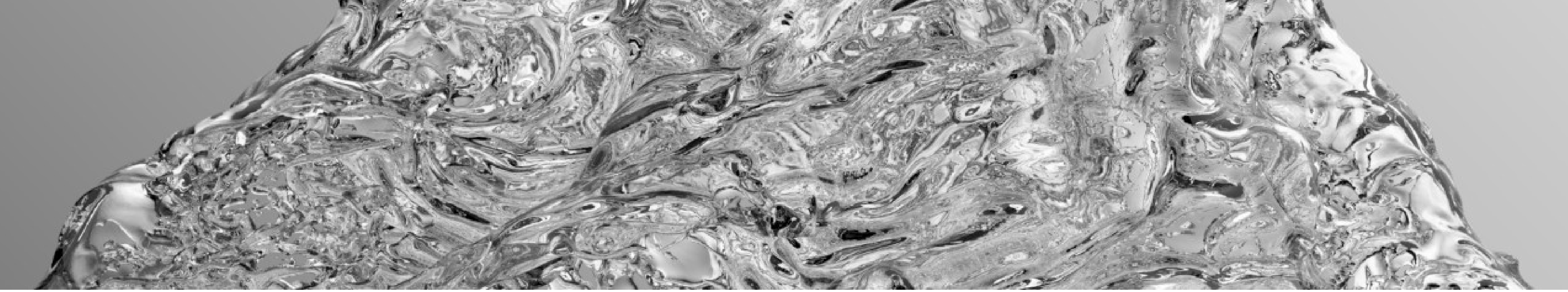


EEN-E2001 Computational Fluid Dynamics

Lecture 1: Partial Differential Equations and Finite Difference Method

Prof. Ville Vuorinen

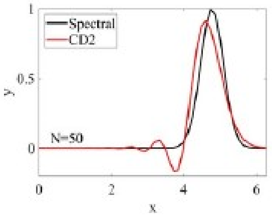
January 16th 2023

Aalto University, School of Engineering

Lecture 1: Linear PDEs and finite difference method

$$\frac{\partial T}{\partial t} + \nabla \cdot T\boldsymbol{u} = \alpha \nabla^2 T$$

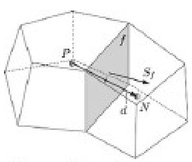
$$\frac{\partial T}{\partial x} \approx \frac{T_{i+1} - T_{i-1}}{2\Delta x}$$



Lecture 2: Gauss' theorem and finite volume method

$$\int_{\Omega} \nabla \cdot (T\boldsymbol{u})\, d\Omega = \int_{\partial\Omega} (T\boldsymbol{u}) \cdot \boldsymbol{n}\, dS$$

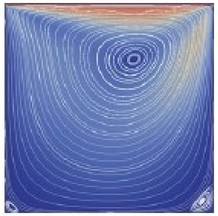
$$\int_{\partial\Omega} \boldsymbol{u} \cdot \boldsymbol{n}\, dS \approx \Sigma_f \boldsymbol{u}_f \cdot \boldsymbol{n}_f\, dS_f$$



Lecture 3: Navier-Stokes equation and pressure

$$\frac{\partial \boldsymbol{u}}{\partial t} + \nabla \cdot \boldsymbol{u}\boldsymbol{u} = -\nabla p + \nu \nabla^2 \boldsymbol{u}$$

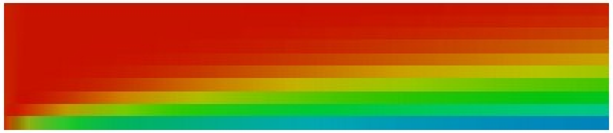
$$-\nabla^2 p = \nabla \cdot \nabla \cdot \boldsymbol{u}\boldsymbol{u}$$

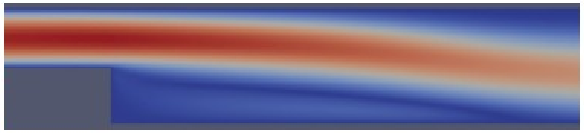


Lecture 4: OpenFOAM code and structure

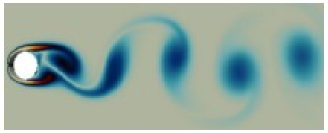
```
fvVectorMatrix UEqn
(
      fvm::ddt(U)
    + fvm::div(phi, U)
    - fvm::laplacian(nu, U)
);
```

Lecture 5: Simulating fluid physical phenomena: part A





Lecture 6: Simulating fluid physical phenomena: part B



CFD simulation and PDE solution includes at least the following aspects covered on the course

1) **Physics** identification. System length and timescales.

2) **Mathematical equations and physics interpretation** boundary/initial conditions.

3) **Objectives, feasibility, and time-constraints**.

4) **Numerical method and modeling assumptions**.

5) **Geometry and mesh generation**.

6) **Computing** i.e. running simulation.

7) **Visualization and post-processing**.

8) **Validation and verification, reference data**. Reporting, analysis and discussion of the results. Are the results sane?

Background

Introduction

Prof. V.Vuorinen

2004: M.Sc. (Tech.) computational physics/HUT.

2010: D.Sc.(Tech.) computational fluid dynamics/AALTO.

2014: Assistant professor in CFD in energy/AALTO.

