Turbulence and CFD models: Theory and applications

Roadmap to Lecture 10

1. **SRS simulations – Scale-resolving simulations**
2. **LES equations – Filtered Navier-Stokes equations**
3. **Sub-grid scale models for LES**
4. **DES models**
5. **A few mesh resolution guidelines and rough estimates for LES/DES simulations**
6. **Final remarks on LES/DES turbulence models**

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1. **SRS simulations – Scale-resolving simulations**
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6. Final remarks on LES/DES turbulence models

SRS simulations – Scale-resolving simulations

- Overview of the main turbulence modeling approaches.

MODELING APPROACH

RANS
Reynolds-**A**veraged **N**avier-**S**tokes equations

URANS
Unsteady **R**eynolds-**A**veraged **N**avier-**S**tokes equations

- Many more acronyms between **RANS/URANS** and **SRS** simulations.
- Some of the acronyms are used only to differentiate approaches used in commercial solvers.

PANS, **SAS**, **RSM**, **EARSM**, **PITM**, **SBES, ELES**

SRS
Scale-**R**esolving **S**imulations

DES
Detached **E**ddy **S**imulations

LES
Large **E**ddy **S**imulations

DNS
Direct **N**umerical **S**imulations

Increasing computational cost

Increasing modelling and mathematical complexity

It is time to focus our attention on these approaches

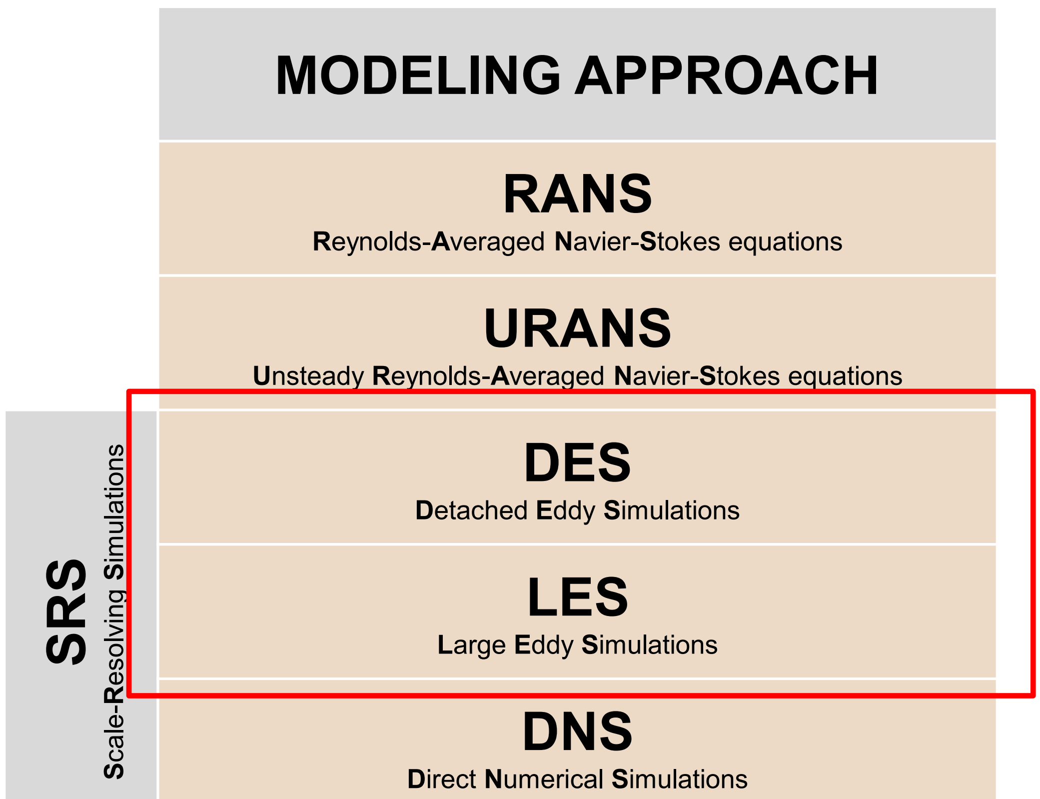
SRS simulations – Scale-resolving simulations

- We have seen so far that DNS requires no mathematical modeling.
- In theory, it is the simplest of the approaches to deal with turbulence.
- The problem relies in the fact that very fine meshes and small time-steps are required to properly solve the turbulent scales.
- Make no mistake, if you run a simulation in laminar mode (with no turbulence models), you will get a solution, but unless you are using an extremely fine mesh, the results will be highly over or under predicted.

