$[\cdot]$ denotes a measure (norm) for the error

Then:

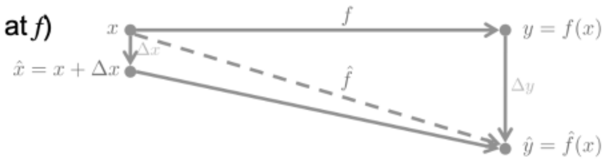
$$\boxed{[\Delta y] \leq \kappa \cdot [\Delta x]}$$

Definition: We call κ the condition number of the problem.

Error Analysis

Forward and Backward Error Analysis

Look at the Algorithm now (or at f)



Definition: An algorithm is stable w.r.t. backward analysis, if $[\Delta x]$ is "small".

Remark: "small" means relative to data error (rounding, etc.), e.g.

$$[\Delta x] \leq (\#flops) \cdot \epsilon$$

Remark: we know (see above): $[\Delta y] \leq \kappa[\Delta x]$

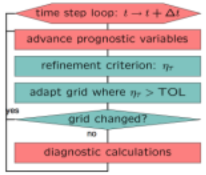
Definition: An algorithm is stable w.r.t. forward analysis, if

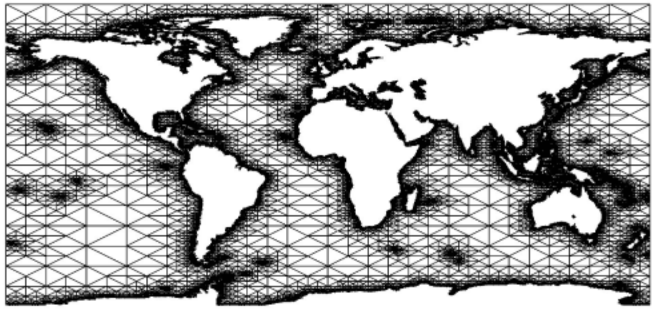
$$[\Delta y] \leq \kappa(\#flops) \cdot \epsilon$$

Steps in Scientific Computing

Utilize Computer

Find Algorithm

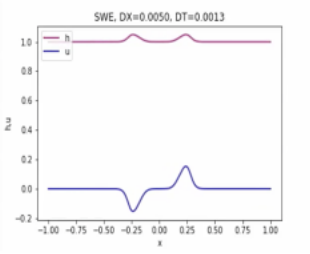




Understand the Problem

$$(hu)_t + ((hu)u)_x = -(\frac{g}{2}h^2)_x$$

$$h_t + (uh)_x = 0$$



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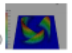
Recap:
Partial Differential Equations

Continuity Equation:

$$\mathbf{F}_{\text{cont}}(\mathbf{u}) := \frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot (\mathbf{v}\mathbf{u})$$



Remark: follows from applying first principle and transport theorem.

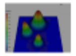
Transport Equation:

$$\mathbf{F}_{\text{trans}}(\mathbf{u}) := \frac{\partial \mathbf{u}}{\partial t} + \mathbf{v}\nabla\mathbf{u}$$

Remark: for divergence free flow field $\mathbf{v}$.

Heat Equation:

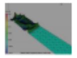
$$\mathbf{F}_{\text{heat}}(\mathbf{u}) := \frac{\partial \mathbf{u}}{\partial t} - \Delta\mathbf{u}$$



Remark: follows from exchanging flux function $q = \mathbf{v}\mathbf{u}$ by $q = \nabla\mathbf{u}$.

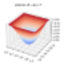
Wave Equation:

$$\mathbf{F}_{\text{wave}}(\mathbf{u}) := \frac{\partial^2 \mathbf{u}}{\partial t^2} - \Delta\mathbf{u}$$



Laplace Equation:

$$\mathbf{F}_{\text{Lapl}}(\mathbf{u}) := -\Delta\mathbf{u}$$



Remark: for time-independence $\frac{\partial u}{\partial t} = 0$.

Definition: (Quasilinear PDE)
A partial differential equation $F(y,u,\nabla u) = 0$ is called quasi-linear, if F is linear in ∇u, but not in y and u, i.e.,

$$F(y,w,p) = a(y,w)\cdot p - b(y,w),$$

where $a, b \in C(U \times \mathbb{R})$.

Definition: (Characteristic System, Characteristic Curve)
Let $a, b \in C(U \times \mathbb{R})$. Then we denote by $y = y(\tau)$ and $w = w(\tau)$, $\tau \in I \subset \mathbb{R}$ the (local) solution of the initial value problem given by

$$\frac{dy}{d\tau} = a(y,w), \quad y(0) = y_0,$$
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This system is called characteristic system of the partial differential equation

$$a(y,u)\cdot\nabla u - b(y,u) = 0.$$

Solutions of the system are called characteristic curves, and the projections of these curves to U, i.e. the curves $y = y(\tau)$ are the ground curves.