2021: Research team ~ 8 PhD students, 6 Postdocs, 1 Senior researcher

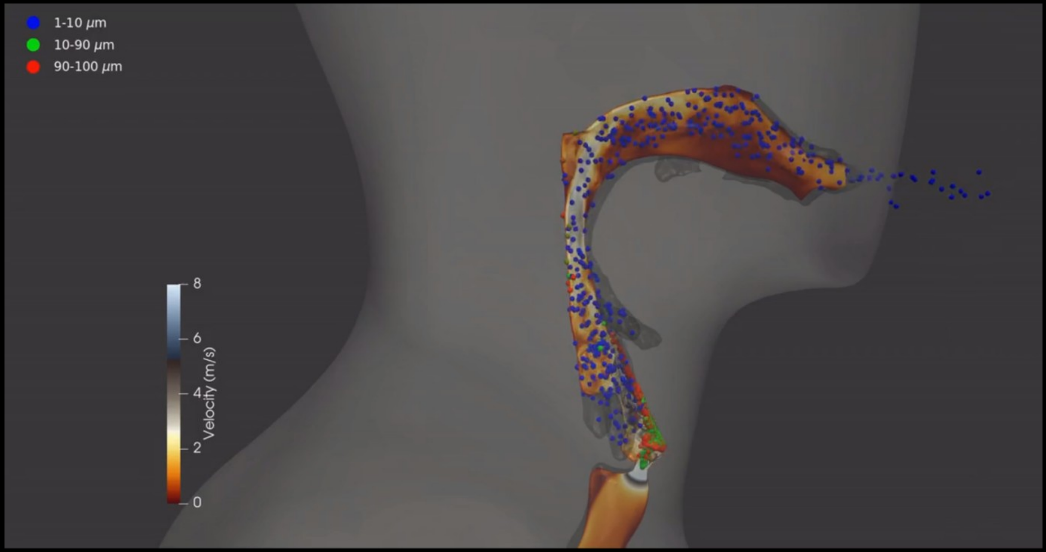
2021: Supervised 9 PhD thesis. Co-supervised additionally 3 PhD thesis

2021: ~90 journal publications, focus on scale-resolving CFD.

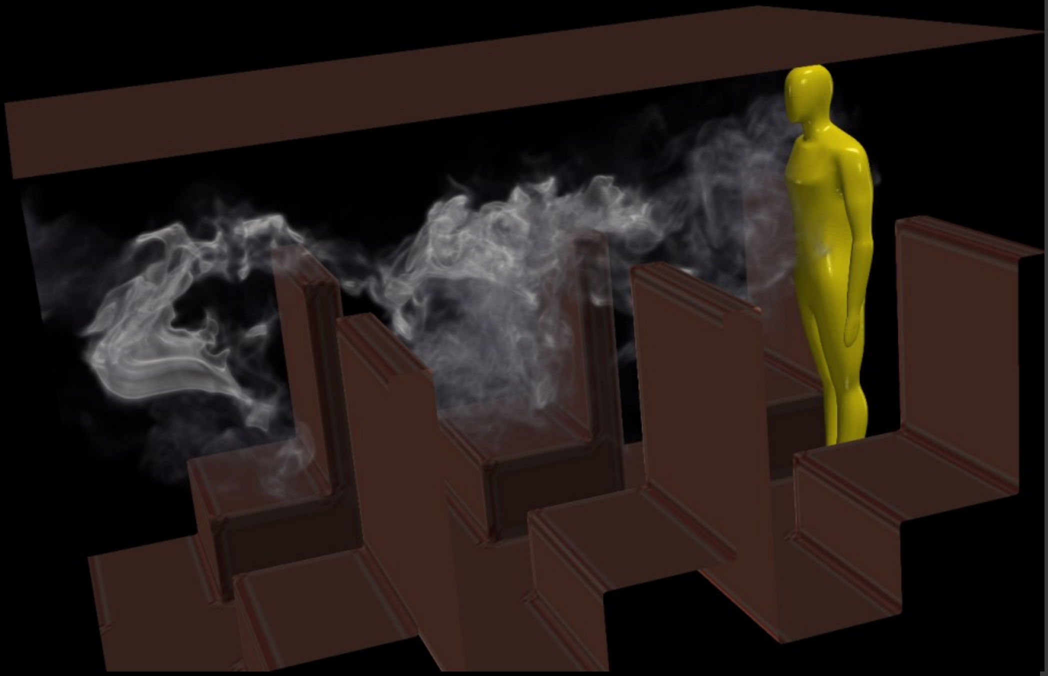
3/2020: Research on COVID-19
→ Early discovery of aerosol transmission and the “droplet paradigm”
→ 220+ media articles & SCICOM on #COVIDisAirborne

