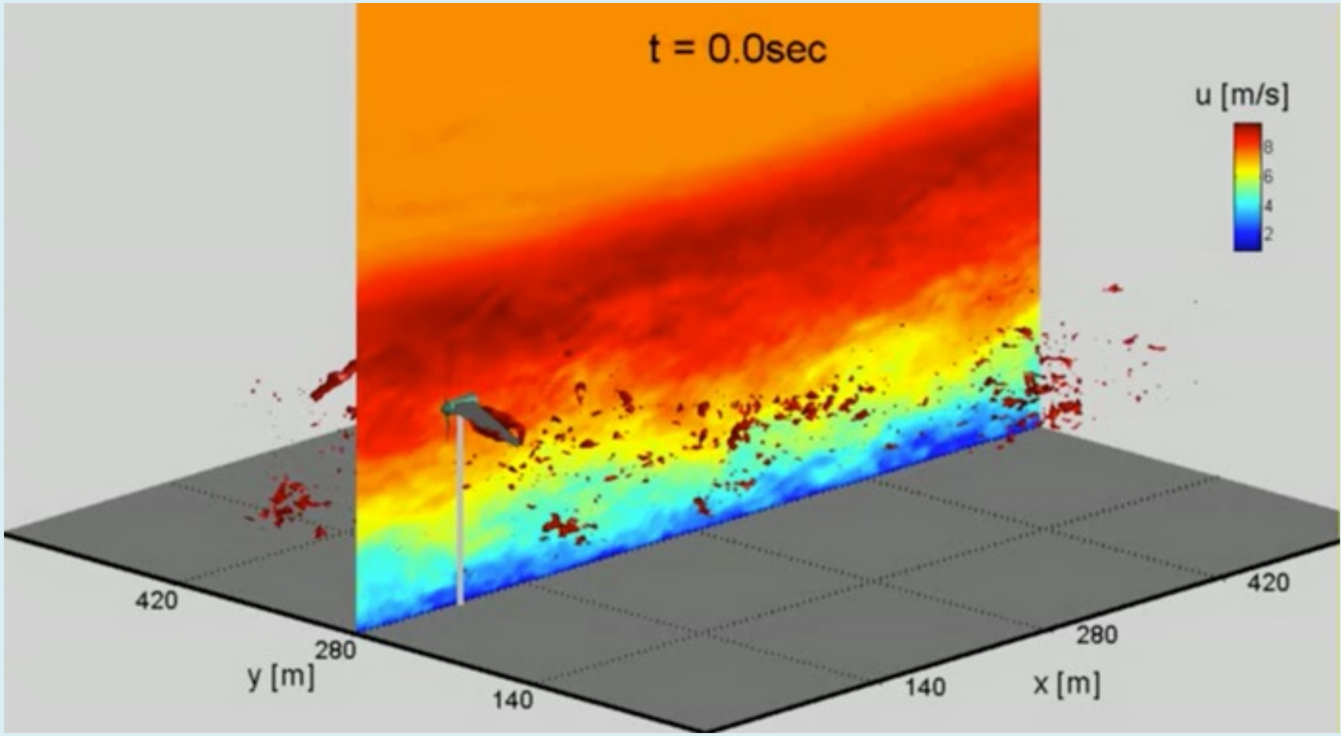
Environmental Transport Phenomena

Computational Fluid Dynamics



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Computational Fluid Dynamics (CFD)

I. Approaches for simulating turbulent flows

II. Direct Numerical Simulation (DNS)

III. RANS and the closure problem

IV. Large-Eddy Simulation (LES)

Reference: Lecture + Handout (handout optional)

Motivation

- For turbulent flows, we know the transport equations (advection-diffusion equations in 3D), but there is **no analytical solution**
- In computational fluid dynamics (CFD), equations are discretized (in time and space) and **solved numerically (with computers)**
- To resolve all eddy motions (from integral scale to Kolmogorov scale)**, one needs a resolution as fine as the Kolmogorov scale in 3-D** [this is called Direct Numerical Simulation].

<u>Question</u>: Is this possible for all turbulent flows?

Governing Transport (Advection-Diffusion) Equations

Incompressible flow

$$\frac{\partial u_i}{\partial x_i} = 0$$

Mass conservation (continuity)

$$\frac{\partial u_i}{\partial t} + \frac{\partial}{\partial x_j}\left(u_i u_j\right) = -\frac{1}{\rho}\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j}\left(\nu\left[\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right]\right) + F_i$$

Momentum conservation (Navier-Stokes equations)

$$\frac{\partial C}{\partial t} + \frac{\partial}{\partial x_i}\left(u_i C\right) = +\frac{\partial}{\partial x_i}\left(D_m \frac{\partial C}{\partial x_i}\right) + Q$$

Advection-diffusion equation for conservation of Scalars (e.g. pollutant, temperature)

Note: F_i is any external forcing;
Q is any source or sink of scalar.

Steps in CFD:

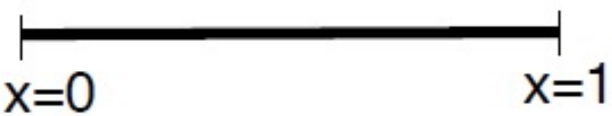
- **STEP 1: Meshing**
- **STEP 2: Discretize equations**
- **STEP 3: Solve discretized equations**

General Strategy in CFD (generally in numerical methods)

The general strategy consists of replacing a **continuous domain** with a **discrete domain** using a grid

Continuous Domain

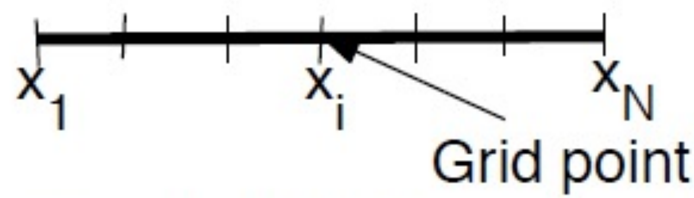
$0 \le x \le 1$



Coupled PDEs + boundary conditions in continuous variables

Discrete Domain

$x = x_1, x_2, \ldots, x_N$

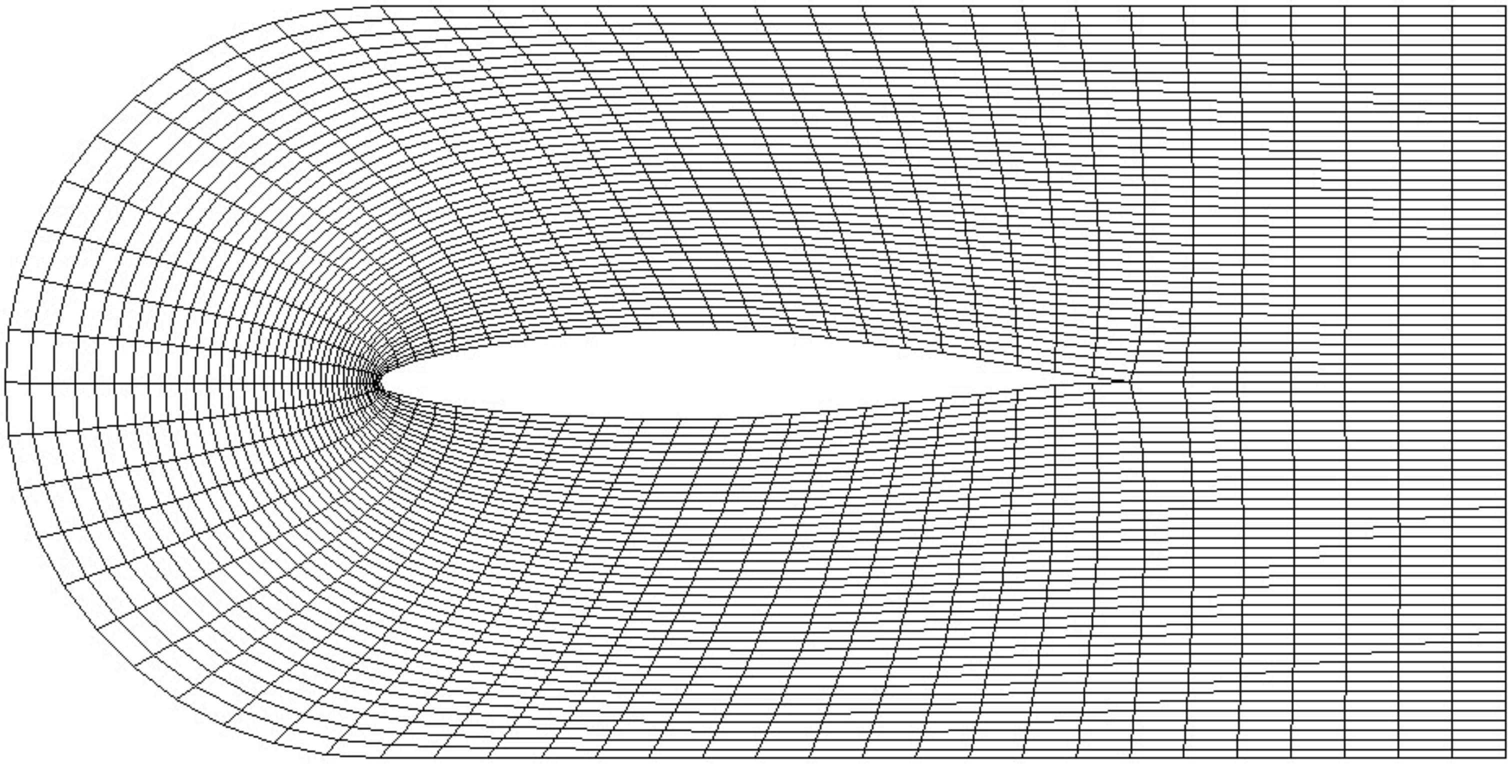


Coupled algebraic eqs. in discrete variables

Variables are only defined at the grid points

Step 1: Define a mesh (points where equations are solved)

Example of 2-D computational mesh to simulate flow around an airfoil (more details in FLUENT project)

