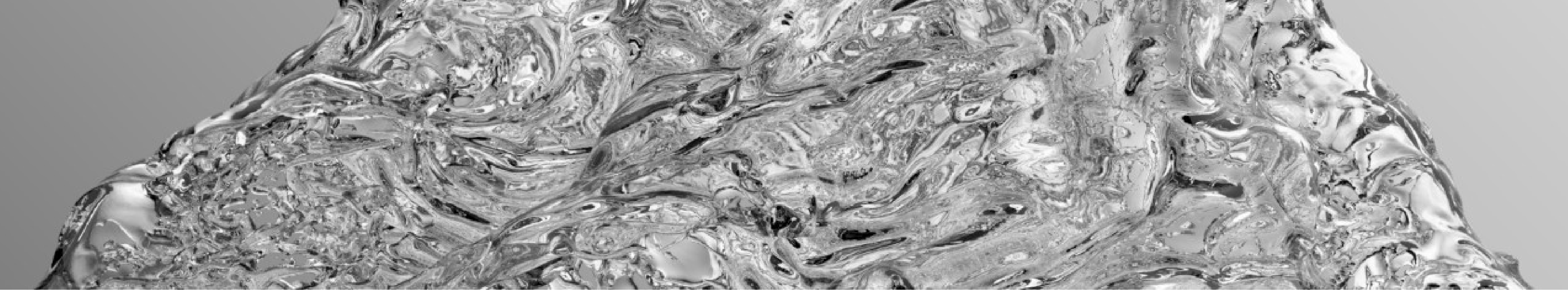

EEN-E2001 Computational Fluid Dynamics

Lecture 2: Gauss' Theorem and Finite Volume Method

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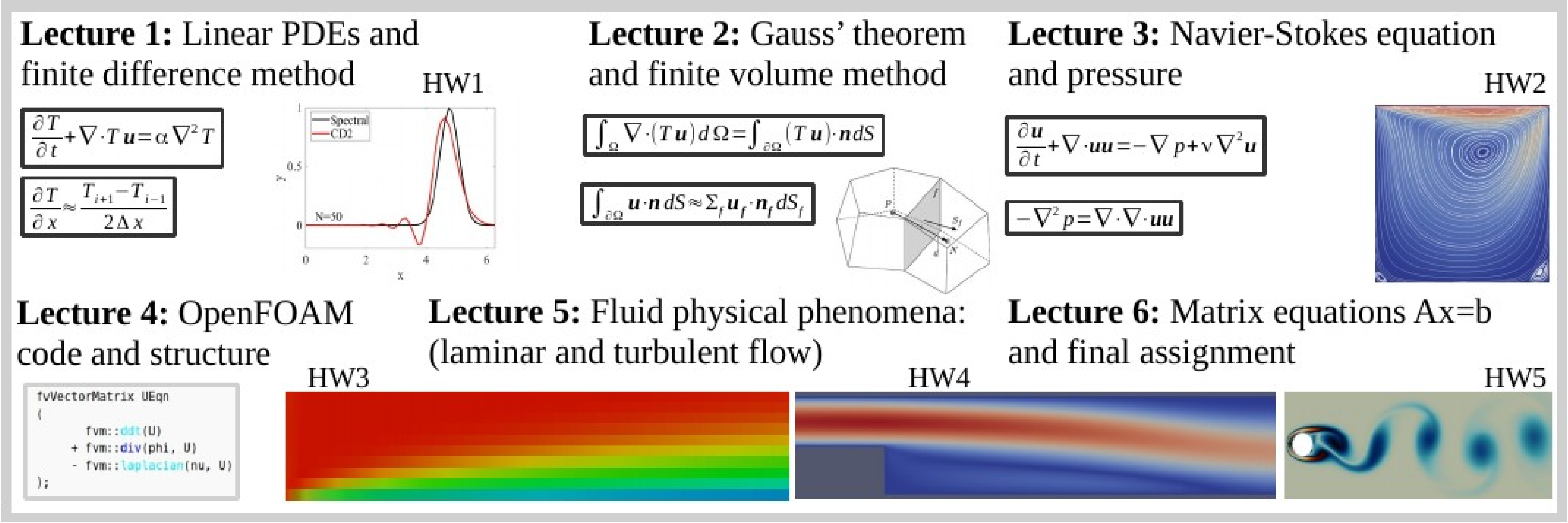
Aalto University, School of Engineering



Intended learning objectives of the full lecture

After the lecture the student:

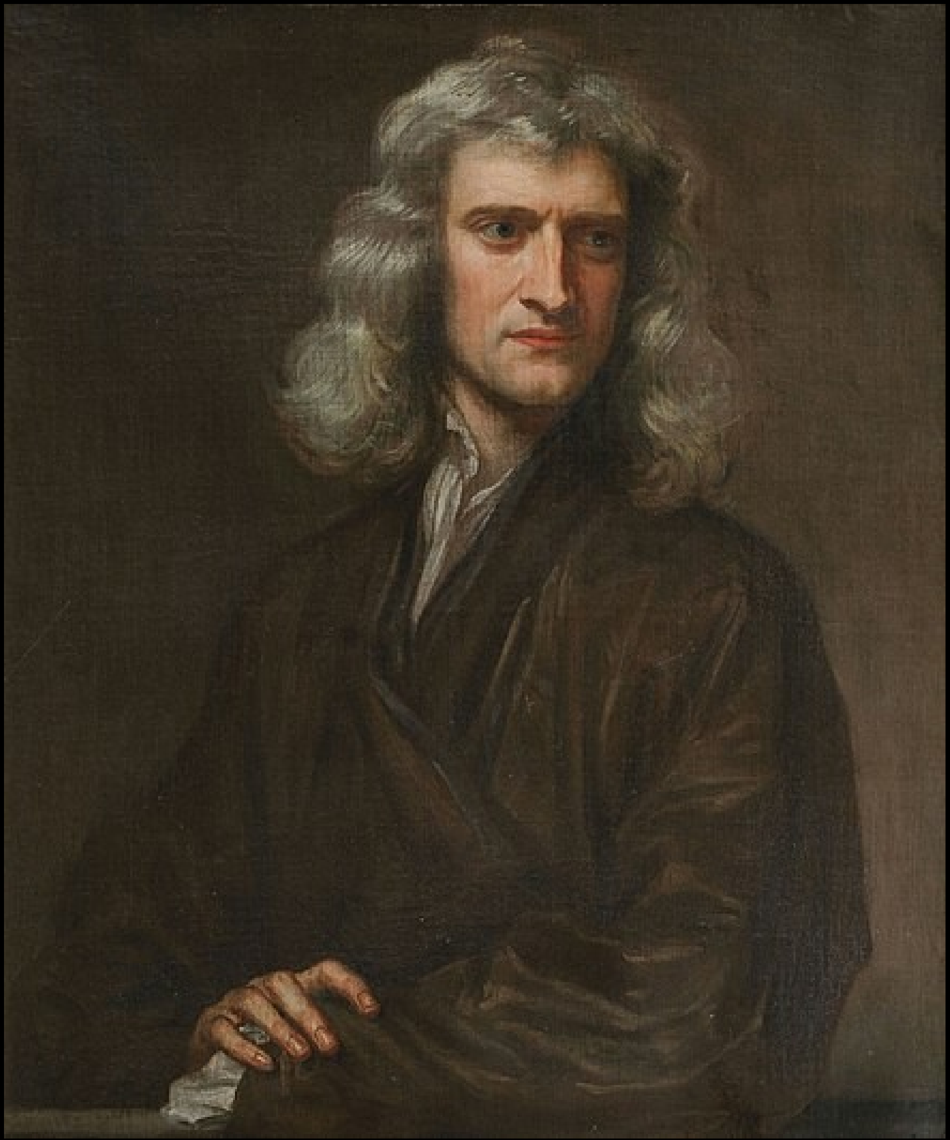
- Can explain connection between Gauss' theorem and the finite volume method (fvm)

