Scientific Computing I

Module 10: Case Study – Computational Fluid Dynamics

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Fluid mechanics as a Discipline

Prominent discipline of application for numerical simulations:

- *experimental* fluid mechanics: wind tunnel studies, laser Doppler anemometry, hot wire techniques, ...
- *theoretical* fluid mechanics: investigations concerning the derivation of turbulence models, e.g.
- *computational* fluid mechanics (CFD): numerical simulations

Many fields of application:

- aerodynamics: aircraft design, car design,. . .
- thermodynamics: heating, cooling,. . .
- process engineering: combustion
- material science: crystal growth
- astrophysics: accretion disks
- geophysics: mantle convection, climate/weather prediction, tsunami simulation, . . .

Part I: Modelling

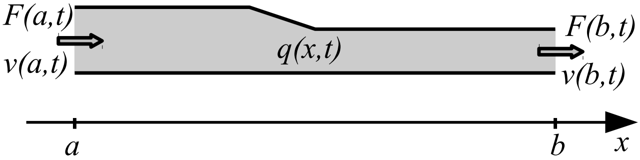
Fluids and Flows

- *ideal* or *real* fluids
  $\rightarrow$ "ideal": no resistance to tangential forces
- *compressible* or *incompressible* fluids
  $\rightarrow$ volume change of gases (vs. liquids?) under pressure
- *viscous* or *inviscid* fluids
  $\rightarrow$ think of the different characteristics of honey and water
- *Newtonian* and *non-Newtonian* fluids
  $\rightarrow$ the latter may show some elastic behaviour (e.g. in liquids with particles like blood)
- *laminar* or *turbulent* flows
  $\rightarrow$ turbulence: unsteady, 3D, high vorticity, vortices of different scales, high transport of energy between scales

Mathematical Models for CFD

- typically: all require different models
- our focus here: incompressible, viscous, Newtonian, laminar
  - $\rightarrow$ **incompressible Navier-Stokes Equations**
  - $\rightarrow$ **Shallow Water Equations**
- starting point: continuum mechanics
  - $\rightarrow$ macroscopic properties (pressure, density, velocity field)
  - $\rightarrow$ compared to stochastic or micro-/mesoscopic approaches (lattice Boltzman method, e.g.)
- relies on basic conservation laws (remember the heat equation): conservation of *mass* and *momentum* (and energy)
- additionally: slight focus on *Finite Volume Methods*

Advection Equation



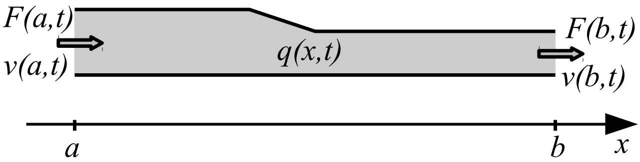
Conservation of some quantity q in a fluid domain $\Omega = [a, b]$ with given velocity $v(x, t)$:

- total amount/mass of q in $\Omega = [a, b]$ is given by $\int_a^b q(x, t)\,\mathrm{d}x$
- change of mass can only happen due to in-/outflow at a and b:

$$\frac{\partial}{\partial t}\int_a^b q(x, t)\,\mathrm{d}x = F(a, t) - F(b, t) = -F(x, t)\big|_a^b = -\int_a^b \frac{\partial}{\partial x}F(x, t)\,\mathrm{d}x$$

- note: $F(a, t)$ and $-F(b, t)$ denote an inflow into the domain Ω

Advection Equation (2)



Consider

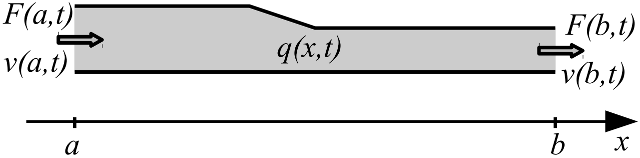
- flux function $F(x,t)$ depends on velocity $v(x,t)$, density $q(x,t)$ and the pipe's cross-sectional area $A(x)$:

$$F(x,t) = A(x)v(x,t)q(x,t)$$

- for simplicity, we set $A(x) = 1$, and obtain:

$$\frac{\partial}{\partial t}\int_a^b q(x,t)\,\mathrm{dx} = -\int_a^b \frac{\partial}{\partial x}F(x,t)\,\mathrm{dx} = -\int_a^b \frac{\partial}{\partial x}\big(v(x,t)q(x,t)\big)\,\mathrm{dx}$$

Advection Equation (3)



Advection Equation:

- for smooth functions, we may write:

$$\int_a^b \frac{\partial}{\partial t} q(x,t)\,\mathrm{dx} = \frac{\partial}{\partial t}\int_a^b q(x,t)\,\mathrm{dx} = -\int_a^b \frac{\partial}{\partial x}\big(v(x,t)q(x,t)\big)\,\mathrm{dx}$$

- as this equation has to hold for any $\Omega = [a,b]$, we demand:

$$\frac{\partial}{\partial t} q(x,t) = -\frac{\partial}{\partial x}\big(v(x,t)q(x,t)\big) \quad \text{or short:} \quad q_t + (vq)_x = 0$$