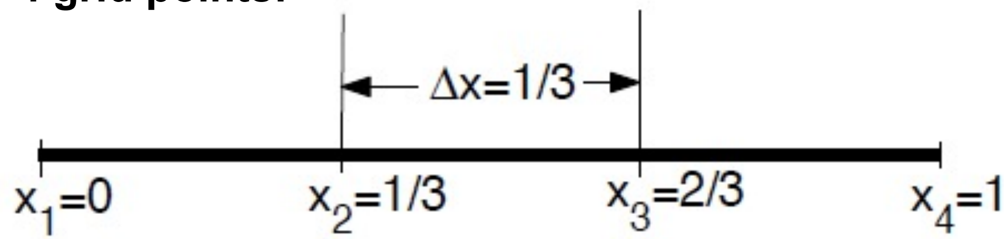


Step 2: Discretize the governing equations

A very simple example: 1-D equation

$$\frac{du}{dx} + u = 0; \quad 0 \leq x \leq 1; \quad u(0) = 1$$

In this case, using a mesh with only 4 grid points:



$$\left(\frac{du}{dx}\right)_i + u_i = 0$$

Discretizing each term of the governing partial differential equation using for example a *finite difference* approximation:

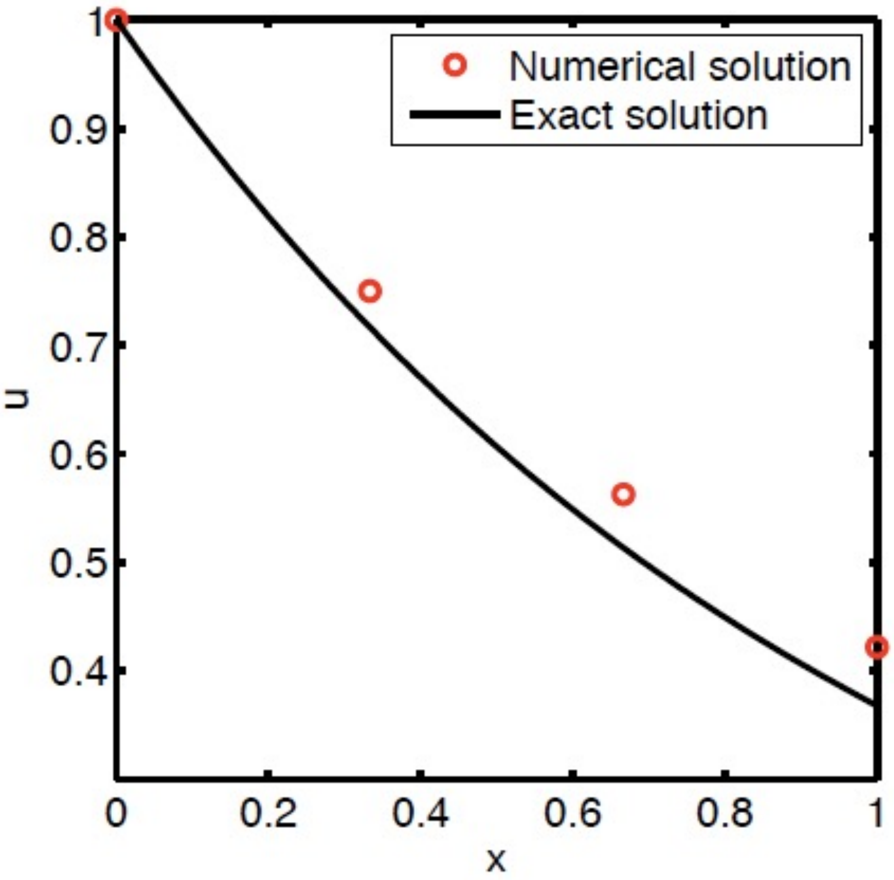
$$\left(\frac{du}{dx}\right)_i = \frac{u_i - u_{i-1}}{\Delta x} + O(\Delta x)$$

Discretization Error

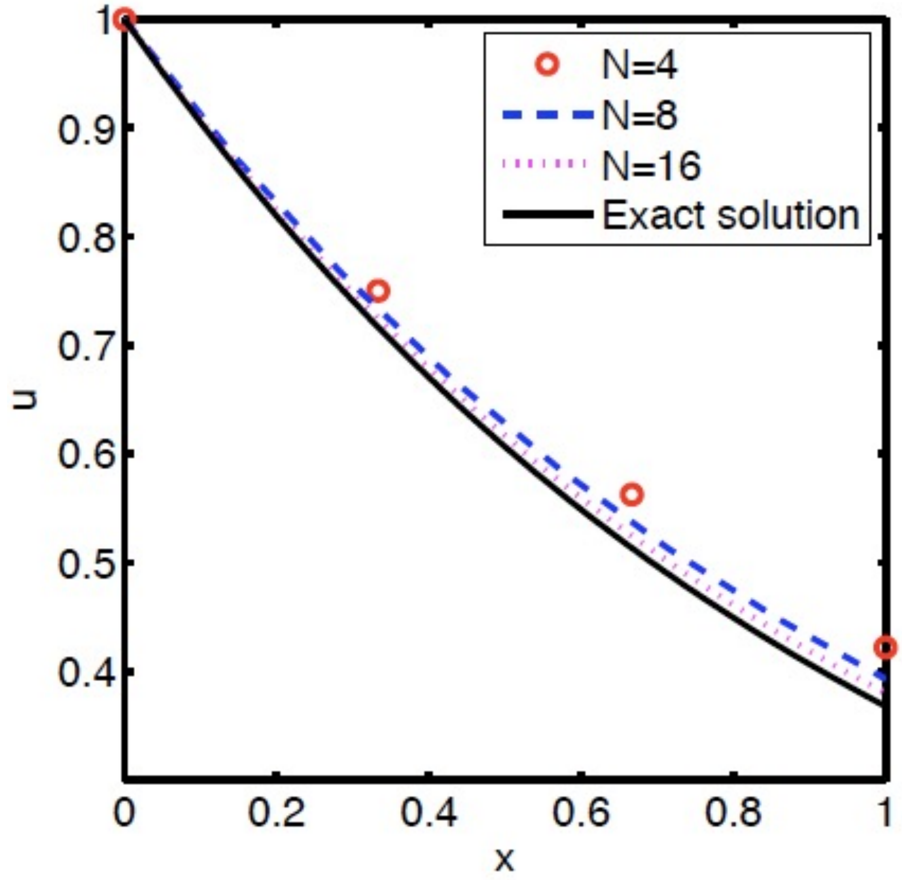
In this case, first order approximation

Spatial and temporal discretization of the equations

NUMERICAL ERROR (due to discretization)



