Introduction to CFD modelling of source terms and local-scale atmospheric dispersion (Part 1 of 2)

Atmospheric Dispersion Modelling Liaison Committee (ADMLC) meeting

15 February 2018

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Outline

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- Concepts: domain, grid, boundary conditions, finite-volume method
- Turbulence Modelling
  - Reynolds-Averaged Navier Stokes (RANS): steady and unsteady
  - Large Eddy Simulation (LES)

Part 1

- Atmospheric boundary layers
- CFD Software
- Case studies
  - Source terms: flashing jets, overfilling tanks
  - Local-scale atmospheric dispersion: Jack Rabbit II

Part 2

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Concepts: Geometry and Domain

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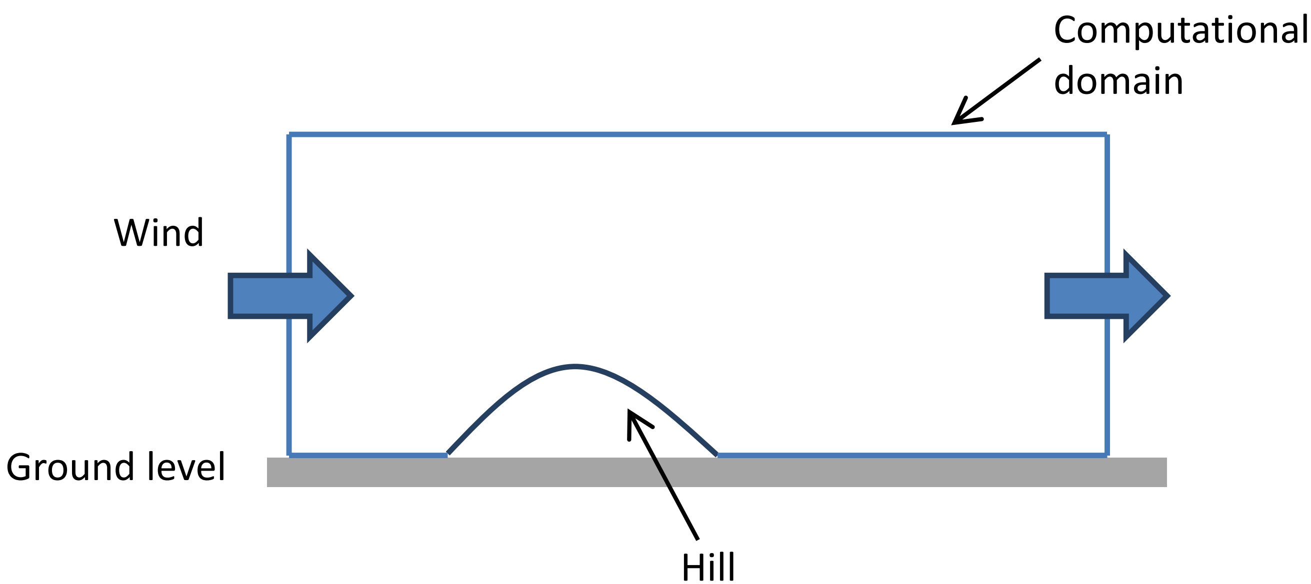
Task: to model air flow over a hill



- Position of domain boundaries should not influence the aspect of the flow of interest, e.g. gas cloud size in dispersion simulations
- Guidance on domain size is given in Franke *et al*. COST Action 732 "Best practice guidelines for the CFD simulation of flows in the urban environment"

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Concepts: Boundary Conditions

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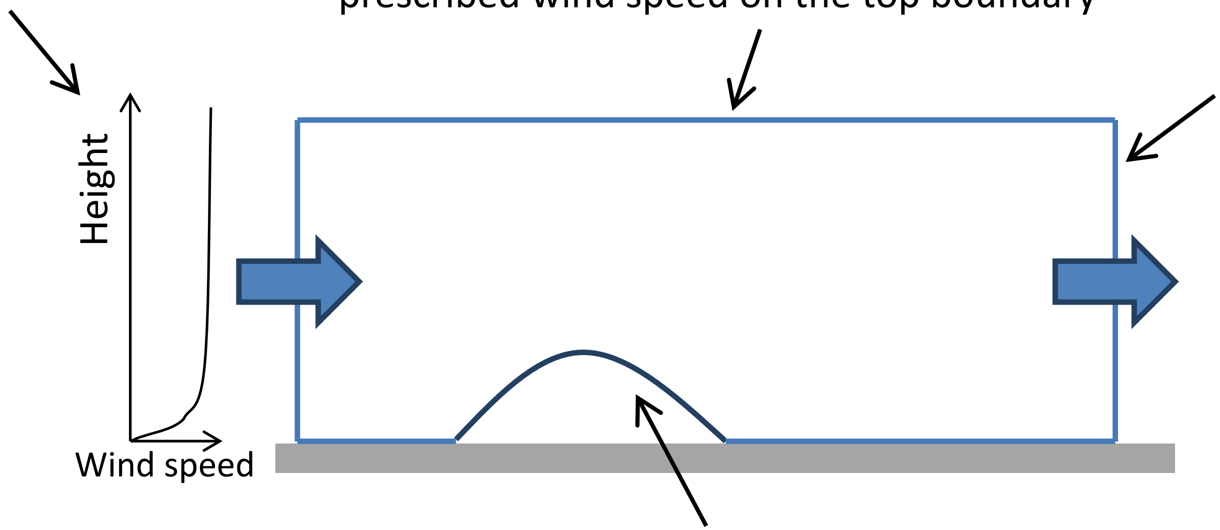
Wind speed profile specified on inlet boundary

“Slip” conditions, prescribed shear-stress or prescribed wind speed on the top boundary

Constant pressure conditions applied on outflow boundary

(needs to account for density variation with height if air is treated as an ideal gas or temperature variations are modelled)



Air velocity set to zero on the ground boundary

- Choice of boundary conditions for Atmospheric Boundary Layers (ABLs) is complicated
- Maintaining realistic ABL profiles along flat, empty terrain is often not possible
- This is covered in more detail in “Part 2” of my talk

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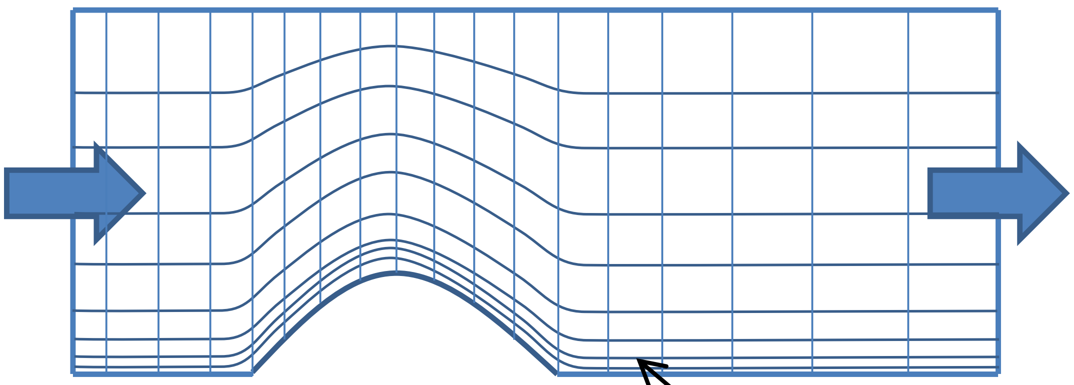
Concepts: Grid or Mesh