	MODELING APPROACH
	RANS **R**eynolds-**A**veraged **N**avier-**S**tokes equations
	URANS **U**nsteady **R**eynolds-**A**veraged **N**avier-**S**tokes equations
SRS **S**cale-**R**esolving **S**imulations	**DES** **D**etached **E**ddy **S**imulations
	LES **L**arge **E**ddy **S**imulations
	DNS **D**irect **N**umerical **S**imulations

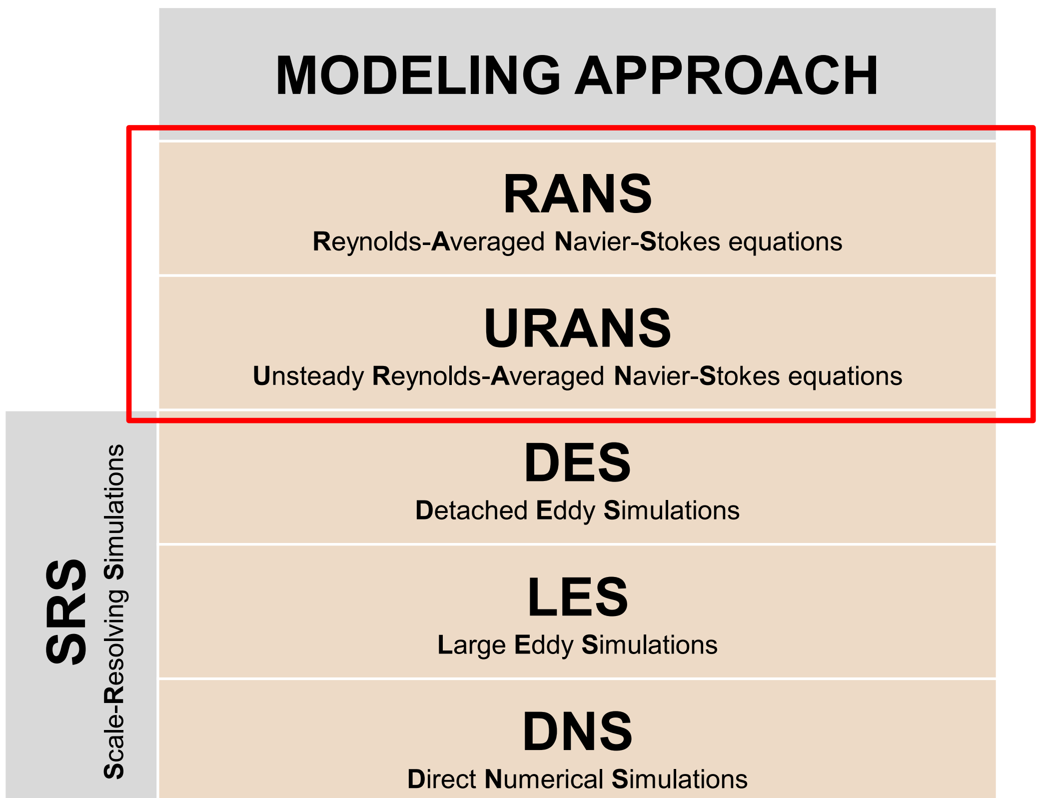
SRS simulations – Scale-resolving simulations

- LES/DES simulations are midway DNS and RANS.
- They are much affordable than DNS, but they still they require large computational resources and low dissipative numerical methods.
- In LES/DES simulations the large scales are fully resolved with the mesh and a small amount of turbulent viscosity is added to model the scales smaller than the local cell size.
- In LES/DES simulations, the mesh resolution determines the fraction of the energy spectrum directly resolved.



SRS simulations – Scale-resolving simulations

- RANS/URANS simulations are very affordable and very reliable (if good standard practices are followed).
- You can use RANS/URANS models with 2D and 3D cases, and steady and unsteady solvers.
- Using RANS/URANS turbulence models all scales are modeled.
- You can use RANS/URANS solutions as starting point for LES/DES simulations.
- The workhorse in CFD is RANS/URANS.



