Advanced Turbulence Modelling for CFD

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About Me

- Ba in Mechanical and Aerospace Engineering from UQ (2010-2013)
- PhD in Hypersonic Combustion Simulations (2014-2018))
- Presently researching high speed combustion for Center for Hypersonics
- Open source programmer and TTRPG player
- Research Interests: Fluid Dynamics, High Performance Computing, Space

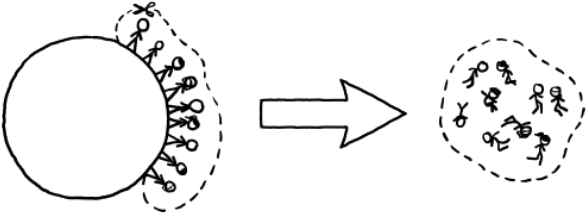


Figure 1: "Everybody Out Plan", *what-if.xkcd.com/7/*

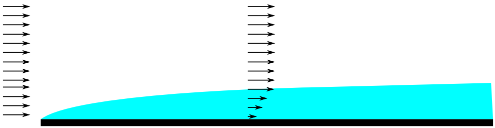
Outline

- What even is turbulence modelling?
- Traditional Turbulence Modelling and Its Discontents (RANS)
- Advanced Technique 1: Direct Numerical Simulation (DNS)
  - DNS requirements
  - Case Study: DNS of Supersonic Shear Layer
- Advanced Technique 2: Large Eddy Simulation (LES)
  - LES requirements
  - Case Study: LES of Scramjet Model

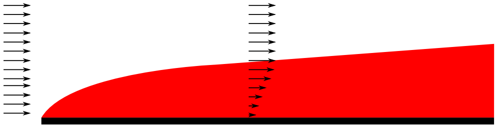
What even is Turbulence Modelling?

- The most common type of turbulence models are Reynolds Averaged Navier-Stokes (RANS) type
- RANS turbulence models add extra equations to the fluid mechanics to roughly account for turbulence
- Typically they add an increase in viscosity μ in places where turbulence is expected

Laminar Simulation



Turbulent Simulation



What even is Turbulence Modelling?

- Real turbulence is a seething tangle of vortices
- RANS models compute a smeared-out time-average of this unsteady flow

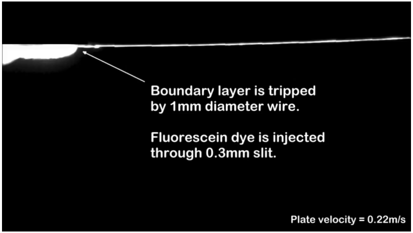


Figure 2: "Spatially developing turbulent boundary layer on a flat plate", J. H. Lee, Y. S. Kwon, N. Hutchins, and J. P. Monty, *arxiv.org/abs/1210.3881*

Traditional Turbulence Modelling and Its Discontents

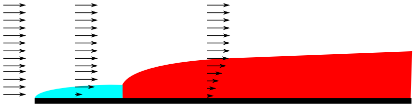
- In spite of more than a hundred years of research, turbulence is still an enigma
- Millennium Prize Problem No. Six (US$1,000,000 yet unclaimed)

Prove or give a counter-example of the following statement:

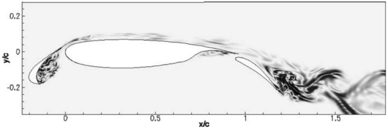
In three space dimensions and time, given an initial velocity field, there exists a vector velocity and a scalar pressure field, which are both smooth and globally defined, that solve the Navier-Stokes equations.

