Practical Quality Measures for Large-Eddy Simulation

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- Health and Safety Context
- LES/DES/SAS Quality
  - Grid Resolution
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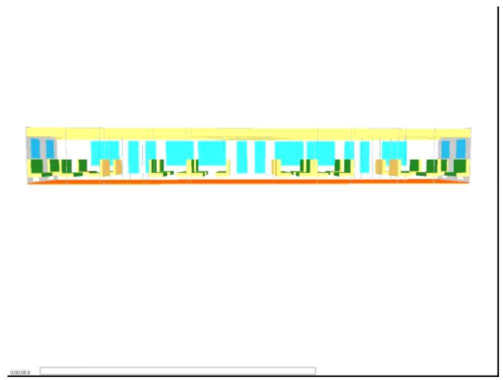
LES in Health and Safety

- Fire Dynamics Simulator (FDS) from NIST



- Used extensively in fire investigation, e.g. collapse of World Trade Center twin towers
- OECD Best Practice Guidelines for CFD in Nuclear Reactor Safety Applications:

"Obviously, more advanced scale-resolving CFD methods based on LES, DES, or SAS are required for such cases."

LES/DES/SAS Quality Issues

Differences compared to RANS quality issues:

- Subgrid-scale model
- Wall treatment
- Unsteady inflow conditions
- Numerical schemes
- Grid dependence ←
- Temporal treatment

Grid Resolution

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- Complex issue: dynamic interaction of model and discretization errors
- In the limit:
  - Overly coarse grids produce poor results
  - Very fine grid, LES results tend to DNS
- What practical guidance exists on grid resolution?

1. Rules of thumb ← e.g. 20 cells across characteristic fire diameter
2. Measures based on prior RANS
3. Single-grid estimators
4. Multi-grid estimators

2. Measures based on RANS

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- Ratio of integral turbulence length scale to grid cell size: $$\frac{\left(k^{3/2}/\varepsilon\right)}{\Delta} > 10$$

- Ratio of grid cell size to Kolmogorov length scale: $$\frac{\Delta}{\eta} = \frac{\Delta}{\left(\nu^{3}/\varepsilon\right)^{1/4}} < 25$$

- Near-wall spacing, for wall-resolving LES:

$$(x^{+}, y^{+}, z^{+}) < (100, 2, 20)$$

"Young person's guide to DES Grids", Spalart 2001

3. Single-grid estimators

- Viscosity ratio, ν_{eff}/ν < 20 for $Re_t \sim 1200$

  < 5 for $Re_t \sim 300$

- Relative effective viscosity index
- Subgrid activity parameter
- Proportion of resolved turbulent kinetic energy:

$$\frac{k_{res}}{k_{res} + k_{sgs} + k_{num}} > 0.8$$

- Power spectral density (-5/3 slope)

4. Multi-grid estimators

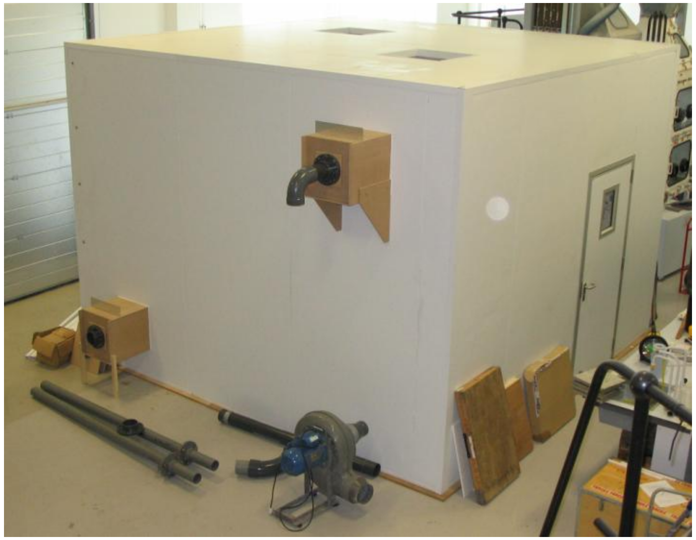
- “Index of Quality” of Celik *et al*. (2005)
- Grid and Model variation of Klein (2005)

- Both based on Richardson extrapolation using multiple LES solutions

Known Limitations

- Accuracy of RANS model, esp. in transitional or massively separated flows.
- Subgrid activity parameter close to 1.0 in most industrial LES
- Resolved TKE can be higher on coarse grid than on fine grid
- Magnitude of numerical dissipation?
- Multi-grid methods: resolution not in asymptotic range for *RE*, interaction of errors
- Spectra: modified by buoyancy, only found at points and in low-*Re* flows?

Application



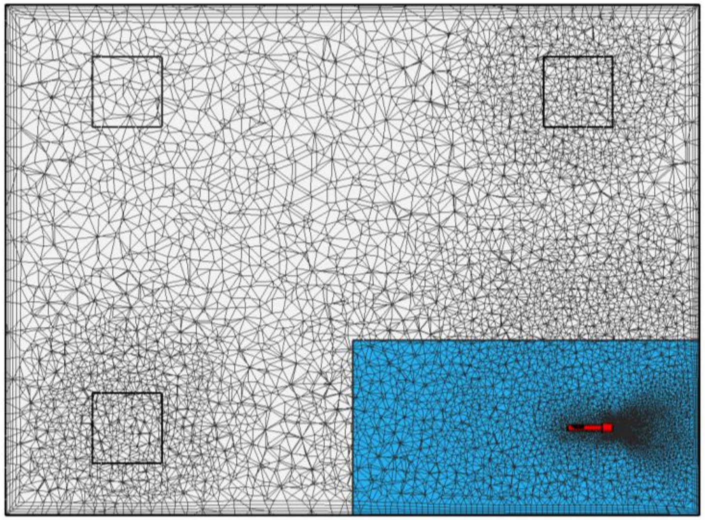
Continuous methane gas release in a ventilated room