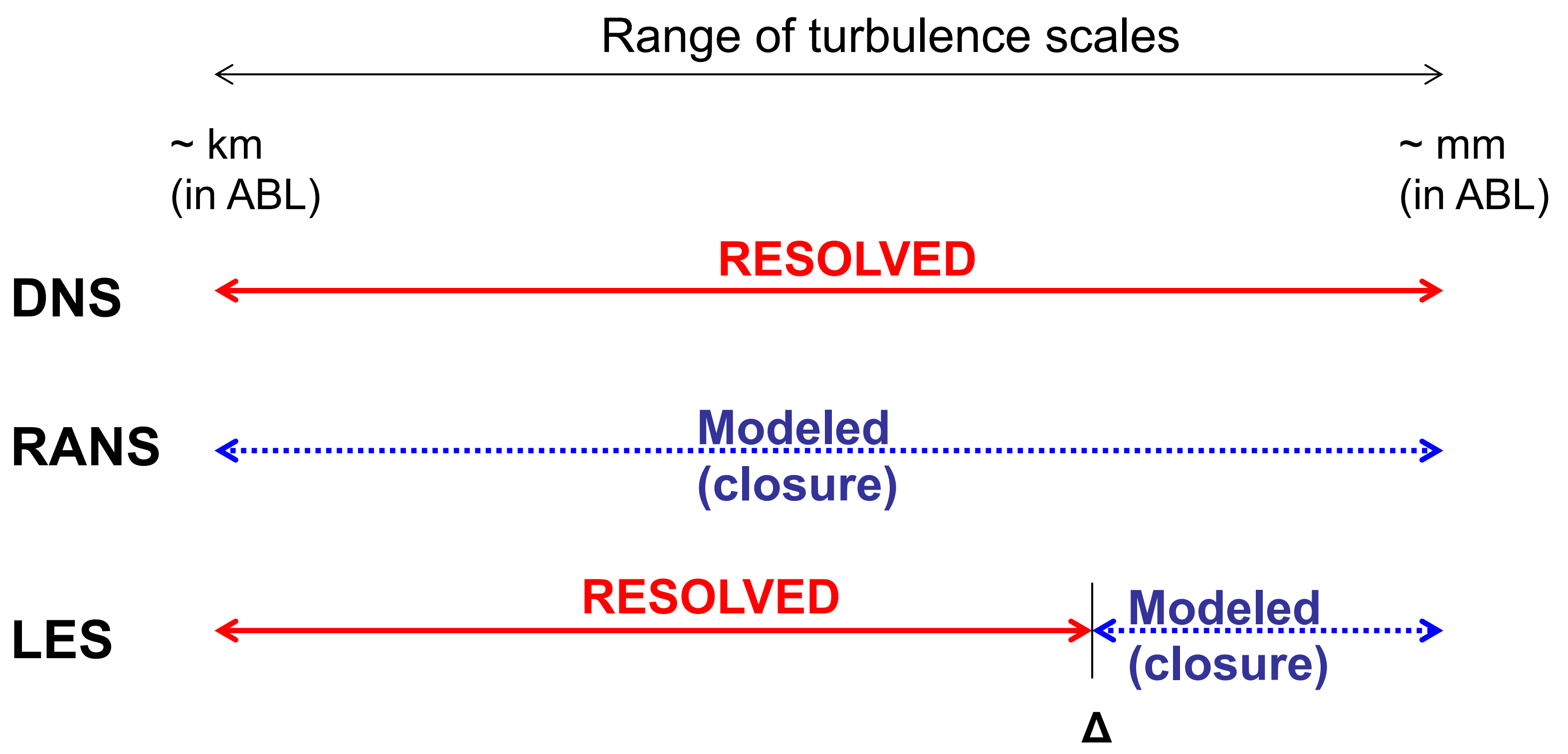
GRID CONVERGENCE



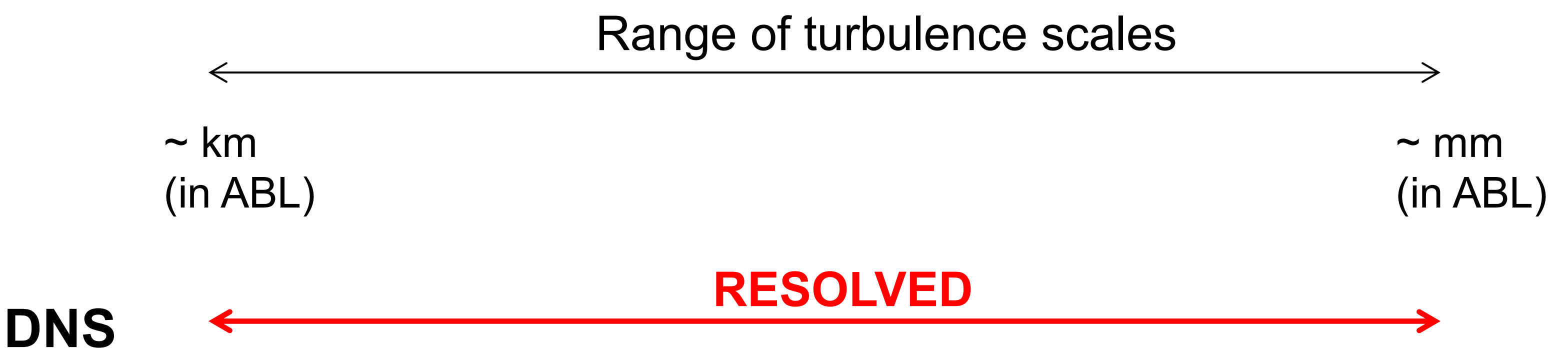
Effect of Grid Refinement (resolution): The finer the grid (smaller Δx), the smaller the discretization (numerical) error.

Approaches for simulation/modeling of turbulent flows

- **DNS** (Direct Numerical Simulation)
- **RANS** (Reynolds-Averaged Navier Stokes)
- **LES** (Large-Eddy Simulation)



Direct Numerical Simulation (DNS)



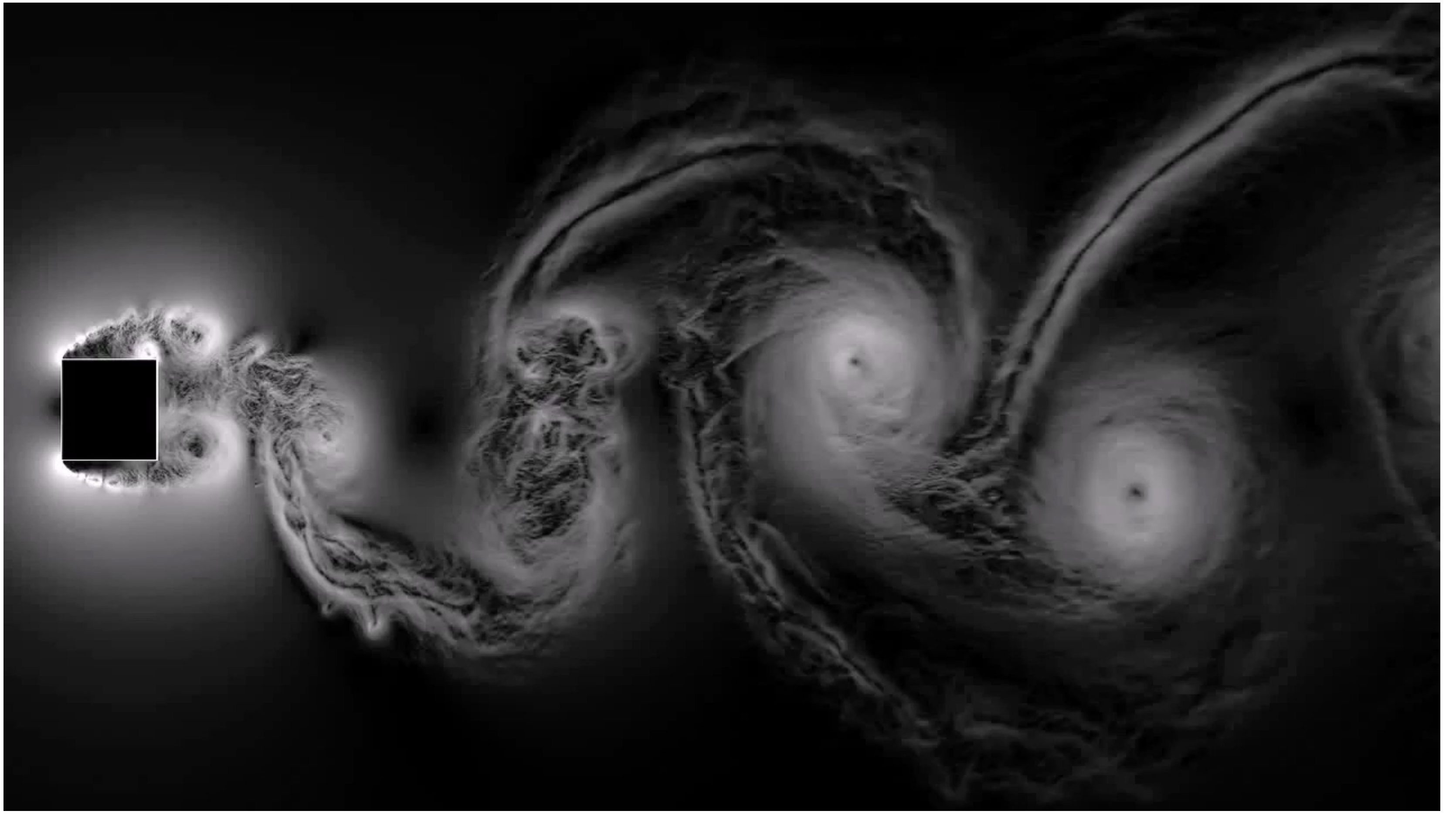
- **<u>All the eddy motions are resolved in 3D</u>** (from the integral scale to the Kolmogorov scale). **No need for turbulence model.**

- To achieve that, the governing (advection-diffusion) equations are discretized in space (using resolution Δx, Δy, Δz) and time (using resolution Δt) such that:

(a) The total **computational domain is large enough to capture the largest eddies** (need to simulate all the eddy sizes).

(b) **Resolution Δ is FINE ENOUGH to capture the smallest eddy motions**

Direct Numerical Simulation (DNS): Example



DNS of the turbulent flow around a square cylinder at Re=22000

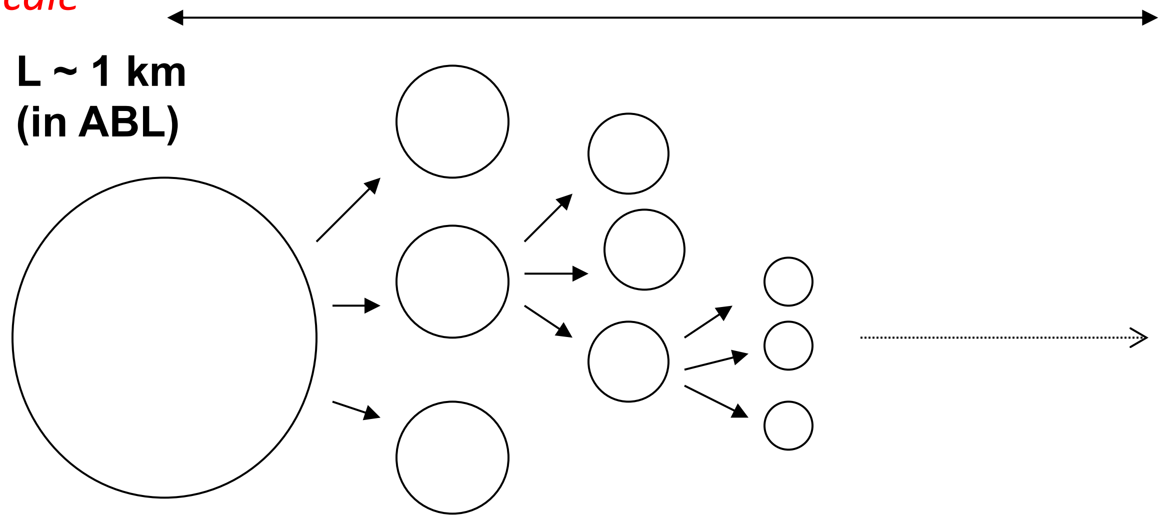
(Number of grid points: 325×10^6)

https://www.youtube.com/watch?v=c8zKWaxohng

Direct Numerical Simulation (DNS): Example

DNS of a turbulent hydraulic jump

https://www.cambridge.org/core/journals/journal-of-fluid-mechanics/article/direct-numerical-simulation-of-a-turbulent-hydraulic-jump-turbulence-statistics-and-air-entrainment/84800BF335F44F8A13EE5C648CDC388D#fndtn-supplementary-materials



$$\frac{L_I}{L_K} \sim \mathrm{Re}^{3/4}$$

Energy production → ***(Energy cascade)*** → ***Energy dissipation***

(Inertial effects) *(Viscous effects)*

- **Full resolution (Direct Numerical Simulation):**

How many grid points are required for ABL simulations?