Advection and Diffusion

Diffusion

- even in a fluid at rest, an inhomogeneous density $q(x,t)$ will slowly change towards a uniform density q_0 due to molecular processes $\rightarrow$ **diffusion**
- *Fick's law of diffusion*: resulting flux is prop. to gradient of q

$$-F_{\text{diff}} = \beta q_x$$

- to model both advection and diffusion, we have $-F = -vq + \beta q_x$, and thus

$$q_t + (vq)_x = \beta q_{xx}$$

- special case $q_t = 0 \rightsquigarrow$ **"advection-diffusion equation"**:

$$-\beta q_{xx} + (vq)_x = 0$$

1D Euler Equations

- with our quantity q being the mass density ρ, we obtain an equation for the **conservation of mass**:

$$\rho_t + (v\rho)_x = 0$$

- another conservation property is that of momentum ρv; here, the flux term includes the pressure p:

$$F_{\text{mom}} = \rho v^2 + p$$

- thus, we obtain as equation for the **conservation of momentum**:

$$(\rho v)_t + (\rho v^2 + p)_x = 0$$

- we obtain a system of two PDEs, the **1D Euler Equations**
- to close the system, we need a relation between ρ and p (using the ideal gas law, e.g.)
- we might add an equation for temperature (derived from the conservation of internal energy)

Conservation Laws in Higher Dimensions

- in 2D, a conservation law for quantity q takes the form:

$$q_t + F(q)_x + G(q)_y = 0$$

- or similar in 3D:

$$q_t + F(q)_x + G(q)_y + H(q)_z = 0$$

- for advection, the flux functions are

$$F(q) = uq \qquad G(q) = vq \qquad H(q) = wq$$

  where u, v, w are the velocity components in the three space dimensions x, y, z
- hence, for 2D we obtain a conservation law such as

$$q_t + (uq)_x + (vq)_y = 0$$

2D Euler Equations

- in 2D, with velocity components $u(x, y, t)$ and $v(x, y, t)$ the equation for **conservation of mass** reads:

$$\rho_t + (\rho u)_x + (\rho v)_y = 0$$

- similar, the two equation for **conservation of momentum** are:

$$(\rho u)_t + (\rho u^2 + p)_x + (\rho uv)_y = 0$$
$$(\rho v)_t + (\rho uv)_x + (\rho v^2 + p)_y = 0$$

- again, we assume constant temperature, and we need a relation between ρ and p to close the system
- the Euler equations model an inviscid (ideal) fluid
- we also neglect additional source terms, such as for gravity forces, etc.

Navier-Stokes Equations

- mass conservation/continuity equation is the same as for the Euler equations:

$$\rho_t + (\rho u)_x + (\rho v)_y + (\rho w)_z = 0$$

or, written in vector notation:

$$\frac{\partial}{\partial t}\rho + \nabla \cdot (\rho \vec{u}) = 0, \qquad \nabla \cdot \vec{u} = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z}$$

- momentum conservation/momentum equations

$$\frac{\partial}{\partial t}(\rho \vec{u}) + \nabla \cdot (\vec{u} \otimes \rho \vec{u}) - \nabla \sigma - f = 0$$

- with σ being the *stress tensor*, which includes the pressure p and viscous forces: $\sigma = -pI + \ldots$
- f models external (volume) forces (gravity, e.g.)

Navier-Stokes Equations

Conservation and Convection Form

- the equations for mass and momentum, on the previous slide, are given in the so-called **conservation form**
- with the equations

  $$\nabla\cdot(\rho\vec{u}) = \vec{u}\cdot\nabla\rho+\rho\nabla\cdot\vec{u} \quad \text{and} \quad \nabla\cdot(\rho\vec{u}\otimes\vec{u}) = \vec{u}\big(\nabla\cdot(\rho\vec{u})\big)+(\rho\vec{u}\cdot\nabla)\vec{u},$$

  we obtain:

  $$\frac{\partial}{\partial t}\rho + \vec{u}\cdot\nabla\rho + \rho\nabla\cdot\vec{u} = 0$$

  $$\frac{\partial}{\partial t}(\rho\vec{u}) + \vec{u}\big(\nabla\cdot(\rho\vec{u})\big) + (\rho\vec{u}\cdot\nabla)\vec{u} - \nabla\sigma - f = 0$$

- with $\frac{\partial}{\partial t}(\rho\vec{u}) = \rho\frac{\partial}{\partial t}\vec{u} + \vec{u}\frac{\partial}{\partial t}\rho$

  and applying $\vec{u}\frac{\partial}{\partial t}\rho + \vec{u}\big(\nabla\cdot(\rho\vec{u})\big) = \vec{u}\big(\frac{\partial}{\partial t}\rho + \nabla\cdot(\rho\vec{u})\big) = 0$,

  we obtain for the momentum equation in **convection form**

  $$\rho\left(\frac{\partial}{\partial t}\vec{u} + (\vec{u}\cdot\nabla)\vec{u}\right) - \nabla\sigma - f = 0$$

Navier-Stokes Equations

Incompressible Equations

- in the convective forms

$$\frac{\partial}{\partial t}\rho + \vec{u} \cdot \nabla\rho + \rho\nabla \cdot \vec{u} = 0$$

$$\rho\left(\frac{\partial}{\partial t}\vec{u} + (\vec{u} \cdot \nabla)\vec{u}\right) - \nabla\sigma - f = 0$$

  we assume that the density ρ is constant: $\frac{\partial}{\partial t}\rho = 0$, $\nabla\rho = 0$

- we obtain obtain the **incompressible Navier-Stokes equations**:

$$\nabla \cdot \vec{u} = 0$$

$$\rho\left(\frac{\partial}{\partial t}\vec{u} + (\vec{u} \cdot \nabla)\vec{u}\right) - \nabla\sigma - f = 0$$

- "incompressible": the density does not change due to pressure or temperature, e.g.