Application of CFD to airborne transmission investigations

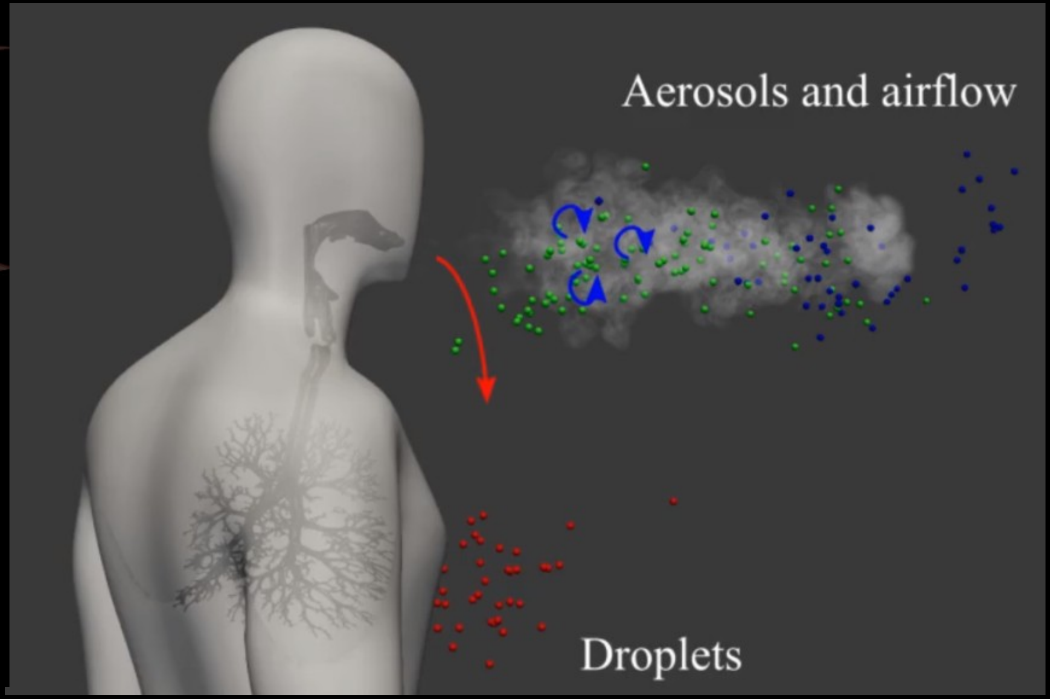
Simulation by:
M.Auvinen &A.Hellsten/FMI



Courtesy: E.Laurila
(submitted)



Simulation: V.Vuorinen
Visualization: M.Gadalla



Courtesy: M.Korhonen

Partial differential equations

Convection and diffusion as transport mechanisms

In fluid dynamics, we are interested in understanding how different variables – e.g. velocity/concentration/temperature - change in space (x,y,z) and time (t). Unknown functions below could be typically velocity and concentration fields.

Transport mechanisms: convection (velocity) and diffusion (molecular)

$$c = c(x, y, z, t)$$

$$\vec{u} = \vec{u}(x, y, z, t)$$

Ordinary differential equations (ODEs) describe commonly <u>time dependency</u> of physical system. No space coordinate dependency.

ODE for $y=y(t)=?$ (e.g. radioactivity decay/Newton's cooling law)

$$\frac{dy}{dt}=-\lambda y(t)$$

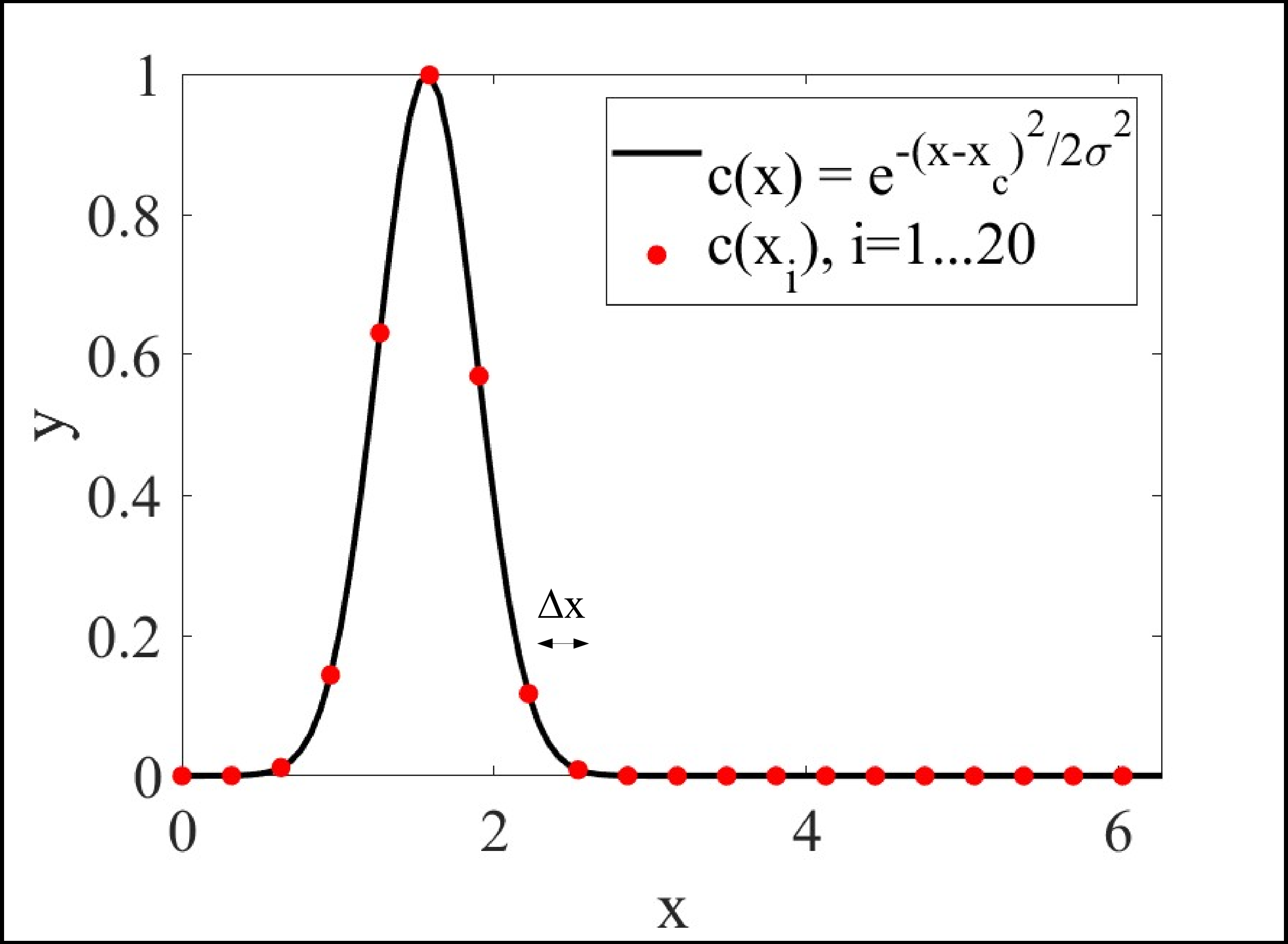
Initial condition

$$y(t=0)=y_o$$

Analytical solution

$$y(t)=y_o e^{-\lambda t}$$

First of all, to resolve space-dependent functions, we need enough many grid points i.e. high enough resolution.



