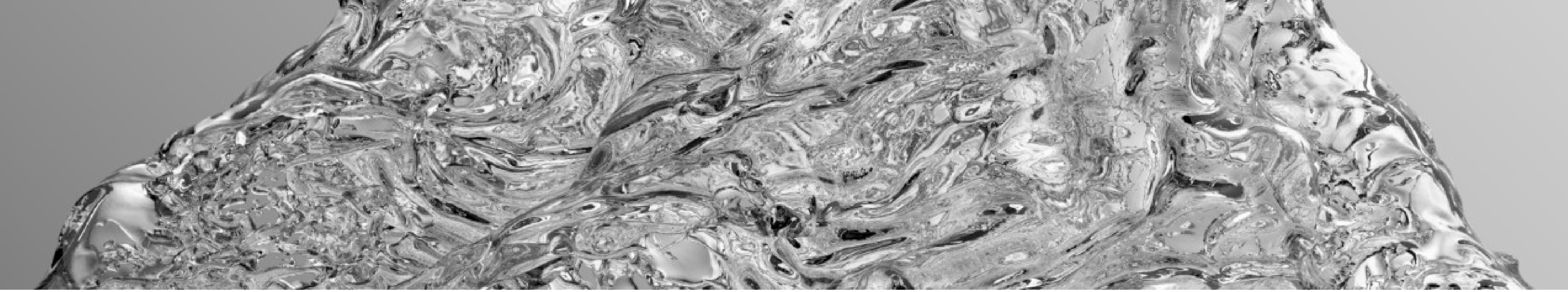


EEN-E2001 Computational Fluid Dynamics

Lecture 2: Gauss' Theorem and Finite Volume Method

Prof. Ville Vuorinen, M.Eng. Ilya Morev

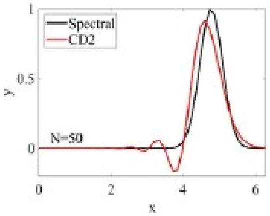
January 23rd 2023

Aalto University, School of Engineering

Lecture 1: Linear PDEs and finite difference method

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

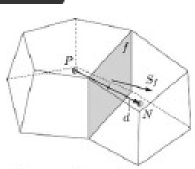
$$\frac{\partial T}{\partial x}\approx\frac{T_{i+1}-T_{i-1}}{2\Delta x}$$



Lecture 2: Gauss' theorem and finite volume method

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

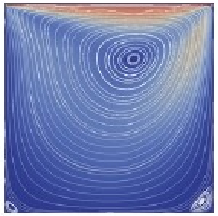
$$\int_{\partial\Omega}\boldsymbol{u}\cdot\boldsymbol{n}\,dS\approx\Sigma_f\boldsymbol{u}_f\cdot\boldsymbol{n}_f\,dS_f$$



Lecture 3: Navier-Stokes equation and pressure

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

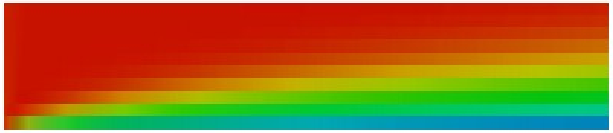
$$-\nabla^2 p=\nabla\cdot\nabla\cdot\boldsymbol{u}\boldsymbol{u}$$

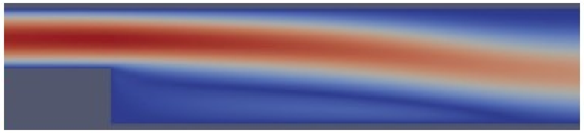


Lecture 4: OpenFOAM code and structure

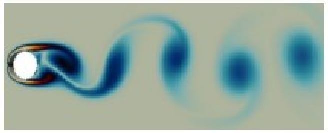
```
fvVectorMatrix UEqn
(
      fvm::ddt(U)
    + fvm::div(phi, U)
    - fvm::laplacian(nu, U)
);
```

Lecture 5: Simulating fluid physical phenomena: part A





Lecture 6: Simulating fluid physical phenomena: part B



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.

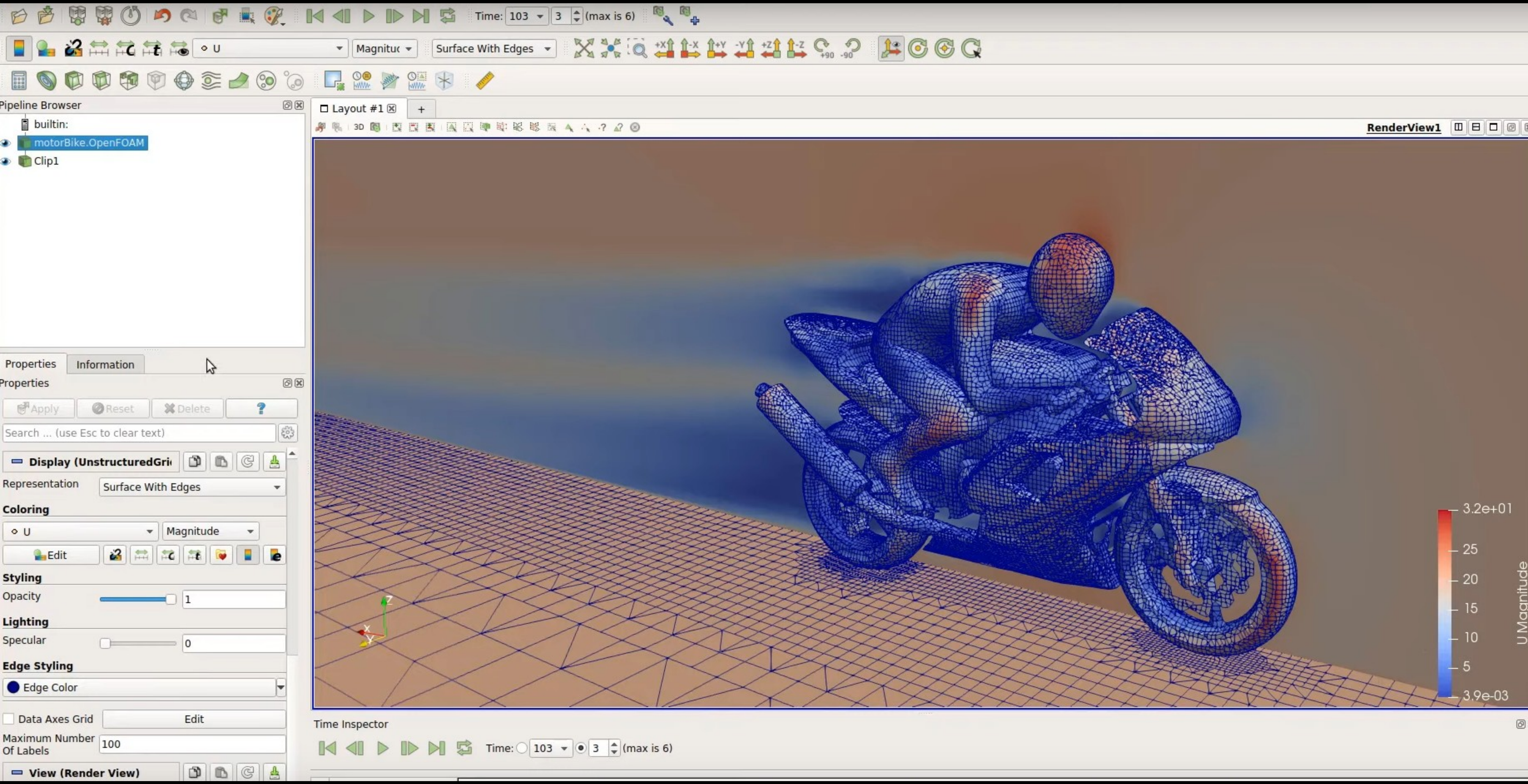
7) **Visualization and post-processing**.