Viscous Forces

Open question: stress tensor σ

- σ includes pressure p and viscosity tensor τ: $\sigma = -pI + \tau$
- *Newtonian* fluids: viscous stresses proportional to the strain rate (first derivatives)
- isotropic, **incompressible** fluids, Stokes assumption (no volume viscosity), then $\nabla\sigma = -\nabla p + \mu\Delta\vec{u}$
- μ the dynamic viscosity

Incompressible Navier-Stokes equations:

$$\nabla \cdot \vec{u} = 0$$

$$\rho\left(\frac{\partial}{\partial t}\vec{u} + (\vec{u}\cdot\nabla)\vec{u}\right) = -\nabla p + \mu\Delta\vec{u} + f$$

Dynamic Similarity of Flows

Dimensionless Form of the Navier-Stokes Equations

- we scale our unknowns to typical length scale L and velocity u_∞:

$$x \to \frac{x}{L} \qquad t \to \frac{u_\infty t}{L} \qquad u \to \frac{u}{u_\infty} \qquad p \to \frac{p - p_\infty}{\rho u_\infty^2}$$

- and obtain the dimensionless form of the Navier-Stokes equations:

$$\nabla \cdot \vec{u} = 0$$

$$\frac{\partial}{\partial t}\vec{u} + (\vec{u} \cdot \nabla)\vec{u} = -\nabla p + \frac{1}{\mathrm{Re}}\Delta \vec{u} + f$$

introducing the **Reynolds number** $\mathrm{Re} := \frac{\mu}{\rho u_\infty L}$

- important corollary: flows with the same Reynolds number will show the same behaviour

Boundary Conditions (here only velocity)

- **no-slip:** the fluid can not penetrate the wall and sticks to it
$$\vec{u} = 0.$$
- **free-slip:** the fluid can not penetrate the wall but does not stick to it
$$u_{\vec{n}} = 0, \frac{\partial \vec{u}_{\|}}{\partial \vec{n}} = 0.$$
- **inflow:** both tangential and normal velocity components are prescribed
$$\vec{u} = \vec{u}_{\text{inflow}}.$$
- **outflow:** should be "do nothing"; simple option: all velocity components do not change in normal direction
$$\frac{\partial \vec{u}}{\partial \vec{n}} = 0.$$
- **periodic:** same velocity and pressure at inlet and outlet
$$\vec{u}_{\text{in}} = \vec{u}_{\text{out}}.$$

Part II: A Finite Difference/Volume Method for the Incompressible Navier-Stokes Equations

Numerical Treatment – Spatial Derivatives

Finite Volume Discretisation and Upwind Flux
Marker-and-Cell Method, Staggered Grid
Discretization of Continuity Equation
Discretization of Momentum Equation

Time Discretization

Chorin Projection

Implementation

Finite Volume Discretisation – Advection-Diffusion Equation

- compute tracer concentration q with diffusion β and convection v:

  $$-\beta q_{xx} + (vq)_x = 0 \qquad \text{on } \Omega = (0,1)$$

  with boundary conditions $q(0) = 1$ and $q(1) = 0$.
- equidistant grid points $x_i = ih$, grid cells $[x_i, x_{i+1}]$
- back to representation via conservation law (for one grid cell):

  $$\int_{x_i}^{x_{i+1}} \frac{\partial}{\partial x} F(x)\,\mathrm{d}x = F(x)\Big|_{x_i}^{x_{i+1}} = 0$$

  with $F(x) = F(q(x)) = -\beta q_x(x) + vq(x)$.
- we need to compute the flux F at the boundaries of the grid cells; however, assume $q(x)$ piecewise constant within the grid cells

Finite Volume Discretisation – Advection-Diffusion Equation (2)

- wanted: compute $F(x_i)$ with $F(q(x)) = -\beta q_x(x) + vq(x)$
- where $q(x) := q_i$ for each $\Omega_i = [x_i, x_{i+1}]$
- computing the diffusive flux is straightforward:

$$-\beta q_x\big|_{x_{i+1}} = -\beta \frac{q(x_{i+1}) - q(x_i)}{h}$$

- options for advective flux vq:
  - symmetric flux:

$$vq\big|_{x_{i+1}} = \frac{vq(x_i) + vq(x_{i+1})}{2}$$

  - "upwind" flux:

$$vq\big|_{x_{i+1}} = \begin{cases} vq(x_i) & \text{if } v > 0 \\ vq(x_{i+1}) & \text{if } v < 0 \end{cases}$$

Finite Volume Discretisation – Advection-Diffusion Equation (3)

- system of equations: for all i

$$F(x)\Big|_{x_i}^{x_{i+1}} = F(x_{i+1}) - F(x_i) = 0$$

- for symmetric flux:

$$-\beta \frac{q(x_{i+1}) - 2q(x_i) + q(x_{i-1})}{h^2} + v \frac{q(x_{i+1}) - q(x_{i-1})}{2h} = 0$$

  leads to non-physical behaviour as soon as $\beta < \frac{vh}{2}$
  (observe signs of matrix elements!)