- Can write down & derive the fvm discretized 1d convection-diffusion problem (relevance: HW2)

In fact, Gauss (left) and Newton (right) developed much of the mathematics and physics tools & thinking that we use nowadays in our CFD simulations

https://en.wikipedia.org/wiki/Carl_Friedrich_Gauss
https://en.wikipedia.org/wiki/File:Carl_Friedrich_Gauss_1840_by_Jensen.jpg

https://en.wikipedia.org/wiki/Isaac_Newton
https://en.wikipedia.org/wiki/File:Portrait_of_Sir_Isaac_Newton,_1689.jpg



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

1) **Physics** identification.

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**.

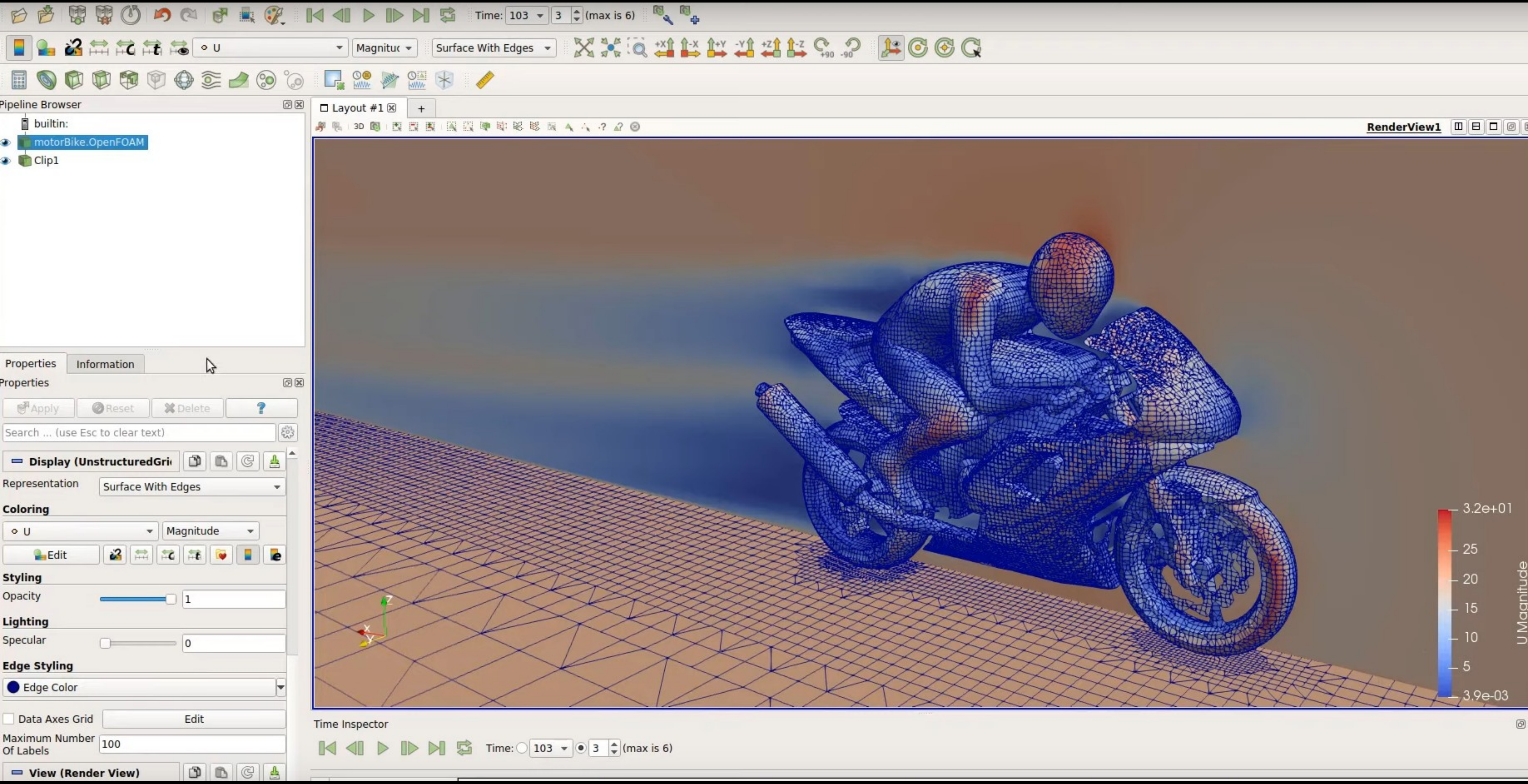
8) **Validation and verification, reference data**. Reporting, analysis and discussion of the results. Are the results sane?