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

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

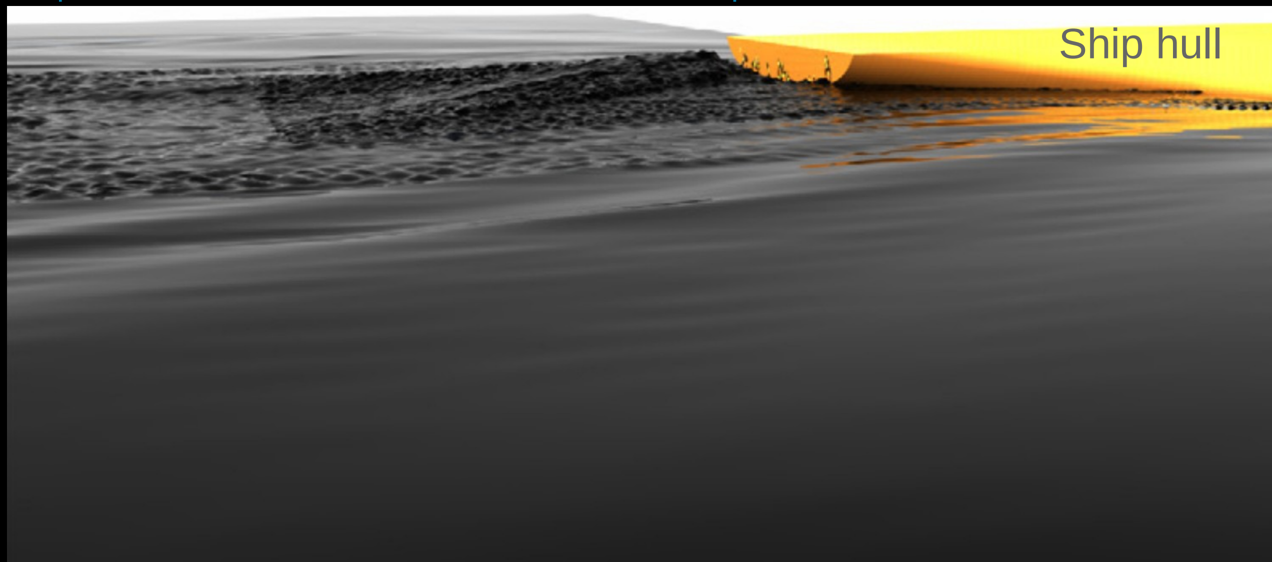
The Motorbike tutorial and steady state velocity field

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



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

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

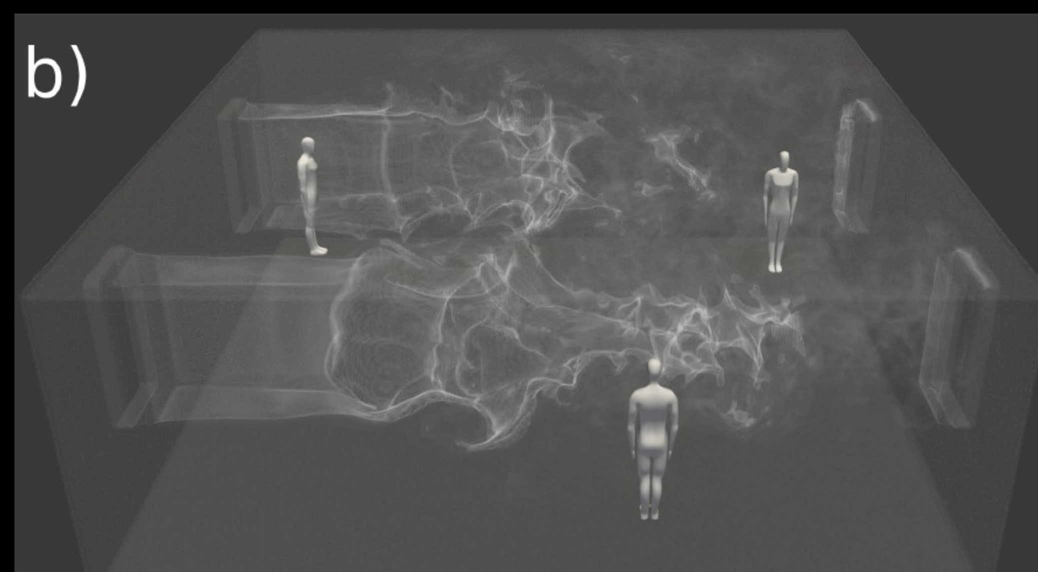
Navier-Stokes (Newton's 2nd law)

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

a)

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

b)



Indoor airflow simulation by: M.Korhonen

“Computational cost” depends on numerous aspects:

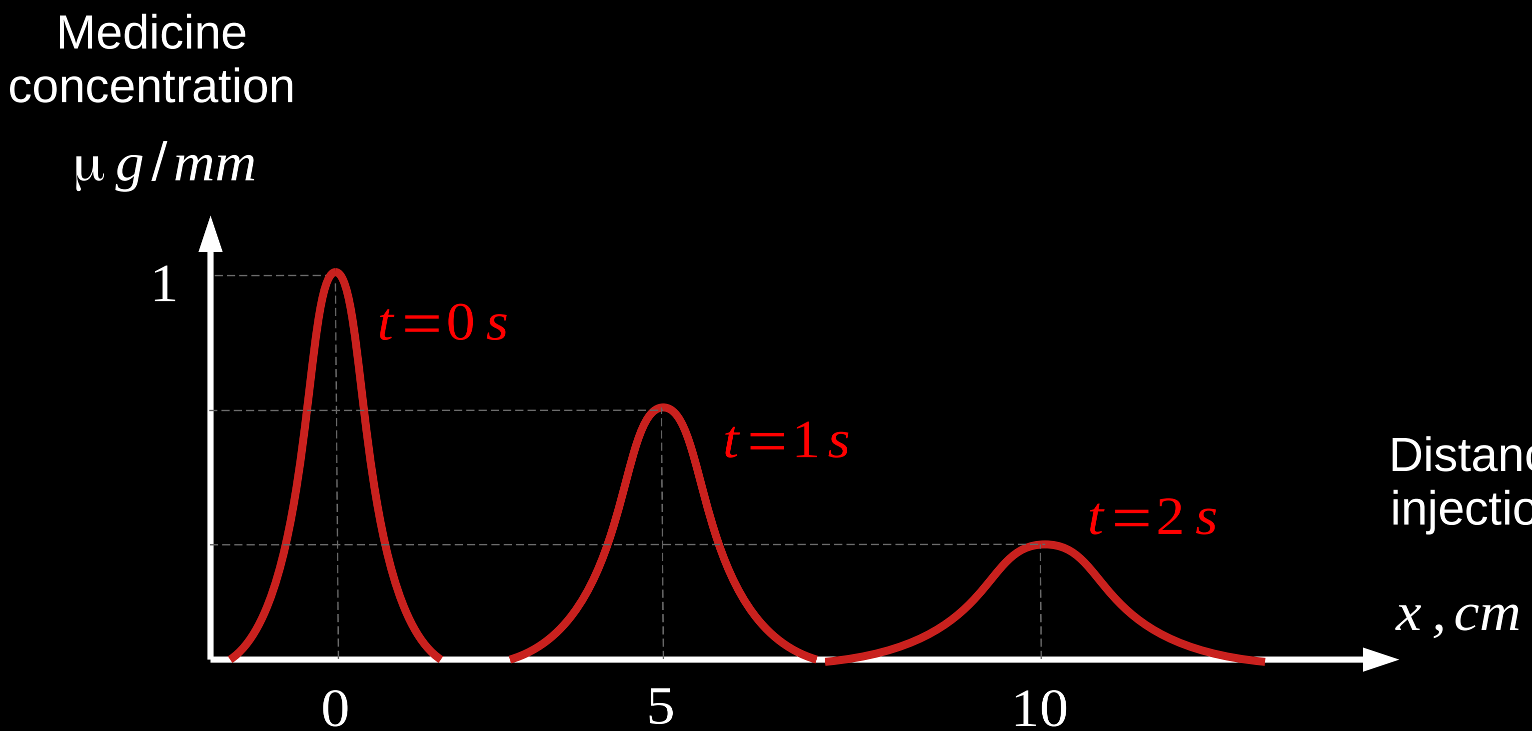
Type of software, computing infrastructure, how long can you wait, method, resolution, how long we need to simulate physical time, steady vs transient, physics (e.g. refinement need at boundary layers/wakes), what is the intention of the simulation (e.g. visualization of known physics, quick design insight, 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	Published in a journal.
Ship hydro	Medium ~60M cells	**~10 days** (Supercomputer)	Transient LES method	Published in a journal.

1d convection-diffusion of a Gaussian

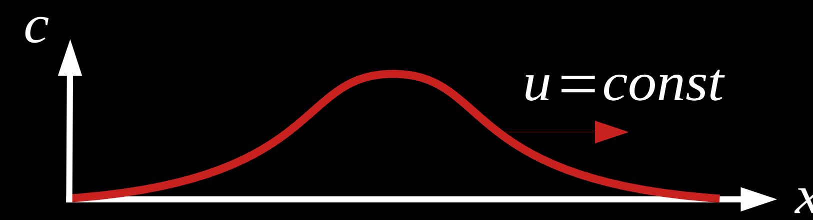
Example: medicine injection into a blood vessel (very fast and small quantity)

3D smoke cloud moving with air



1d convection-diffusion equation

1) **Physics** identification.



2) **Mathematical equations and physics interpretation.**

$$\frac{\partial c}{\partial t}+\nabla\cdot\boldsymbol{u}\,c=\nabla\cdot(\alpha\nabla c)$$

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

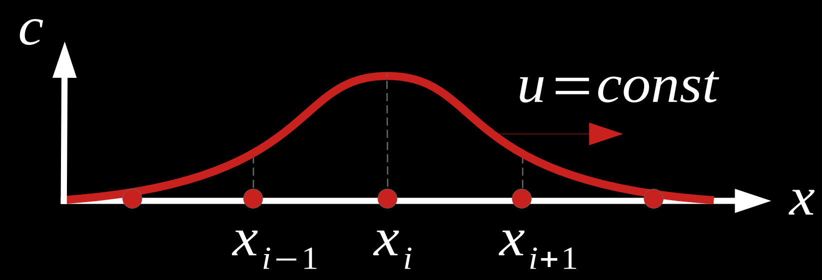
Find the concentration field after 1, 5, and 10s

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

Finite-**difference** method (Lecture 1)

Finite-**volume** method (Lecture 2)

Finite-**difference** method (Lecture 1)



c_i^n: n - time coordinate, i - space coordinate

$$\frac{\partial c}{\partial t} + \nabla \cdot \boldsymbol{u} c = \nabla \cdot (\alpha \nabla c)$$

⬇

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

⬇

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

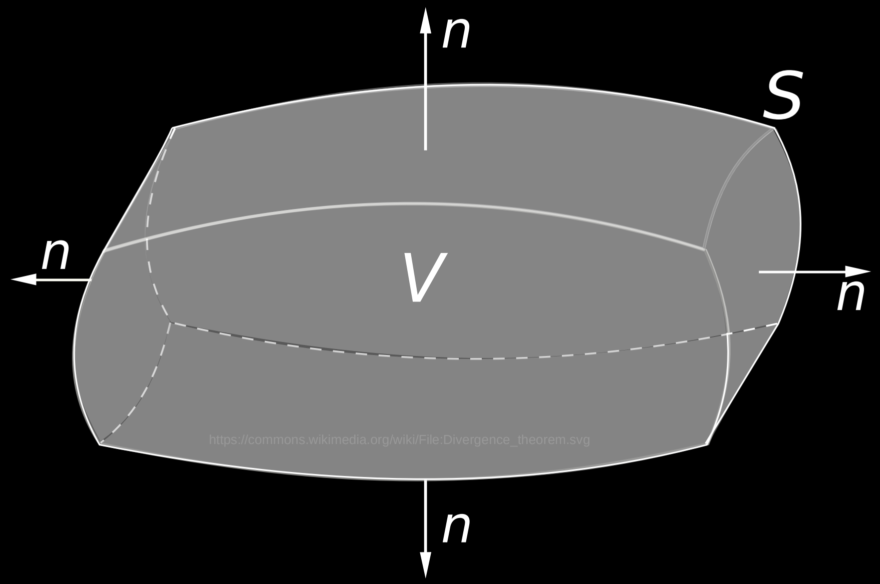
Finite-difference method: discretize space with points and solve for values of field in these points

Gauss' (Ostrogradsky's) theorem

General formulation

$$\int_V \nabla \cdot \boldsymbol{a}\, dV = \int_S \boldsymbol{a} \cdot \boldsymbol{n}\, dS$$