$$\left(\frac{L_I}{L_K}\right)^3 \sim \mathrm{Re}^{9/4} \sim 10^{20}$$

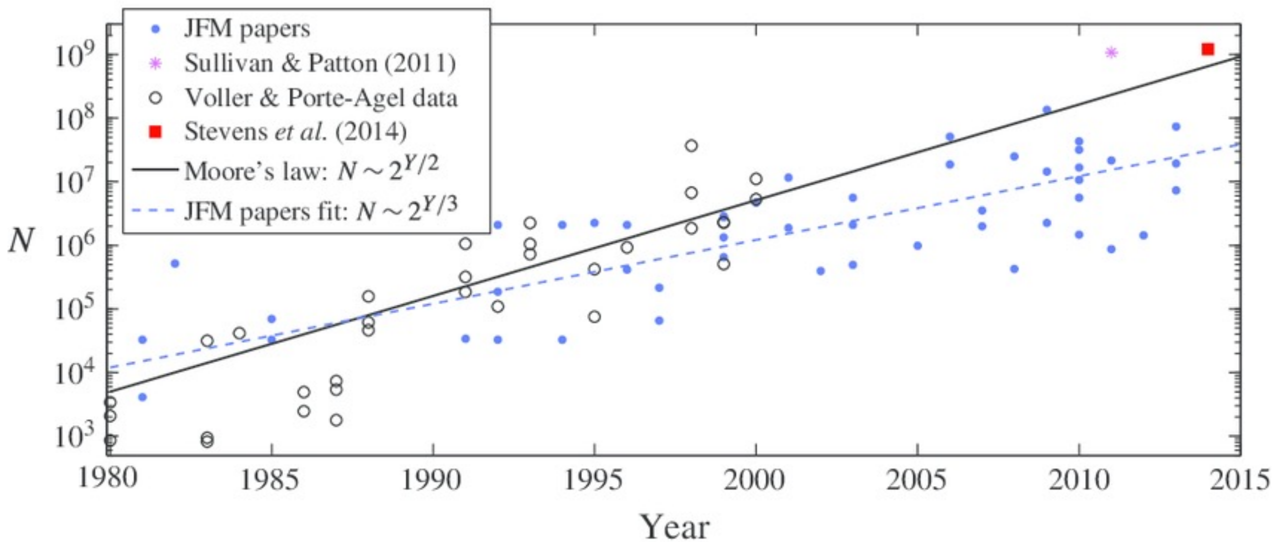
Atmospheric BL: $Re \sim 10^8 - 10^9$

Computational Resources

- Direct Numerical Simulation is **IMPOSSIBLE** for many high-Re flows
- Example: ABL: (needs Δx~1 mm ; Δt~ 1 ms)

➔ It requires $Re^{9/4}$ ~ 10^{20} grid points!!

[Using best available supercomputers: maximum number of grid points in DNS ~ 10^{12}]



Bou-Zeid et al. (2015)

If Moore's law on computer power [doubling every 18 months] holds:

DNS of atmospheric turbulence over a 10 km x 10 km x 1 km domain may be possible in ~ year **2080**.

Reynolds-Averaged Navier Stokes (RANS) Approach

Range of turbulence scales

~ km (in ABL) ←→ ~ mm (in ABL)

RANS ←······→ **Modeled (closure)**

- **<u>RANS</u>**: It solves 'Reynolds-Averaged Navier Stokes' equations.
  - *When the flow is 'steady' ($\partial \overline{C} / \partial t = 0$) → average=time average.*

- **<u>URANS (Unsteady RANS)</u>:** It also solves the RANS equations, but including the time evolution of the averaged quantities (with time derivative).

➢ ***<u>Question</u>: What type of averaging allows to do that?***

RANS (Reynolds-Averaged Navier Stokes)

Incompressible flow

$$\frac{\partial \bar{u}_i}{\partial x_i} = 0$$

$$\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial}{\partial x_j}\left(\bar{u}_i \bar{u}_j\right) = -\frac{1}{\rho}\frac{\partial \bar{p}}{\partial x_i} - \frac{\partial \tau_{ij}}{\partial x_j} + \frac{\partial}{\partial x_j}\left(\nu\left[\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i}\right]\right) + \bar{F}_i$$

Turbulent (Reynolds) stress

$$\tau_{ij} = \overline{u_i' u_j'}$$

$$\frac{\partial \bar{C}}{\partial t} + \frac{\partial}{\partial x_i}\left(\bar{u}_i \bar{C}\right) = -\frac{\partial q_i}{\partial x_i} + \frac{\partial}{\partial x_i}\left(D_m \frac{\partial \bar{C}}{\partial x_i}\right) + \bar{Q}$$

Turbulent flux

$$q_i = \overline{u_i' C'}$$

Effect of turbulent fluctuations on the average fields

<u>CLOSURE PROBLEM</u>: **Fundamental problem in turbulence (equations are not closed: more unknowns than equations)**

Reynolds-Averaged Navier Stokes (RANS) Approach

Reynolds decomposition:

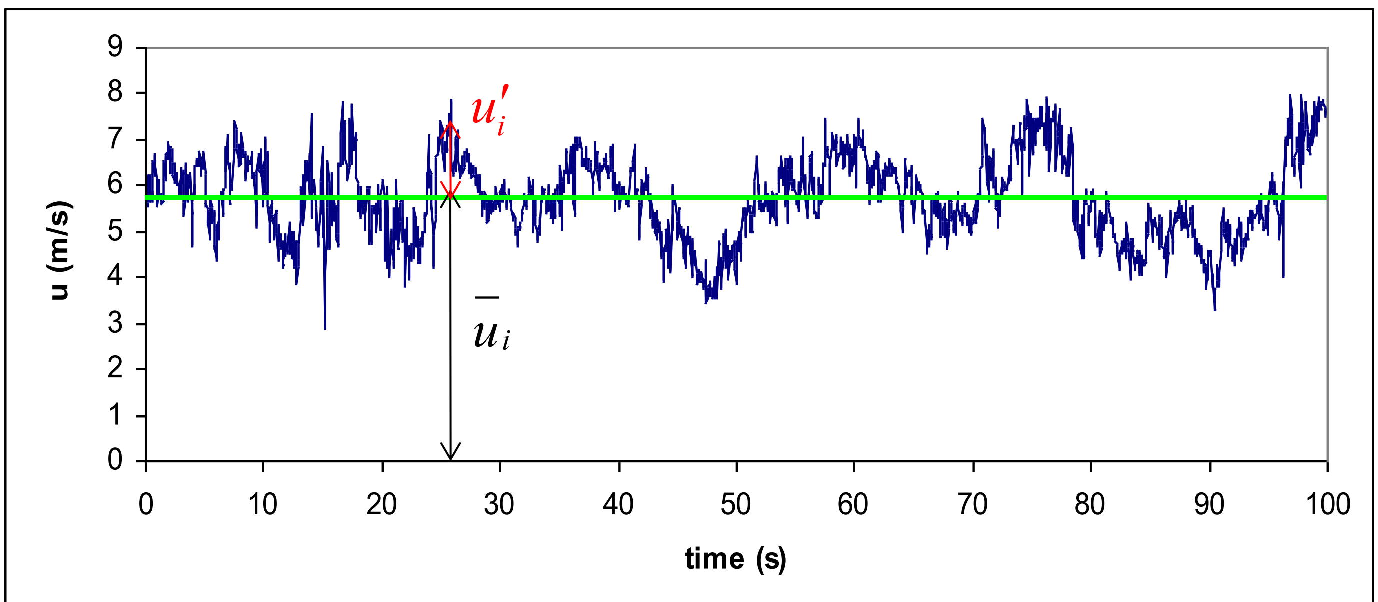
$$u_i = \overline{u}_i + u'_i$$
$$C = \overline{C} + C'$$

Types of averages:

- **Time Averaging**
- **Ensemble Averaging** (over different realizations of the same 'experiment')

Note: for turbulent **stationary** flows, time averages are equal to ensemble averages

Example of time averaging



Turbulence models: Eddy-viscosity/diffusivity models

NOTE: In laminar flows, energy dissipation and transport of mass, momentum and energy normal to the streamlines is mediated by molecular viscosity/diffusivity

EFFECT of TURBULENCE can be represented as an INCREASED VISCOSITY/DIFFUSIVITY

EDDY-VISCOSITY/DIFFUSIVITY MODEL

$$\overline{u_i'\xi'} = -D_{t,\xi} \frac{\partial \overline{\xi}}{\partial x_i}$$

TURBULENT FLUX: sought to mimic the molecular gradient diffusion process

Note: Although the eddy viscosity hypothesis is NOT CORRECT in detail, it is easy to implement and can provide REASONABLY GOOD RESULTS

CHALLENGE: How to specify the eddy viscosity/diffusivity D_t ?

Turbulence models: Eddy-viscosity/diffusivity models

$$\overline{u_i'\xi'} = -D_{t,\xi}\frac{\partial\overline{\xi}}{\partial x_i}$$

D_t has units of m^2/s

$$\overline{u'w'} = -D_{t,mom}\frac{\partial\overline{u}}{\partial z}$$

Eddy-viscosity model (for momentum); *Eddy viscosity:* $D_{t,mom} = \nu_t$

$$\overline{w'\theta'} = -D_{t,\theta}\frac{\partial\overline{\theta}}{\partial z}$$

Eddy-diffusivity model (for scalars like temperature or pollutants)

Analogy with molecular viscosity/diffusivity

- Reynolds stress modeled like viscous stress
- Turbulence more effective than viscosity at mixing:

$$D_{t,mom} >> \nu$$

$$D_{t,mom} \sim 0.1 - 2\times10^3\, m^2 s^{-1}$$

$$\nu \sim 1.5\times10^{-5}\, m^2 s^{-1}$$

$D_{t,\theta}$ **Eddy-diffusivity**

Reynolds analogy (Pr_t=1)

$$D_{t,\theta} = \frac{D_{t,mom}}{\Pr_t} \approx D_{t,mom}$$

<u>Example:</u>

Using a combination of a length scale (l_{scale}) and a velocity scale (u_{scale})

$$D_{t,mom} \propto u_{scale} \cdot l_{scale}$$

<u>**CHALLENGE**</u>: **How to specify the scales l_{scale} and u_{scale} ?**

- In **channel flow:** *See previous lecture*

- In **boundary layers:**

$$l_{scale} \approx k \cdot z$$

$$u_{scale} \approx u_*$$

k = von Karman constant (k≈0.4)