Partial differential equations (PDEs) describe space-time dependency of a physical system.

Convection-diffusion (CD) eqn is the key PDE of fluid dynamics.

CD-eqn is a general conservation law (mass, momentum, energy,..)

Transported function $c=c(x,y,z,t)$

For example:
- virus concentration
- molecular concentration
- velocity component

Diffusivity [m^2/s]

Convection term

$$\frac{\partial c}{\partial t}+\vec{u}\cdot\nabla c=\alpha\nabla^2 c$$

Diffusion term

Velocity [*m/s*]

Smoke cloud moving in air can be accurately modeled by solving Navier-Stokes equation and CD-eqn for smoke concentration

$\vec{u} = \vec{u}(x, y, z, t)$

$c = c(x, y, z, t)$

$$\frac{\partial c}{\partial t} + \vec{u} \cdot \nabla c = \alpha \nabla^2 c$$

For a PDE problem to be well posed, it is necessary to have boundary and initial conditions.

E.g. convection-diffusion equation (1d)

$$\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x} = \alpha \frac{\partial^2 c}{\partial x^2}$$

Initial condition

$$c(x, t=0) = c_o(x)$$

Boundary conditions. **For example:** fixed values,

$$c(x=0) = c_1 \quad c(x=L) = c_2$$

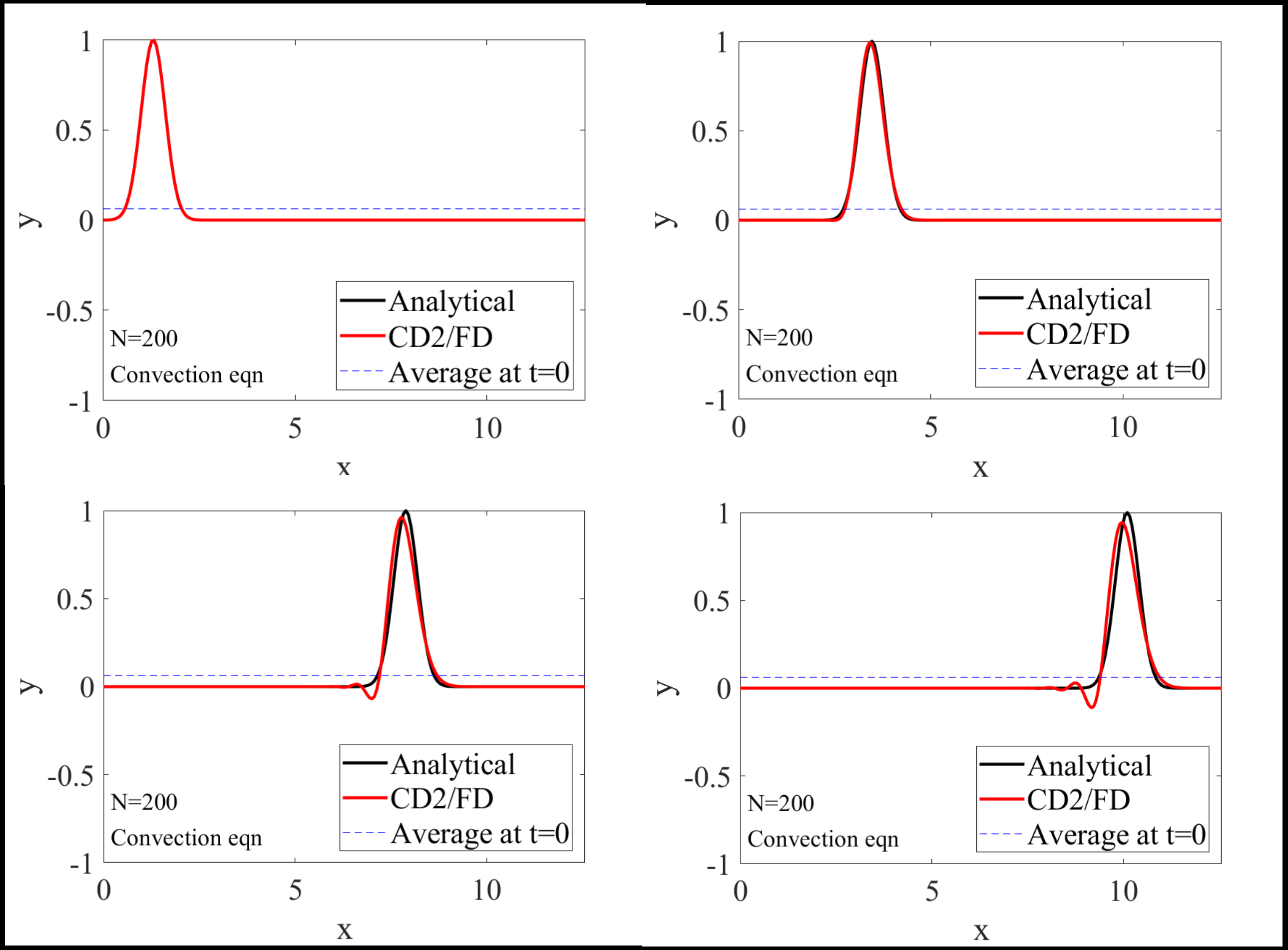
Convection equation (1d)