Preliminary Remark: (Non-linear Conservation Law)
In this session we will consider Cauchy problems for non-linear conservation laws:

$$\begin{cases} u_t + f(u)_x &= 0 \quad \text{in } \mathbb{R}\times(0,\infty), \\ u &= u_0 \quad \text{on } \mathbb{R}\times\{t=0\}, \end{cases}$$

where $f : \mathbb{R} \to \mathbb{R}$ a given non-linear flux function.

Definition: (Weak Solution)
A function $u \in L^\infty(\mathbb{R}\times(0,\infty))$ is called weak solution (sometimes *integral solution*), of a conservation law $u_t + f(u)_x = 0$, if it satisfies for all v the following weak problem

$$\int_0^\infty \int_{-\infty}^\infty u v_t + f(u) v_x \, dx dt + \int_{-\infty}^\infty u_0(x) v(x,0)\, dx = 0.$$

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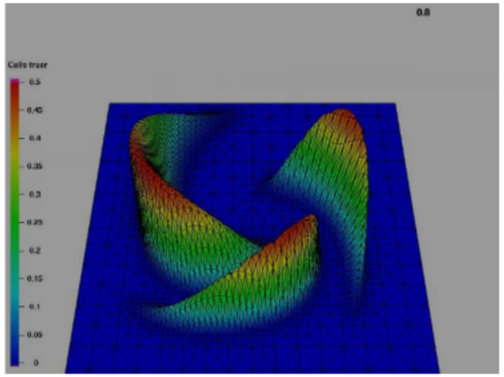

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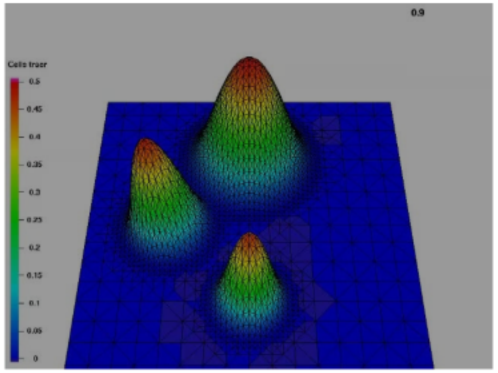

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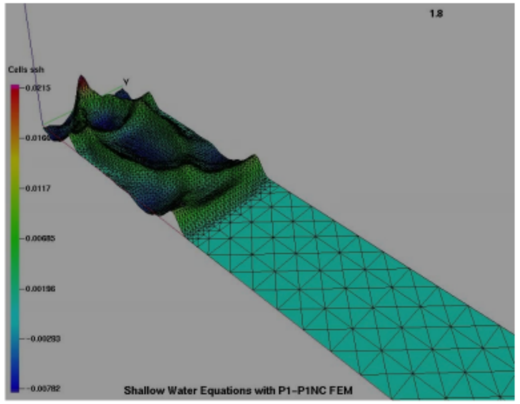

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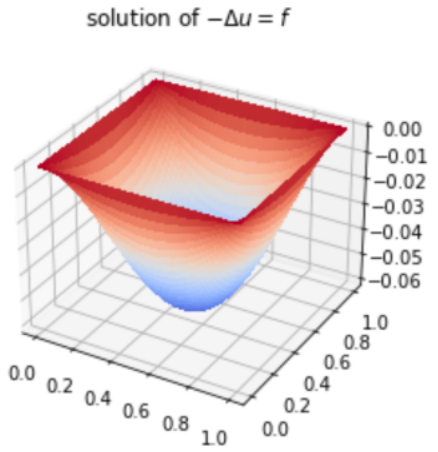

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Simple Example of Caution

Consider: Transport Equation:

$$\frac{\partial \rho}{\partial t} + v\frac{\partial \rho}{\partial x} = 0,$$

where $\rho : \mathbb{R} \times (0,T] \to \mathbb{R}$, is unknown function (e.g. a density);
$v \equiv 1$ is a constant unit velocity.
Furthermore, let $\rho(x,0) = \rho_0$ and initial condition.

Definition: (Grid Function)
For a function $f : [a,b] \to \mathbb{R}$, $[a,b] \subset \mathbb{R}$, we define a subdivision, called grid:

$$x_i = i \cdot \Delta x,$$

where $i = 0, \ldots, N$, $\Delta x = \frac{b-a}{N}$, such that $x_0 = a$ and $x_N = b$ and x_i are equi-spaced.