Sub-divide domain into thousands or millions of cells, using a grid or mesh



Smaller grid cells near the ground to resolve the steep gradients in velocity near the ground

- Velocity, temperature, pressure etc. calculated at a point within each cell
- Some CFD software packages allow use of tetrahedral or polyhedral cells for flexibility
- Cells near the ground should be hexahedral or prisms as otherwise boundary layer will not be accurately predicted`

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Concepts: Finite-Volume Method

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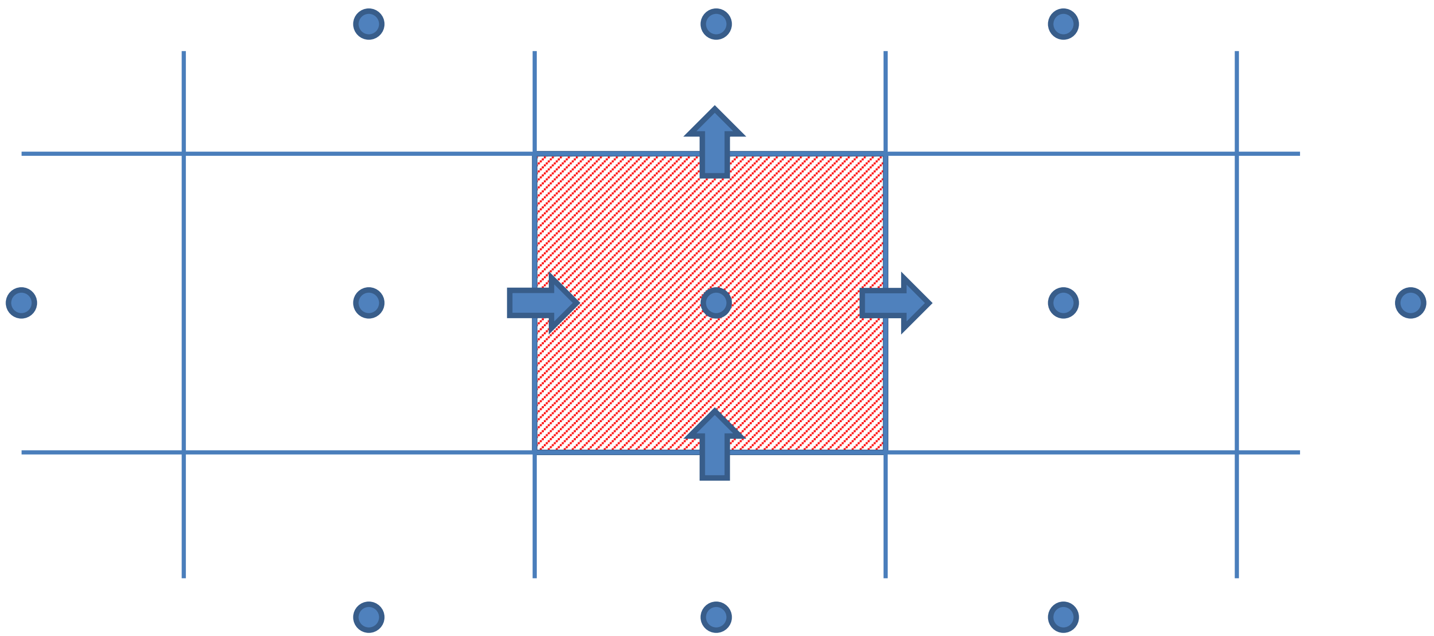
Conservation of Mass Mass flux into cell = Mass flux out of cell

(Assuming no mass created inside the cell)



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Concepts: Finite-Volume Method

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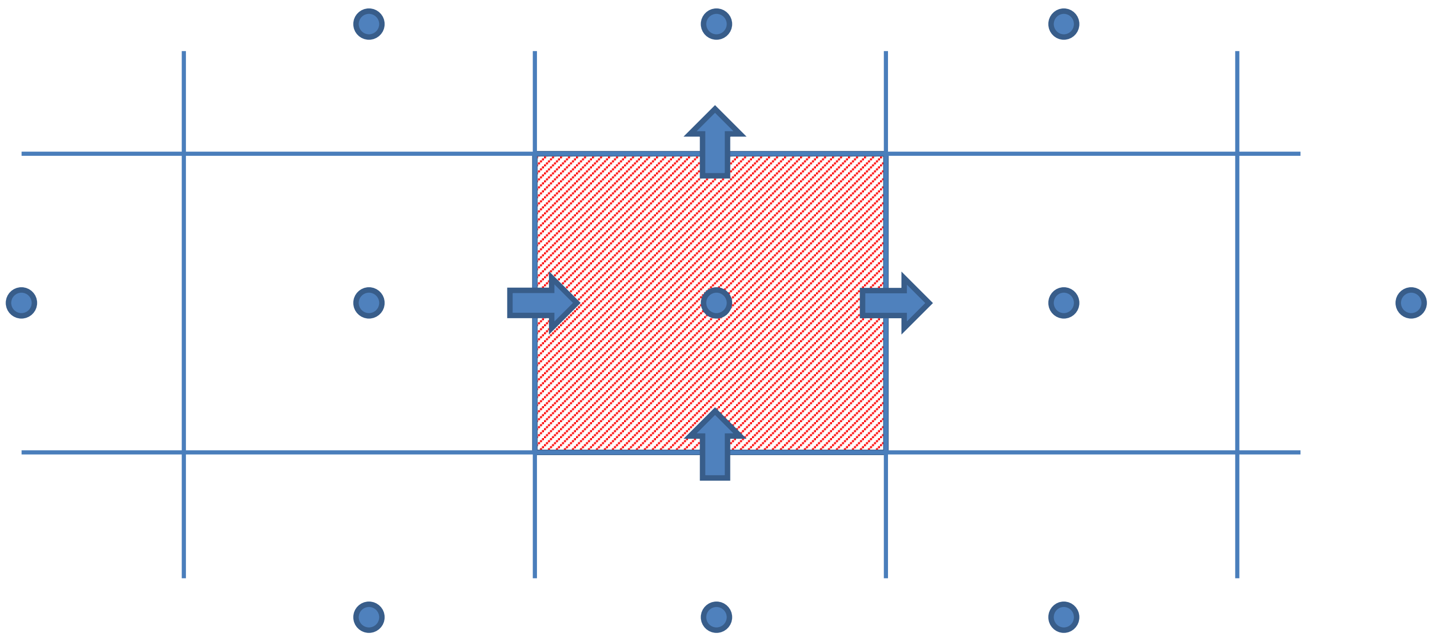
Conservation of Momentum

Momentum flux into cell – Momentum flux out of cell = Sum of pressure and viscous forces



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WARNING: Equations ahead

If in doubt, mentally substitute the words “blah blah blah” for the equations

Aim of next slides is to show:

- Numerical methods in CFD are important
- Example: international turbulence model inter-comparison exercise discussed by Roache*: results dominated by numerical errors, not choice of models
- Sometimes choice of numerical method is “art” not “science” – depends on skill/experience of modeller
- Terminology: What are “discretization errors”? What are “residuals”? What is “convergence”?