Example applications on finite volume method CFD simulations

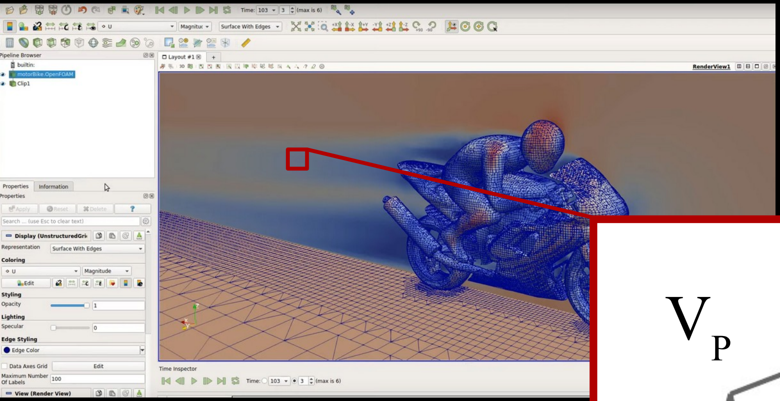
Visual example: Aerodynamics CFD simulation using the finite volume method (OpenFOAM)

The Motorbike tutorial and steady state velocity field

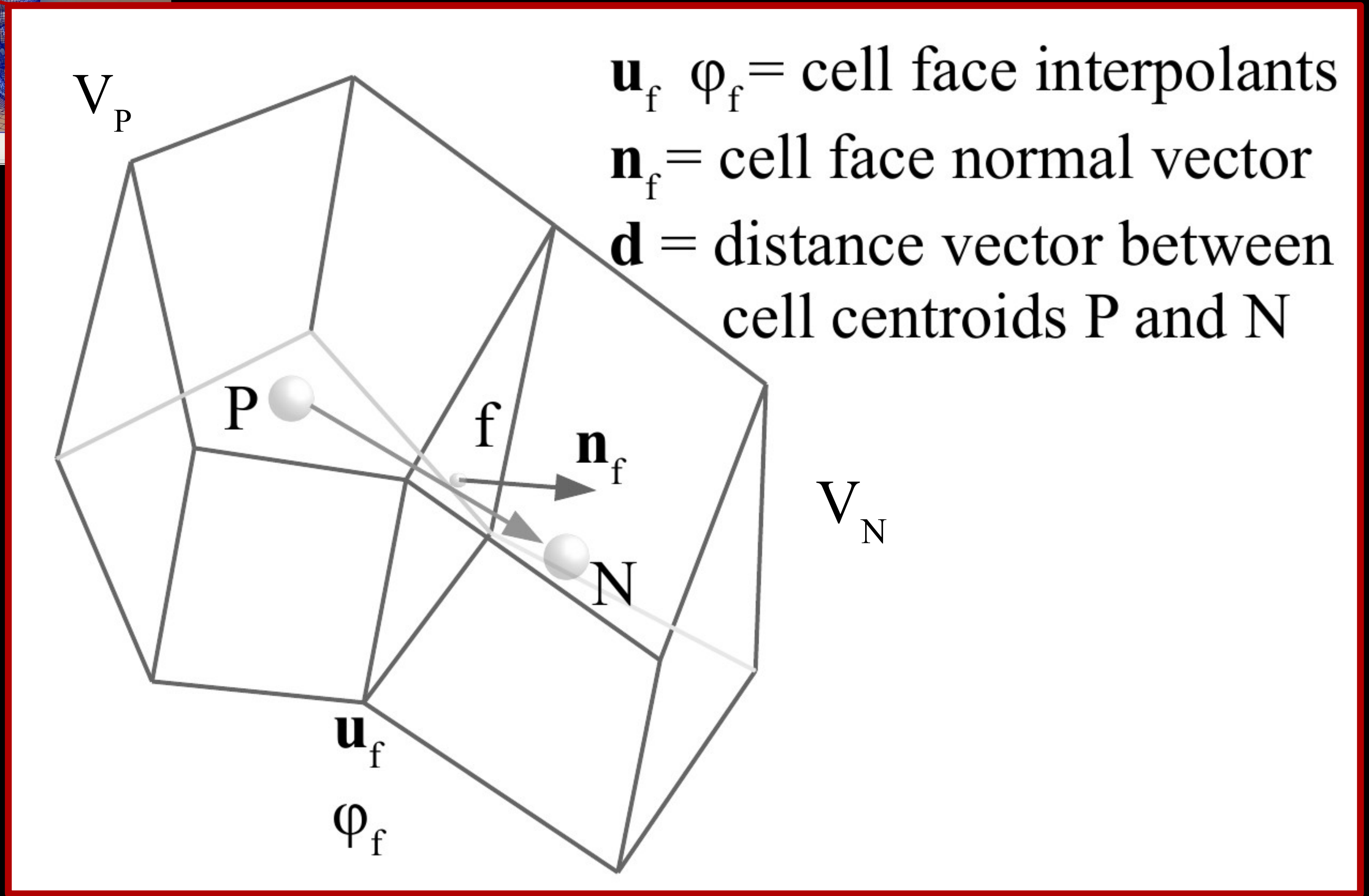
https://www.youtube.com/watch?v=1C4Av_yCfpw&list=RDCMUCDuQsPzfqxcYKVp_uuKCzqw&start_radio=1&rv=1C4Av_yCfpw&t=6



Basic idea of finite volume method: divide geometry into small volumes and update numerical solution at volume centroids by estimating e.g. mass & momentum fluxes through the faces of the control volumes during small time intervals