- In **complex flows: CHALLENGING**

Note: More on RANS turbulence models during Fluent Project sessions

A common RANS turbulence model: the k-ε model

(Jones and Launder, 1972)

$$D_{t,mom} \propto u_{scale} \cdot l_{scale}$$

- **It requires solving two additional equations:**

(1) One p.d.e. for TKE: k

Note: $[k] = L^2T^{-2}$

$$\frac{Dk}{Dt} = \underbrace{\frac{\partial}{\partial x_i}\left[\frac{\mu_{\text{eff}}}{\sigma_k}\frac{\partial k}{\partial x_i}\right]}_{\text{diffusion}} + \underbrace{\left[\mu_t\left(\frac{\partial U_i}{\partial x_j}+\frac{\partial U_j}{\partial x_i}\right)-\frac{2}{3}\rho\,\delta_{ij}k\right]\frac{\partial U_j}{\partial x_i}}_{\text{production}} - \underbrace{c_D\frac{\rho\,k^{3/2}}{\ell_m}}_{\text{dissipation}}$$

to obtain *velocity scale*

velocity scale

$$u_{scale} \approx \sqrt{2k}$$

(2) One p.d.e. for energy dissipation ε

Note: $[\varepsilon] = L^2T^{-3}$

$$\frac{D\epsilon}{Dt} = \underbrace{\frac{\partial}{\partial x_i}\left[\frac{\mu_{\text{eff}}}{\sigma_\epsilon}\frac{\partial \epsilon}{\partial x_i}\right]}_{\text{diffusion}} + \underbrace{c_{\epsilon,1}\left[\mu_t\left(\frac{\partial U_i}{\partial x_j}+\frac{\partial U_j}{\partial x_i}\right)-\frac{2}{3}\rho\,\delta_{ij}k\right]\frac{\partial U_j}{\partial x_i}}_{\text{production}} - \underbrace{c_{\epsilon,2}\frac{\rho\,\epsilon^2}{k}}_{\text{dissipation}}$$

to obtain *length scale*

length scale

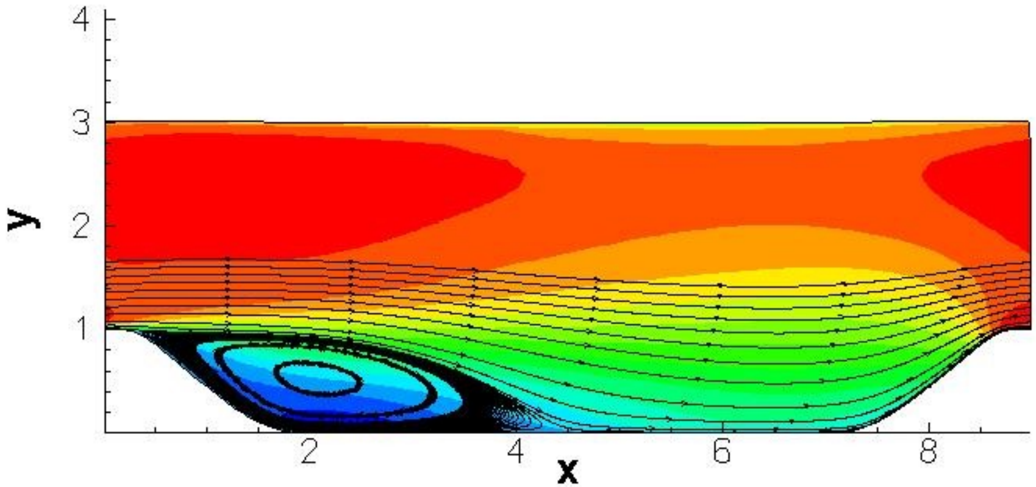
$$l_{scale} \approx \frac{k^{3/2}}{\varepsilon}$$

$$D_{t,m} \propto \frac{k^2}{\varepsilon}$$

Also: $\mu_t = C_\mu \dfrac{k^2}{\varepsilon}$ (Note: Momentum diffusivity = kinematic viscosity: $D_{t,m} = \nu_t = \frac{\mu_t}{\rho}$)

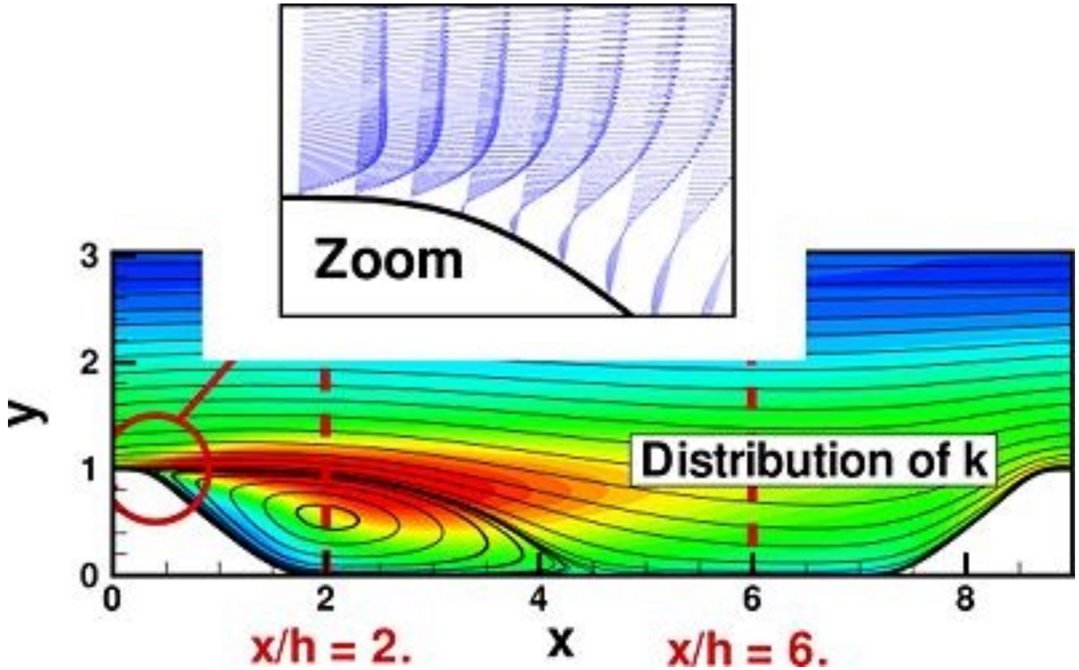
Model coefficients (**obtained by data fitting** for several flows): $C_\mu = 0.09$ $\sigma_k = 1.00$ $\sigma_\epsilon = 1.30$ $C_{1\epsilon} = 1.44$ $C_{2\epsilon} = 1.92$

RANS example: flow over complex terrain



Mean velocity and streamlines

(Red: high; Blue: low)

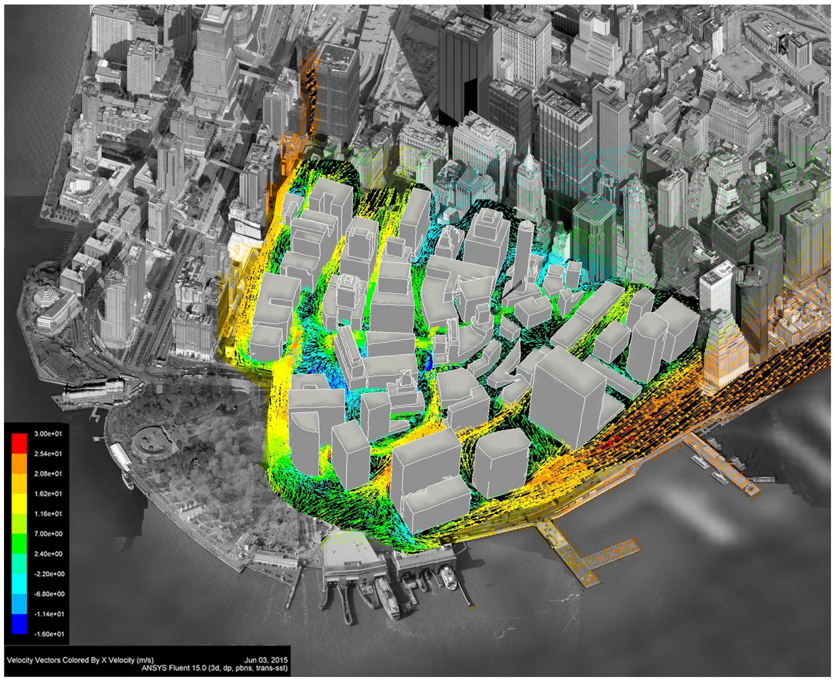


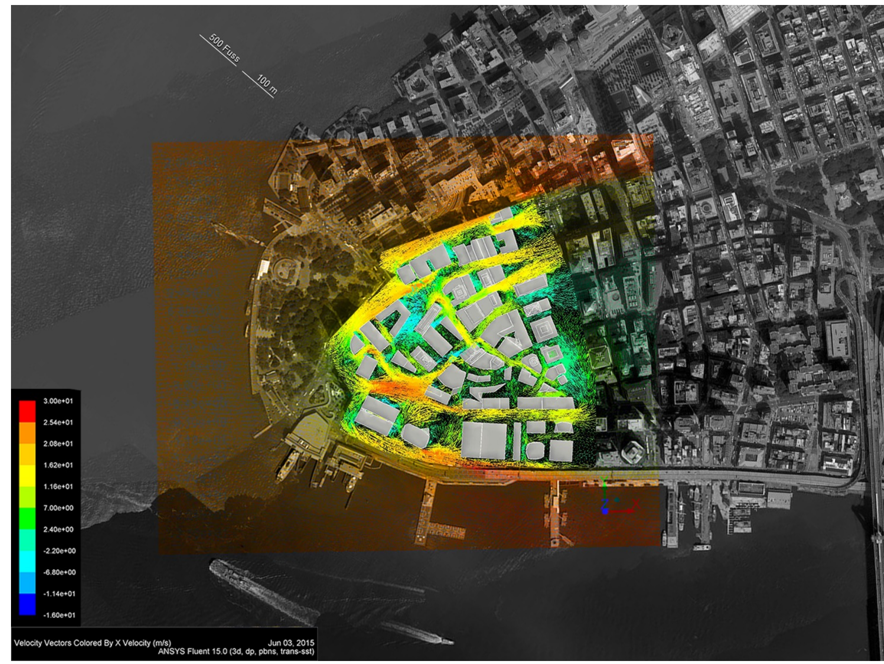
Turbulence Kinetic Energy k (T.K.E.)