* Roache, P.J., *Verification and validation in computational science and engineering,* Hermosa Publishers, 1998.

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Concepts: Navier-Stokes equation

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<u>Conservation of Momentum</u>: Newton's second law of motion

$$F = m\,a$$

Force

Mass

Acceleration

$$F = \underbrace{\frac{d}{dt}(m\,v)}$$

Force

Rate of change of momentum

$$\frac{d}{dt}(m\,v) = F$$

Rate of change of momentum

Force

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Concepts: Navier-Stokes equation

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<u>Conservation of Momentum</u>: Newton's second law of motion

$$\underbrace{\frac{d}{dt}(m\,v)}_{\text{Rate of change of momentum}} = \underbrace{F}_{\text{Force}}$$

Navier-Stokes (one-dimensional):

$$\underbrace{\frac{\partial}{\partial t}(\rho U) + \frac{\partial}{\partial x}(\rho U U)}_{\text{Rate of change of momentum}} = \underbrace{-\frac{\partial P}{\partial x}}_{\text{Pressure force}} + \underbrace{\frac{\partial}{\partial x}\left(\mu \frac{\partial U}{\partial x}\right)}_{\text{Viscous force}}$$

U = velocity, ρ = density, x = distance, P = pressure, μ = viscosity

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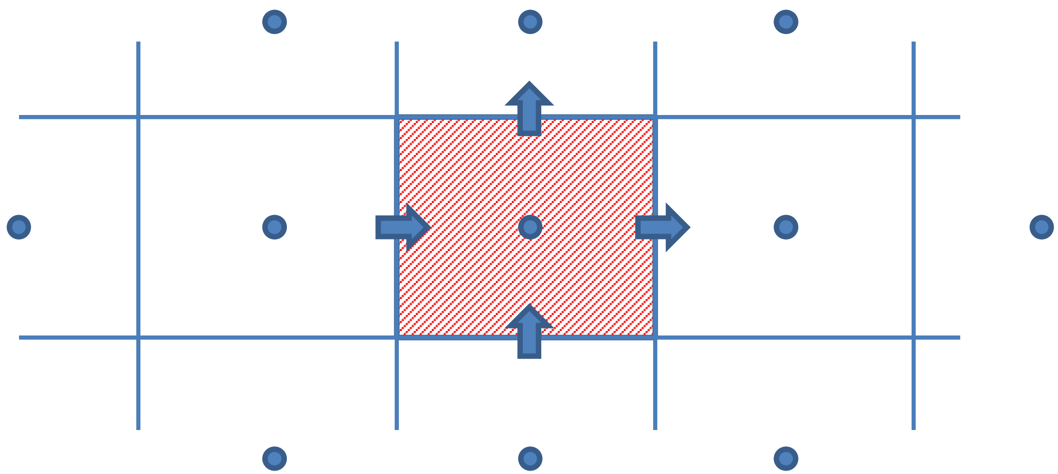
Concepts: Other transport equations

Similar method used for conservation of energy, conservation of gas concentration etc.

$$\underbrace{\frac{\partial}{\partial t}(\rho\varphi)}_{\text{Rate of change over time}} + \underbrace{\frac{\partial}{\partial x}(\rho U\varphi)}_{\text{Convection}} = \underbrace{\frac{\partial}{\partial x}\left(\Gamma\frac{\partial\varphi}{\partial x}\right)}_{\text{Diffusion}} + \underbrace{S}_{\text{Source (or sink)}}$$



$\varphi =$ Concentration

$\Gamma =$ Diffusivity

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Concepts: Discretization

Finite-volume method

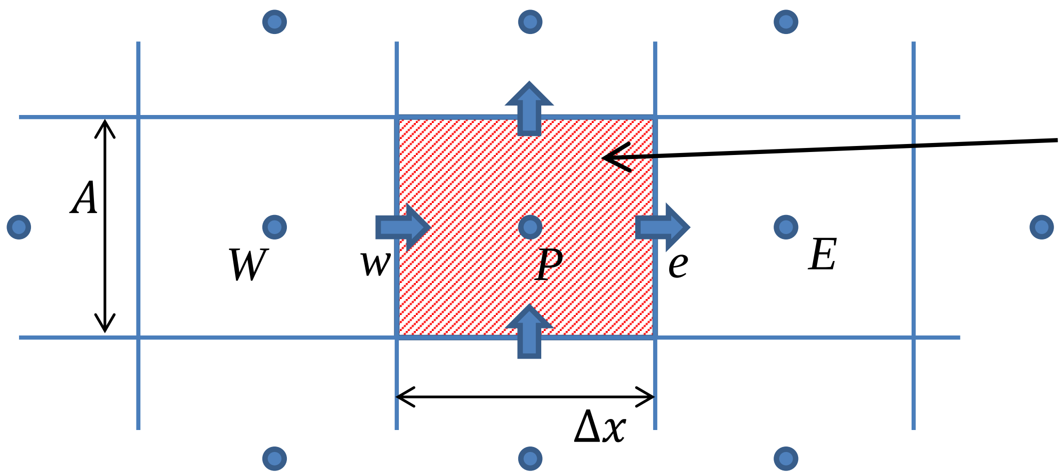
- Integrate each term in the conservation equations over the cell volume, $dVol$

Convection term: $$\int \frac{\partial}{\partial x}(\rho U \varphi)\, dVol$$

Discretized: $$\frac{(\rho U \varphi)_e - (\rho U \varphi)_w}{\Delta x} A \Delta x$$

Flux of φ through west face of cell

How do we calculate this? See next slide…



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Concepts: Discretizing Convection

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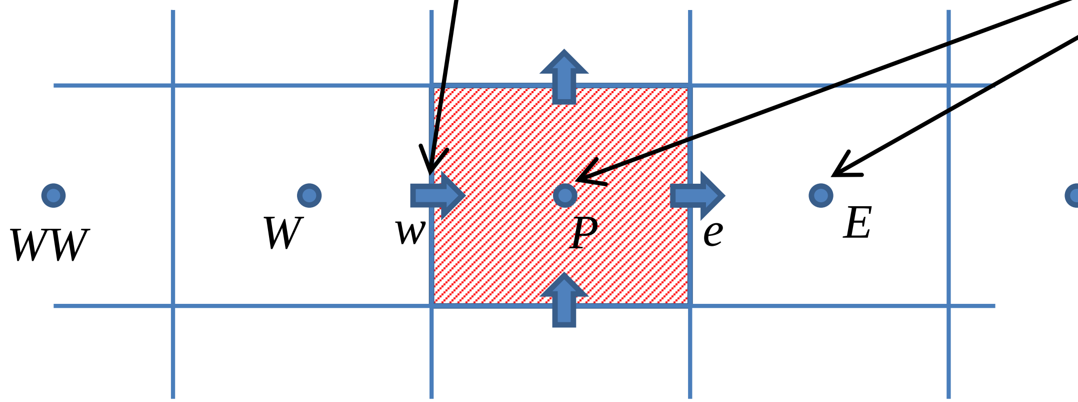
Problem: how to estimate the value of φ_w on cell face using the values of φ at nodes?