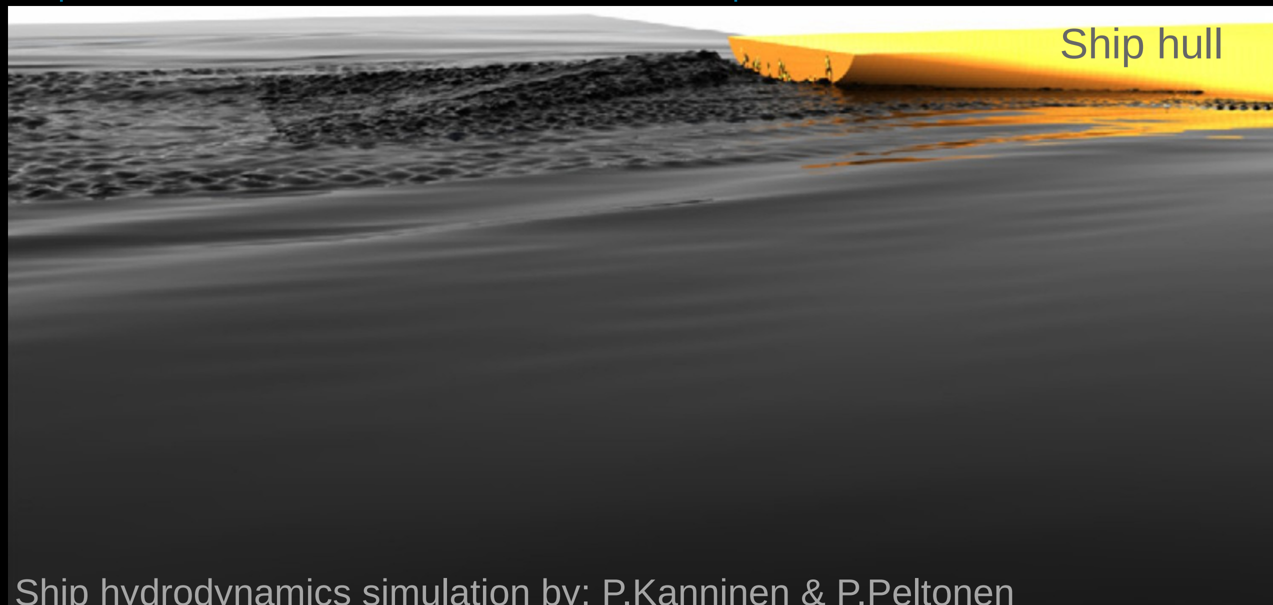


Control volume



Visual research examples: recent high-performance computing applications using finite volume method (OpenFOAM) in my team

https://www.sciencedirect.com/science/article/abs/pii/S0029801821017194?via%3Dihub



Ship hydrodynamics simulation by: P.Kanninen & P.Peltonen

Velocity

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

Concentration

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

Convection-Diffusion eqn

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

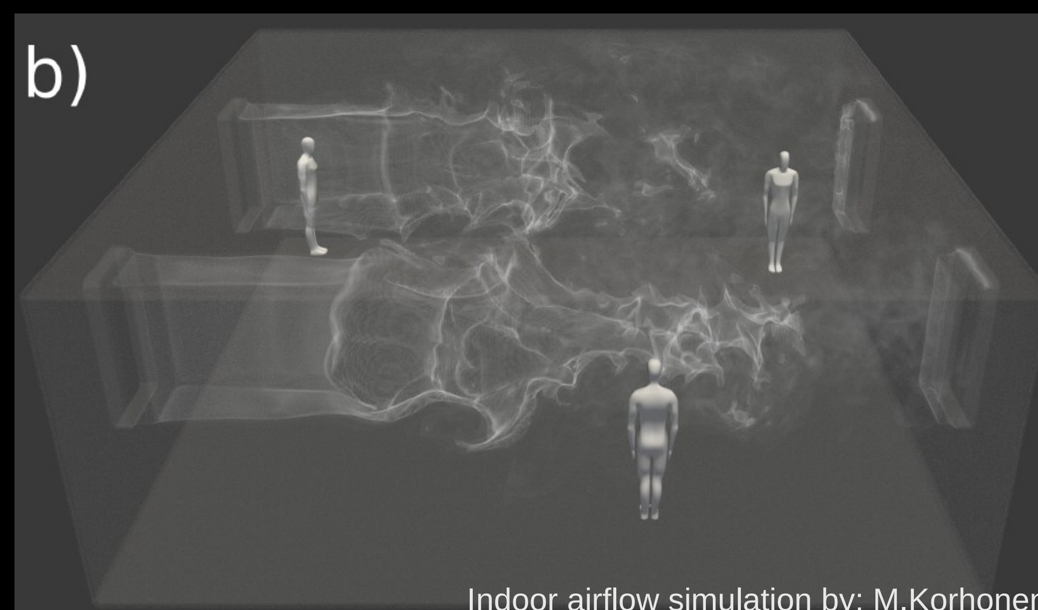
Navier-Stokes (Newton's 2nd law)

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

a)


Indoor airflow simulation by: V.Vuorinen. Visualization: M.Gadalla

b)


Indoor airflow simulation by: M.Korhonen

“Computational cost” depends on numerous aspects:

Type of software, computing infrastructure, how long can you wait, method, resolution, how long we need to simulate physical time, steady vs transient, physics (e.g. refinement need at boundary layers/wakes), what is the intention of the simulation (e.g. visualization of known physics, quick design insight, exact matching of an experiment with publication quality) etc

Case	Resolution	Computational cost	Method	Comment
Motorbike	Very coarse ~0.1M cells	**~1 min** (Laptop CPU)	Steady state RANS - method	A basic tutorial. Intention: demo
Airflow in a room	Medium ~30M cells	**~2 days** (GPU)	Transient LES method	To be submitted to a journal.
Ship hydro	Medium ~60M cells	**~10 days** (Supercomputer)	Transient LES method	Published in a journal.

Finite volume method in a nutshell

The core problem in solving convection-diffusion type equations (PDE's):
In CFD, we would like to find a $\Delta\varphi=\Delta t(-C+D)$ to update solution as $\varphi_{n+1} = \varphi_n + \Delta\varphi$.
→ Need to numerically calculate divergence terms i.e. convection $C=C(x,y,z,t)$ & diffusion $D=D(x,y,z,t)$ $(t=n\Delta t)$.

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

$$\boxed{D=\alpha\nabla\cdot\nabla\phi}$$

Gauss' theorem: enables converting volume integrals into surface integrals (B.Sc. math)

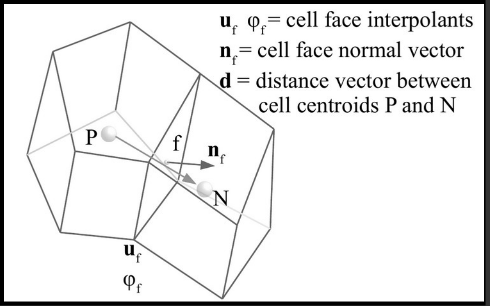
$$\boxed{\int_V \nabla\cdot(\boldsymbol{u}\phi)\,dV=\int_A (\boldsymbol{u}\phi)\cdot\boldsymbol{n}\,dA}$$

dA = differential area element on the outer surface A of volume V
$\boldsymbol{n}$ = the surface outer normal vector

Gauss' theorem + volume averaging: divergence terms C and D can be converted into surface integrals which can be numerically computed via summations.