Interest: to predict the flammable gas cloud size

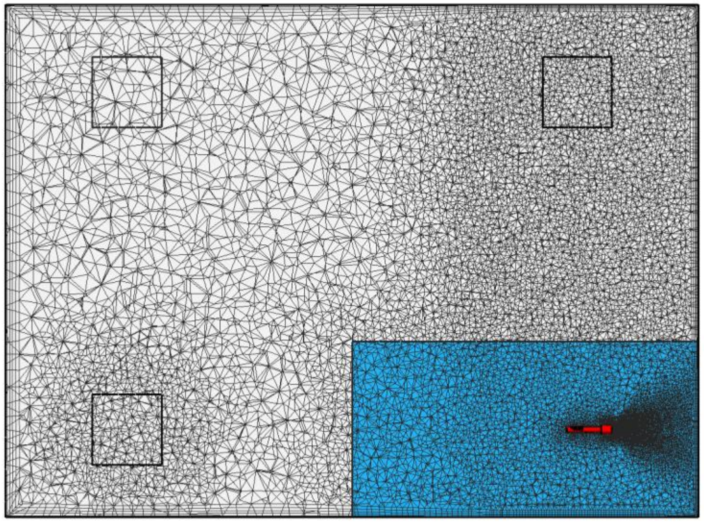
Flow Behaviour

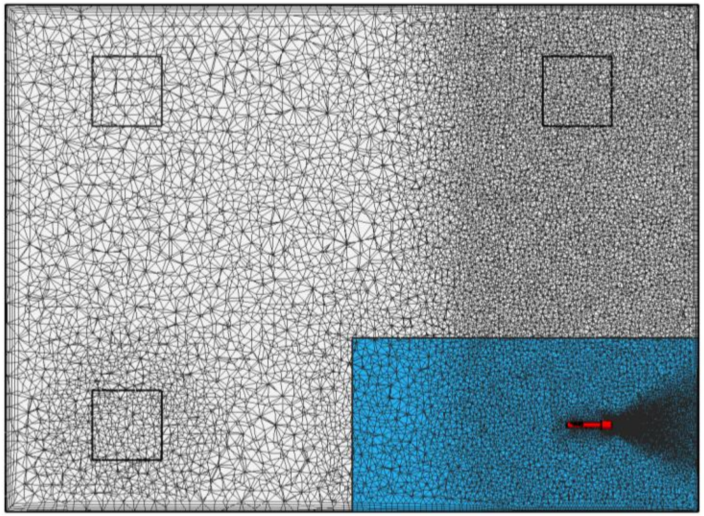
Grids

Coarse (0.2M nodes)



Medium (0.4M nodes)

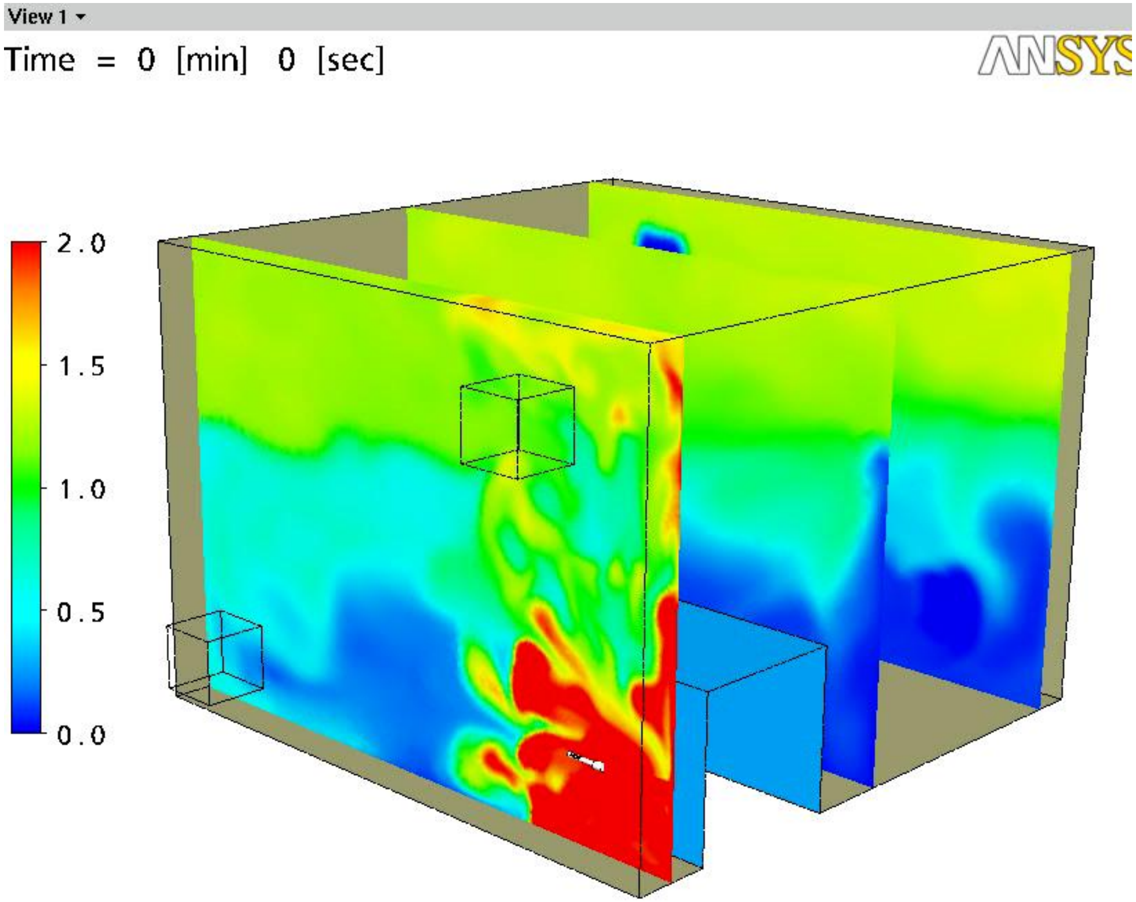




Fine

(0.7M nodes)