Traditional Turbulence Modelling and Its Discontents

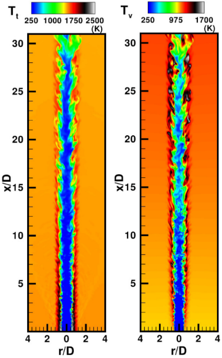
- Because of this RANS models are often a mix of guesswork, empiricism, and calibrations to data
- Things RANS models are not very good at:



Transitional Flow



Complicated Geometries
Spalart et al. (2006), Figure 9



Extra Physics

Koo, Raman, and Varghese (2015), Figure 6

Advanced Turbulence Modelling 1: Direct Numerical Simulation

- Turbulent fluctuations are driven by viscous shearing forces
- These forces are correctly simulated in CFD, but usually we don't have enough resolution to see them
- With enough grid points however, turbulence appears with no modelling required

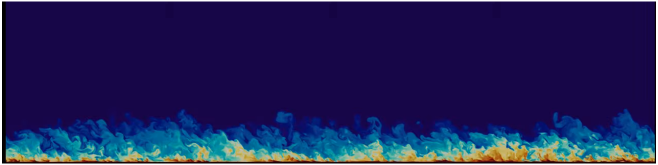


Figure 3: "Passive Scalar Mixing in Turbulent Boundary Layer", 10 billion cell Direct Numerical Simulation, Nagoya University Fluid Dynamics Laboratory, *https://www.youtube.com/watch?v=_fM5Ad9TcR8*

Direct Numerical Simulation: Requirements

DNS requires a *LOT* of cells

- Flow Problem must be:
  - Small domain/low Reynolds number
  - Simple geometry
  - Domain must be 3D (Important!)
- Fluid Dynamics Code must be:
  - Multi-process parallel with good scalability
  - High spatial accuracy to minimise numerical dissipation
  - Efficient evaluation of timesteps

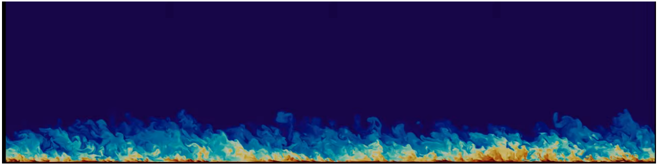
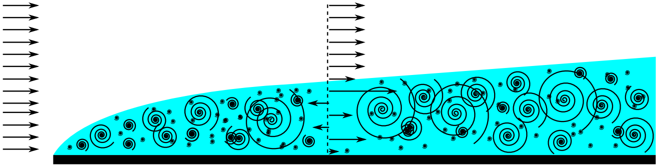


Figure 4: "Passive Scalar Mixing in Turbulent Boundary Layer", 10 billion cell Direct Numerical Simulation, Nagoya University Fluid Dynamics Laboratory, *https://www.youtube.com/watch?v=_fM5Ad9TcR8*

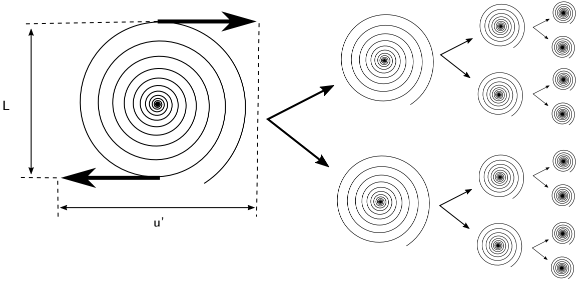
Direct Numerical Simulation: Requirements

- First attempt at DNS requires some guesswork about cell density
- After one attempt, check the resolution and iterate
- Evaluating the discretisation requires estimating the size of turbulent structures
- Imagine the turbulence being composed of a fractal of interlocking turbulent structures



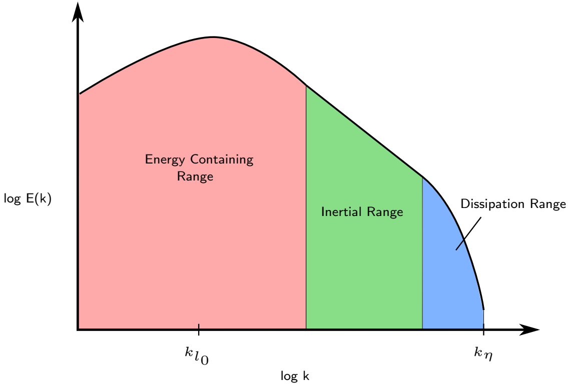
Direct Numerical Simulation: Requirements