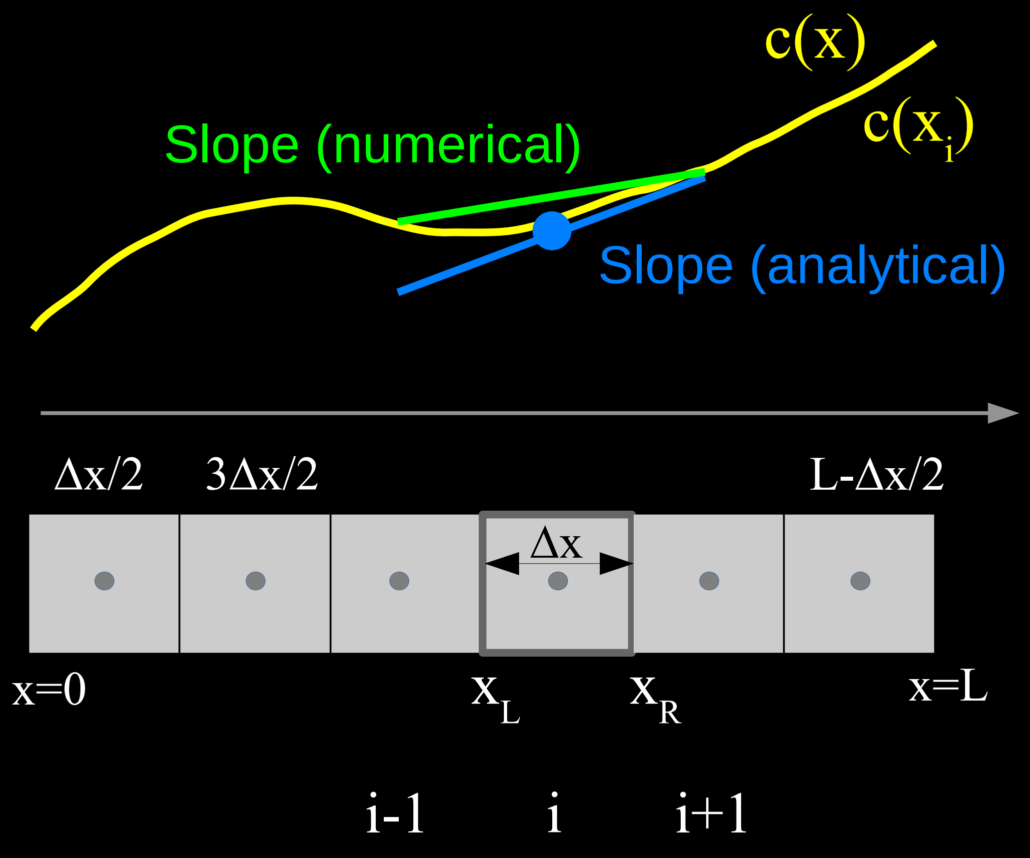
$$\boxed{C_{ave}=\frac{1}{V}\int_V \nabla\cdot(\boldsymbol{u}\phi)\,dV=\frac{1}{V}\int_A (\boldsymbol{u}\phi)\cdot\boldsymbol{n}\,dA\approx\frac{1}{V}\Sigma_{faces}(\boldsymbol{u_f}\,\phi_f)\cdot\boldsymbol{n_f}\,dA_f}$$

$$\boxed{D_{ave}=\frac{1}{V}\int_V \alpha\nabla\cdot\nabla\phi\,dV=\frac{1}{V}\int_A \nabla\phi\cdot\boldsymbol{n}\,dA\approx\frac{1}{V}\Sigma_{faces}\nabla\phi_f\cdot\boldsymbol{n_f}\,dA_f}$$



Recall: discretization methods (FDM, FVM, FEM) needed to numerically calculate space derivatives appearing in PDE's

(derivative = slope of the function)



E.g. with CD2/FD: $c'(x_i) = \dfrac{\partial c}{\partial x} \approx \dfrac{c_{i+1} - c_{i-1}}{2\,\Delta x}$

Next, we derive fvm discretization for the derivative $c'(x)$.

Keywords: "volume averaging & Gauss' theorem"

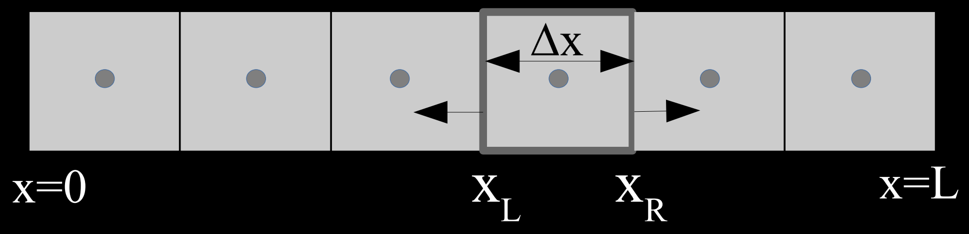
Let us integrate $c'(x)$ over $x_L < x < x_R$ ($\Delta x = x_R - x_L$):

$$\boxed{\int_{x_L}^{x_R} c'(x)\,dx = +c(x_R) - c(x_L)}$$

To obtain "volume average" of $c'(x)$, divide both sides by Δx:

$$\boxed{\frac{1}{\Delta x}\int_{x_L}^{x_R} c'(x)\,dx = \frac{+c(x_R) - c(x_L)}{\Delta x}}$$

Volume average of $c'(x)$ over Δx — Looks essentially like CD2/FD



Note:
Cell face outer normal vectors point to (+1,0) and (-1,0) directions so actually the +/- signs in 1d integration originate from the Gauss' theorem.

This leads to a finite volume discretization formula for $c'(x)$

Interpolating fluxes linearly $c(x_L) = 0.5(c_i + c_{i-1})$ and $c(x_R) = 0.5(c_i + c_{i+1})$ yields the fvm discretization:

$$\boxed{\left(\frac{\partial c}{\partial x}\right)_{fvm} = \frac{1}{\Delta x}\int_{x_L}^{x_R} c'(x)\,dx = \frac{+c(x_R) - c(x_L)}{\Delta x} = \frac{c_{i+1} - c_{i-1}}{2\Delta x}}$$

… being exactly the CD2/FD formula (week 1).