Gas Cloud



	Timescale (s)
Gas jet	10^{-5}
Vent inlet	2 – 3
Plume	3
Air change	300

- Time-step $\Delta t = 0.1$ s
- Averaging period ≈ 7 mins

Grid Resolution

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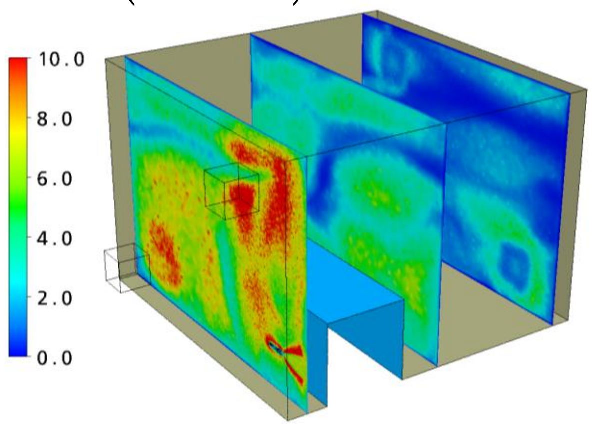
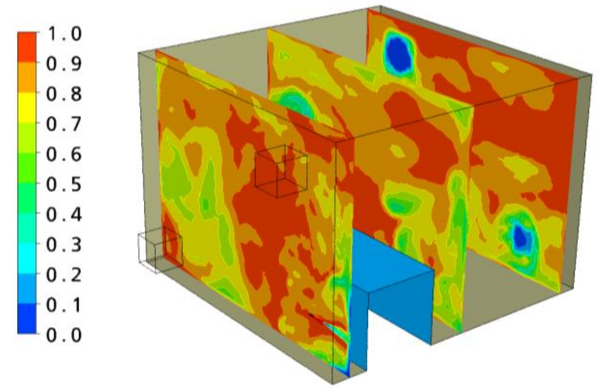
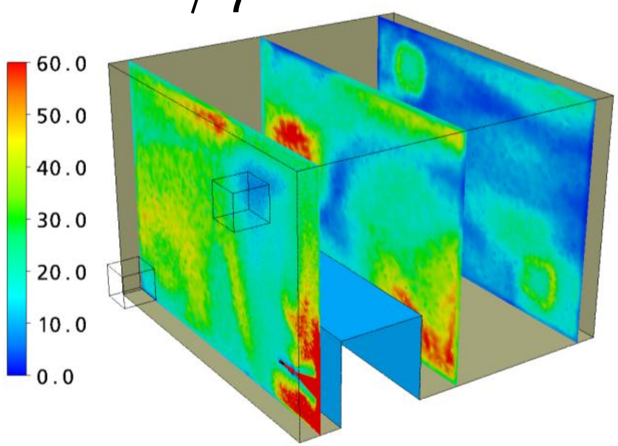
$$\left(k^{3/2}/\varepsilon\right)/\Delta > 10$$