- Energy cascade hypothesis: Large structures extract energy from the flow and are broken apart into smaller ones (Kolmogorov (1961))
- These smaller structures are unstable and break down in turn, until eventually the smallest structures are dissipated by viscous forces
- Viscous forces get stronger at smaller scales due to the larger gradients involved



Direct Numerical Simulation: Requirements

- Rather than being random, the spectrum of structure sizes has a recognisable shape
- Spectra of the cascade are usually expressed in terms of wave number: $k \sim \frac{1}{L}$

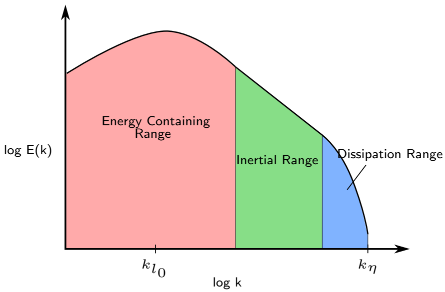


Direct Numerical Simulation: Requirements

- Under ideal conditions (isotropic, homogeneous, high Reynolds number), the cascade process is self similar
- This leads to an 'inertial range' with predictable behaviour, characterised by a single value of the dissipation ϵ:

$$E \sim \epsilon^{2/3} k^{-5/3}$$

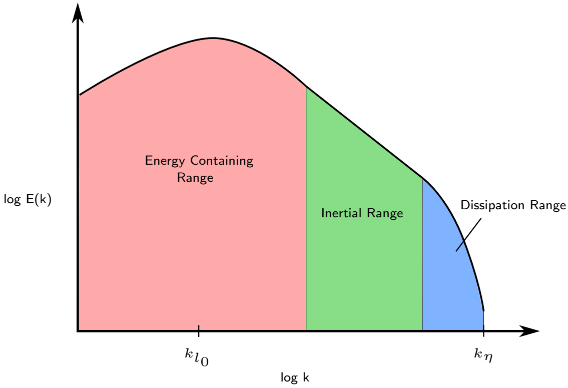
$$u' \sim (\epsilon L)^{1/3}$$



Direct Numerical Simulation: Requirements

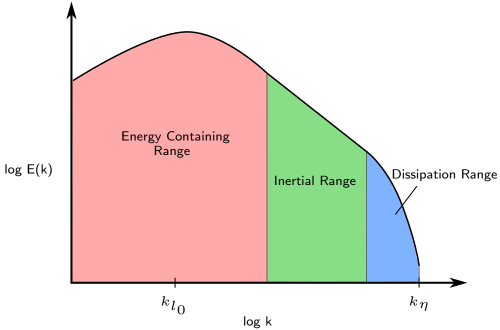
Real turbulence differs from this ideal at high and low wave numbers, but the approximation is good enough to define some useful scales. Using k_t (turbulent kinetic energy), ν (normal laminar viscosity):

- Integral Scale (Largest Structures): $l_0 = \frac{k_t^{3/2}}{\epsilon}$
- Kolmogorov Microscale (Smallest Structures): $\eta = (\frac{\nu^3}{\epsilon})^{\frac{1}{4}}$



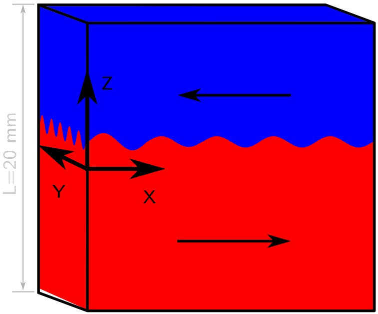
Direct Numerical Simulation: Requirements