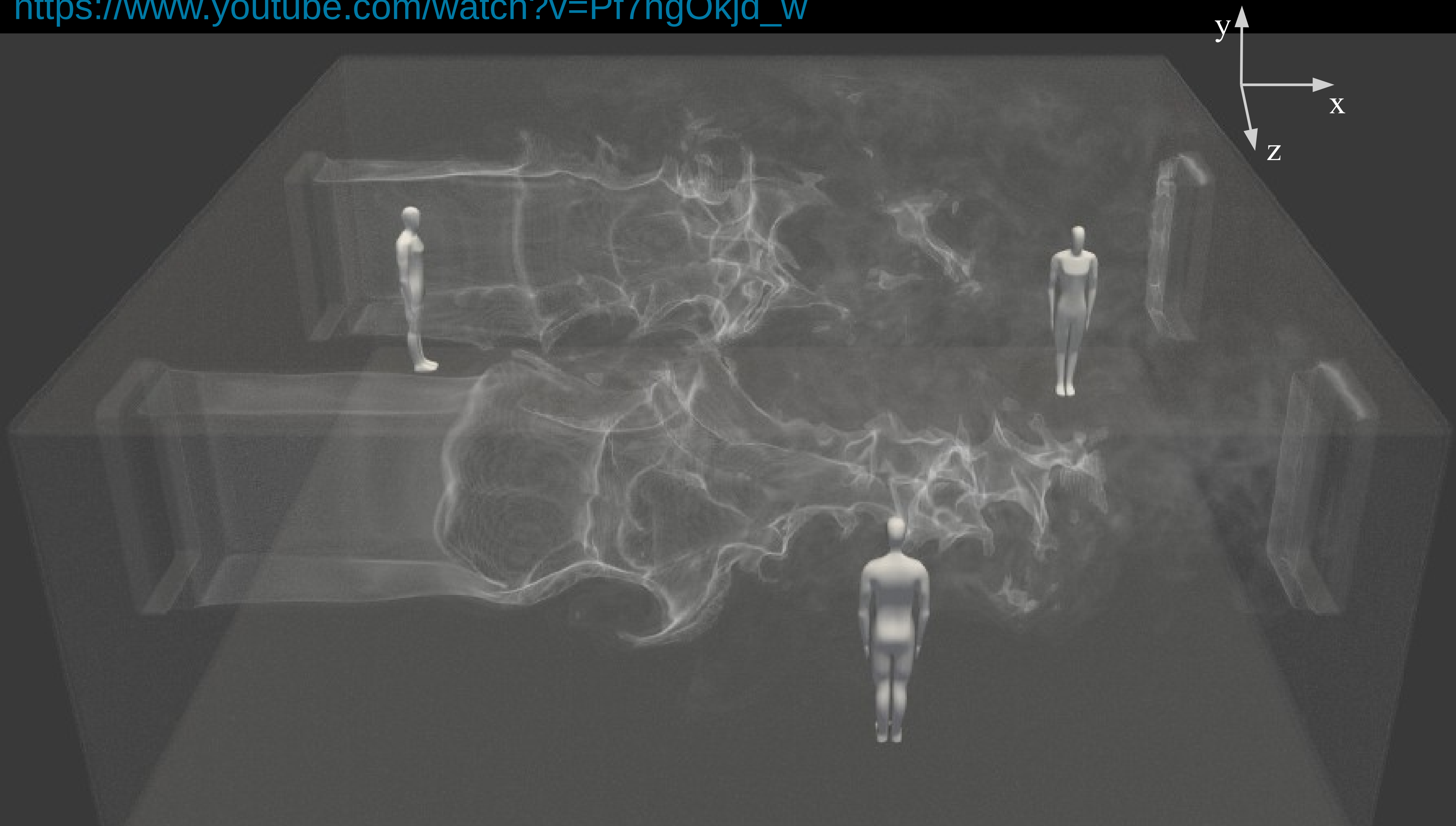
Notes:

→ Averaging derivative over an interval (1d) or volume (3d) we can find finite volume discretization formulae. On uniform grids, and linear interpolation, FVM and FDM give exactly the same 2^{nd} order central difference (CD2) formula (see: Week 1).

→ Face interpolation of $c(x_L)$ and $c(x_R)$ is one of the most essential parts to pay attention on in CFD (the numerical uncertainty and error contained in the interpolation details). In HW1 you will compare three interpolation procedures: linear (CD2) vs upwind (UW1) vs a flux limiter. Flux limiters “try” to be as close to CD2 but still diffusive enough to stabilize the numerical solution.

Recap discussions: Gauss' theorem, conservation of mass and a room with cross-draught. Flow enters 1m/s from the left windows and exits from right. Window area = constant.

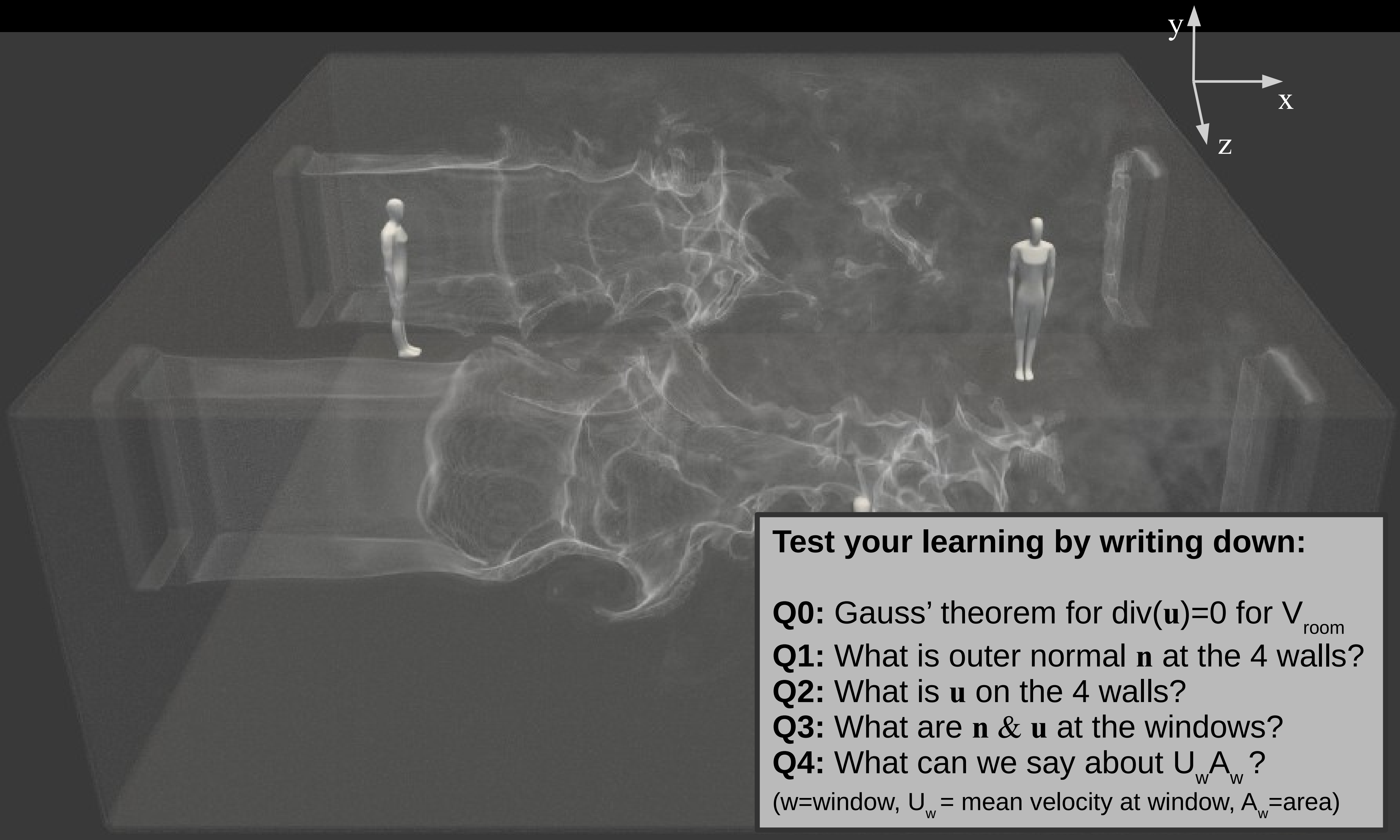
https://www.youtube.com/watch?v=Pf7hgOkjd_w