Taylor-series truncation error on uniform grid

1.) Upwind: $\varphi_w = \varphi_W$ First-order accurate

2.) Central differencing: $\varphi_w = \dfrac{\varphi_W + \varphi_P}{2}$ Second-order accurate

3.) Quadratic Upwind (QUICK): $\varphi_w = \dfrac{6}{8}\varphi_W + \dfrac{3}{8}\varphi_P - \dfrac{1}{8}\varphi_{WW}$ Third-order accurate

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Concepts: Discretizing Convection

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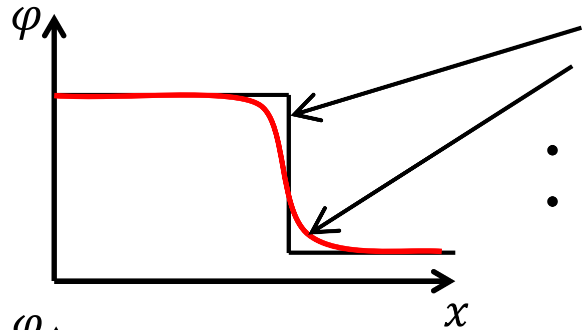
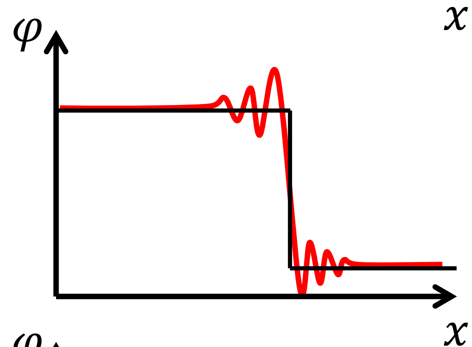
Approximations for φ_w produce different numerical errors:

1.) Upwind:



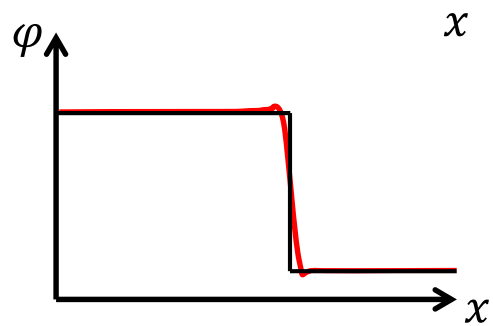
- Bounded (no overshoots)
- Diffusive

2.) Central differencing:



- Easily becomes unbounded (requires low velocity, high viscosity or fine grid to remain bounded)
- Less diffusive than upwind scheme

3.) Quadratic Upwind (QUICK):



- Smaller under/overshoots than central differencing
- Less diffusive than upwind

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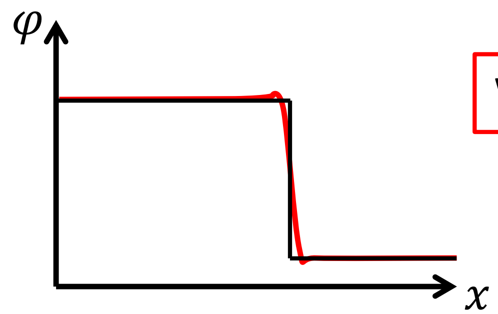
Concepts: Discretizing Convection

3.) Quadratic Upwind (QUICK):



Why not always use QUICK?

- Small under/overshoots may be acceptable for the velocity
- But for some parameters it can produce non-physical values, e.g. negative energy? negative concentration? negative turbulent viscosity?
- Potential solution: Total Variation Diminishing (TVD) schemes or flux limiters
- Problem: some higher-order schemes need to know values of φ in cells further away (difficult in unstructured grids with tetrahedral or polyhedral cells)
- Common approach: high-order upwind-biased scheme for velocity, upwind for other quantities

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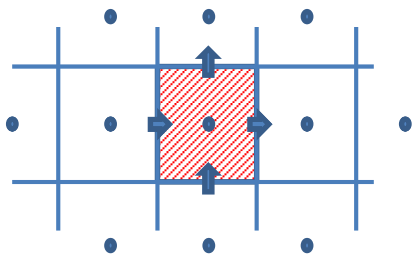
Solving Discretized Equations

Final discretized equations relate the parameter value in one cell (φ_P) to the values in the neighbouring cells (φ_E, φ_W...) and a source term (S)

Discretized equations for all cells assembled together into a large matrix:

$$\begin{bmatrix} a_{1P} & a_{1E} & \cdots \\ \cdots & \cdots & \cdots \\ \cdots & a_{nW} & a_{nP} \end{bmatrix} \begin{bmatrix} \varphi_1 \\ \cdots \\ \varphi_n \end{bmatrix} = \begin{bmatrix} S_1 \\ \\ S_n \end{bmatrix}$$



Initial values of φ are assumed ⟵ Important!

Matrix solver iterates to find new values of φ until "residuals" fall to tolerable levels and results are then said to have "converged"

$$\begin{bmatrix} a_{1P} & a_{1E} & \cdots \\ \cdots & \cdots & \cdots \\ \cdots & a_{nW} & a_{nP} \end{bmatrix} \begin{bmatrix} \varphi_1 \\ \cdots \\ \varphi_n \end{bmatrix} - \begin{bmatrix} S_1 \\ \\ S_n \end{bmatrix} = residuals$$

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Finite-Volume Method

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Commonly-used convergence criteria:

- Total residuals: need to fall by 3 or more orders of magnitude from initial level
- Plot solution from one iteration to the next, watch how the flow evolves (particularly useful if residuals are not falling). Converged solution should no longer change with successive iterations.

If the solver experiences convergence problems (residuals do not fall):

- Increase the degree of under-relaxation: slow the update from one iteration to the next (use more of the last iteration's values)
- Refine the grid (use smaller cells) in the region where there are problems
- Use a more realistic initial (assumed) flow field
- Run the simulation as transient (time-varying) instead of steady
- Reduce the time-step for transient simulations

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- Turbulence Modelling
  - Reynolds-Averaged Navier Stokes (RANS): steady and unsteady
  - Large Eddy Simulation (LES)
- Atmospheric boundary layers
- CFD Software
- Case studies
  - Source terms: flashing jets, overfilling tanks
  - Local-scale atmospheric dispersion: Jack Rabbit II

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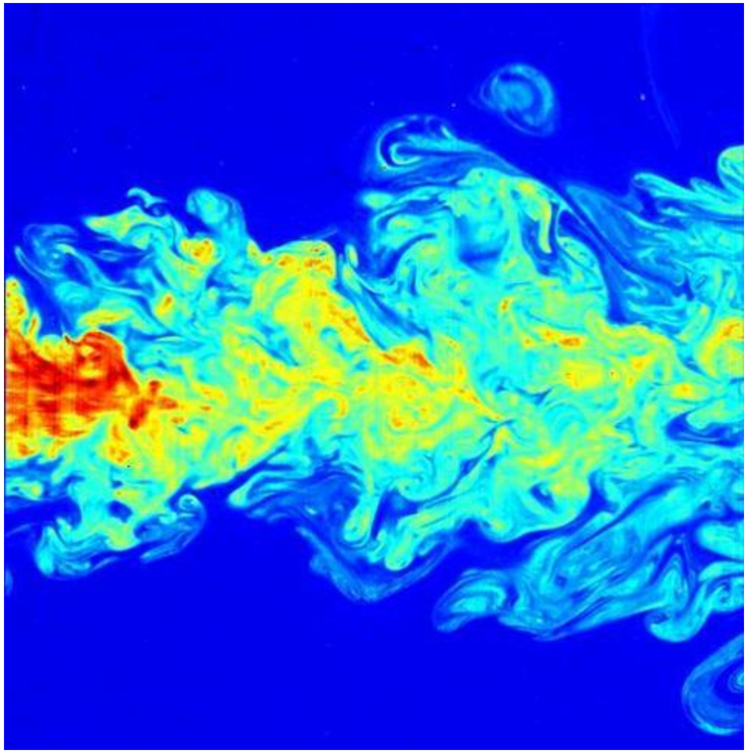
Turbulence