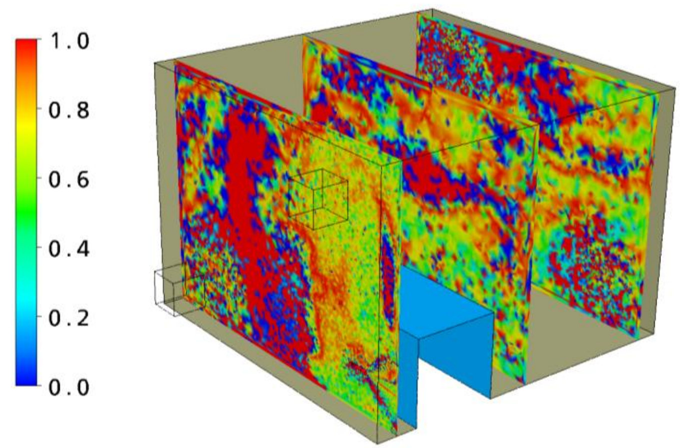
$$k_{res}/(k_{res} + k_{sgs}) > 0.8$$



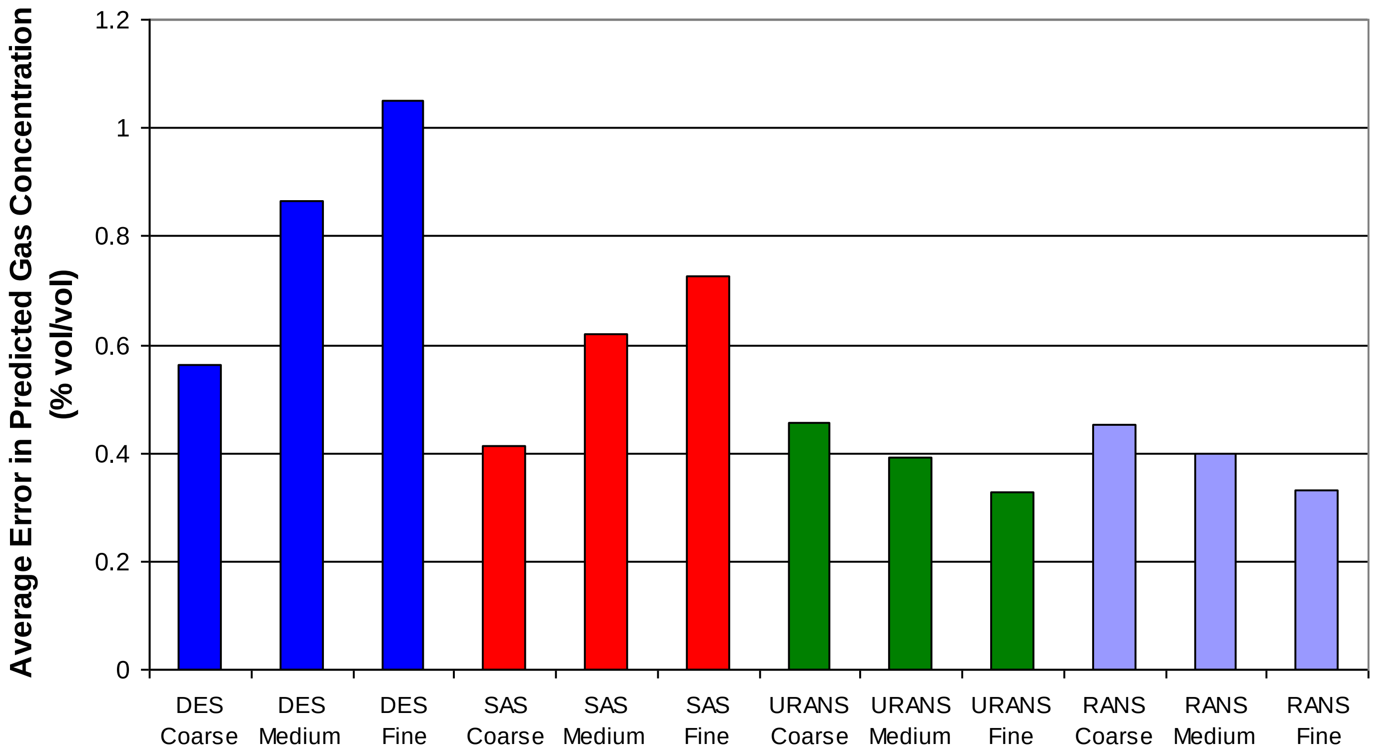
$$\Delta/\eta < 25$$



$$LES\_IQ_k > 0.8$$

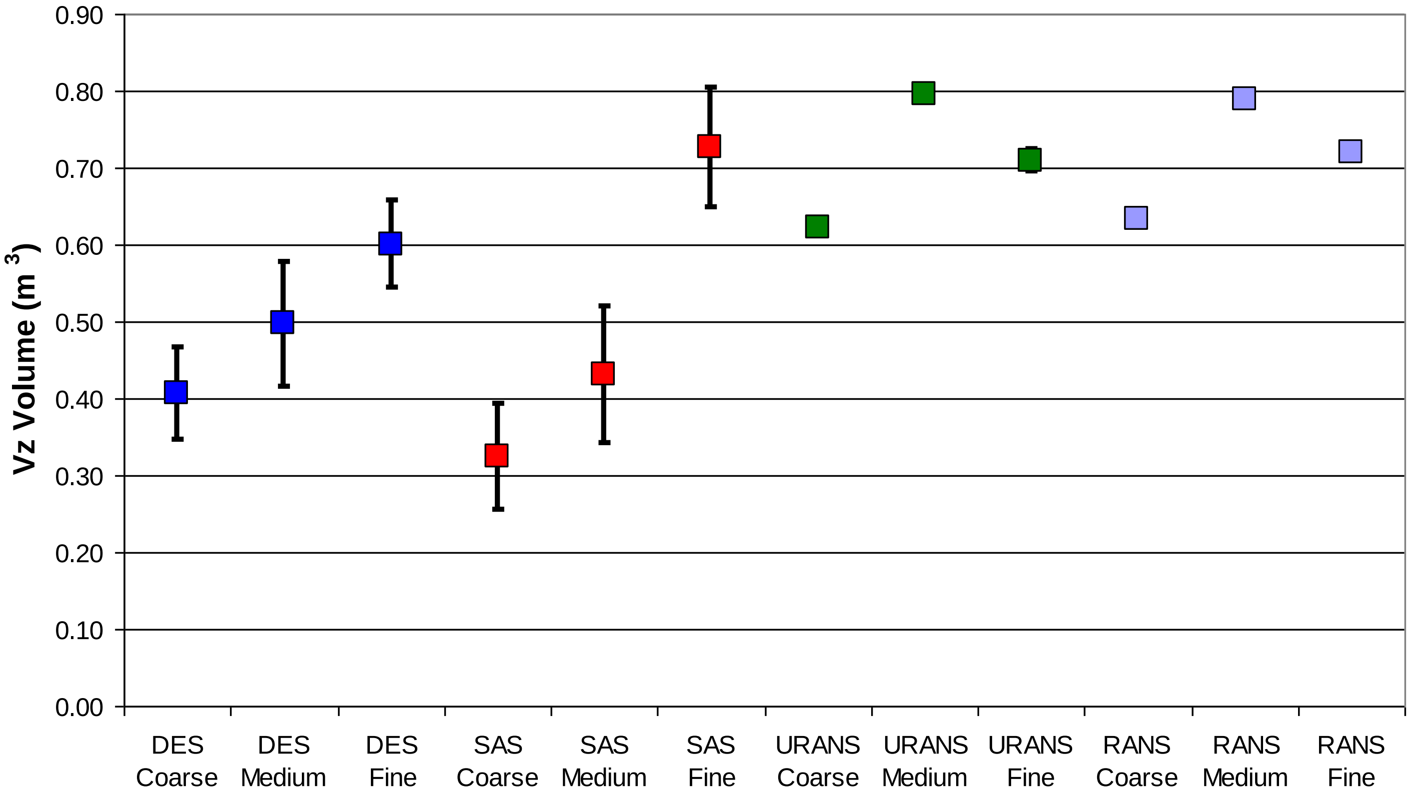


Results



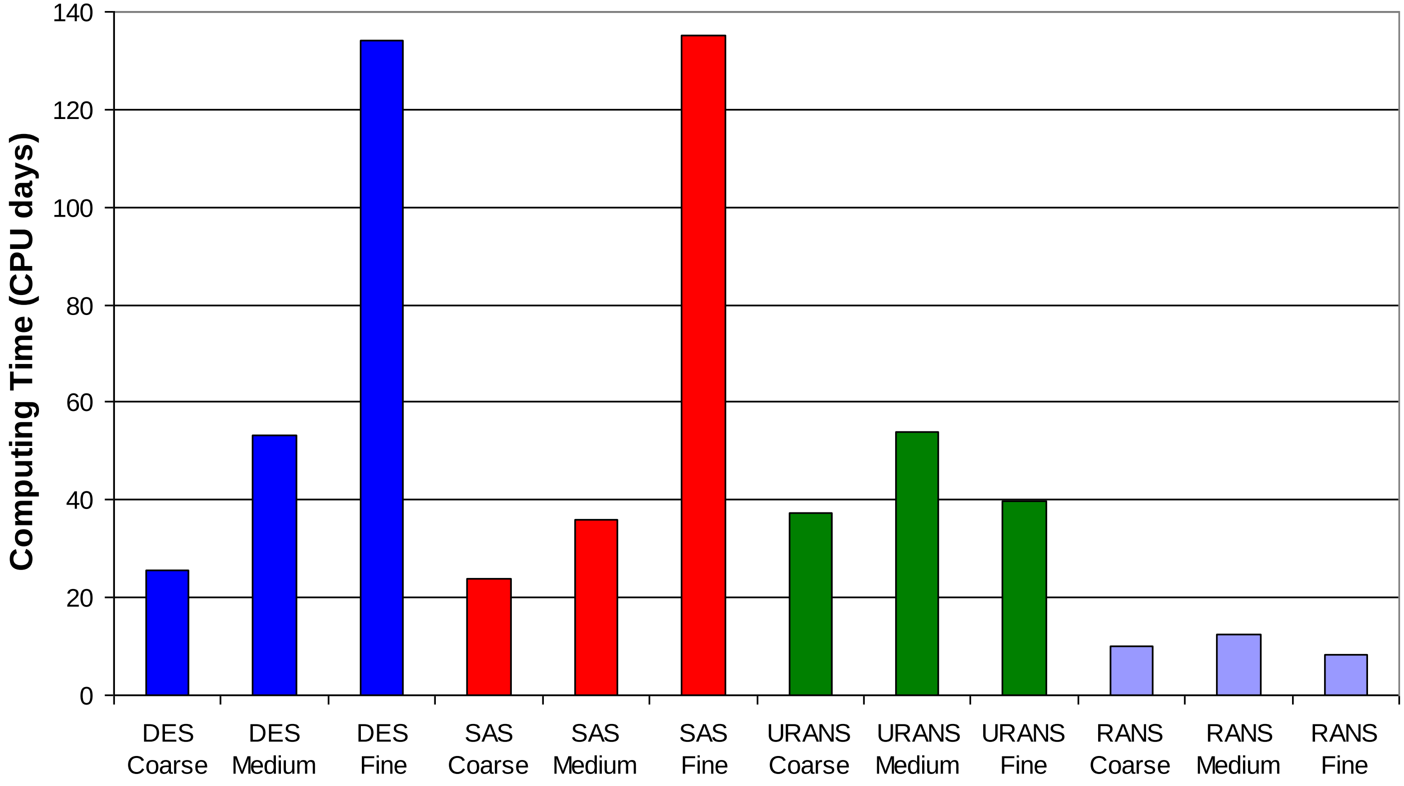
Average error between CFD and experiments

Results



Predicted mean gas cloud size and 95% confidence intervals

Computing Time



Computing time in CPU days

Conclusions

- Number of grid resolution indices in literature.
- Each has advantages/limitations, none ideal.
- Results for test case show that DES/SAS can be worse than SST if grid resolution marginal.
- SAS appears sensitive to grid resolution.
- Confidence Intervals useful to identify statistical uncertainty and define duration of simulation.
- Further research in LES/DES/SAS/URANS quality and trust required: cohort studies?
- Suggestion: document grid resolution and statistical uncertainty in future results.