- To perform a DNS, the grid must contain sufficient space to resolve the largest structures (l_0) and sufficient cell density to resolve most of the dissipation range.
- η is actually quite small, it marks the lower end of the dissipation range.
- 90% of the dissipation happens between 8η and 50η.
- Resolving too little of the dissipation range can cause the energy to pile up in the turbulent cascade. (Bad)



Direct Numerical Simulation: Case Study

- 2cm cubic Supersonic Shear Layer, periodic reacting flow with 299^3 cells
- Computed with Unstructured 3D code on 496 cores using the *Magnus* supercomputer in Perth



Air:	
p	101,000 (Pa)
T	1,400 (K)
u	-1,168.89 (m/s)
Y_{N_2}	0.767
Y_{O_2}	0.233

Fuel:	
p	101,000 (Pa)
T	1,500 (K)
u	1,665.89 (m/s)
Y_{H_2}	1.0

Figure 5: Supersonic Shear Layer Initial Conditions.

Direct Numerical Simulation: Case Study

- High resolution dataset for studying interaction between turbulence and chemistry

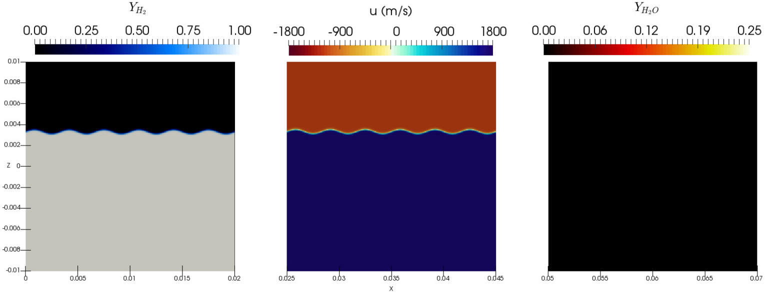
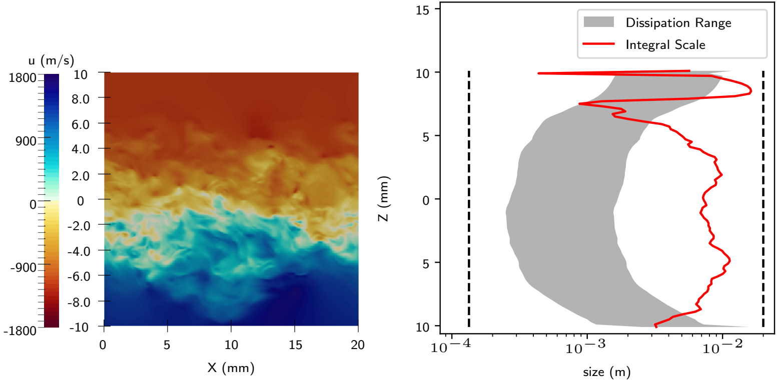


Figure 6: Animation of Supersonic Shear Layer. Left: Fuel Mass Fraction. Middle: Streamwise Velocity. Right: Product Mass Fraction.

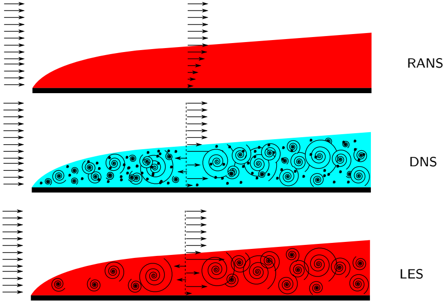
Direct Numerical Simulation: Case Study

- Supersonic Shear Layer: Velocity field and turbulent scales @ 100 μs



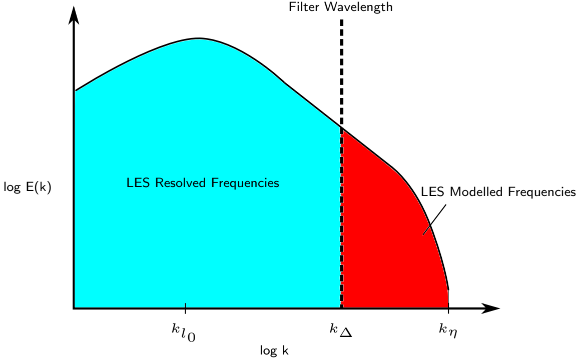
Advanced Turbulence Modelling 2: Large Eddy Simulation