Analytical solution: shape maintained and function travels/shifts at velocity u

CD2/FD (central difference, 2nd order, finite difference): **numerical dispersion** is additionally noted at later times

E.g. concentration cloud moves due to wind.

$$\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x} = 0$$



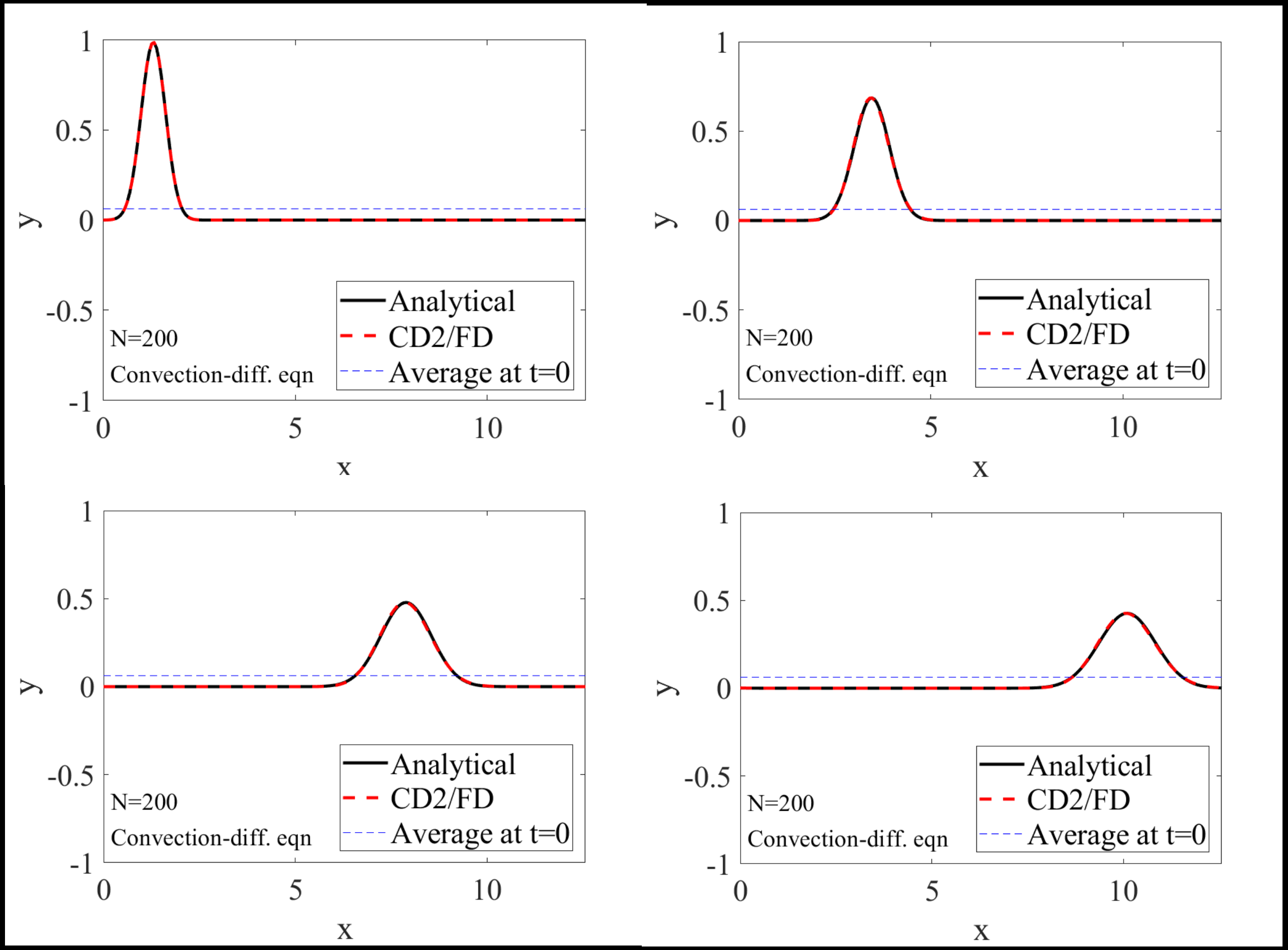
Convection-diffusion equation (1d)

Solutions travel at velocity u while amplitude decreases

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} = \alpha \frac{\partial^2 c}{\partial x^2}$$

c=e.g. temperature, concentration

α=diffusivity [m²/s]