- system of equations for upwind flux (assume $v > 0$):

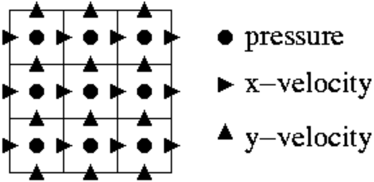
$$-\beta \frac{q(x_{i+1}) - 2q(x_i) + q(x_{i-1})}{h^2} + v \frac{q(x_i) - q(x_{i-1})}{h} = 0$$

  $\rightarrow$ stable, but overly diffusive solutions (positive definite matrix)

Marker-and-Cell Method – Staggered Grid

Marker-and-Cell method (Harlow and Welch, 1965):

- discretization scheme: Finite Differences
- can be shown to be equivalent to Finite Volumes, however
- based on a so-called **staggered grid**:
    - *Cartesian* grid (rectangular grid cells), with cell centres at $x_{i,j} := (ih, jh)$, e.g.
    - pressure located in cell centres
    - velocities (those in normal direction) located on cell edges



Spatial Discretisation – Continuity Equation:

- mass conservation: discretise $\nabla \cdot \vec{u}$
  $\rightarrow$ evaluate derivative at cell centres, allows central derivatives:

$$(\nabla \cdot \vec{u})\big|_{i,j} = \left.\frac{\partial u}{\partial x}\right|_{i,j} + \left.\frac{\partial v}{\partial y}\right|_{i,j} \approx \frac{u_{i,j} - u_{i-1,j}}{h} + \frac{v_{i,j} - v_{i,j-1}}{h}$$

  remember: $u_{i,j}$ and $v_{i,j}$ located on cell edges
- notation: $(\nabla \cdot \vec{u})\big|_{i,j} := (\nabla \cdot \vec{u})\big|_{x_{i,j}}$
  (evaluate expression at cell centre $x_{i,j}$)

Spatial Discretisation – Pressure Terms

- note: velocities located on midpoints of cell edges

$$\left.\frac{\partial u}{\partial t}\right|_{i+\frac{1}{2},j} = \ldots \qquad \left.\frac{\partial v}{\partial t}\right|_{i,j+\frac{1}{2}} = \ldots$$

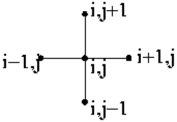
  thus, all derivatives need to be approximated at midpoints of cell edges!

- pressure term ∇p: central differences for first derivatives (as pressure is located in cell centres)

$$\left.\frac{\partial p}{\partial x}\right|_{i+\frac{1}{2},j} \approx \frac{p_{i+1,j} - p_{i,j}}{h} \qquad \left.\frac{\partial p}{\partial y}\right|_{i,j+\frac{1}{2}} \approx \frac{p_{i,j+1} - p_{i,j}}{h}$$

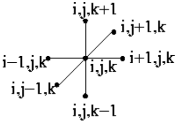
Spatial Discretisation – Diffusion Term

- for diffusion term $\Delta\vec{u}$: use standard 5- or 7-point stencil
- 2D:



$$\Delta u\Big|_{i,j} \approx \frac{u_{i-1,j} + u_{i,j-1} - 4u_{i,j} + u_{i+1,j} + u_{i,j+1}}{h^2}$$

- 3D:



$$\Delta u\Big|_{i,j,k} \approx \frac{u_{i-1,j,k} + u_{i,j-1,k} + u_{i,j,k-1} - 6u_{i,j,k} + u_{i+1,j,k} + u_{i,j+1,k} + u_{i,j,k+1}}{h^2}$$

Spatial Discretisation – Convection Terms

- treat derivatives of nonlinear terms $(\vec{u} \cdot \nabla)\vec{u}$:
- central differences (for momentum equation in x-direction):

$$u \frac{\partial u}{\partial x}\bigg|_{i+\frac{1}{2},j} \approx u_{i,j} \frac{u_{i+1,j} - u_{i-1,j}}{2h} \qquad v \frac{\partial u}{\partial y}\bigg|_{i+\frac{1}{2},j} \approx v\big|_{x_{i+\frac{1}{2},j}} \frac{u_{i,j+1} - u_{i,j-1}}{2h}$$

with $v\big|_{x_{i+\frac{1}{2},j}} = \frac{1}{4}\left(v_{i,j} + v_{i,j-1} + v_{i+1,j} + v_{i+1,j-1}\right)$