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for assistance with bootstrapping

Questions?

DES Blending Function

Turbulence Model

$$\varepsilon = \beta^* k \omega F_{DES}$$

$$F_{DES} = \max\left[\frac{k^{3/2}/\varepsilon}{C_{DES}\Delta}\left(1 - F_{SST}\right), 1\right]$$

Set to zero to recover Strelets (2001) model

$$C_{DES} = 0.61$$

Discretization Scheme

$$\varphi_{ip} = \sigma \varphi_{ip,U} + (1-\sigma)\varphi_{ip,C}$$

$$\sigma = \tanh\left(A^3\right)$$

$$A = \max\left(\frac{C_{DES}\Delta_{\max}}{L_{turb}\, g} - 0.5, 0\right)$$

$$L_{turb} = \frac{\sqrt{k}}{c_\mu \omega}$$

$$g = \max\left[\tanh\left(B^4\right), 10^{-10}\right]$$

$$B = 2\Omega \frac{\max(S, \Omega)}{\max\left(\frac{S^2 + \Omega^2}{2}, 10^{-10}\right)}$$

$$\sigma^{\lim} = \max\left[\sigma, 1 - \min\left(\frac{5}{CFL}, 1\right)\right]$$

DES Blending Function

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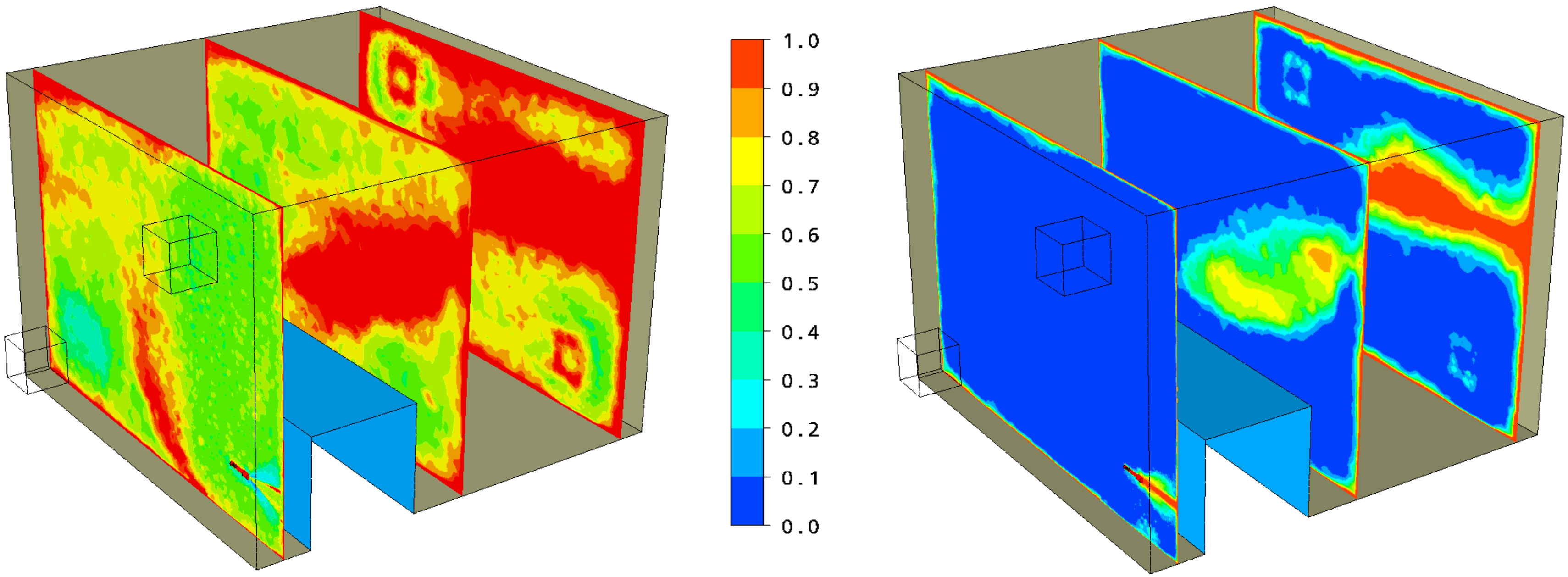
Turbulence Model