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- Turbulence involves time-varying flow behaviour with a range of scales
  - Large eddies
  - Smaller eddies
- Solving Navier-Stokes equations with sufficiently fine grid to resolve all scales is nearly always too computationally demanding
- Direct Numerical Simulation (DNS) only possible at low Reynolds numbers, i.e. when there is a limited range of scales
- We are often not interested in the motion of every turbulent eddy: just the mean flow or the large eddies

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Turbulence Modelling

Three common engineering approaches for simulating turbulent flows:

1.) Steady RANS

Roughly an order of magnitude increase in computing time

2.) Unsteady RANS

Roughly an order of magnitude increase in computing time

3.) Large-Eddy Simulation (LES)

For some flows you cannot use "steady RANS" because:

- Flow is too unsteady, e.g. flapping wakes or puffing buoyant plumes
- Transient behaviour is important, e.g. puff release from catastrophic tank failure

For some flows: LES may be just as fast to run as unsteady RANS, e.g. fire modelling

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Turbulence Modelling

What is Steady/Unsteady RANS and LES?

P.R. Spalart / Int. J. Heat and Fluid Flow 21 (2000) 252–263

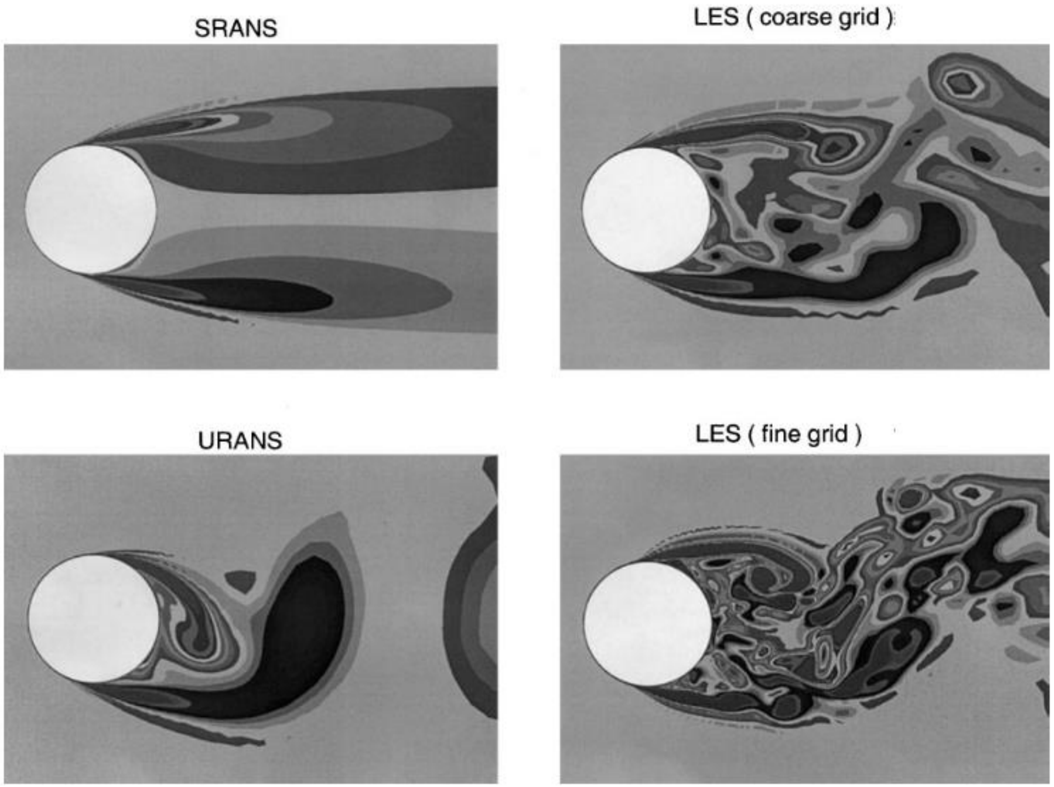

Fig. 4. Simulation of flow past circular cylinder by various approaches (Shur et al., 1996; Travin et al., 2000).

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Reynolds-Averaged Navier Stokes (RANS)

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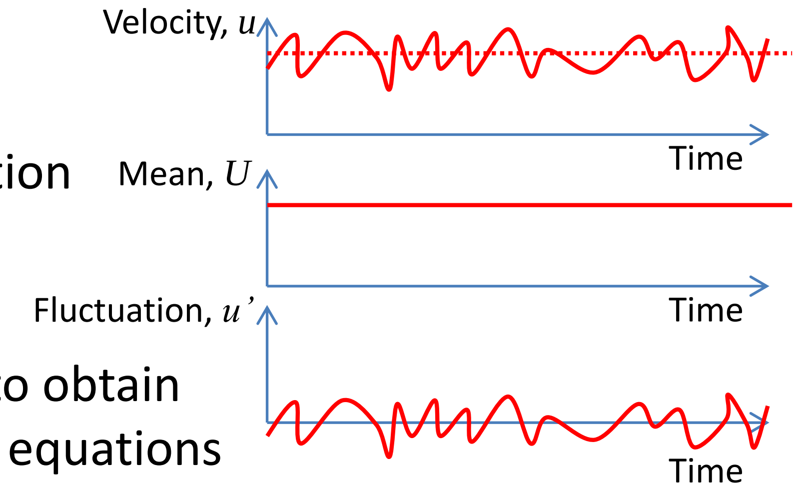
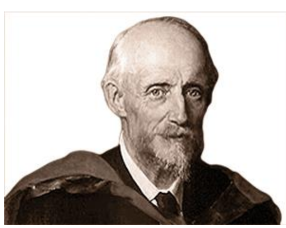
- Osborne Reynolds (1842-1912)
- Decompose velocity into mean + fluctuation

$$u = U + u'$$



- Substitute into Navier-Stokes equations to obtain Reynolds-averaged Navier Stokes (RANS) equations
- Mean velocity, U, calculated from:

$$\frac{\partial}{\partial t}(\rho U) + \frac{\partial}{\partial x}(\rho U U) = -\frac{\partial P}{\partial x} + \frac{\partial}{\partial x}\left(\mu \frac{\partial U}{\partial x}\right) - \underbrace{\frac{\partial}{\partial x}\left(\rho \overline{u' u'}\right)}$$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Additional unknown term is the "Reynolds stress"
It represents the effect of the turbulent fluctuations on the mean flow