$\boldsymbol{a}$ - vector field
V - control volume
S - control surface



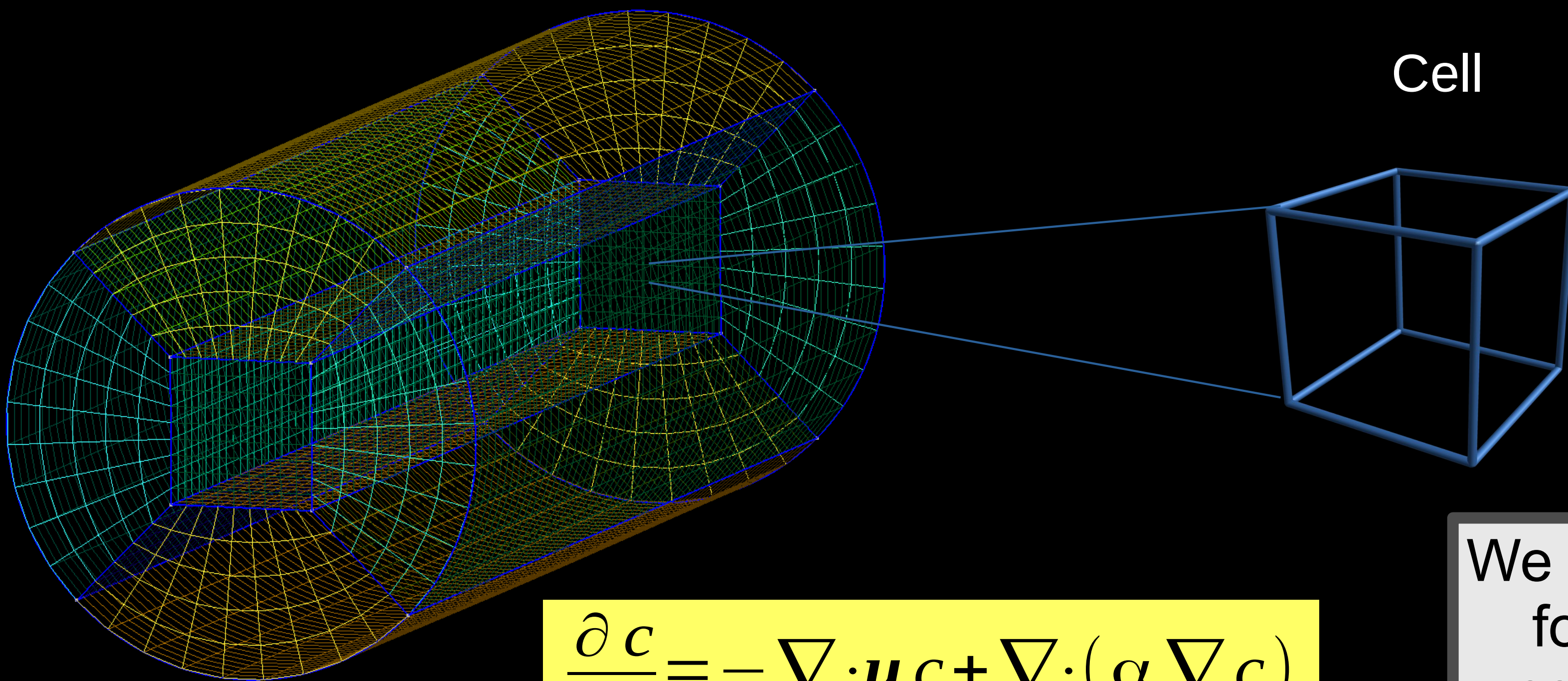
Using general flux $\boldsymbol{u}\phi$

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

$\boldsymbol{u}$ - velocity field
ϕ - scalar field (density, concentration,...)

Meaning: change of transported scalar quantity in any volume equals sum of fluxes through boundaries
Thus, we can transform any volume integral of a divergence of a vector field to a surface integral

Divide domain into control volumes (cells)



We are now solving for an average concentration in each cell

$$\frac{\partial c}{\partial t} = -\nabla \cdot \boldsymbol{u} c + \nabla \cdot (\alpha \nabla c)$$

Key step!

Apply volume integral:

$$\frac{1}{V}\int_V \frac{\partial c}{\partial t} dV = -\frac{1}{V}\int_V \nabla \cdot \boldsymbol{u} c \, dV + \frac{1}{V}\int_V \nabla \cdot (\alpha \nabla c) dV$$

Rate of change of c in a cell: $\left.\frac{\partial c}{\partial t}\right|_{cell}$

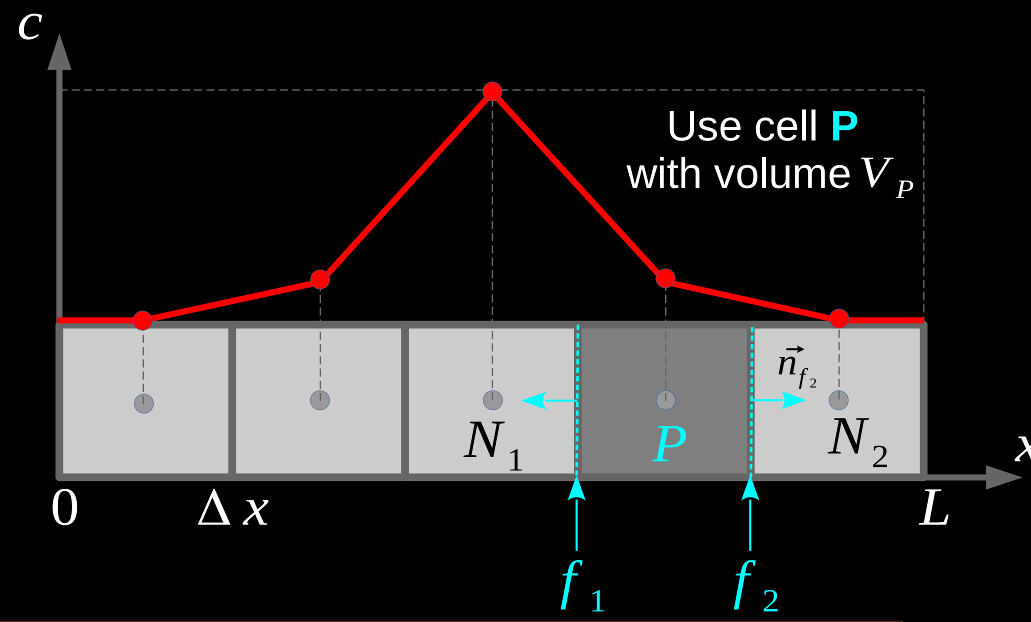
Change due to **convection**: C_{ave}

Change due to **diffusion**: D_{ave}

1d convection of a Gaussian

Goal: calculate field *c* after Δt

$u = const > 0$, $t_1 = t_0 + \Delta t$, **5 cells**



- Initial condition: average concentration values for each cell is given (based on Gaussian)
- Boundary condition: periodic (last and first cells are connected)
- Grid: uniform and has 5 cells
- Velocity: constant positive
- How can we calculate change of the concentration field after some small time step Δt?