Indoor airflow simulation by: M.Korhonen

Basic fluid dynamics (M.Sc.): Velocity field of incompressible fluids, such as low speed air and water, satisfies the mass conservation equation:

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



Test your learning by writing down:

Q0: Gauss' theorem for div($\mathbf{u}$)=0 for V_{room}

Q1: What is outer normal $\mathbf{n}$ at the 4 walls?

Q2: What is $\mathbf{u}$ on the 4 walls?

Q3: What are $\mathbf{n}$ & $\mathbf{u}$ at the windows?

Q4: What can we say about $U_w A_w$?

(w=window, U_w = mean velocity at window, A_w=area)

Gauss theorem + mass conservation:

$$\int_{V_{room}} \nabla \cdot \vec{u}\, dV = \int_{A_{room}} \vec{u} \cdot \boldsymbol{n}\, dA = 0$$

Finite volume method for the 1d convection-diffusion equation

(relevance: small theory question in HW2)

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

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

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

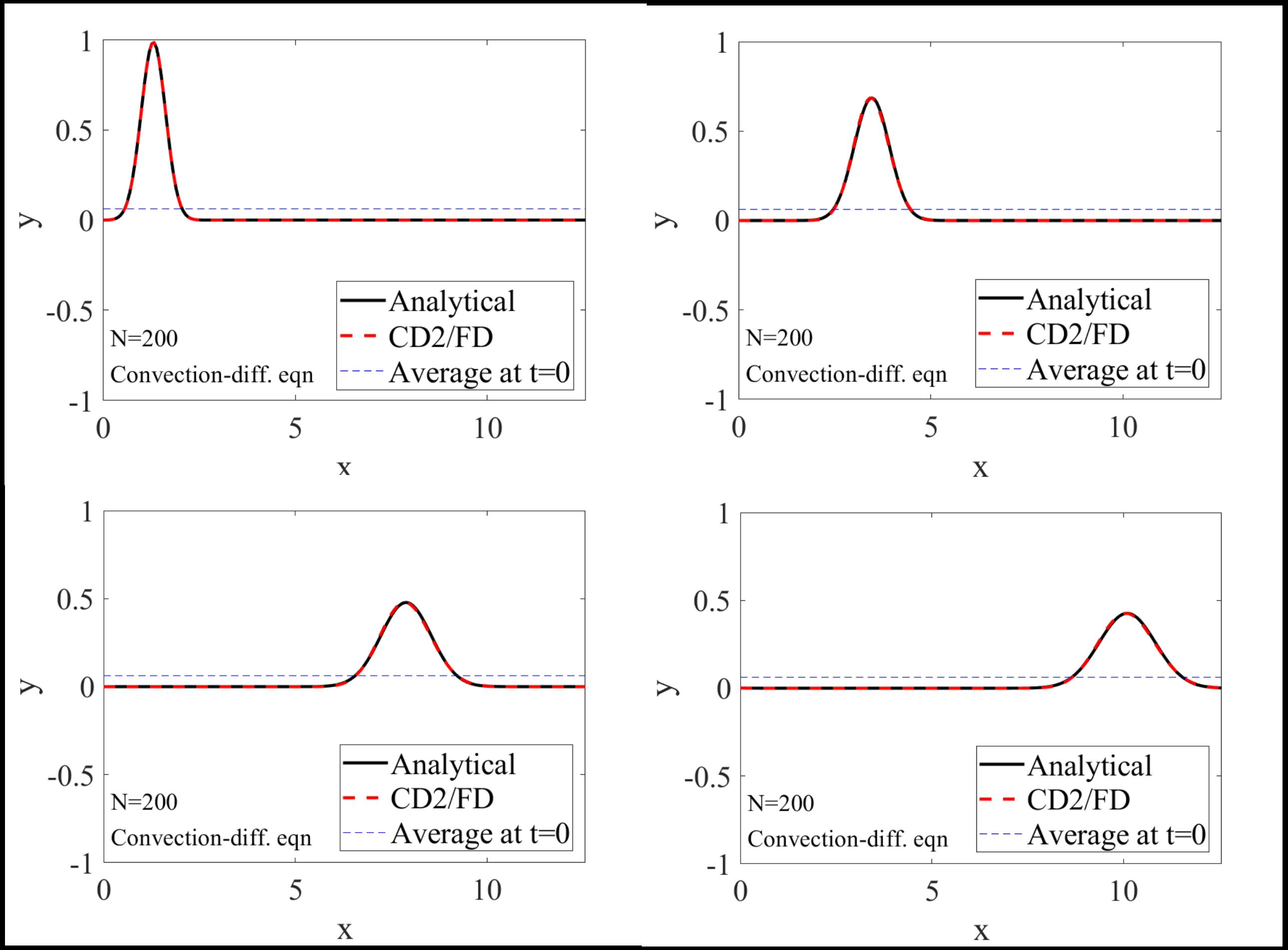
$$c = c(x, y, z, t)$$

3D smoke cloud moving in air

Let us model the smoke cloud motion in a simple way using the 1D convection-diffusion equation (u=constant)