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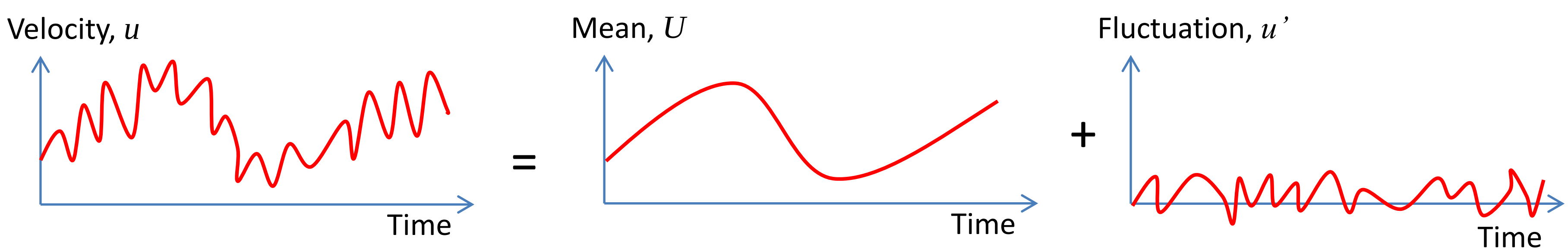
Reynolds-Averaged Navier Stokes (RANS)

- What does the “mean” in Reynolds averaging represent?
- For steady flows: a long time average
- For time-varying flows:
  - Separation in scales of motion: rapid fluctuations from turbulence, slower changes from mean flow behaviour
  - Reynolds averaging is an average over the rapid turbulent fluctuations, the mean is the slowly-evolving mean flow behaviour
  - … but what if there is no clear separation of time scales?
  - Think of mean as ensemble average over multiple repeats of the same flow?
  - No matter how you want to visualise it – the equations are the same



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Reynolds-Averaged Navier Stokes (RANS)

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- Many RANS turbulence models developed in the period 1920's – 2000's
  - GI Taylor and Prandtl mixing length model (1924)
  - One-equation Prantl model
  - Two-equation models: k-ε, k-ω, k-L etc.

  Reynolds stress is linearly proportional to the local strain rate

  - Non-linear eddy-viscosity models (two to four equations?)
  - Reynolds stress transport models (seven eqns: Reynolds stresses and dissipation)
  - Triple moment closure…
- Each has strengths and weaknesses
- Empirically-derived coefficients
- Goal: to develop a universal "general-purpose" model that gives accurate results across a wide range of flows

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Reynolds-Averaged Navier Stokes (RANS)

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- *k-ε* is probably the most widely used model for industrial flow analysis
  - Simplest “complete” turbulence model – applicable to broad range of flows
  - Fairly easy to implement and numerically robust
  - Widely recognized weaknesses
    - Over-prediction of turbulent kinetic energy at stagnation point
      (Order of magnitude over-prediction of turbulent heat transfer)
    - Poor prediction of boundary layer separation
    - Poor performance in swirling flows: linear swirl velocity in pipe, but non-linear in reality
    - No secondary flows in square ducts
    - Over-prediction of spreading rate in round jets (the round/plane jet anomaly)
  - Tuning of model constants was a compromise
  - Many corrections to *k-ε* model have been proposed for specific flows
    - e.g. jets, stagnation points, atmospheric boundary layers
    - But these ad-hoc corrections usually degrade the overall model performance in other flows
  - Used in popular industrial CFD codes: FLACS, KFX, Fluidyn-Panache

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Example: turbulent wall jet

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CFD Forum 2005
Bad Nauheim, Deutschland

Implementation and comparison of different turbulence models
for three dimensional wall jets with FLUENT

Implementation and comparison of different turbulence models for three dimensional wall jets with FLUENT

Ch. Heschl[1], W. Sanz[2] and P. Klanatsky[1]

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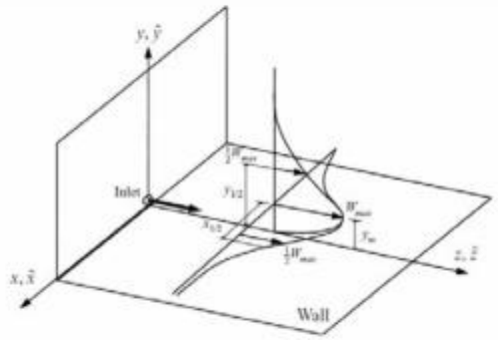

Figure 6: Investigated flow situation (Craft and Launder, 1992)

TCL pressure strain model by Craft and Launder (2001)

$$\phi_{ij,1} = -c_1\varepsilon\left(a_{ij} + c_1'\left(a_{ik}a_{jk} - \frac{1}{3}A_2\delta_{ij}\right)\right) - \varepsilon a_{ij}$$

$$\begin{aligned}\phi_{ij,2} = &-0.6\left(P_{ij} - \frac{1}{3}\delta_{ij}P_{kk}\right) + 0.3a_{ij}P_{kk} \\ &-0.2\left[\frac{\overline{u_k'u_j'}\,\overline{u_l'u_i'}}{k}\left(\frac{\partial u_k}{\partial x_l} + \frac{\partial u_l}{\partial x_k}\right) - \frac{\overline{u_l'u_k'}}{k}\left(\overline{u_i'u_k'}\frac{\partial u_j}{\partial x_l} + \overline{u_j'u_k'}\frac{\partial u_i}{\partial x_l}\right)\right] \\ &-c_2\left[A_2\left(P_{ij} - D_{ij}\right) + 3a_{mi}a_{nj}\left(P_{mn} - D_{mn}\right)\right] \\ &+c_2'\left(\Pi_1 + \Pi_2 + \Pi_3 + \Pi_4 + \Pi_5\right)\end{aligned}$$

$$\Pi_1 = \left(\frac{7}{15} - \frac{A_2}{4}\right)\left(P_{ij} - \frac{1}{3}\delta_{ij}P_{kk}\right)$$

$$\Pi_2 = 0.1\left[a_{ij} - \frac{1}{2}\left(a_{ik}a_{kj} - \frac{1}{3}\delta_{ij}A_2\right)\right]P_{kk} - 0.05a_{ij}a_{lk}P_{kl}$$

$$\Pi_3 = 0.1\left[\left(\frac{\overline{u_i'u_m'}}{k}P_{mj} + \frac{\overline{u_j'u_m'}}{k}P_{mi}\right) - \frac{2}{3}\delta_{ij}\frac{\overline{u_l'u_m'}}{k}P_{ml}\right] \quad (35)$$

$$\Pi_4 = 0.2\frac{\overline{u_l'u_i'}\,\overline{u_k'u_j'}}{k^2}\left(D_{lk} - P_{lk}\right)$$

$$\Pi_5 = 0.1\left[\frac{\overline{u_l'u_i'}\,\overline{u_k'u_j'}}{k^2} - \frac{1}{3}\delta_{ij}\frac{\overline{u_l'u_m'}\,\overline{u_k'u_m'}}{k^2}\right] \times \left[6D_{lk} + 13k\left[\frac{\partial u_l}{\partial x_k} + \frac{\partial u_k}{\partial x_l}\right]\right]$$

$$c_1 = 3.1\left(A_2A\right)^{1/2},\ c_1' = 1.1$$

$$c_2 = \min\left(0.55\left(1 - \exp\left(-A^{1.5}R_t/100\right)\right), 3.2A/(1+S)\right)$$

$$c_2' = \min(0.6, A) + 3.5(S - \Omega)/(3 + S + \Omega) - 2S_I$$

$$S = \frac{k}{\varepsilon}\sqrt{S_{ij}S_{ij}/2},\ \Omega = \frac{k}{\varepsilon}\sqrt{\Omega_{ij}\Omega_{ij}/2},\ S_I = S_{ij}S_{jk}S_{ki}/\left(S_{st}S_{st}/2\right)^{1.5}$$