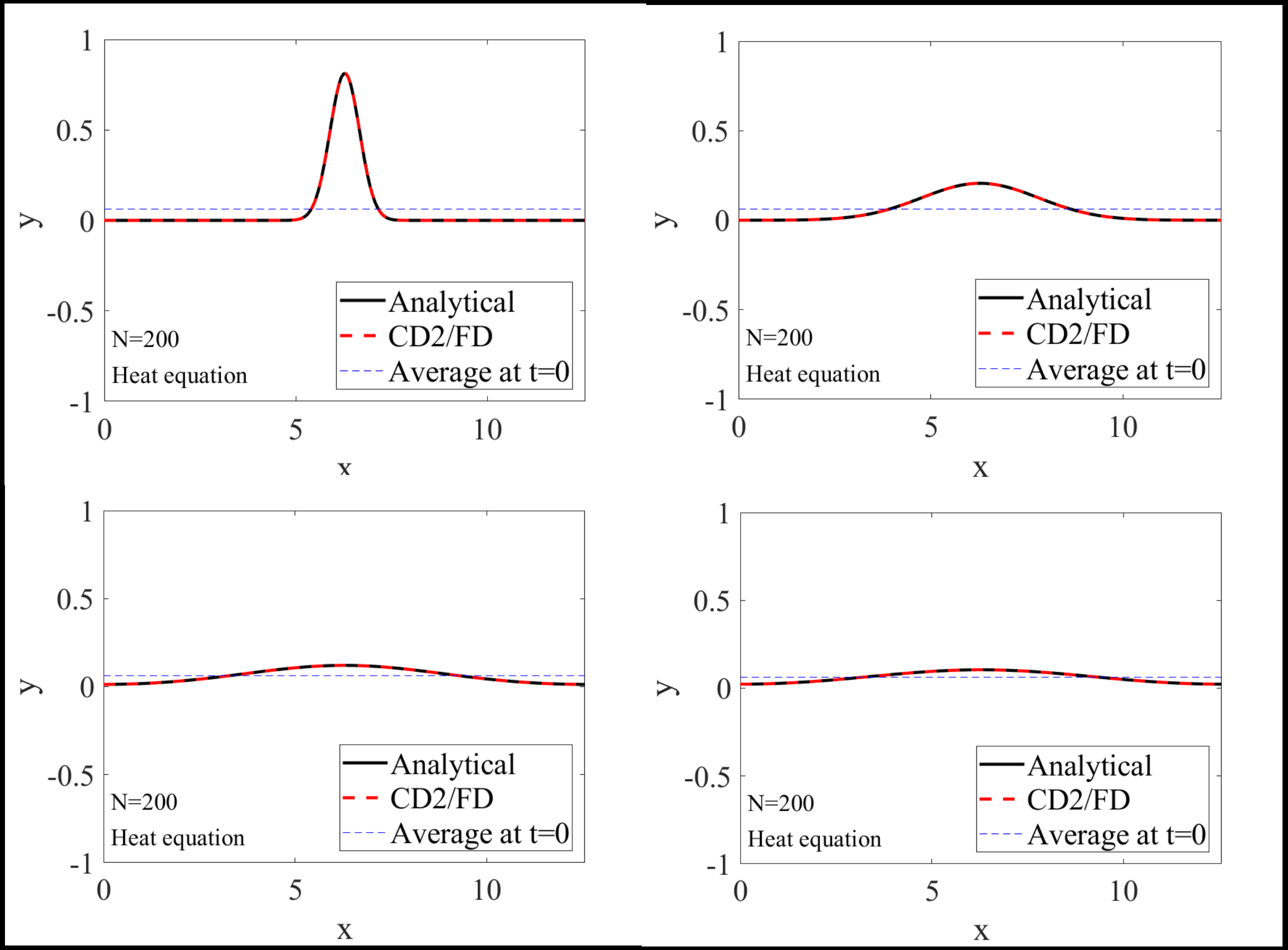


Diffusion equation i.e. heat equation (1d)

Solution amplitude decreases and the diffusion spreads the function
E.g. heat conducts from more hot towards cooler parts

$$\frac{\partial c}{\partial t} = \alpha \frac{\partial^2 c}{\partial x^2}$$

c=e.g. temperature, concentration
α=diffusivity [m²/s]



Wave equation (1d)

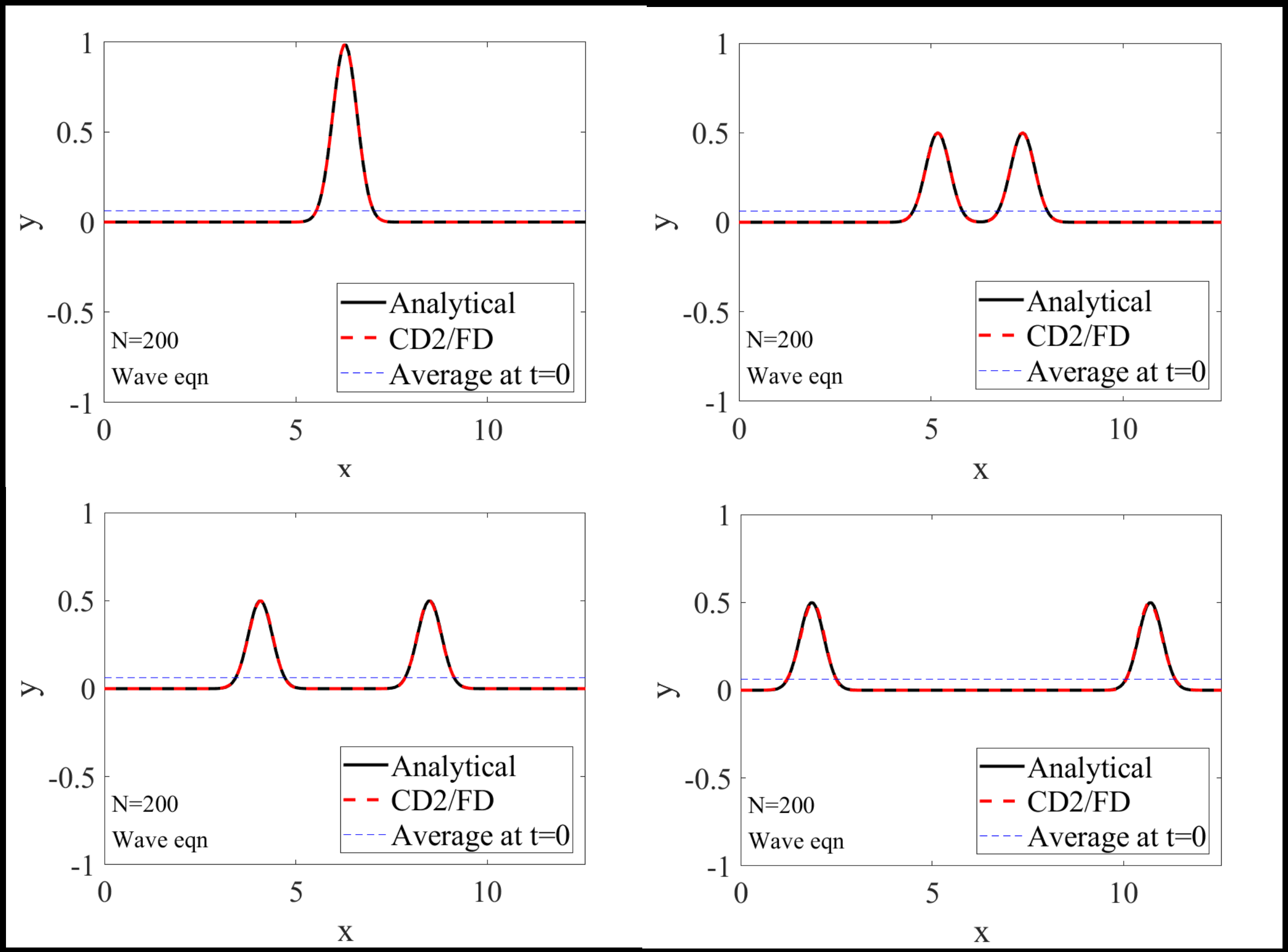
Waves start traveling in opposite directions with velocities $\pm u$