Time-marching

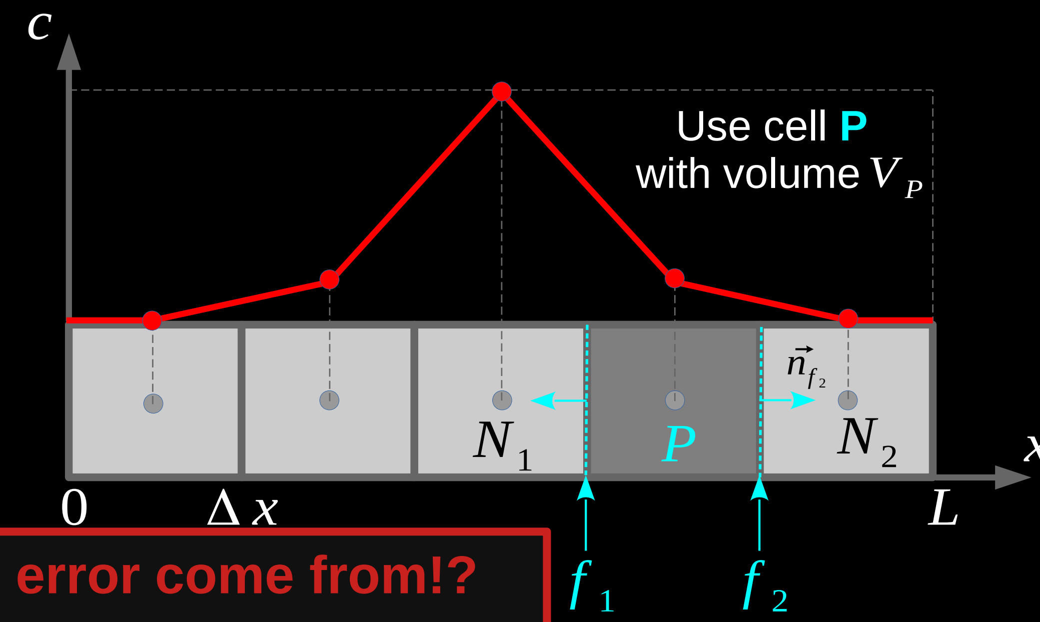
1. Equations are integrated over some time step.
2. New values of fields (u, p, T…) are obtained and then used as initial values for next iteration.

1d convection of a Gaussian

Goal: calculate field *c* after Δt

$u = const > 0,\ t_1 = t_0 + \Delta t,$ **5 cells**

$$\underbrace{\frac{1}{V}\int_V \frac{\partial c}{\partial t} dV}_{} = \underbrace{-\frac{1}{V}\int_V \nabla\cdot \boldsymbol{u}\, c\, dV}_{C_{ave}} + \underbrace{\frac{1}{V}\int_V \nabla\cdot(\alpha \nabla c)\, dV}_{C_{ave}}$$



C_{ave} Convectio[n]

From where does the error come from!?

$$\frac{1}{V_P}\int_{V_P} \nabla\cdot(\vec{u} c)\, dV = \frac{1}{V_P}\int_{A_P} (\vec{u} c)\vec{n}\, dA_P = \frac{1}{V_P}\sum_f (\vec{u}_f c_f)\cdot \vec{n}_f A_f = \frac{u_{f_2} c_{f_2} - u_{f_1} c_{f_1}}{\Delta x} = u\frac{c_{f_2} - c_{f_1}}{\Delta x}$$

Gauss' theorem

Finite number of faces & Use average fluxes

1d uniform mesh

Constant velocity

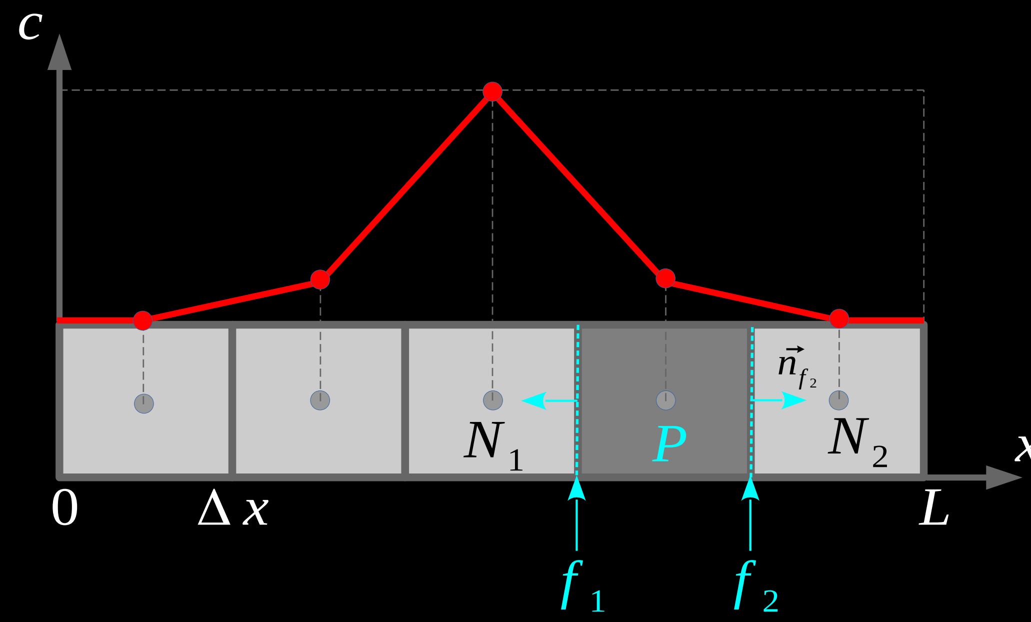
D_{ave} Diffusion

$$\frac{1}{V_P}\int_{V_P} \alpha \nabla\cdot(\nabla c)\, dV = \frac{\alpha}{V_P}\int_{A_P} (\nabla c)\vec{n}\, dA_P = \frac{\alpha}{V_P}\sum_f (\nabla c_f)\cdot \vec{n}_f A_f = \alpha\frac{(\partial c/\partial x)_{f_2} - (\partial c/\partial x)_{f_1}}{\Delta x}$$

1d convection of a Gaussian

Goal: calculate field *c* after Δt

$u = const > 0\,,\ t_1 = t_0 + \Delta t\,,$ **5 cells**



We started with:

$$\frac{\partial c}{\partial t} = -\nabla \cdot \boldsymbol{u} c + \nabla \cdot (\alpha \nabla c)$$

After volume averaging and Gauss theorem

$$\left.\frac{\partial c}{\partial t}\right|_{cell\ P} = -u \frac{c_{f_2} - c_{f_1}}{\Delta x} + \alpha \frac{(\partial c / \partial x)_{f_2} - (\partial c / \partial x)_{f_1}}{\Delta x}$$