1 = RANS ; <1 = DES

$(C_{DES}\,\Delta) / (k^{3/2} / \varepsilon)$

Discretization Scheme

0 = central ; 1 = upwind-biased



Results

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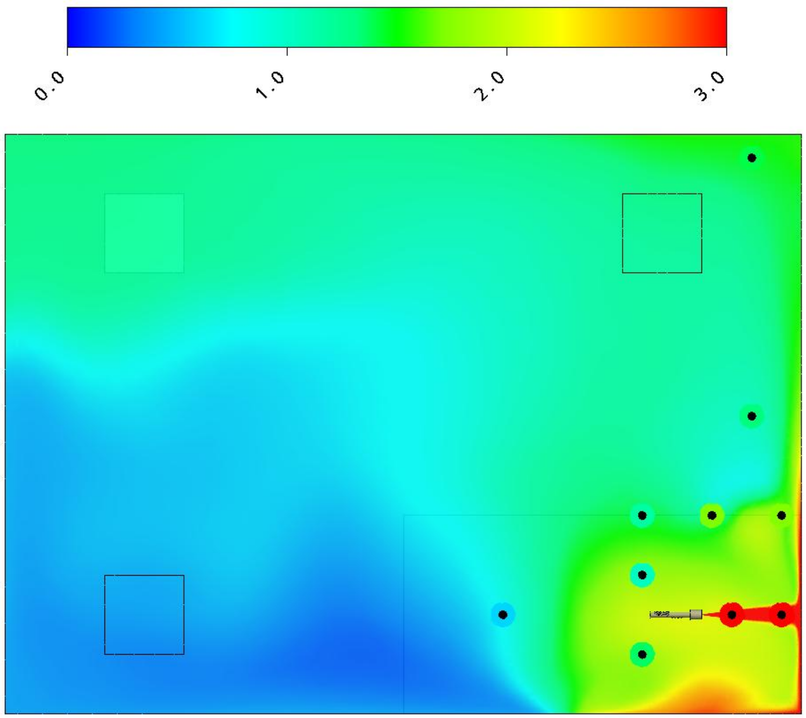
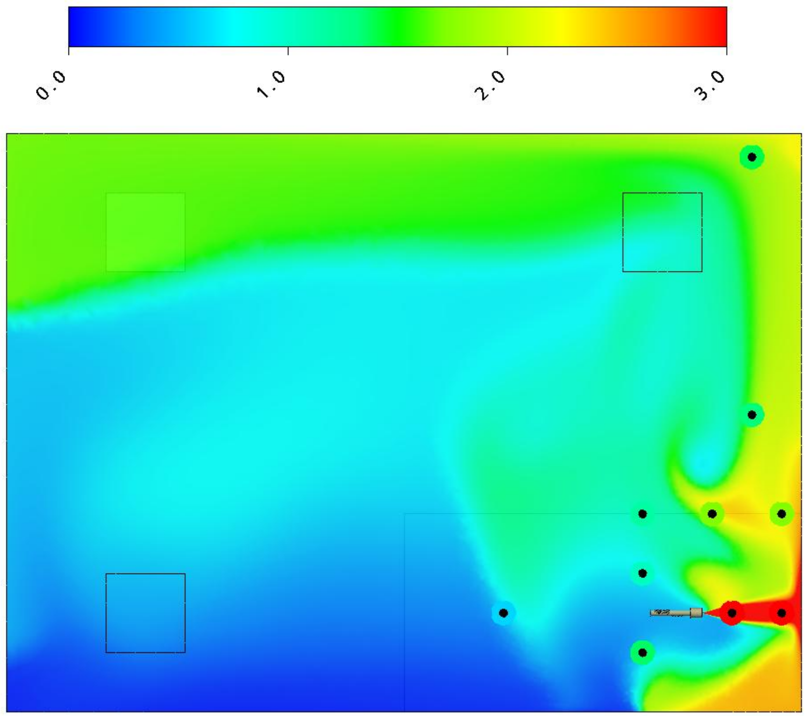


DES



RANS (SST)

Mean Gas Concentrations (% vol/vol)

Results

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LES "Index of Quality"

$$LES\_IQ_k = 1 - \frac{|k_{tot} - k_{res}|}{k_{tot}}$$

$$k_{tot} = k_{res} + a_k h^p$$

$p = 2$

Cell size

$$a_k = \frac{(k_{res})_1 - (k_{res})_2}{h_2^2 - h_1^2}$$

Subscript: 1= Medium, 2 = fine

Problems when:

$(k_{res})_1 > (k_{res})_2$

→ $a_k < 0$

→ $k_{res} + a_k h^p < | a_k h^p |$

→ $\frac{|k_{tot} - k_{res}|}{k_{tot}} > 1$

→ $LES\_IQ_k < 0$

or when:

$(k_{res})_1 >> (k_{res})_2$

→ $a_k << 0$

→ $k_{tot} < 0$

→ $LES\_IQ_k > 1$

2. Measures based on RANS

- Ratio of integral turbulence length scale to grid cell size: $$\frac{\left(k^{3/2}/\varepsilon\right)}{\Delta}$$

Baggett *et al*. (1997)	Channel flow	3.5
Jiménez & Moser (1998)	Channel flow	3.5 – 7
Pope (2000)	High-*Re* isotropic turbulence	12 – 17
Addad *et al*. (2004)	Buoyancy opposed wall jet	12 – 30
Van Maele & Merci (2008)	Tunnel fires	12

2. Measures based on RANS

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- Ratio of grid cell size to Kolmogorov length scale

$$\frac{\Delta}{\eta} = \frac{\Delta}{\left(\nu^3 / \varepsilon\right)^{1/4}}$$

Celik *et al*. (2005)	Rule of thumb	< 25
Hadžiabdić & Hanjalić (2008)	Impinging Jet	< 21

3. Single-grid estimators

- Subgrid activity parameter

  (Geurts & Fröhlich, 2002)

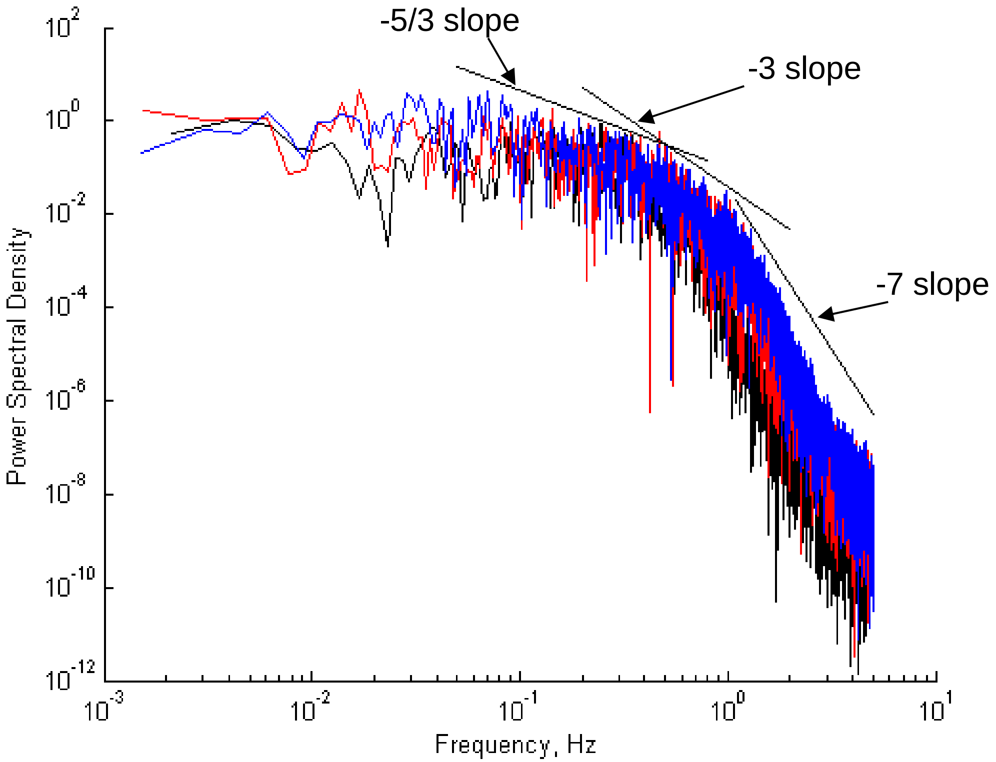
$$s = \frac{\overline{\varepsilon_t}}{\overline{\varepsilon_t} + \overline{\varepsilon_\mu}} = \frac{\overline{\nu_t S^2}}{\overline{(\nu + \nu_t) S^2}}$$