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Example: turbulent wall jet

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Using a more sophisticated/complicated Reynolds stress transport model (tcl) does not necessarily give you more accurate results than a simple two-equation *k-ε* model (ske)

model	$\frac{dy_{1/2}}{dz}$	$\frac{dx_{1/2}}{dz}$	$\frac{\dot{x}_{1/2}}{\dot{y}_{1/2}}$
Experiment (Abrahamsson et al. 1997)	0.065	0.320	4.94
cubic	0.039	0.743	19.04
ip	0.043	0.913	21.36
ip-hyb	0.044	0.550	12.43
ip-without wr	0.078	0.089	1.15
ip-with-wr-LS	0.032	0.723	22.37
ske	0.074	0.070	0.95
ssg	0.057	0.049	0.85
tcl	0.038	0.743	19.30
ske-ewt	0.071	0.068	0.96
v2f-nonlinear	0.071	0.420	1.07

Table 3: Comparison of spreading rate anlong the jet

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Reynolds-Averaged Navier Stokes (RANS)

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Conclusions

- There is no general-purpose or “universal” RANS model that gives accurate predictions in all flows
- Different RANS models have different strengths and weaknesses
- Important to understand the limitations of your chosen RANS model and validate your model against experimental data for relevant flows
- Source of information:
  - ERCOFTAC
    - Best Practice Guide
    - Knowledge Base Wiki
  - Franke *et al.* COST Action 732 “Best Practice Guideline for CFD simulation of flows in the urban environment”

ERCOFTAC
Knowledge Base Wiki

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Some examples:

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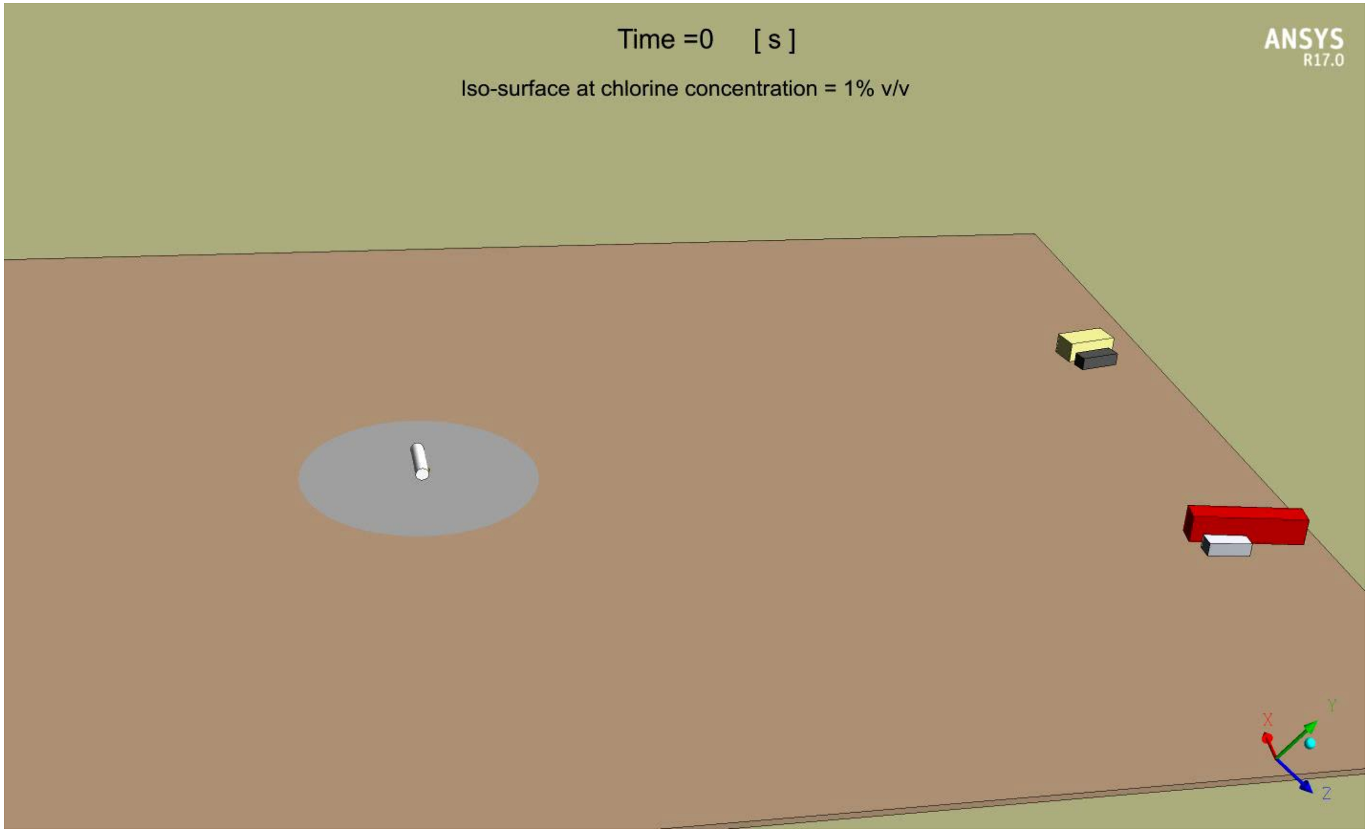
Unsteady RANS simulation of chlorine dispersion for Jack Rabbit II chlorine trials



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Some examples:

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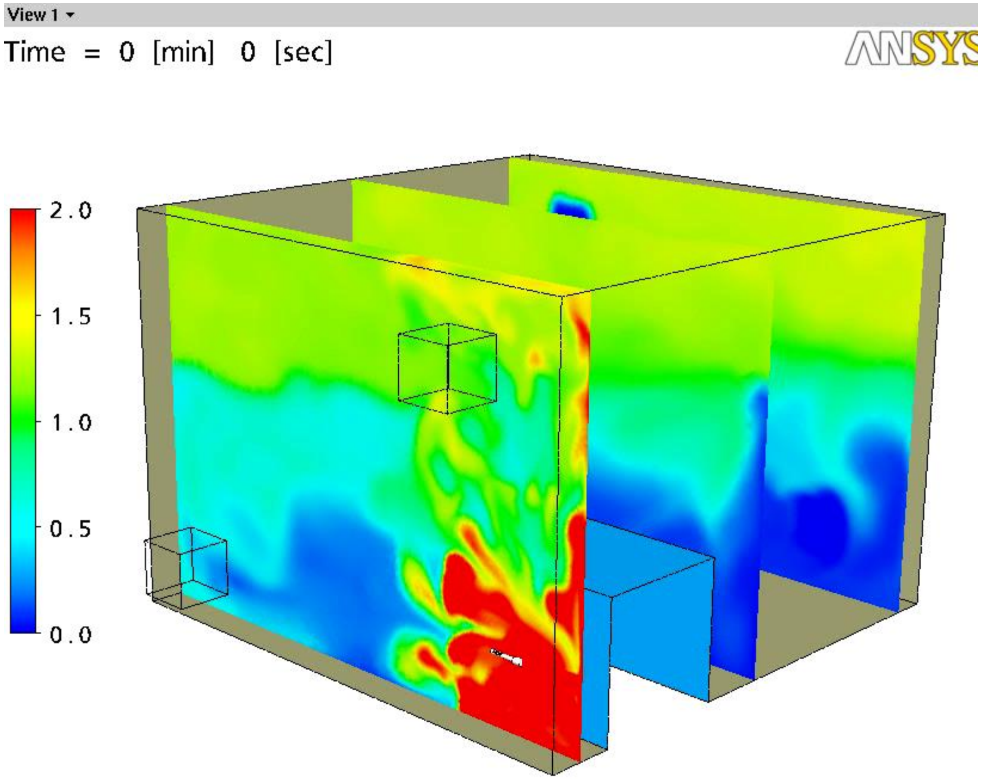
Large Eddy Simulation (LES) of gas dispersion in a ventilated room