(Red: high; Blue: low)

Reynolds-Averaged Navier Stokes (RANS): Example

Simulated mean wind velocity vectors (color represents magnitude) in Manhattan (New York)

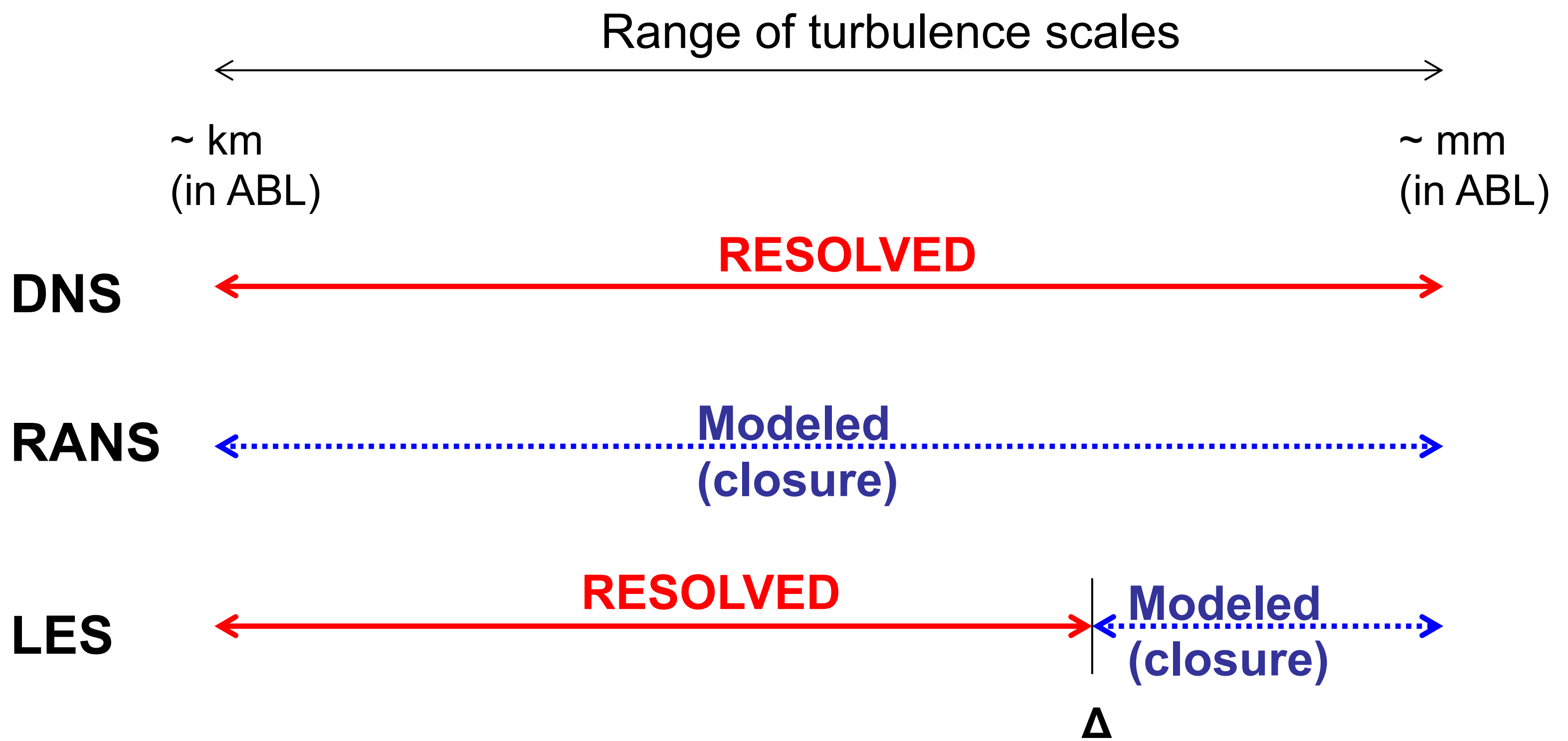




(Red: high; Blue: low)

Approaches for simulation/modeling of turbulent flows

- **DNS** (Direct Numerical Simulation)
- **RANS** (Reynolds-Averaged Navier Stokes)
- **LES** (Large-Eddy Simulation)



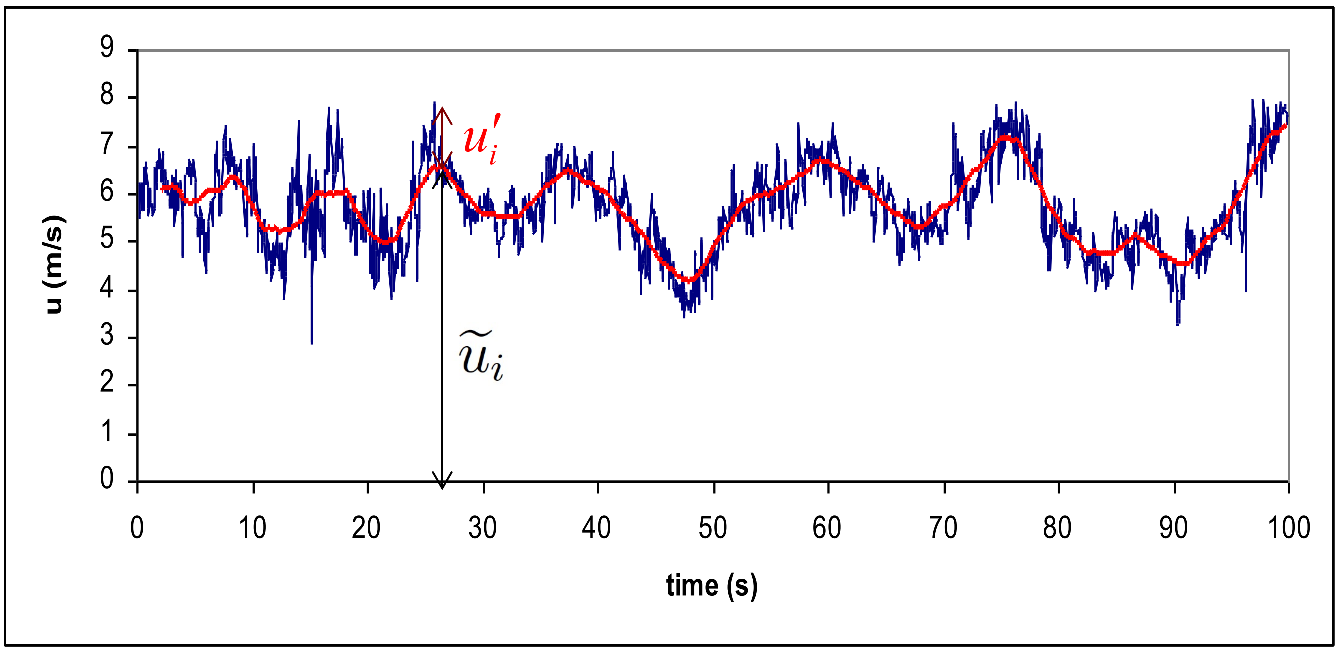
Large-Eddy Simulation (LES)

- **DNS (Direct Numerical Simulation)**
- **LES (Large-Eddy Simulation)**

$$u_i = \tilde{u}_i + u_i'$$

$$\tilde{u}_i(x) = \int G(x, x')\, u_i(x')\, dx'$$

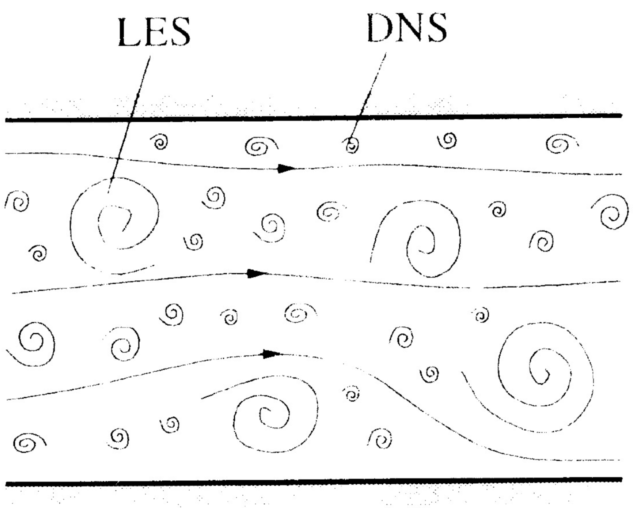
Note: In LES, the 'tilde' denotes a filtering operation (a local spatial average in 3D)