- DNS is very expensive, those small eddies require very small cells
- Most of the energy is contained in the large eddies, which vary from flow to flow
- In contrast the small eddies are more universal and homogeneous
- Large Eddy Simulation is a compromise that directly simulates large structures like in DNS, and models small ones like in RANS



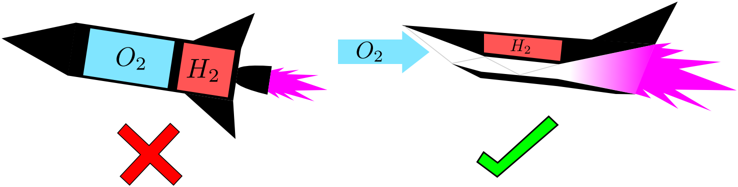
Large Eddy Simulation: Requirements

- Low-to-Moderate Reynolds Number
- Fluid dynamics code with High Order Spatial Accuracy
- Three dimensional domain (Also important for LES! 2D Turbulence behaves differently)
- High cell density grid, with smallest cells in the inertial range
- Special LES turbulence model, in this case IDDES (Shur et al. (2008))



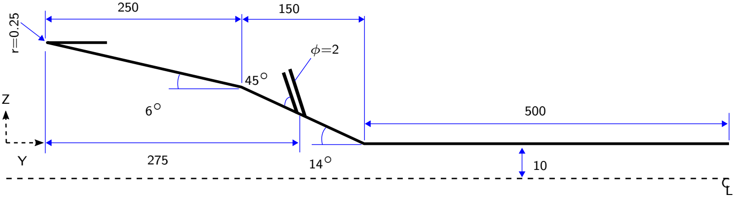
Large Eddy Simulation: Case Study

- LES of model scramjet experiment to compute combustion data
- Motivation: Air-breathing space launch systems



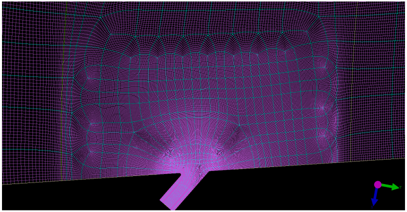
Large Eddy Simulation: Case Study, Geometry

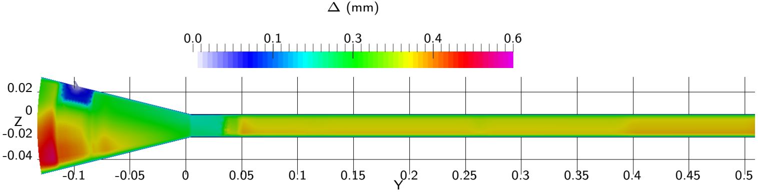
- Based on 2018 experiment in T4 at UQ by Augusto Moura
- Planar scramjet model with a single hydrogen fuel injector
- Flight conditions approximate 30-40 km altitude, Mach 10, 0.49 Equivalence Ratio