With the grid, we can define a grid function $f_\Delta : \{x_i\}_{i=1,\ldots,N} \to \mathbb{R}^N$ with

$$f_\Delta(x_i) := f(x_i).$$

We will often write $f_i = f_\Delta(x_i)$.

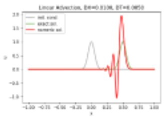
Result: We obtain an explicit formula to compute:

- $t = 0$: Start with $\rho_i^0 = \rho_0(x_i)$, $i = 0, \ldots, N$.
- $0 < t \leq T$: We propagate $t^j \to t^{j+1}$ $(j = 0, \ldots, L-1)$ by

$$\rho_i^{j+1} = \rho_i^j - \frac{\Delta t \cdot v_i^j}{2\Delta x}\left(\rho_{i+1}^j - \rho_{i-1}^j\right).$$

Note: on the right hand side only ρ^j appears.

Beware!



The computation is wrong!

Remark: (Finite Difference)
Later in this lectures, we will formally define a finite difference approximation.
Recall: the definition of a derivative of a C^1-function $f : \mathbb{R} \to \mathbb{R}$

$$\frac{df}{dx} = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}.$$

From this, we define a finite difference operator:

$$\delta_h f = \frac{f(x+h) - f(x)}{h} \approx \frac{df}{dx}.$$

Remark: Using grid $t^j = j \cdot \Delta t$, $j = 0, L$, $\Delta t = \frac{T}{L}$, and $x_i = i \cdot \Delta x$, $i = 0, N$, $\Delta x = \frac{b-a}{N}$, we can derive a finite difference approximation to transport equation

$$\frac{\partial \rho}{\partial t} + v\frac{\partial \rho}{\partial x} = 0,$$

by

$$\begin{aligned} &\delta_{\Delta t}^f \rho + v_i^j \delta_{\Delta x}^c \rho = 0, \\ \Rightarrow \quad &\frac{\rho_i^{j+1} - \rho_i^j}{\Delta t} + v_i^j \frac{\rho_{i+1}^j - \rho_{i-1}^j}{2\Delta x} = 0. \end{aligned}$$

Remark: Using a grid function f_i on a grid $x_i = i\Delta x$ $(i = 0, N)$, we may write

- forward finite difference: $\delta_h^f f_i = \frac{f_{i+1} - f_i}{\Delta x}$;
- backward finite difference: $\delta_h^b f_i = \frac{f_i - f_{i-1}}{\Delta x}$;
- centered finite difference: $\delta_h^c f_i = \frac{f_{i+1} - f_{i-1}}{2\Delta x}$;

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Remark: We may derive a

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- **backward finite difference**: $\delta_h^{\mathsf{b}} f = \frac{f(x)-f(x-h)}{h}$;
- **centered finite difference**: $\delta_h^{\mathsf{c}} f = \frac{f(x+h)-f(x-h)}{2h}$;

Remark: Using a grid function f_i on a grid $x_i = i\Delta x$ $(i = 0, N)$, we may write

- forward finite difference: $\delta_h^{\mathsf{f}} f_i = \frac{f_{i+1} - f_i}{\Delta x}$;
- backward finite difference: $\delta_h^{\mathsf{b}} f_i = \frac{f_i - f_{i-1}}{\Delta x}$;
- centered finite difference: $\delta_h^{\mathsf{c}} f_i = \frac{f_{i+1} - f_{i-1}}{2\Delta x}$;

Remark: Extension to partial derivatives is straight forward.

Remark: Using grid $t^j = j \cdot \Delta t$, $j = 0, L$, $\Delta t = \frac{T}{L}$, and $x_i = i \cdot \Delta x$, $i = 0, N$, $\Delta x = \frac{b-a}{N}$, we can derive a finite difference approximation to transport equation

$$\frac{\partial \rho}{\partial t} + v \frac{\partial \rho}{\partial x} = 0,$$

by

$$\begin{aligned} \delta^{\mathsf{f}}_{\Delta t} \rho + v_i^j \delta^{\mathsf{c}}_{\Delta x} \rho = 0, \\ \Rightarrow \quad \frac{\rho_i^{j+1} - \rho_i^j}{\Delta t} + v_i^j \frac{\rho_{i+1}^j - \rho_{i-1}^j}{2\Delta x} = 0. \end{aligned}$$