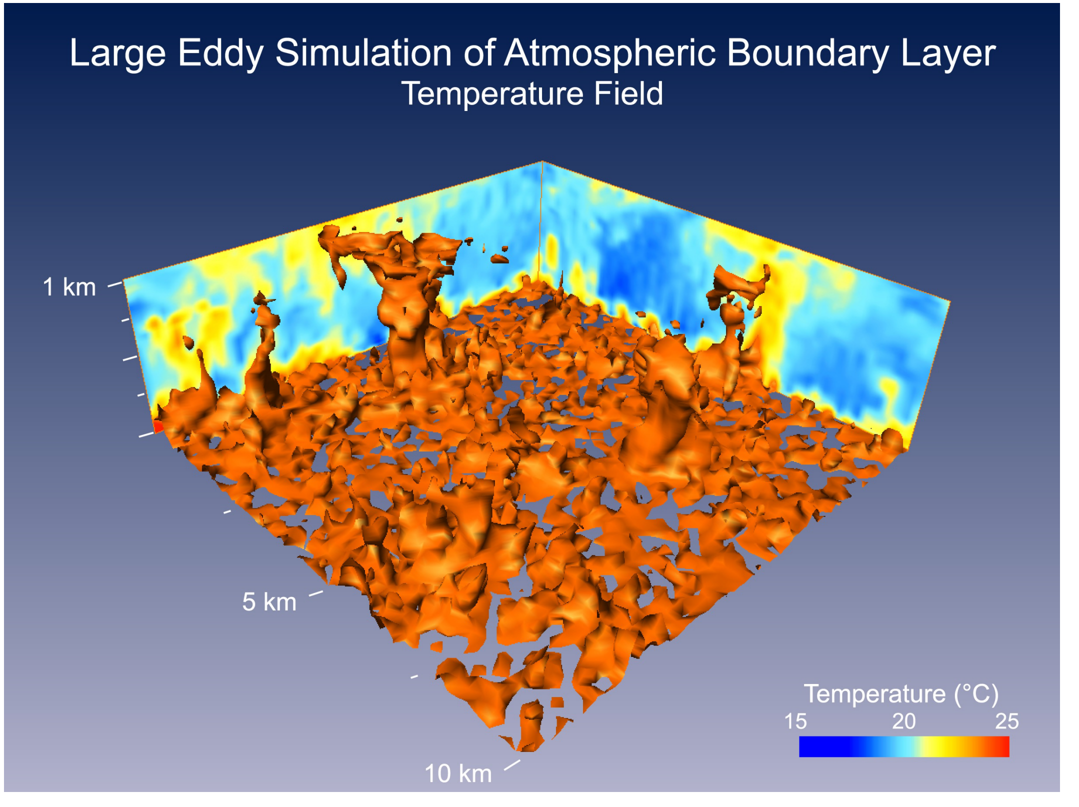


Large-Eddy Simulation (LES)

Resolved scales | Subgrid scales (SGS)

$L_I \sim 1$ km | Δ (filter size ~10 m) | $L_K \sim 1$ mm





LES (filtered) transport equations

$$\frac{\partial \tilde{u}_i}{\partial x_i} = 0$$

$$\frac{\partial \tilde{u}_i}{\partial t} + \frac{\partial}{\partial x_j}\left(\tilde{u}_i \tilde{u}_j\right) = -\frac{1}{\rho}\frac{\partial \tilde{p}}{\partial x_i} - \frac{\partial \tau_{ij}}{\partial x_j} + F_i$$

SGS stress

$$\tau_{ij} = \widetilde{u_i u_j} - \tilde{u}_i \tilde{u}_j$$

$$\frac{\partial \tilde{C}}{\partial t} + \frac{\partial}{\partial x_i}\left(\tilde{u}_i \tilde{C}\right) = -\frac{\partial q_i^{sgs}}{\partial x_i} + \tilde{Q}$$

(Derivation in next slide)

SGS flux

$$q_i^{sgs} = \widetilde{u_i C} - \tilde{u}_i \tilde{C}$$

Effect of sub-grid scales on the resolved (filtered) scales

EXAMPLES of LES: All movies shown of ABL simulations in next lectures.

LES (filtered) scalar transport equation: derivation

Starting with advection-diffusion equation:

$$\frac{\partial C}{\partial t}+\frac{\partial}{\partial x_i}\left(u_i C\right)=\frac{\partial}{\partial x_i}\left[D_m\frac{\partial C}{\partial x_i}\right]+Q$$

[Note: Q is a source/sink term]

Applying LES filtering operation (of size Δ):

$$\frac{\partial \tilde{C}}{\partial t}+\frac{\partial}{\partial x_i}\left(\widetilde{u_i C}\right)=\frac{\partial}{\partial x_i}\left[D_m\frac{\partial \tilde{C}}{\partial x_i}\right]+\tilde{Q}$$

Adding and substracting the same term:

$$\frac{\partial \tilde{C}}{\partial t}+\frac{\partial}{\partial x_i}\left(\widetilde{u_i C}-\tilde{u}_i\tilde{C}+\tilde{u}_i\tilde{C}\right)=\frac{\partial}{\partial x_i}\left[D_m\frac{\partial \tilde{C}}{\partial x_i}\right]+\tilde{Q}$$

Rearranging:

$$\frac{\partial \tilde{C}}{\partial t}+\frac{\partial}{\partial x_i}\left(\tilde{u}_i\tilde{C}\right)=-\frac{\partial}{\partial x_i}\left(\widetilde{u_i C}-\tilde{u}_i\tilde{C}\right)+\frac{\partial}{\partial x_i}\left[D_m\frac{\partial \tilde{C}}{\partial x_i}\right]+\tilde{Q}$$

$$q_i^{sgs}=\widetilde{u_i C}-\tilde{u}_i\tilde{C}$$

SUBGRID-SCALE (SGS) FLUX

- Represents the effect of subgrid-scales (eddies smaller than Δ)
- Closure Problem
- Need a model (**SGS Model**)
- ***Q: What could be a reasonable model?****
- Note:

$$q_i^{sgs}<\overline{u_i'C'}$$

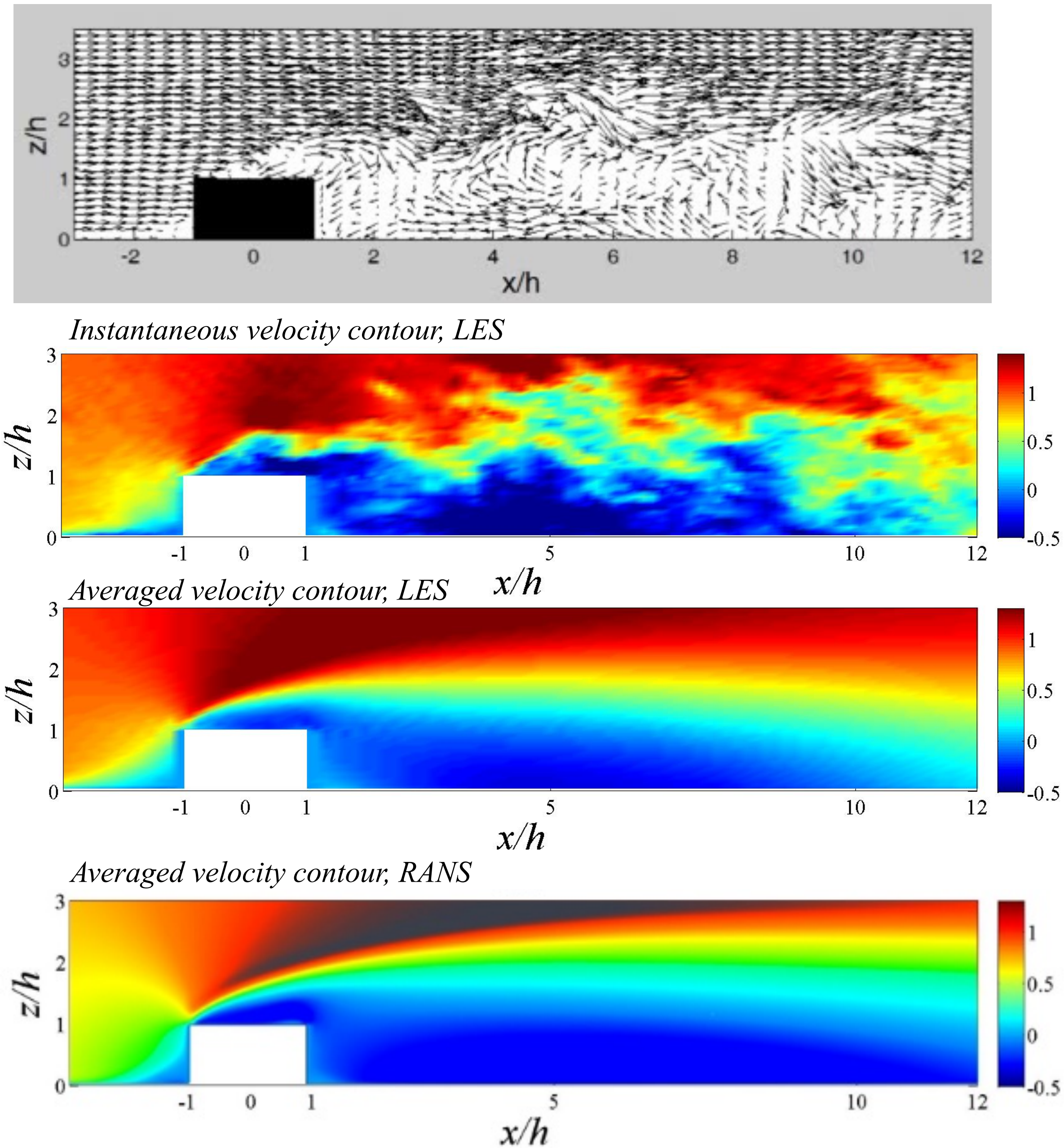
Represents the effect of **only subgrid scale (SGS) eddies (smaller than** Δ)