Actually this is a Detached Eddy Simulation, but more on that later…

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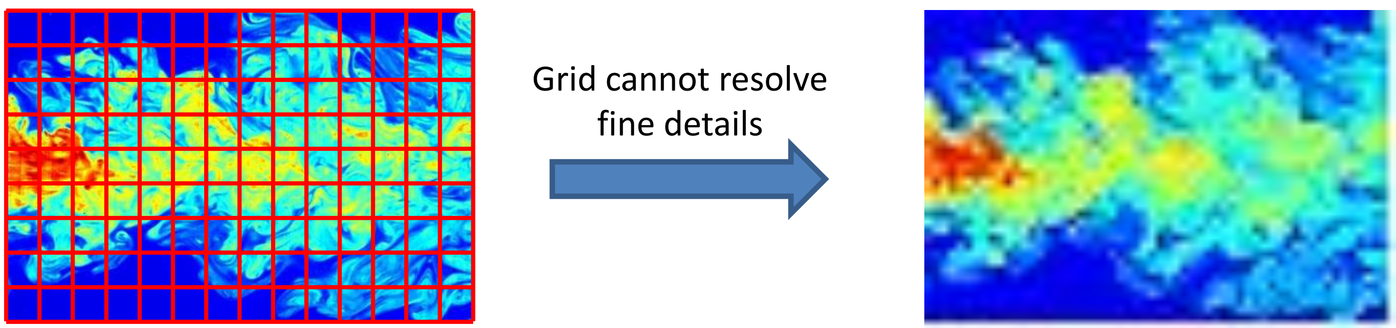
Large-Eddy Simulation

- Concept:
  - Rather than average over time (like in RANS) you average over space in LES
  - LES simulations are always time-varying
  - Basically you use a grid that is too coarse to resolve the fine eddies
  - Formally the averaging process over space is called a spatial “filter”



- Applying spatial filter to Navier-Stokes equations results in unknown term:
  - Sub-Grid-Scale (SGS) stress – a similar type of term to Reynolds stress in RANS
  - SGS stress represents the interaction between larger (resolved) eddies and smaller (unresolved) eddies

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Large-Eddy Simulation

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- Theoretical advantages of LES over RANS
  - Smaller eddies are more uniform (isotropic) and therefore it should be easier to develop a “universal” LES model
    - In contrast, RANS models need to approximate all the scales of turbulent motion (including both large and small eddies)
  - As you refine the grid, the LES resolves more of the turbulence and the model is responsible for a smaller fraction of total turbulence energy
    - In the limit of a very fine grid, you resolve all the turbulence (DNS)
    - Fine grid = more accurate simulation
  - In contrast, with RANS when if you refine the grid, the model still approximates the turbulence effects across all scales
    - Fine grid = just as good/bad as coarser grid (provided it is not too coarse and produces numerical errors)

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Large-Eddy Simulation

- Origins of LES: large-scale atmospheric dynamics
  - Smagorinsky (1963) *General circulation experiments with the primitive equations*, Mon. Weather Review, 91(3) p99-164
- SGS turbulence models
  - Like RANS, there are various models of different sophistication
  - Smagorinsky model: stress proportional to local rate of strain
    - Similar in concept to Prandtl mixing length RANS model with length = filter width
    - Problem: Smagorinsky constant in the model is not really “constant”
  - One-equation models: transport equation for turbulent kinetic energy
  - Dynamic models: filter at two scales and extrapolate from one scale to the other scale

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- LES in commercial CFD software?
  - Fire Dynamics Simulator (FDS): most widely-used software for simulating fires, e.g. building fires, large pool fires (and it's free!)
  - General-purpose CFD software usually provide options for various LES and RANS models: ANSYS-Fluent/CFX, OpenFOAM, Star-CCM+

- Strengths of LES
  - Often more accurate than RANS (provided grid is fine enough), particularly for flows with inherent large-scale unsteadiness
    - Vortex shedding in wakes behind bluff obstacles (buildings, vehicles etc.)
    - Puffing plume instabilities from fires
  - Useful detail from resolving time-varying turbulent flow behaviour
  - Aero-acoustics: predicting noise from turbulent fluctuations in jets
  - Great videos!

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Limitations/issues with LES

- LES requires time-varying solution and fine grid:
  - Need a fast computer, and expect long computing times
  - Steady flows: need to monitor simulations over time to ensure statistical convergence (confidence intervals on mean values are useful)
  - Transient flows (e.g. puff release): LES simulation provides just one realisation, need to repeat simulations to obtain an ensemble mean
- Fine grid: how fine does it need to be?
  - Common approach: use the finest grid you can afford
  - Grid quality indices, e.g. fraction of turbulence energy resolved

    Gant S.E. "*Reliability issues of LES-related approaches in an industrial context*" Flow, Turbulence and Combustion, 84(2), p325-335, 2010.

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Limitations/issues with LES (continued)

- Inflow boundary conditions usually need to be time-varying (turbulent)
  - Different options: periodic inflow/outflow boundaries?
  - “Auxiliary” simulation: separate LES simulation with periodic inflow/outflow
  - Synthetic eddy methods
  - RANS simulation with imposed random fluctuations

Problem: it often takes time for the inflow profiles to develop into realistic turbulence downstream from the inlet boundary

- Numeric methods
  - Upwind-biased discretization schemes tend to damp-out turbulent fluctuations
  - Unable to use same approach commonly used for RANS models
  - Ideally need to use central differencing (but can be difficult to keep stable)

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Other turbulence modelling topics

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- Hybrid RANS-LES models
  - Detached Eddy Simulation
  - Scale Adaptive Simulation
- Wall functions
  - Models to approximate the flow in the boundary-layer (near walls) to avoid having to use a very fine grid, and reduce computing times

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Outline

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- Concepts: domain, grid, boundary conditions, finite-volume method
- Turbulence Modelling
  - Reynolds-Averaged Navier Stokes (RANS): steady and unsteady
  - Large Eddy Simulation (LES)

Part 1

- Atmospheric boundary layers
- CFD Software
- Case studies
  - Source terms: flashing jets, overfilling tanks
  - Local-scale atmospheric dispersion: Jack Rabbit II

Part 2

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Acknowledgements

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