Rate of change of c in a cell

Change due to **convection** C_{ave}

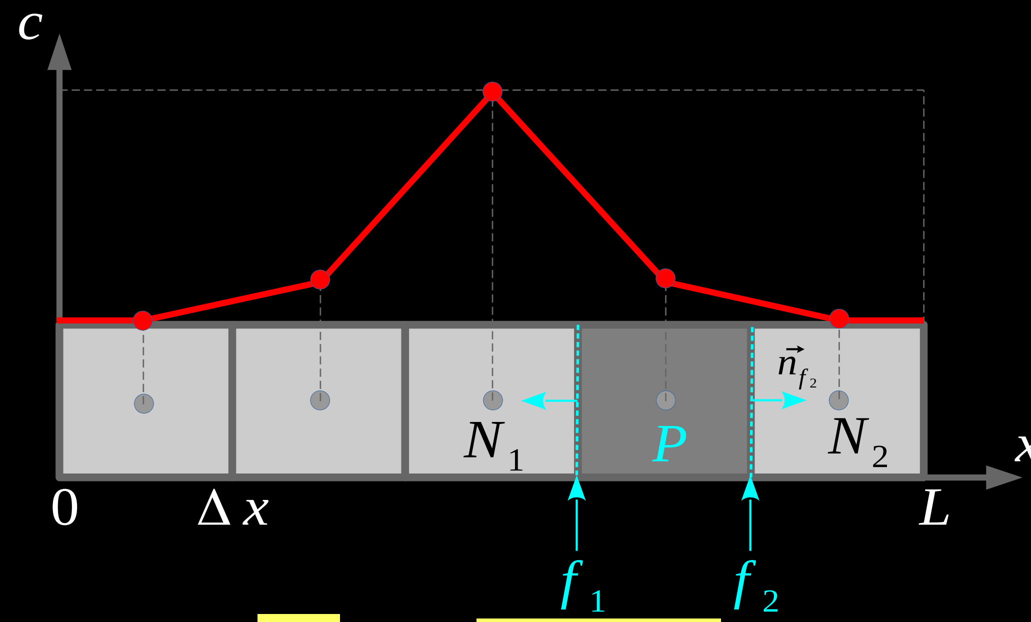
Change due to **diffusion** D_{ave}

How do we calculate face values of c and $\partial c / \partial x$?

1d convection of a Gaussian

Goal: calculate field *c* after Δt

$u = const > 0$, $t_1 = t_0 + \Delta t$, **5 cells**



How do we calculate **face values** of c and $\partial c / \partial x$?

Linear

$$c_{f_1 LIN} = \frac{c_P + c_{N_1}}{2}$$

Upwind

$$c_{f_1 UW} = \begin{cases} c_P \ \text{if } u < 0 \\ c_{N_1} \ \text{if } u > 0 \end{cases}$$

Flux limiting

$$c_{f_1} = c_{f_1 UW} - \phi(r_{N_1})(c_{f_1 UW} - c_{f_1 LIN})$$

$\phi(r_P)$ - flux limiter function

$$r_P = \frac{c_P - c_{N_1}}{c_{N_2} - c_P}$$

- ratio of successive gradients

Blended

$$c_{f_1 BL} = (1-\gamma) c_{f_1 UW} + \gamma c_{f_1 LIN}$$

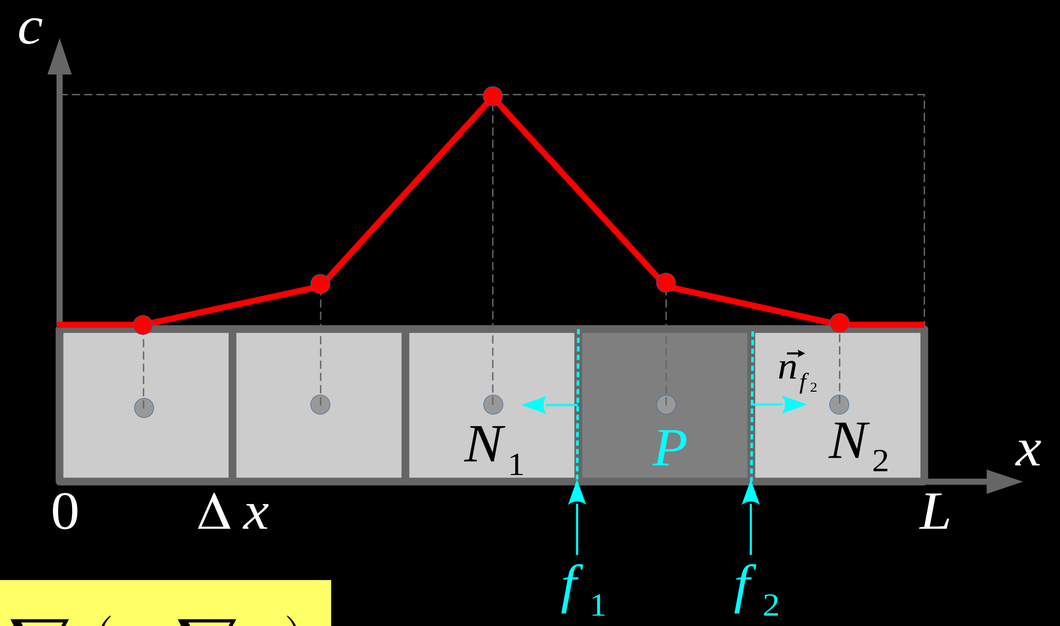
$$\left(\frac{\partial c}{\partial x}\right)_{f1} = \frac{1}{\Delta x} \int_{x_{N_1}}^{x_P} c'(x)\, dx \approx \frac{c_P - c_{N_1}}{\Delta x}$$

Note: face interpolation is one of the most essential parts to pay attention on in CFD!
We will study the effect of different interpolation tecniques in Assignment 1.

1d convection of a Gaussian

Goal: calculate field *c* after Δt

$u = const > 0\,,\ t_1 = t_0 + \Delta t\,,$ **5 cells**



Are we done?
Or is there something missing still?

We started with:

$$\frac{\partial c}{\partial t} = -\nabla \cdot \boldsymbol{u} c + \nabla \cdot (\alpha \nabla c)$$

Volume averaging + Gauss' theorem

$$\left.\frac{\partial c}{\partial t}\right|_{cell\,P} = -u \frac{c_{f_2} - c_{f_1}}{\Delta x} + \alpha \frac{(\partial c / \partial x)_{f_2} - (\partial c / \partial x)_{f_1}}{\Delta x}$$

Euler + linear

$$\frac{c_P^{n+1} - c_P^n}{\Delta t} = -u \frac{c_{N_2} - c_{N_1}}{2 \Delta x} + \alpha \frac{c_{N_2} - 2 c_P + c_{N_1}}{\Delta x^2}$$