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

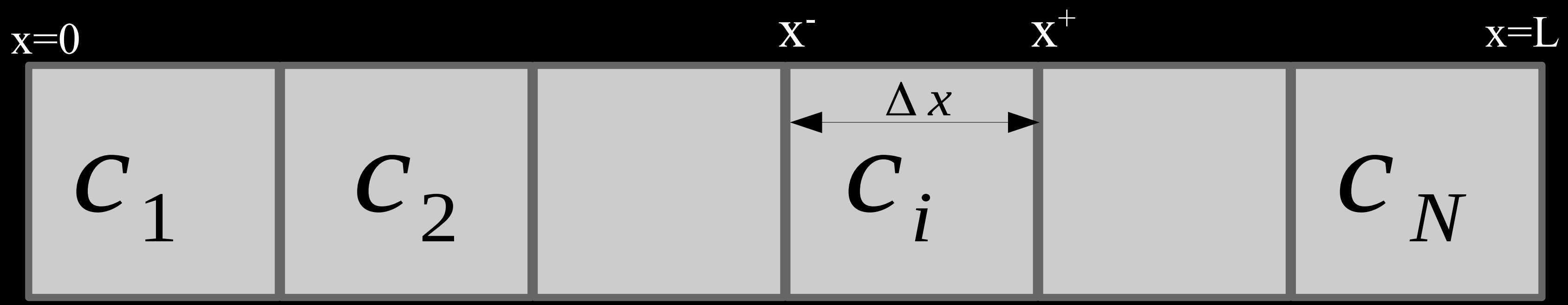
c=smoke concentration
α=diffusivity [m²/s]
u=mean wind velocity [m/s]



We average the 1d CD-eqn over finite intervals of length Δx.

Definition: average of a function in 1d over the interval Δx

$$\boxed{f_{ave} = \frac{1}{\Delta x}\int_{\Delta x} f\, dx}$$



Averaged CD-eqn over the interval Δx

$$\boxed{\frac{1}{\Delta x}\int_{x^-}^{x^+} \frac{\partial c}{\partial t}\, dx + \frac{1}{\Delta x}\int_{x^-}^{x^+} u \frac{\partial c}{\partial x}\, dx = \frac{1}{\Delta x}\int_{x^-}^{x^+} \alpha \frac{\partial^2 c}{\partial x^2}\, dx}$$

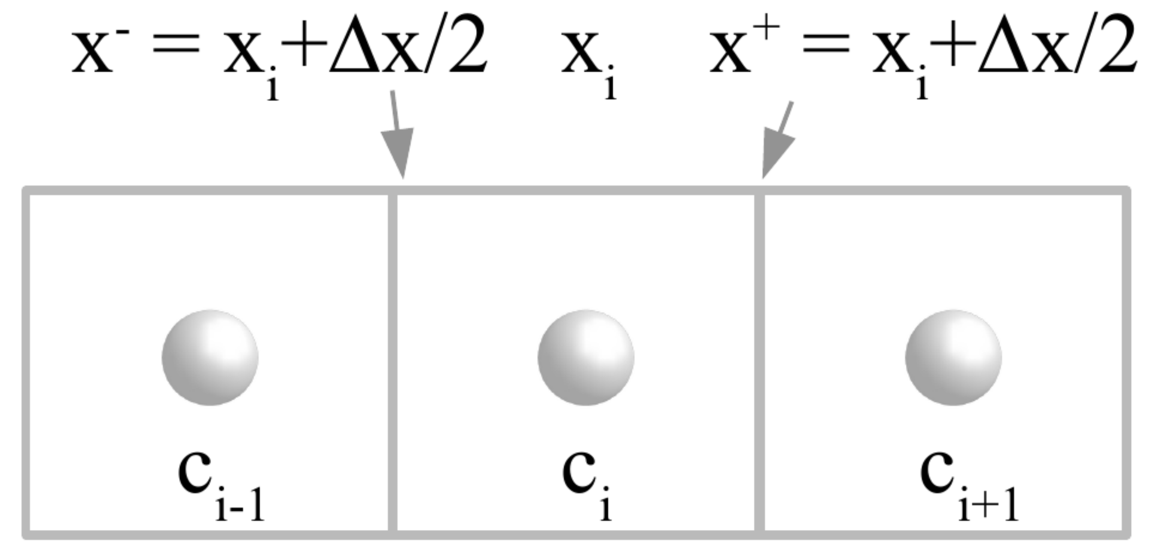
We average the 1d CD-eqn over a finite interval of length Δx.

Assuming Δx is small, we assume:

$$\boxed{c \approx \frac{1}{\Delta x}\int_{x^-}^{x^+} c\,dx}$$

The resulting form:

$$\boxed{\frac{\partial c}{\partial t} + u\,\frac{c(x^+,t) - c(x^-,t)}{\Delta x} = \alpha\left[\frac{\partial c(x^+,t)}{\partial x} - \frac{\partial c(x^-,t)}{\partial x}\right]\frac{1}{\Delta x}}$$



Estimation of quantities at the cell face

The terms below require **interpolation** of c to the cell face from adjacent cells

$$\boxed{c(x^{+}), c(x^{-})}$$

The terms below require **estimation of the gradients** of c on the cell face

$$\boxed{\alpha \frac{\partial c(x^{+})}{\partial x}, \alpha \frac{\partial c(x^{-})}{\partial x}}$$

How could we get those values ?

→ On uniform grid one could simply linearly **interpolate**

$$\boxed{c(x^{+}) \approx 0.5(c_{i+1} + c_i)} \qquad \boxed{c(x^{-}) \approx 0.5(c_i + c_{i-1})}$$

$$\boxed{\alpha \frac{\partial c(x^{+})}{\partial x} \approx \alpha \frac{c_{i+1} - c_i}{\Delta x}} \qquad \boxed{\alpha \frac{\partial c(x^{-})}{\partial x} \approx \alpha \frac{c_i - c_{i-1}}{\Delta x}}$$

Gathering the interpolants into the cell averaged equations and discretizing time with Euler method gives...

$$\frac{\partial c}{\partial t}+u\frac{c(x^{+},t)-c(x^{-},t)}{\Delta x}=\alpha\left[\frac{\partial c(x^{+},t)}{\partial x}-\frac{\partial c(x^{-},t)}{\partial x}\right]\frac{1}{\Delta x}$$

$$\downarrow$$

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

$$\downarrow$$

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

Observation: Finite volume method boils down to the finite difference method (week 1) on uniform grids.

Numerical stability: Courant number (Co) and Courant-Friedrichs-Lewy (CFL) number should be below one.

Co is relevant to the stability of the convection term (e.g. velocity is not allowed to transport over distances larger than grid spacing during timestep)

$$\boxed{Co = \frac{\Delta t\, u}{\Delta x} < 1}$$

CFL is relevant to the stability of the diffusion term (e.g. concentration is not allowed to diffuse over distances larger than grid spacing during timestep)

$$\boxed{CFL = \frac{\Delta t\, \alpha}{\Delta x^2} < 1}$$