Represents the effect of **ALL turbulent eddies**

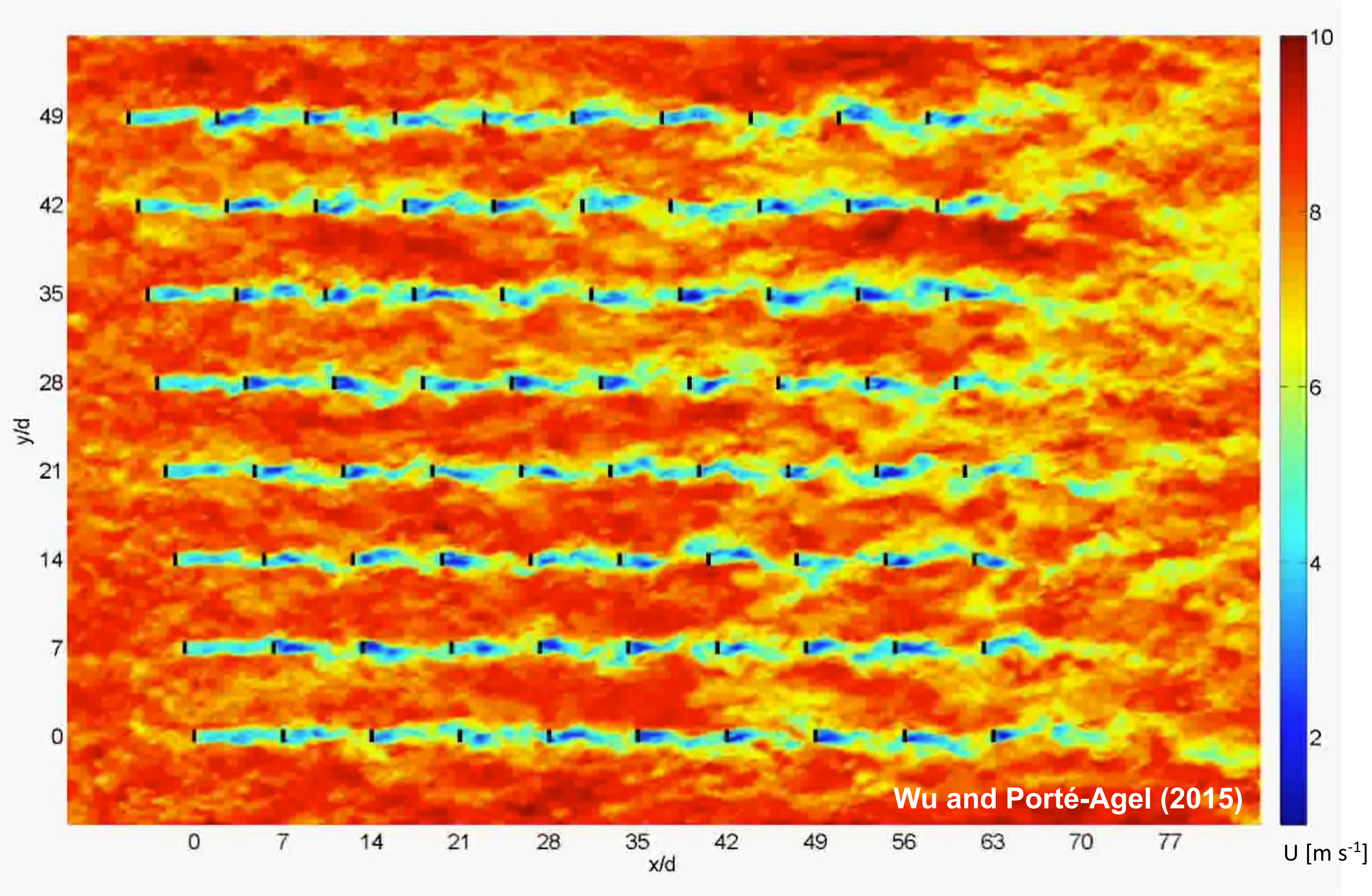
* Standard SGS model: Eddy-diffusion model

$$q_i^{sgs}=-D_{sgs}\frac{\partial \tilde{C}}{\partial x_i}$$

LES example: Flow around a building

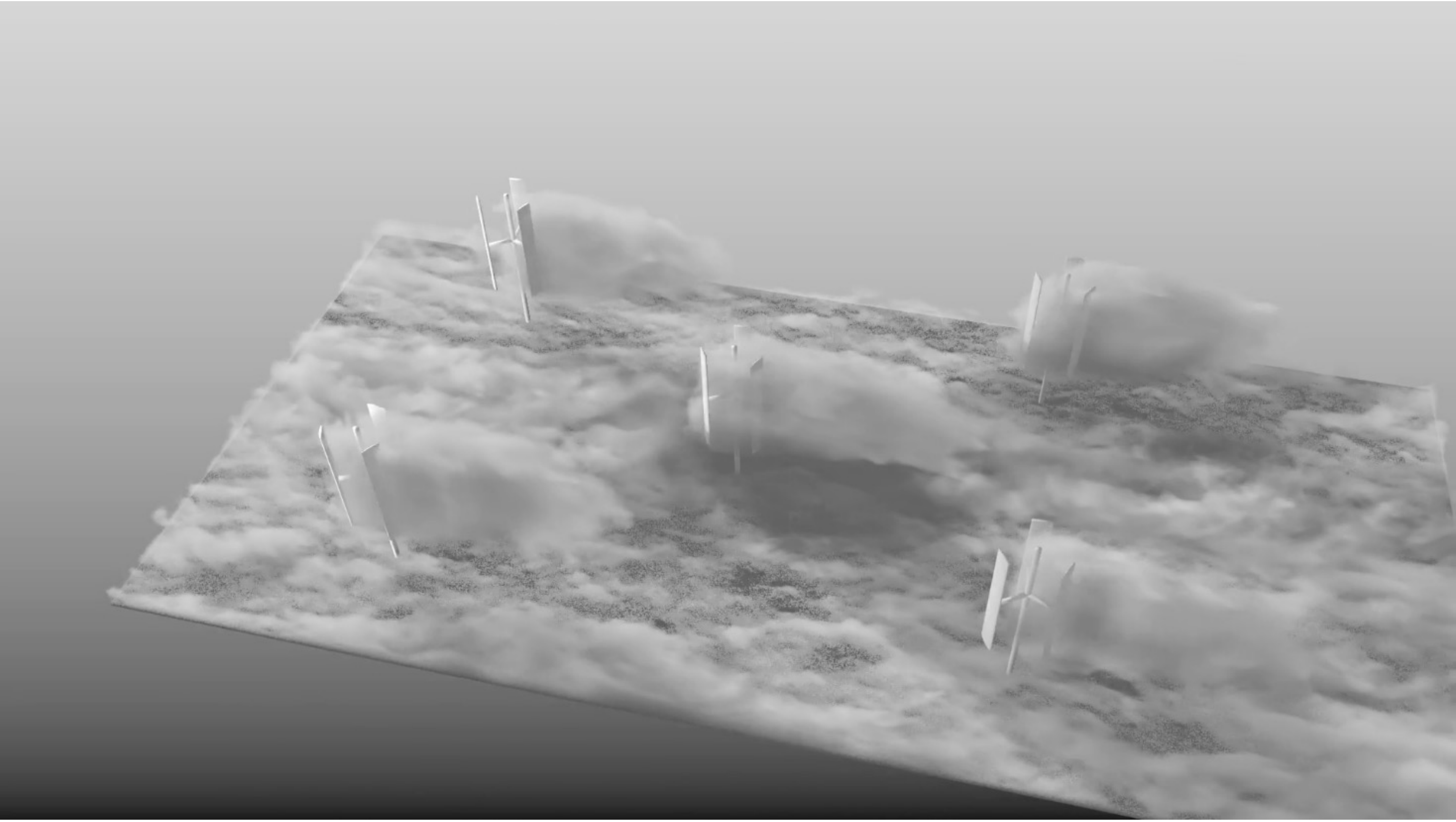


LES of flow inside a wind farm



Simulation with the highly-parallelized WiRE LES code using 1000 CPU-hours (100 processors, 10 hours)

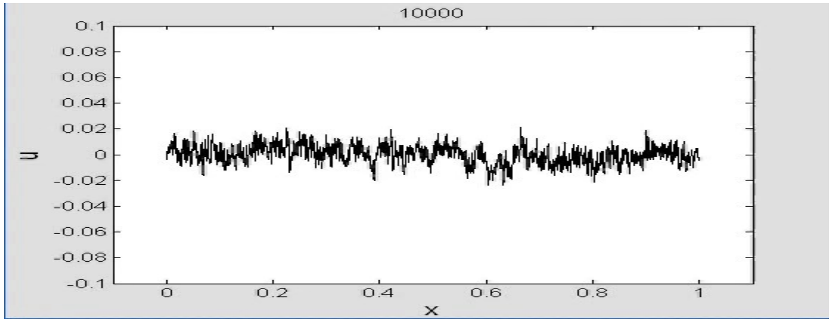
LES example: Flow inside a wind farm or vertical-axis wind turbines



https://youtu.be/ferySLHLocw

1-D Burgers Equation (a simple example – similar to turbulence)

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = \nu\frac{\partial^2 u}{\partial x^2} + F$$



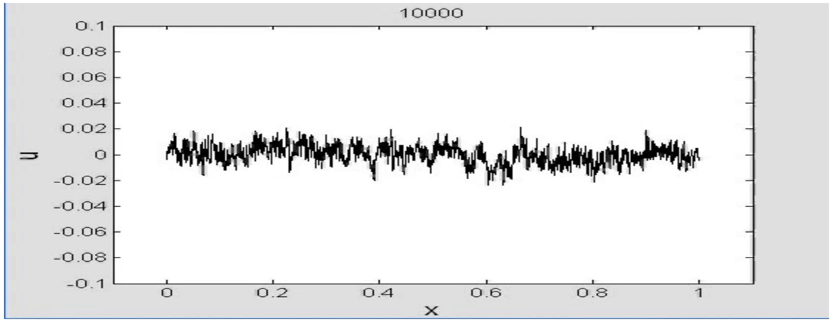
Direct Numerical Simulation – 1D Burgers equation

All scales are resolved

L_I/L_k=8192

1-D Burgers Equation (a simple example – similar to turbulence)

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = \nu \frac{\partial^2 u}{\partial x^2} + F$$

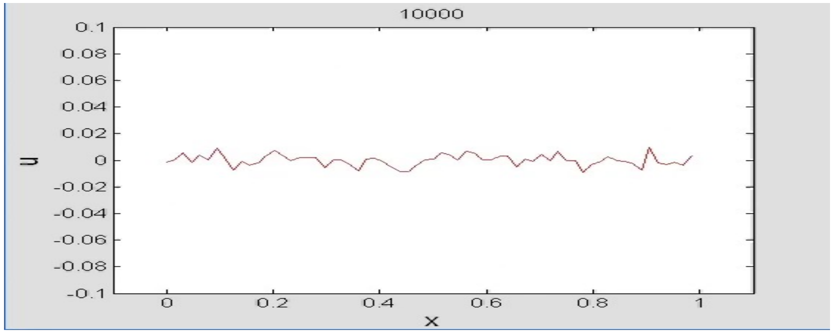


Direct Numerical Simulation – 1D Burgers equation

All scales are resolved

L_I/L_k=8192

Coarser resolution without subgrid model: Wrong statistics



Coarse resolution – 1D Burgers equation

NO subgrid model

L_I/L_k=64

Question: Why without SGS model there is an unrealistic accumulation of energy?