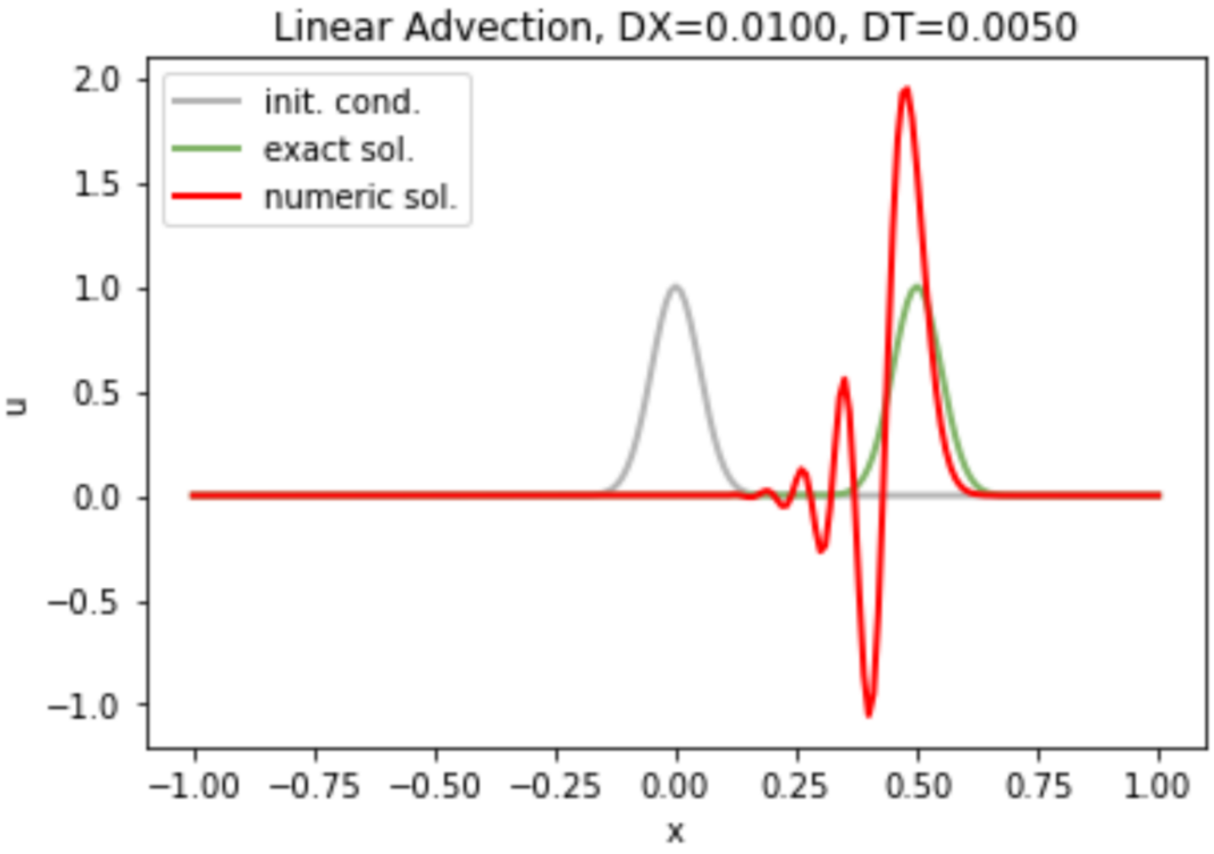
Result: We obtain an explicit formula to compute:

- $t = 0$: Start with $\rho_i^0 = \rho_0(x_i)$, $i = 0, \ldots, N$.
- $0 < t \leq T$: We propagate $t^j \to t^{j+1}$ $(j = 0, \ldots, L-1)$ by

$$\rho_i^{j+1} = \rho_i^j - \frac{\Delta t \cdot v_i^j}{2\Delta x}\left(\rho_{i+1}^j - \rho_{i-1}^j\right).$$

Note: on the right hand side only ρ^j appears.

Beware!



The computation is wrong!

Recap: Numerical Methods

Solution of Linear Systems

Interpolation and Quadrature

Condition and Stability

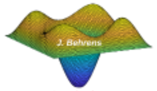
Steps in Scientific Computing

Mantra of Numerical Analysis

1. Is there a solution?
2. Is the solution unique?
3. Is there an algorithm?
4. Is the algorithm efficient?
5. Is the solution accurate?

Recap: Partial Differential Equations

Numerical Approximation of Partial Differential Equations
Finite Difference and Finite Volume Methods



Introduction

Motivation

Geometry

Dimensionality

Complexity

Applicability

Knowledge Gain

Simple Example of Caution

Beware!