= 0 for DNS

= 1 for high-*Re* LES

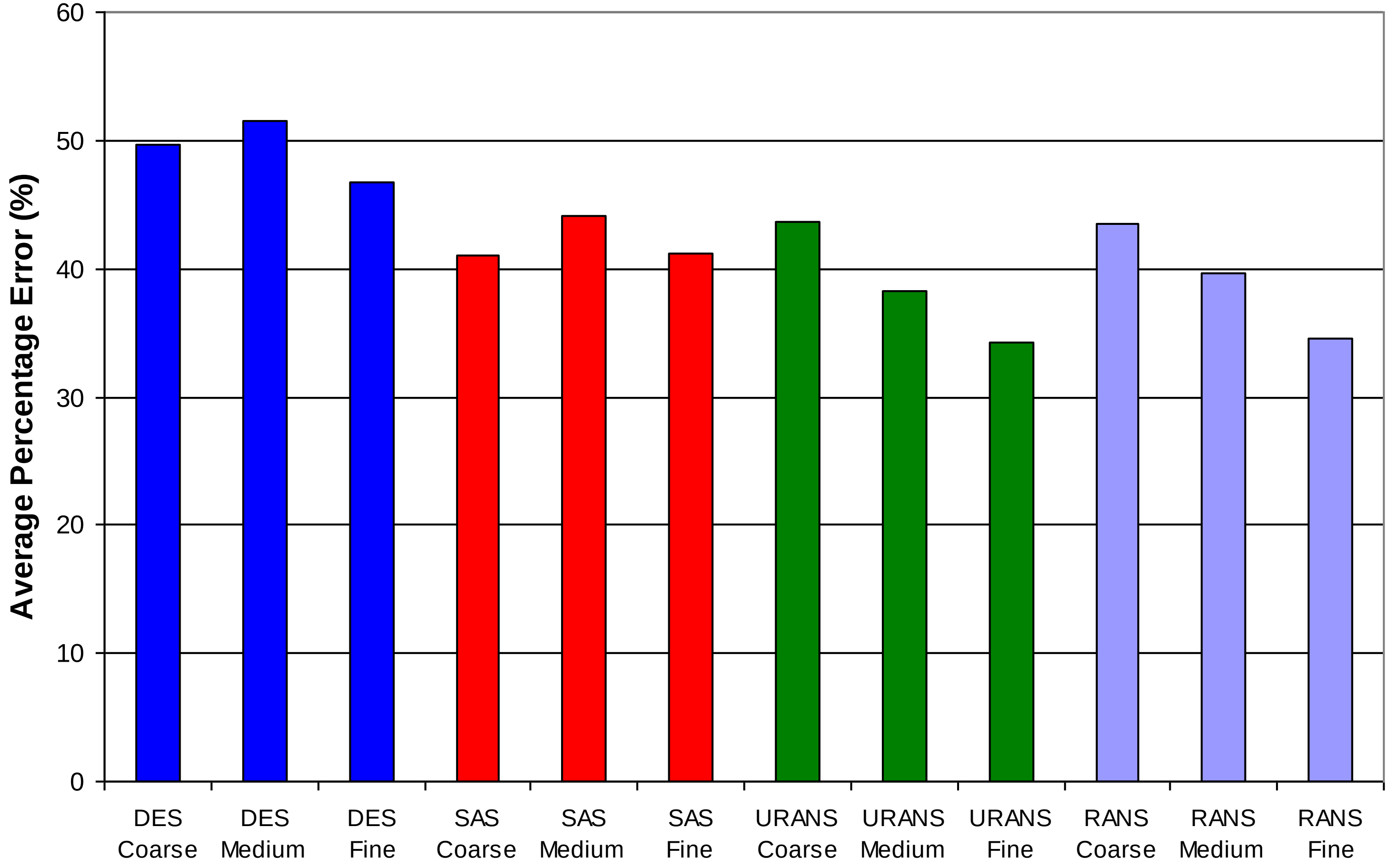
3. Single-grid estimators

Power spectral density based on concentration fluctuations



DES results: – coarse, – medium, – fine

Error in Percentage Terms



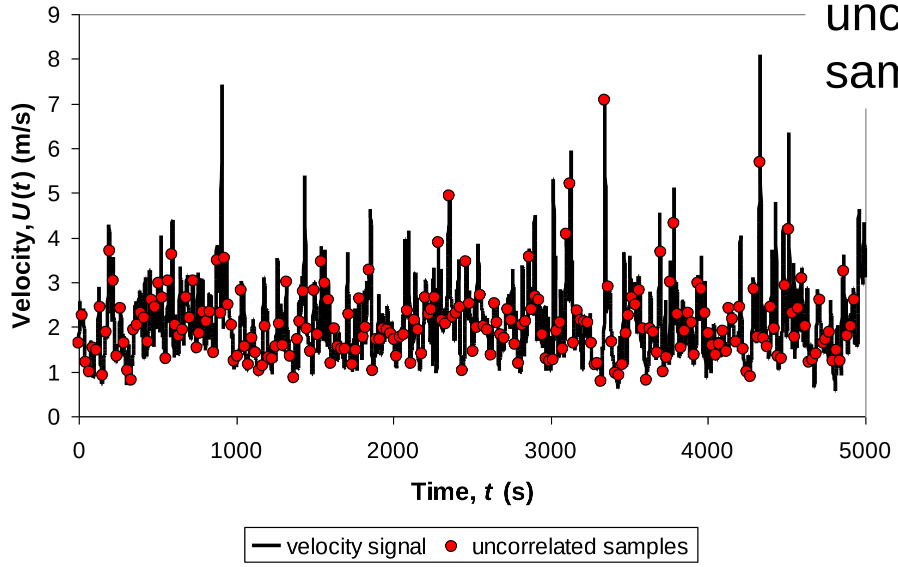
Statistical Uncertainty

- How long should the LES calculation be continued?
- Assess uncertainty in mean values using Confidence Intervals
- "95% confident that mean lies between *x* and *y* m/s"
- Fractional error:

$$e_s = \frac{k\sqrt{\overline{u^2}/n}}{U}$$

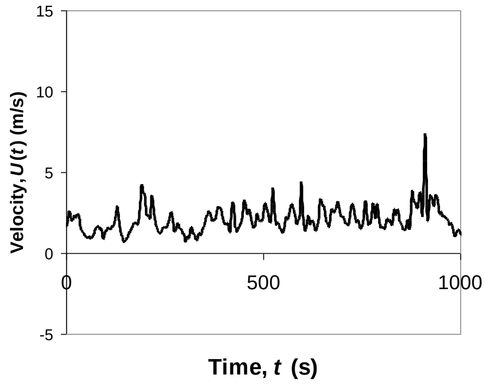
Variance

Number of uncorrelated samples



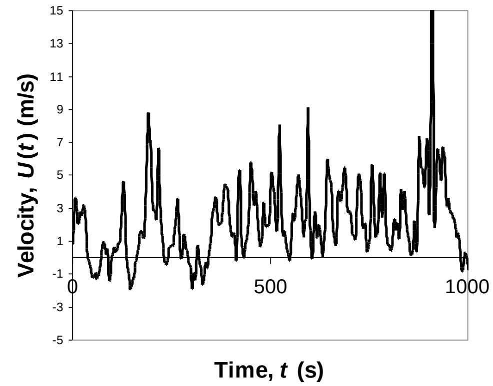
Statistical Uncertainty

- If the turbulence intensity $I = \sqrt{\overline{u^2}} / U$ doubles:



I = 4%

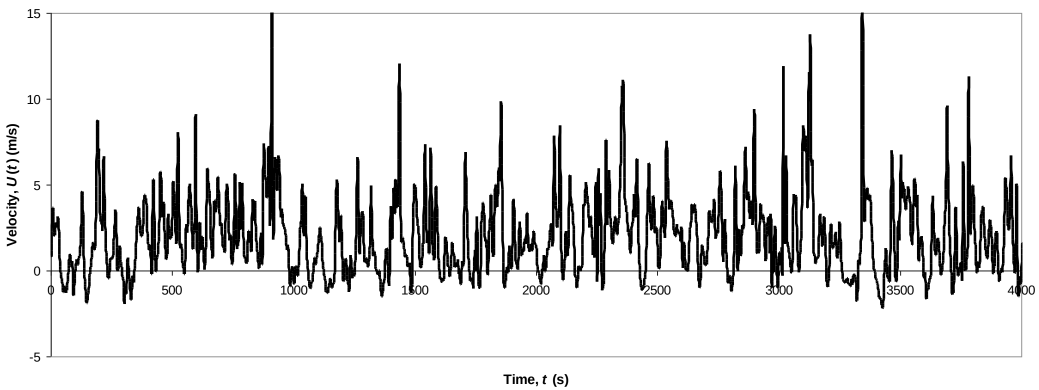
e_s = 5%



I = 8%

e_s = 10%

- Need to increase number of samples by factor of 4 to maintain same confidence level.



I = 8%

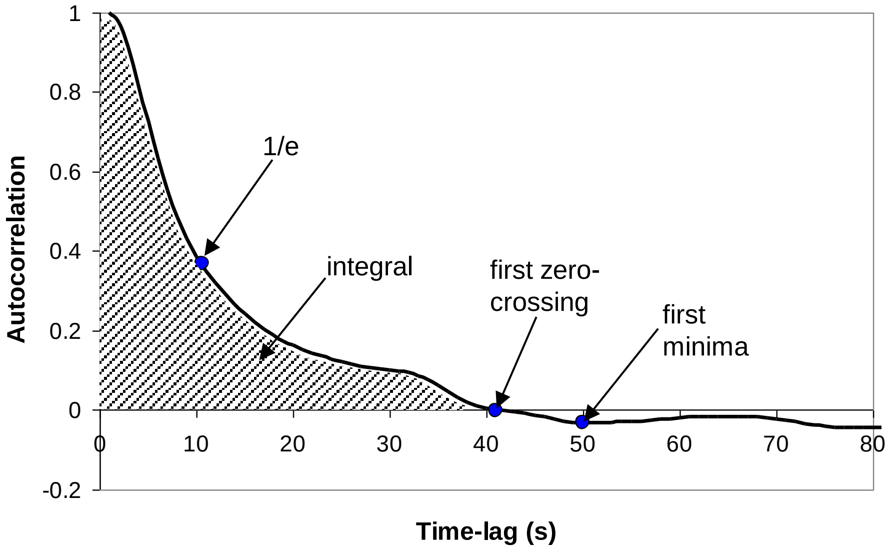
e_s = 5%

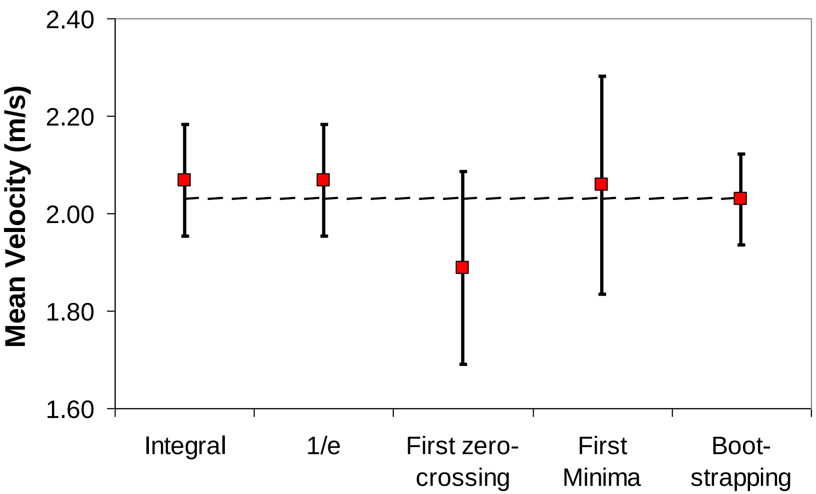
Statistical Uncertainty

- Classical approaches to calculate *CI* rely on *uncorrelated* data
  - Problem: need to sample signal at intervals spaced τ apart
  - How to calculate τ ? Various approaches possible which produce different e_s
- Alternative: *bootstrapping*
  - Can handle correlated data
  - Automatic block length selector means no user-defined parameters
  - Can also be used to calculate confidence intervals on Reynolds stresses etc.

Confidence Intervals

	Interval (s)	Mean ± 95% CI
All data	-	2.03 ± ?
Integral	22	2.06 ± 2.8%
1/e	22	2.06 ± 2.8%
First zero	82	1.90 ± 5.2%
First min	100	2.06 ± 5.4%
Bootstrap	-	2.03 ± 2.3%





Bootstrapping

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  (http://www.economics.ox.ac.uk/members/andrew.patton)