E.g. sound waves in air

$$\frac{\partial^2 c}{\partial t^2} = u^2 \frac{\partial^2 c}{\partial x^2}$$

c=wave amplitude

u=wave speed (e.g. speed of sound)



Example: solution of the convection equation by pen and paper

A smoke cloud concentration c(x,t) is transported by wind along the x-direction. The initial condition c(x,t=0) = g(x) and the wind velocity u>0 and t=time.

$$\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x} = 0$$

We observe that the solution is c=g(x-ut) because if we substitute this expression to the convection eqn above then it fulfills the equation.

Proof:

1) Define a new variable $z=x-ut$
2) By chain rule of derivation applied on $c=g(x-ut)$:

(i) $c_t = c_z z_t = -uc_z$ and
(ii) $c_x = c_z z_x = c_z$

3) **Thus:** $c_t + uc_x = -uc_z + uc_z = 0$

Conclusion: the solution has the same shape as the initial condition and it is just "shifting" in positive x-direction at velocity u (as we saw earlier).

Numerical solution using finite difference method

Common space discretization methods needed to solve PDEs

Finite difference:
Central scheme (CD2)

$$\frac{\partial c}{\partial x} \approx \frac{c_{i+1} - c_{i-1}}{2\Delta x}$$

Finite volume

$$\frac{\partial c}{\partial x} \approx \frac{\int_{\Delta x} \frac{\partial c}{\partial x} dx}{\Delta x} = \frac{c_{i+1/2} - c_{i-1/2}}{\Delta x}$$

Finite difference:
Upwind scheme ($u > 0$)

$$\frac{\partial c}{\partial x} = \frac{c_i - c_{i-1}}{\Delta x}$$

Finite difference:
Downwind scheme ($u < 0$)

$$\frac{\partial c}{\partial x} = \frac{c_{i+1} - c_i}{\Delta x}$$

Common time discretization methods needed to solve PDEs

Euler method (1st order)

$$\frac{\partial c}{\partial t} \approx \frac{c_i^{n+1} - c_i^n}{\Delta t}$$

Backward difference (2nd order)

$$\frac{\partial c}{\partial t} \approx \frac{3c_i^{n+1} - 4c_i^n + c_i^{n-1}}{2\Delta t}$$

Finite difference solution of convection-diffusion equation (Explicit Euler method + central difference CD2)

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} = \alpha\frac{\partial^2 c}{\partial x^2}$$

⇓

$$\frac{c_i^{n+1} - c_i^n}{\Delta t} + u\frac{c_{i+1}^n - c_{i-1}^n}{2\Delta x} = \alpha\frac{c_{i+1}^n - 2c_i^n + c_{i-1}^n}{\Delta x^2}$$

⇓

$$c_i^{n+1} = c_i^n - \Delta t\, u\frac{c_{i+1}^n - c_{i-1}^n}{2\Delta x} + \alpha\Delta t\frac{c_{i+1}^n - 2c_i^n + c_{i-1}^n}{\Delta x^2}$$

→ Can be solved easily by computer (e.g. Week 1 Matlab class).