Rate of change of c in a cell

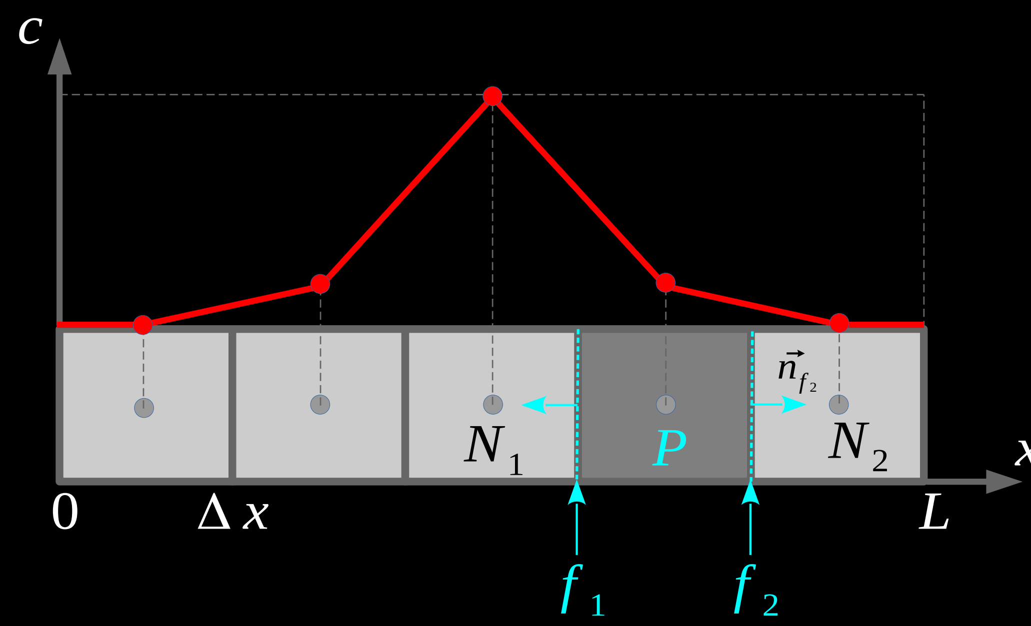
Change due to **convection** C_{ave}

Change due to **diffusion** D_{ave}

1d convection of a Gaussian

Goal: calculate field *c* after Δt

$u = const > 0,\ t_1 = t_0 + \Delta t,$ **5 cells**



Use data from the previous time step (n)

Explicit time stepping:

$$\frac{c_P^{n+1} - c_P^n}{\Delta t} = -u \frac{c_{N_2}^n - c_{N_1}^n}{2\Delta x} + \alpha \frac{c_{N_2}^n - 2c_P^n + c_{N_1}^n}{\Delta x^2}$$

We know everything in the equation and can solve for c_P^{n+1}

However, this method can be quite unstable and thus requires small time steps

Note: this is the formula we obtained for finite-difference:

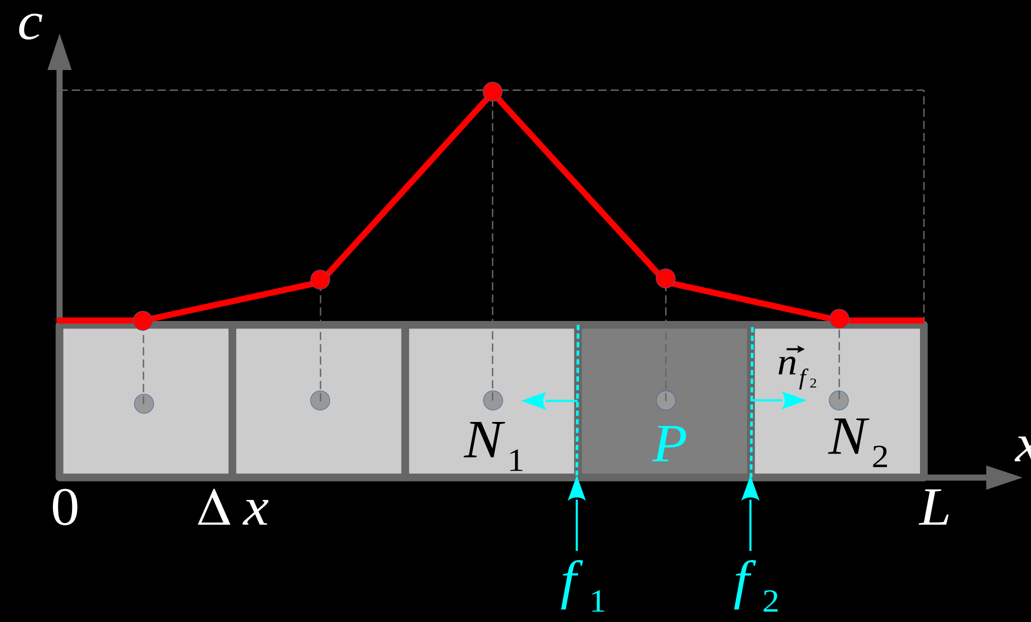
$$\frac{c_i^{n+1} - c_i^n}{\Delta t} = -u \frac{c_{i+1} - c_{i-1}}{2\Delta x} + \alpha \frac{c_{i+1}^n - 2c_i^n + c_{i-1}^n}{\Delta x^2}$$

For 1d uniform grid case FVM and FDM give the same result.

1d convection of a Gaussian

Goal: calculate field *c* after Δt

$u = const > 0\,,\; t_1 = t_0 + \Delta t\,,$ **5 cells**



Use data from the next time step (n+1)

<u>Implicit</u> time stepping:

$$\frac{c_P^{n+1} - c_P^n}{\Delta t} = -u \frac{c_{N_2}^{n+1} - c_{N_1}^{n+1}}{2\Delta x} + \alpha \frac{c_{N_2}^{n+1} - 2c_P^{n+1} + c_{N_1}^{n+1}}{\Delta x^2}$$

Combining unknowns (cell-averaged values c_X^{n+1})

$$a_P c_P^{n+1} + \sum_{N_i} a_{N_i} c_{N_i}^{n+1} = b_P$$

Construct system for all 5 cells

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} & a_{14} & a_{15} \\ a_{21} & a_{22} & a_{23} & a_{24} & a_{25} \\ a_{31} & a_{32} & a_{33} & a_{34} & a_{35} \\ a_{41} & a_{42} & a_{43} & a_{44} & a_{45} \\ a_{51} & a_{52} & a_{53} & a_{54} & a_{55} \end{pmatrix} \cdot \begin{pmatrix} c_1^{n+1} \\ c_2^{n+1} \\ c_3^{n+1} \\ c_4^{n+1} \\ c_5^{n+1} \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \\ b_5 \end{pmatrix} \sim A\vec{c}^{\,n+1} = \vec{b}$$

This method is more stable, but requires iterative linear solvers. It is used by OpenFOAM

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 $D = D(x,y,z,t)$ ($t = n\Delta t$).

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

$$D = \alpha\,\nabla\cdot\nabla\,\phi$$

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

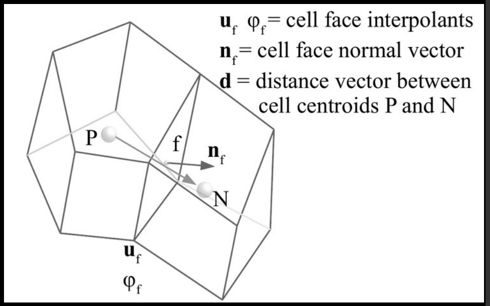
$$\int_V \nabla\cdot(\boldsymbol{u}\phi)\,dV = \int_A (\boldsymbol{u}\phi)\cdot\boldsymbol{n}\,dA$$

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.