- upwind differences (for momentum equation in x-direction):

$$u \frac{\partial u}{\partial x}\bigg|_{x_{i+\frac{1}{2},j}} \approx u_{i,j} \frac{u_{i,j} - u_{i-1,j}}{2h} \qquad v \frac{\partial u}{\partial y}\bigg|_{x_{i+\frac{1}{2},j}} \approx v\big|_{x_{i+\frac{1}{2},j}} \frac{u_{i,j} - u_{i,j-1}}{2h}$$

if $u_{i,j} > 0$ and $v\big|_{x_{i+\frac{1}{2},j}} > 0$

- code for CFD lab will mix central and upwind differences (and is based on conservation form of convection terms)

Time Discretisation

- recall the incompressible Navier-Stokes equations:

$$\nabla \cdot \vec{u} = 0$$

$$\frac{\partial}{\partial t}\vec{u} + (\vec{u} \cdot \nabla)\vec{u} = -\nabla p + \frac{1}{\mathrm{Re}}\Delta\vec{u} + f$$

- note the role of the unknowns:
  - $\rightarrow$ 2 or 3 equations for velocities (x, y, and z component) resulting from momentum conservation
  - $\rightarrow$ 4th equation (mass conservation) to " close" the system; required to determine pressure p
  - $\rightarrow$ however, p does not occur explicitly in mass conservation
- possible approach: **Chorin's projection** method
  - $\rightarrow$ p acts as a variable to enforce the mass conservation as "side condition"

Time Discretisation – Chorin Projection

- explicit Euler scheme for momentum equation:

$$\vec{u}^{(n+1)} = \vec{u}^{(n)} + \tau \left(-\nabla p + \frac{1}{Re} \Delta \vec{u}^{(n)} - \left(\vec{u}^{(n)} \cdot \nabla \right) \vec{u}^{(n)} + \vec{g} \right)$$

- Chorin projection
  $\rightarrow$ compute intermediate velocity that neglects pressure:

$$\vec{u}^{(n+\frac{1}{2})} = \vec{u}^{(n)} + \tau \left(\frac{1}{Re} \Delta \vec{u}^{(n)} - \left(\vec{u}^{(n)} \cdot \nabla \right) \vec{u}^{(n)} + \vec{g} \right),$$

$$\vec{u}^{(n+1)} = \vec{u}^{(n+\frac{1}{2})} - \tau \nabla p$$

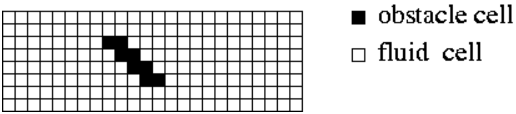
- $\vec{u}^{(n+1)}$ needs to satisfy mass conservation: $\nabla \cdot \vec{u}^{(n+1)} = 0$
  $\rightarrow$ leads to a Poisson equation for the pressure:

$$\nabla \cdot \left(\vec{u}^{(n+\frac{1}{2})} - \tau \nabla p \right) = 0 \quad \Rightarrow \quad \Delta p = \frac{1}{\tau} \left(\nabla \cdot \vec{u}^{(n+\frac{1}{2})} \right)$$

  thus, system of linear equations to be solved in each time step

Implementation

- geometry representation as a flag field *(Marker-and-Cell)*



flag field as an array of booleans:

```
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 1 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 1 1 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 1 1 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 1 1 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
```

- input data (boundary conditions) and output data (computed results) as arrays

Implementation (2)

Lab course *"Scientific Computing – Computational Fluid Dynamics"*:

- modular C-code
- parallelization:
  - simple data parallelism, domain decomposition
  - straightforward MPI-based parallelization (exchange of ghost layers)
- target architectures:
  - parallel computers with distributed memory
  - clusters
- possible extensions:
  - free-surface flows ("the falling drop")
  - multigrid solver for the pressure equation
  - heat transfer or turbulence models

Part III: The Shallow Water Equations and Finite Volumes Revisited

The Shallow Water Equations

$$\frac{\partial}{\partial t}\begin{pmatrix} h \\ hu \\ hv \end{pmatrix} + \frac{\partial}{\partial x}\begin{pmatrix} hu \\ hu^2 + \frac{1}{2}gh^2 \\ huv \end{pmatrix} + \frac{\partial}{\partial y}\begin{pmatrix} hv \\ huv \\ hv^2 + \frac{1}{2}gh^2 \end{pmatrix} = S(t,x,y)$$

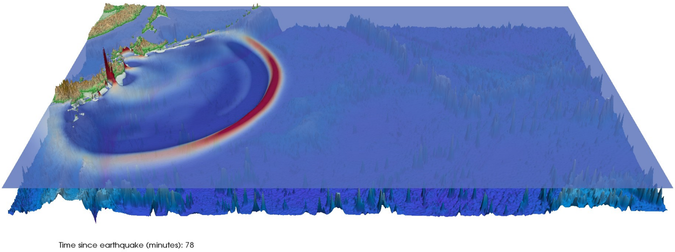
Comments on modelling:

- generalized 2D hyperbolic PDE: $q = (h, hu, hv)^T$

  $$\frac{\partial}{\partial t}q + \frac{\partial}{\partial x}F(q) + \frac{\partial}{\partial y}G(q) = S(t,x,y)$$

  derived from conservations laws for mass and momentum
- may be derived by vertical averaging from the 3D incompressible Navier-Stokes equations
- compare to Euler equations: density ρ vs. water depth h

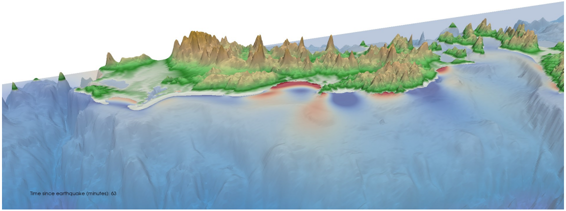
Modelling Scenario: Tsunami Simulation



The Ocean as “Shallow Water”??