Large Eddy Simulation: Case Study, Grid Details

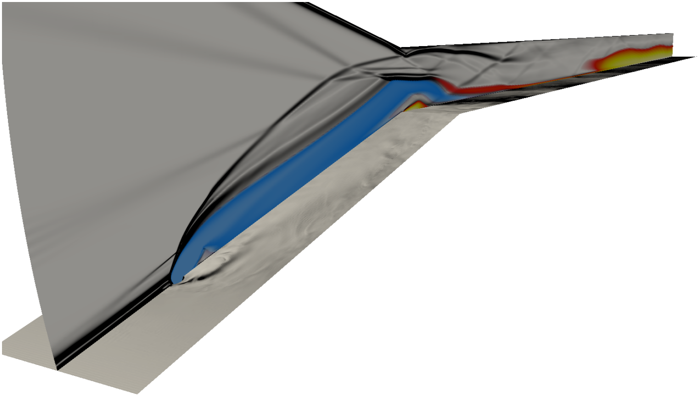
Final Grid Details	
Total Cell Count	37,817,312
Inlet Wall Cell Height	$1\mu m$
Combustor Wall Cell Height	$0.5\mu m$
Injector Cell Size	$0.04mm$
Jet Cell Size	$0.1mm$
Jet Wake Cell Size	$0.25mm$
Combustor Entrance Cell Size	$0.2mm$
Combustor Core Cell Size	$0.4mm$





Large Eddy Simulation: Case Study

Solver Settings	
Solver	UnStructured 3D
Turbulence Modelling	Spalart-Allmaras IDDES (Shur et al. (2008))
Finite Rate Chemistry	13 species, 33 reactions (Jachimowski (1992))
Spatial Derivatives (Smooth)	6th Order Gradient Reconstruction
Spatial Derivatives (Shocks)	Modified Steger-Warming MUSCL
Time Derivatives	2nd Order Implicit Backward Euler
Gas Model	Thermal Equilibrium (McBride, Zehe, and Gordon (2002))



Large Eddy Simulation: Case Study

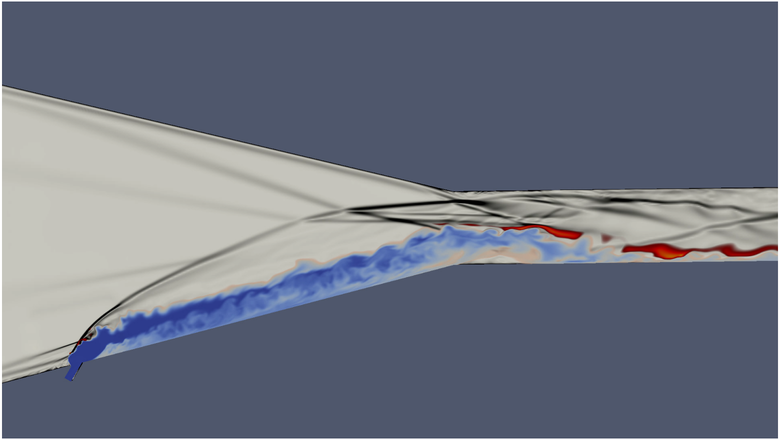
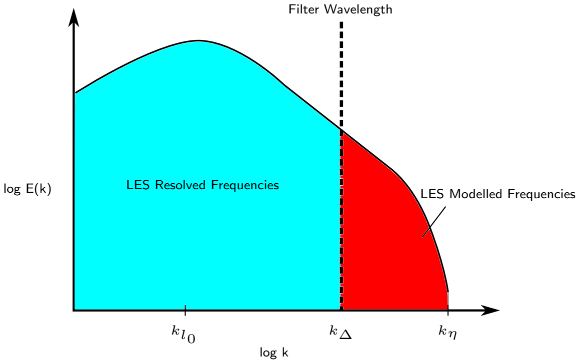


Figure 7: Centerplane colour map of LES case study: Blue (Fuel Mass fraction), Red (OH Mass Fraction), Black (Density Gradients)

Large Eddy Simulation: Case Study

- How to check grid resolution in an LES?
- Various methods: Compare two grids, compare to experiment ...
- Can also check by directly computing turbulent kinetic energy partitioning