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

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



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)

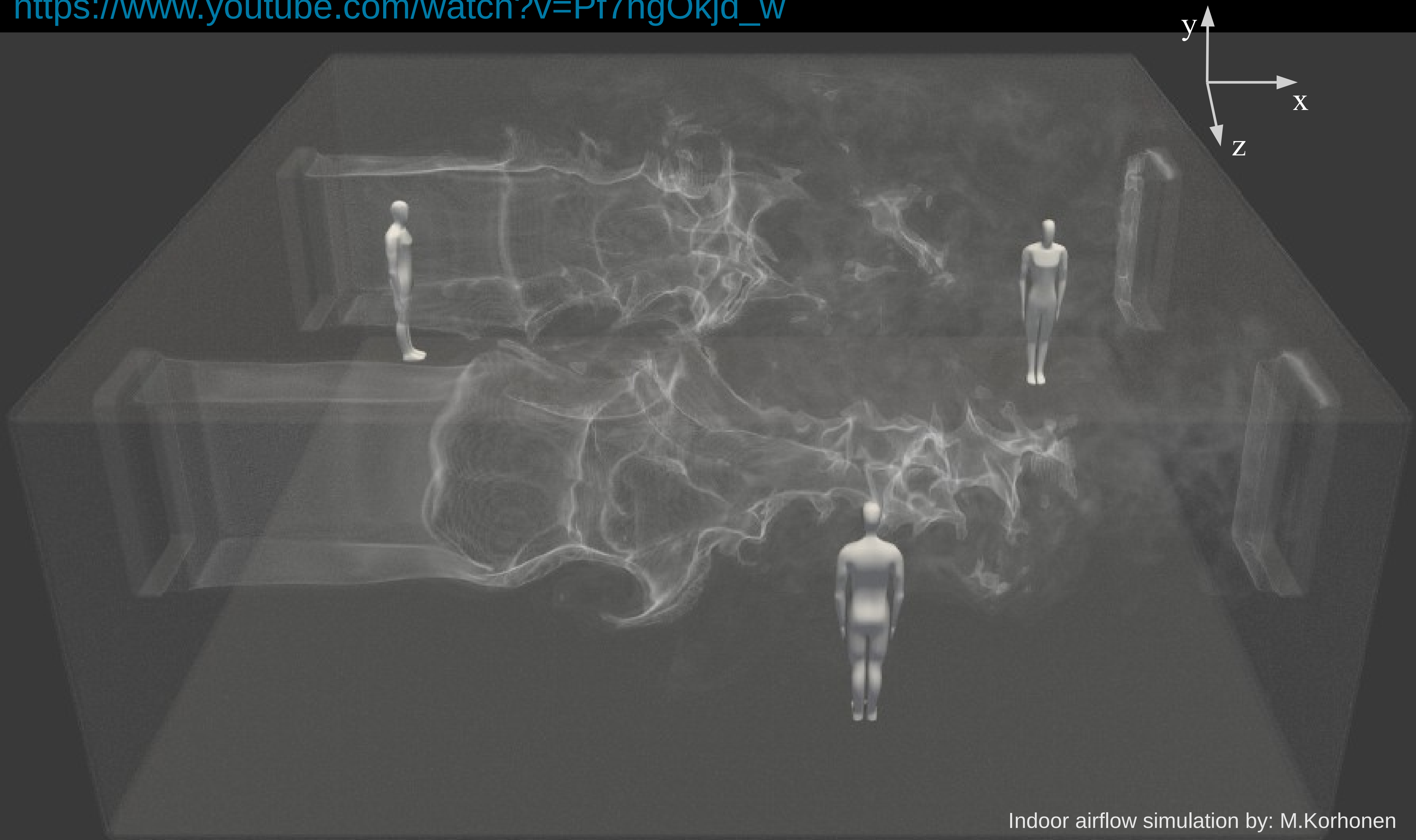
$$Co = \frac{\Delta t\, u}{\Delta x} < 1$$

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)

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

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.

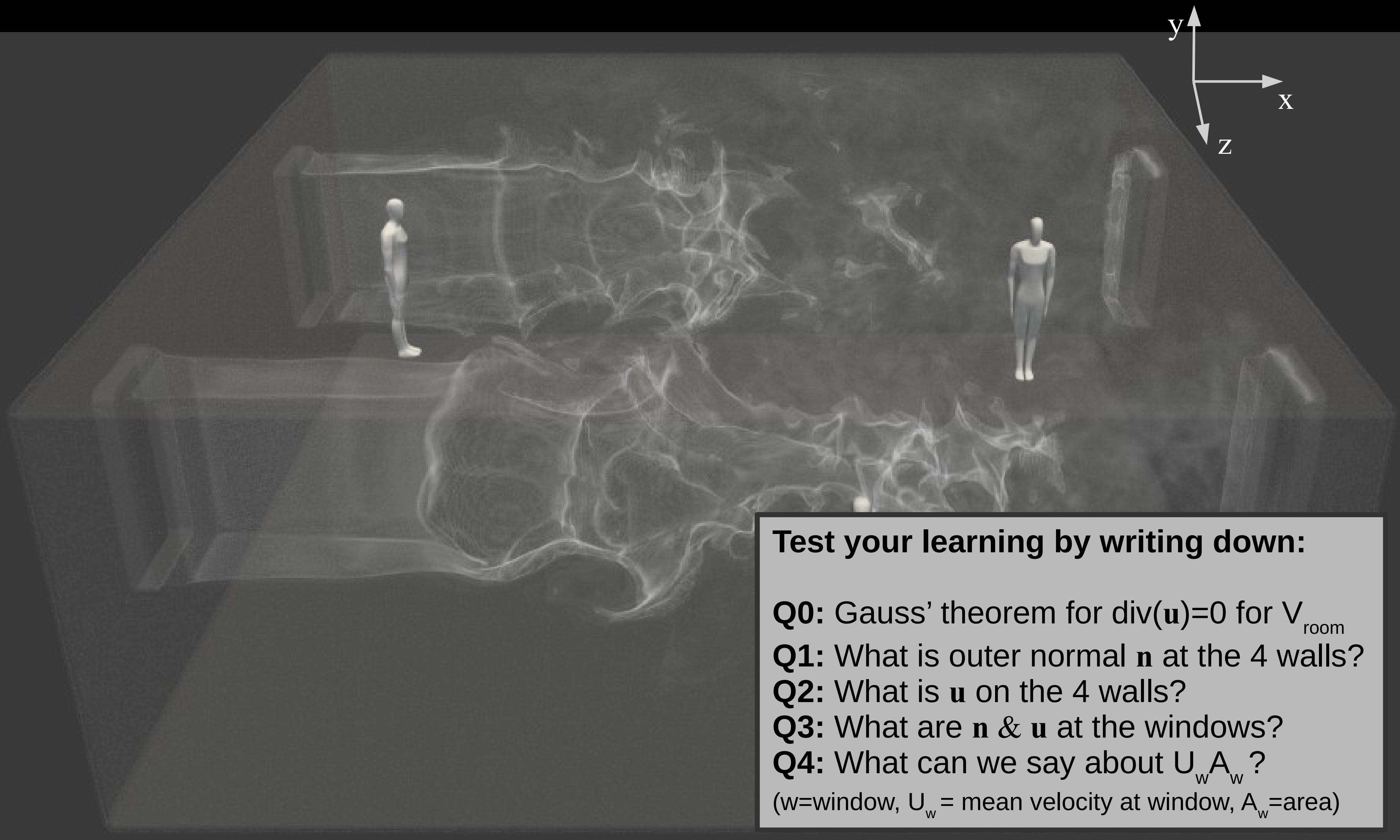
https://www.youtube.com/watch?v=Pf7hgOkjd_w



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:

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



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)