- compare horizontal ($\sim$ 1000 km) to vertical ($\sim$ 5 km) length scale
- wave lengths large compared to water depth
- vertical flow may be neglected; movement of the “entire water column”

Modelling Scenario: Tsunami Simulation (2)



Tsunami Modelling with the Shallow Water equations:

- source term $S(x, y)$ includes bathymetry data (i.e., elevation of ocean floor)
- Coriolis forces, friction, etc., as possible further terms
- boundary conditions are difficult: coastal inundation, outflow at domain boundaries

Finite Volume Discretisation

- discretise system of PDEs

$$\frac{\partial}{\partial t} q + \frac{\partial}{\partial x} F(q) + \frac{\partial}{\partial y} G(q) = S(t, x, y)$$

- with

$$q := \begin{pmatrix} h \\ hu \\ hv \end{pmatrix} \quad F(q) := \begin{pmatrix} hu \\ hu^2 + \frac{1}{2} g h^2 \\ huv \end{pmatrix} \quad G(q) := \begin{pmatrix} hv \\ huv \\ hv^2 + \frac{1}{2} g h^2 \end{pmatrix}$$

- basic form of numerical schemes:

$$Q_{i,j}^{(n+1)} = Q_{i,j}^{(n)} - \frac{\tau}{h}\left(F_{i+\frac{1}{2},j}^{(n)} - F_{i-\frac{1}{2},j}^{(n)}\right) - \frac{\tau}{h}\left(G_{i,j+\frac{1}{2}}^{(n)} - G_{i,j-\frac{1}{2}}^{(n)}\right)$$

where $F_{i+\frac{1}{2},j}^{(n)}$, $G_{i,j+\frac{1}{2}}^{(n)}, \ldots$ approximate the flux functions $F(q)$ and $G(q)$ at the grid cell boundaries

Central and Upwind Fluxes

- define fluxes $F^{(n)}_{i+\frac{1}{2},j}$, $G^{(n)}_{i,j+\frac{1}{2}}$, ... via 1D numerical flux function $\mathcal{F}$:

$$F^{(n)}_{i+\frac{1}{2}} = \mathcal{F}\left(Q^{(n)}_i, Q^{(n)}_{i+1}\right) \qquad G^{(n)}_{j-\frac{1}{2}} = \mathcal{F}\left(Q^{(n)}_{j-1}, Q^{(n)}_j\right)$$

- **central flux**:

$$F^{(n)}_{i+\frac{1}{2}} = \mathcal{F}\left(Q^{(n)}_i, Q^{(n)}_{i+1}\right) := \frac{1}{2}\left(F\left(Q^{(n)}_i\right) + F\left(Q^{(n)}_{i+1}\right)\right)$$

  leads to unstable methods for convective transport

- **upwind flux** (here, for h-equation, $F(h) = hu$):

$$F^{(n)}_{i+\frac{1}{2}} = \mathcal{F}\left(h^{(n)}_i, h^{(n)}_{i+1}\right) := \begin{cases} hu\big|_i & \text{if } u\big|_{i+\frac{1}{2}} > 0 \\ hu\big|_{i+1} & \text{if } u\big|_{i+\frac{1}{2}} < 0 \end{cases}$$

  stable, but includes artificial diffusion

(Local) Lax-Friedrichs Flux

- classical **Lax-Friedrichs method** uses as numerical flux:

$$F^{(n)}_{i+\frac{1}{2}} = \mathcal{F}\left(Q^{(n)}_i, Q^{(n)}_{i+1}\right) := \frac{1}{2}\left(F\left(Q^{(n)}_i\right) + F\left(Q^{(n)}_{i+1}\right)\right) - \frac{h}{2\tau}\left(Q^{(n)}_{i+1} - Q^{(n)}_i\right)$$

- can be interpreted as central flux plus diffusion flux:

$$\frac{h}{2\tau}\left(Q^{(n)}_{i+1} - Q^{(n)}_i\right) = \frac{h^2}{2\tau} \cdot \frac{Q^{(n)}_{i+1} - Q^{(n)}_i}{h}$$

  with diffusion coefficient $\frac{h^2}{2\tau}$, where $c := \frac{h}{\tau}$ is some kind of velocity ("one grid cell per time step")

- idea of **local Lax-Friedrichs** method: use the "appropriate" velocity

$$F^{(n)}_{i+\frac{1}{2}} := \frac{1}{2}\left(F\left(Q^{(n)}_i\right) + F\left(Q^{(n)}_{i+1}\right)\right) - \frac{a_{i+\frac{1}{2}}}{2}\left(Q^{(n)}_{i+1} - Q^{(n)}_i\right)$$