Large Eddy Simulation: Case Study

- Subgrid turbulent kinetic energy: Δ (Cell Size), ν_t (Turbulent Viscosity)
- Based on dimensional analysis, taken from Gehre (2014)

$$k_{sgs} = \frac{\nu_t^2}{(0.07\Delta)^2} \tag{1}$$

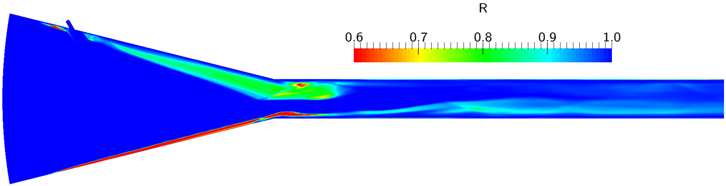
- Resolved turbulent kinetic energy: u, v, w (Velocity Vector Components), $u' = u - \overline{u}$ (Velocity Fluctuations)
- Time averages computed from the actual simulation by averaging over many iterations

$$k_r = \frac{1}{2}({u'}^2 + {v'}^2 + {w'}^2) \tag{2}$$

Large Eddy Simulation: Case Study

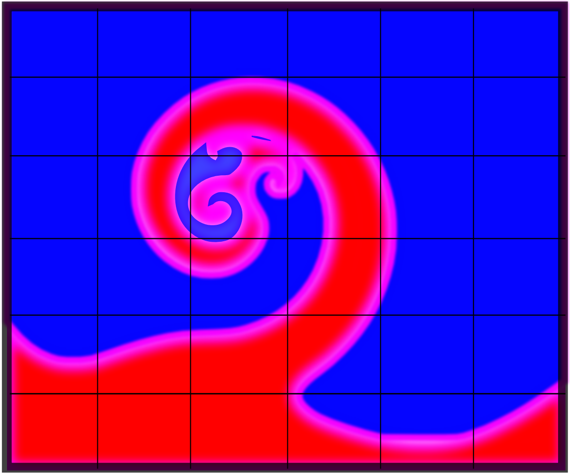
- Rule of thumb for a "good" LES is 80% of the total TKE resolved

$$R = \frac{k_r}{k_r + k_{sgs}} \tag{3}$$



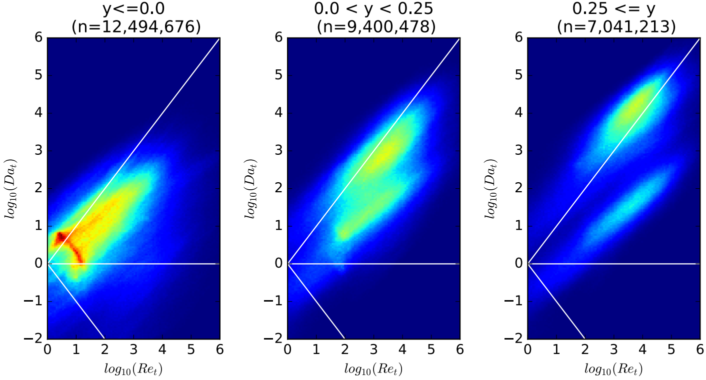
Large Eddy Simulation: Case Study

- Turbulence can affect chemistry too: Turbulent Chemistry models sometimes required
- Combustion regime data from the LES will help choose an appropriate model



Large Eddy Simulation: Case Study

- Combustion characterised Turbulent Reynolds number Re_t: (How intense is the turbulence?)
- And Turbulent Damkohler Number Da_t: (How fast is the chemistry compared to the turbulence?)



Conclusions

- Turbulence modelling is complicated and still not fully understood
- Modern supercomputing has enabled some advanced techniques that are more accurate than RANS
- Direct Numerical Simulation (DNS) uses no models but is only practical for small flows
- Large Eddy Simulation (LES) directly simulates large eddies and models small ones
- Can be applied to actual geometries with reasonable computation times
- Simulated turbulence gives insight into the phenomenon which can help improve simulations in turn

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