Discretization formulae come from Taylor series

- For example, where does the central difference formula (CD2) come from?

$$\frac{\partial f}{\partial x} \approx \frac{f_{i+1} - f_{i-1}}{2\Delta x}$$

- A function can be expanded in Taylor series around point x

$$f(x+\Delta x) = f(x) + \frac{\partial f(x)}{\partial x}\Delta x + \frac{1}{2!}\frac{\partial^2 f(x)}{\partial x^2}\Delta x^2 + \frac{1}{3!}\frac{\partial^3 f(x)}{\partial x^3}\Delta x^3 + \ldots$$

$$f(x-\Delta x) = f(x) - \frac{\partial f(x)}{\partial x}\Delta x + \frac{1}{2!}\frac{\partial^2 f(x)}{\partial x^2}\Delta x^2 - \frac{1}{3!}\frac{\partial^3 f(x)}{\partial x^3}\Delta x^3 + \ldots$$

- We would like to find a numerical, discrete approximation for $f'(x)$ using the values $f(x_i)=f_i$, $f(x_i+\Delta x)=f_{i+1}$ and $f(x_i-\Delta x)=f_{i-1}$
- We see directly that:

$$f(x+\Delta x) - f(x-\Delta x) = 2\frac{\partial f(x)}{\partial x}\Delta x + \frac{2}{3!}\frac{\partial^3 f(x)}{\partial x^3}\Delta x^3 + O(\Delta x^5)$$

$$\frac{f(x+\Delta x) - f(x-\Delta x)}{2\Delta x} + O(\Delta x^2) \approx \frac{\partial f(x)}{\partial x}, \text{ where } O(\Delta x^2) \text{ is the leading error term.}$$

- The CD2 scheme above is said to be “second order” because the leading order term in the error is a polynomial of degree 2 i.e. $O(\Delta x^2)$
- Taking more points would allow to construct more accurate higher degree discretization schemes which would pose less numerical dispersion/diffusion.

Differential operators

Gradient and divergence

Gradient is a vector operator:

$$\nabla = \vec{i}\,\frac{\partial}{\partial x} + \vec{j}\,\frac{\partial}{\partial y} + \vec{k}\,\frac{\partial}{\partial z}$$

Gradient of a scalar function is a vector:

$$\nabla \phi = \vec{i}\,\frac{\partial \phi}{\partial x} + \vec{j}\,\frac{\partial \phi}{\partial y} + \vec{k}\,\frac{\partial \phi}{\partial z}$$

Divergence of a vector is the scalar product of gradient with vector which is a scalar:

$$\nabla \cdot \boldsymbol{u} = \frac{\partial u_1}{\partial x} + \frac{\partial u_2}{\partial y} + \frac{\partial u_3}{\partial z}$$

Divergence of a gradient is the scalar operator i.e. the Laplacian operator:

$$\nabla \cdot \nabla = \Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

In CD-equation, convection and diffusion terms contain divergence

Convection term:

$$\nabla\cdot(\boldsymbol{u}\phi)=\phi\nabla\cdot\boldsymbol{u}+\boldsymbol{u}\cdot\nabla\phi$$

Note:
1st derivatives

Diffusion term (const. diffusivity):

$$\nabla\cdot(\nu\nabla\phi)=\nu\nabla\cdot\nabla\phi=\nu\frac{\partial^2\phi}{\partial x^2}+\nu\frac{\partial^2\phi}{\partial y^2}+\nu\frac{\partial^2\phi}{\partial z^2}$$

Note:
2nd derivatives

Tensors

Used short-hand notation for multiplying vectors $\boldsymbol{u}\boldsymbol{u}$

- If we define u as 3 by 1 vector then how can we multiply two vectors?
- The used short-hand is here understood as matrix product $\boldsymbol{u}\boldsymbol{u}=\boldsymbol{u}\,\boldsymbol{u}^T$
- In the present notation $\boldsymbol{u}\boldsymbol{u}$ defines a 3 by 3 matrix also called a “tensor”

$$\boldsymbol{u}\boldsymbol{u}=[u_i u_j]_{3\times 3}$$

Row index (i) — Column index (j)

Divergence of vector and tensor

Divergence of a vector is a scalar:

$$\nabla \cdot \boldsymbol{u} = \frac{\partial u_1}{\partial x} + \frac{\partial u_2}{\partial y} + \frac{\partial u_3}{\partial z}$$

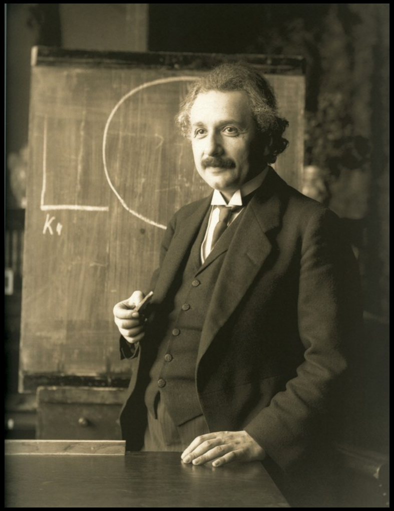
Divergence of a tensor is a vector:

$$\nabla \cdot \boldsymbol{uu} = \vec{C}$$

Thus: we can think that taking divergence reduces the dimensionality of the object.
- divergence of 3 by 3 tensor gives a 3 by 1 vector
- divergence of 3 by 1 vector gives a scalar (think: “1 by 1” matrix)

Einstein summation convention and index notation

Einstein summation convention:
if index appears twice, sum over the index



Divergence of vector:

$$\nabla \cdot \boldsymbol{u} = \frac{\partial u_i}{\partial x_i} = \Sigma_{i=1}^{3} \frac{\partial u_i}{\partial x_i}$$

Divergence of tensor:

$$\nabla \cdot \boldsymbol{uu} = \frac{\partial u_i u_j}{\partial x_j} = u_j \frac{\partial u_i}{\partial x_j} + u_i \frac{\partial u_j}{\partial x_j}$$

Divergence of gradient of scalar:

$$\nu \nabla \cdot \nabla u_i = \nu \frac{\partial^2 u_i}{\partial x_j^2}$$

In incompressible flows the latter term is zero:

$$u_j \frac{\partial u_i}{\partial x_j} = \boldsymbol{u} \cdot \nabla u_i$$

$$u_i \frac{\partial u_j}{\partial x_j} = 0$$