Wave Speed of Tsunamis

- consider the 1D case

$$\frac{\partial}{\partial t}\begin{pmatrix} h \\ hu \end{pmatrix} + \frac{\partial}{\partial x}\begin{pmatrix} hu \\ hu^2 + \frac{1}{2}gh^2 \end{pmatrix} = 0$$

- with $q = (q_1, q_2)^T := (h, hu)^T$, we obtain

$$\frac{\partial}{\partial t}\begin{pmatrix} q_1 \\ q_2 \end{pmatrix} + \frac{\partial}{\partial x}\begin{pmatrix} q_2 \\ q_2^2/q_1 + \frac{1}{2}gq_1^2 \end{pmatrix} = 0$$

- write in convective form:

$$\frac{\partial}{\partial t}\begin{pmatrix} q_1 \\ q_2 \end{pmatrix} + f'\frac{\partial}{\partial x}\begin{pmatrix} q_1 \\ q_2 \end{pmatrix} = 0$$

with

$$f' = \begin{pmatrix} \partial f_1/\partial q_1 & \partial f_1/\partial q_2 \\ \partial f_2/\partial q_1 & \partial f_2/\partial q_2 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -q_2^2/q_1^2 + gq_1 & 2q_2/q_1 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -u^2 + gh & 2u \end{pmatrix}$$

Wave Speed of Tsunamis (2)

- compute eigenvectors and eigenvalues of f':

$$\lambda^{1/2} = u \pm \sqrt{gh} \qquad r^{1/2} = \begin{pmatrix} 1 \\ u \pm \sqrt{gh} \end{pmatrix}$$

- and then with $f' = R \Lambda R^{-1}$, where $R := (r^1, r^2)$ and $\Lambda := \operatorname{diag}(\lambda^1, \lambda^2)$, we can diagonalise the PDE:

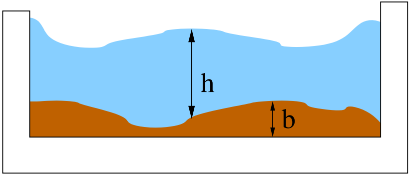
$$\frac{\partial}{\partial t}\begin{pmatrix} w_1 \\ w_2 \end{pmatrix} + \Lambda \frac{\partial}{\partial x}\begin{pmatrix} w_1 \\ w_2 \end{pmatrix} = 0, \qquad w = R^{-1} q$$

- for small changes in h and small velocities, we thus obtain that waves are "advected" (i.e., travel) at speed $\lambda^{1/2} \approx \pm\sqrt{gh}$
- recall local Lax-Friedrichs method:

$$F^{(n)}_{i+\frac{1}{2}} := \frac{1}{2}\left(F\left(Q^{(n)}_i\right) + F\left(Q^{(n)}_{i+1}\right)\right) - \frac{a_{i+\frac{1}{2}}}{2}\left(Q^{(n)}_i - Q^{(n)}_{i-1}\right)$$

$\rightarrow$ choose $a_{i+\frac{1}{2}} = \max\{\lambda^k\}$

Shallow Water Equations with Bathymetry



$$\frac{\partial}{\partial t}\begin{pmatrix} h \\ hu \\ hv \end{pmatrix} + \frac{\partial}{\partial x}\begin{pmatrix} hu \\ hu^2 + \frac{1}{2}gh^2 \\ huv \end{pmatrix} + \frac{\partial}{\partial y}\begin{pmatrix} hv \\ huv \\ hv^2 + \frac{1}{2}gh^2 \end{pmatrix} = \begin{pmatrix} 0 \\ -(ghb)_x \\ -(ghb)_y \end{pmatrix}$$

Questions for numerics:

- treat $(bh)_x$ and $(bh)_y$ as source terms or include these into flux computations?
- preserve certain properties of solutions – e.g., “lake at rest”

Shallow Water Equations with Bathymetry (2)

Consider **"Lake at Rest"** Scenario:

- "at rest": velocities $u = 0$ and $v = 0$
- examine local Lax-Friedrichs flux in h equation:

$$F^{(n)}_{i+\frac{1}{2}} = \frac{1}{2}\left((hu)^{(n)}_i + (hu)^{(n)}_{i+1}\right) - \frac{a_{i+\frac{1}{2}}}{2}\left(h^{(n)}_{i+1} - h^{(n)}_i\right) = 0$$

$$\Rightarrow F^{(n)}_{i+\frac{1}{2}} - F^{(n)}_{i-\frac{1}{2}} = -\frac{a_{i+\frac{1}{2}}}{2}\left(h^{(n)}_{i+1} - h^{(n)}_i\right) + \frac{a_{i-\frac{1}{2}}}{2}\left(h^{(n)}_i - h^{(n)}_{i-1}\right) = 0$$

- note: $a_{i\pm\frac{1}{2}} \approx \sqrt{gh}$ and if $b_{i-1} \neq b_i \neq b_{i+1}$ then $h_{i-1} \neq h_i \neq h_{i+1}$
- thus: "lake at rest" not an equilibrium solution for local Lax-Friedrichs flux

Additional problems:

- complicated numerics close to the shore
- in particular: "wetting and drying" (inundation of the coast)

SWE – An Education-Oriented Shallow Water Code

Model & Discretisation

Simplified setting (no friction, no viscosity, no coriolis forces, etc.):

$$\begin{pmatrix} h \\ hu \\ hv \end{pmatrix}_t + \begin{pmatrix} hu \\ hu^2 + \frac{1}{2}gh^2 \\ huv \end{pmatrix}_x + \begin{pmatrix} hv \\ huv \\ hv^2 + \frac{1}{2}gh^2 \end{pmatrix}_y = S(t,x,y).$$

Finite Volume Discretization:

- generalized 2D hyperbolic PDE: $q = (h, hu, hv)^T$

$$\frac{\partial}{\partial t}q + \frac{\partial}{\partial x}F(q) + \frac{\partial}{\partial y}G(q) = S(t,x,y)$$

- Wave propagation form:

$$\begin{aligned} Q_{i,j}^{n+1} = Q_{i,j}^{n} \quad & - \tfrac{\Delta t}{\Delta x}\left(\mathcal{A}^+\Delta Q_{i-1/2,j} + \mathcal{A}^-\Delta Q_{i+1/2,j}^n\right) \\ & - \tfrac{\Delta t}{\Delta y}\left(\mathcal{B}^+\Delta Q_{i,j-1/2} + \mathcal{B}^-\Delta Q_{i,j+1/2}^n\right). \end{aligned}$$

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Model & Discretisation

Simplified setting (no friction, no viscosity, no coriolis forces, etc.):

$$\begin{pmatrix} h \\ hu \\ hv \end{pmatrix}_t + \begin{pmatrix} hu \\ hu^2 + \frac{1}{2}gh^2 \\ huv \end{pmatrix}_x + \begin{pmatrix} hv \\ huv \\ hv^2 + \frac{1}{2}gh^2 \end{pmatrix}_y = S(t,x,y).$$

Flux Computation on Edges:

- Wave propagation form:

$$\begin{aligned} Q_{i,j}^{n+1} = Q_{i,j}^{n} \quad & - \frac{\Delta t}{\Delta x}\left(\mathcal{A}^+\Delta Q_{i-1/2,j} + \mathcal{A}^-\Delta Q^n_{i+1/2,j}\right) \\ & - \frac{\Delta t}{\Delta y}\left(\mathcal{B}^+\Delta Q_{i,j-1/2} + \mathcal{B}^-\Delta Q^n_{i,j+1/2}\right). \end{aligned}$$

- simple fluxes: Rusanov/(local) Lax-Friedrich
- more advanced: f-Wave or (augmented) Riemann solvers (George, 2008; LeVeque, 2011), no limiters

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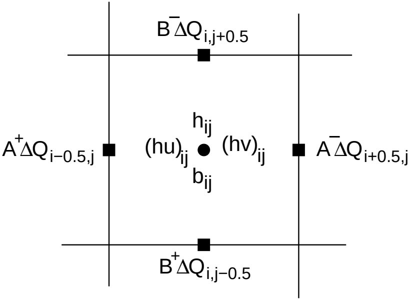
Unknowns and Numerical Fluxes



Unknowns and Numerical Fluxes:

- unknowns h, hu, hv, and b located in cell centers
- two sets of "net updates"/numerical fluxes per edge: $\mathcal{A}^+\Delta Q_{i-1/2,j}$, $\mathcal{B}^-\Delta Q_{i,j+1/2}$, etc.

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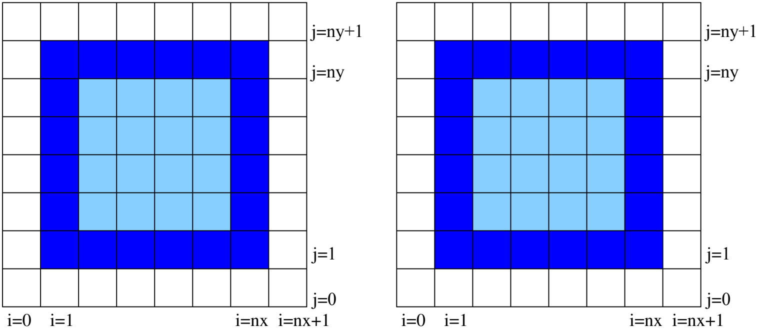
Patches of Cartesian Grid Blocks



Spatial Discretization:

- regular Cartesian meshes; allow multiple patches
- ghost and copy layers to implement boundary conditions, for more complicated domains, and for parallelization

References and Literature

Course material is mostly based on:

- R. J. LeVeque: *Finite Volume Methods for Hyperbolic Equations*, Cambridge Texts in Applied Mathematics, 2002.
- M. Griebel, T. Dornseifer and T. Neunhoeffer: *Numerical Simulation in Fluid Dynamics: A Practical Introduction*, SIAM Monographs on Mathematical Modeling and Computation, SIAM, 1997.

Shallow Water Code SWE:
→ `http://www5.in.tum.de/SWE/`