SRS simulations – Scale-resolving simulations

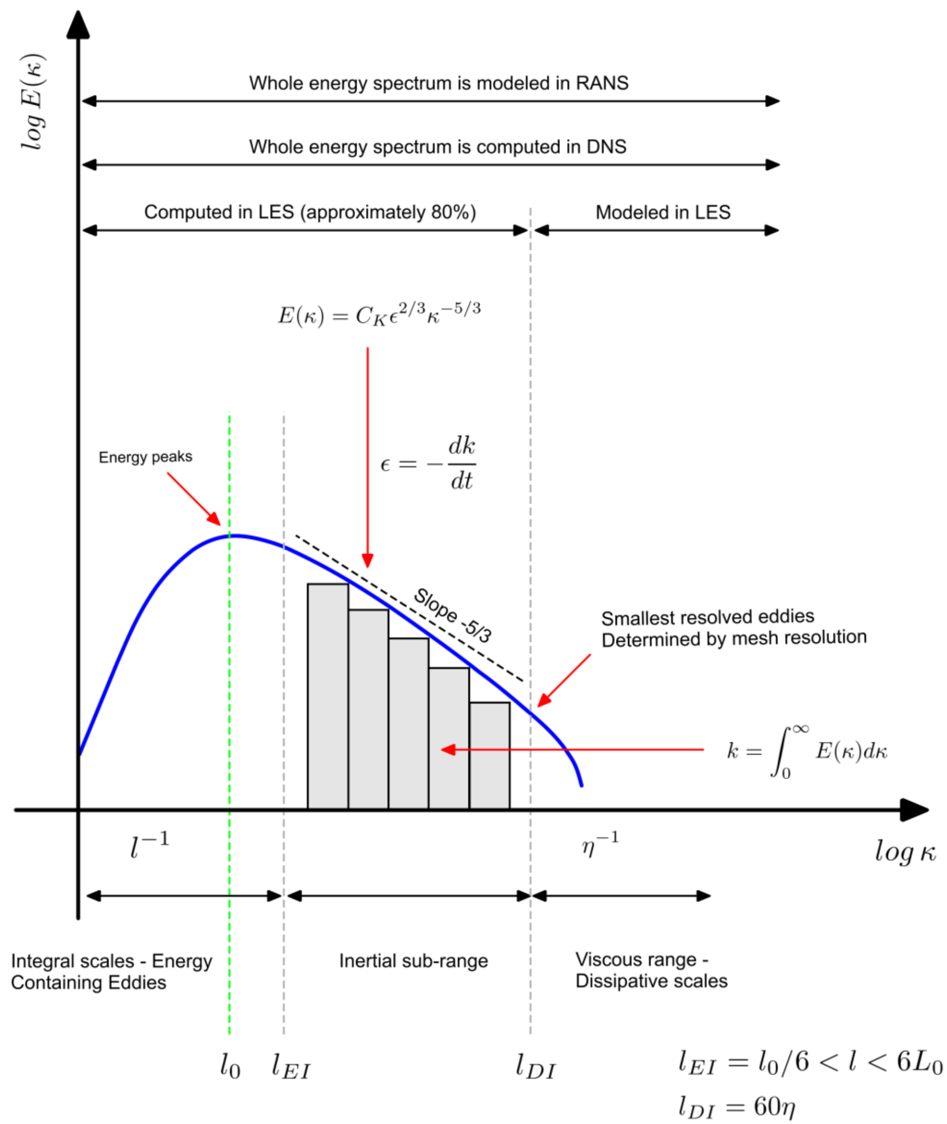
- Scale-resolving simulations or SRS, aim at resolving all or most of the scales in space and time.
- <u>SRS simulations are intrinsically three-dimensional and unsteady.</u>
    - Therefore, the meshing requirements are much larger than those for RANS/URANS simulations.
    - Also, the time-step requirements are more stringent.

- SRS simulations requires good meshes, accurate and robust numerical schemes, and CFL number requirements less than 1 for good accuracy.
    - We must minimize the numerical diffusion due to mesh resolution and numerical discretization.

- Sometimes, the two-dimensional approximation can be taken in SRS, but do it with a lot of care.
- The most well-known SRS approaches are LES (large eddy simulations) and DES (detached eddy simulations).
- DNS simulations also belong to the group of SRS methods.
- DNS simulations do not use any models.
    - They directly resolve all scales in space and time.

SRS simulations – Scale-resolving simulations

- In LES and DES simulations, the large scales are resolved.
- Then, the smallest scales are filtered (or modeled as in RANS/URANS).
- Therefore, the mesh resolution determines the fraction of the energy spectrum directly resolved.
- In a DNS simulation, the whole spectrum is resolved.
- In a good LES simulation, approximately 80% of the spectrum is resolved.
- In a URANS simulation, the whole spectrum is modeled.
- The turbulent power spectrum shown in the figure, represents the distribution of the turbulent kinetic energy k across the various length scales.
- It is a direct indication of how energy is dissipated with eddies size.
- Remember, this plot is local.

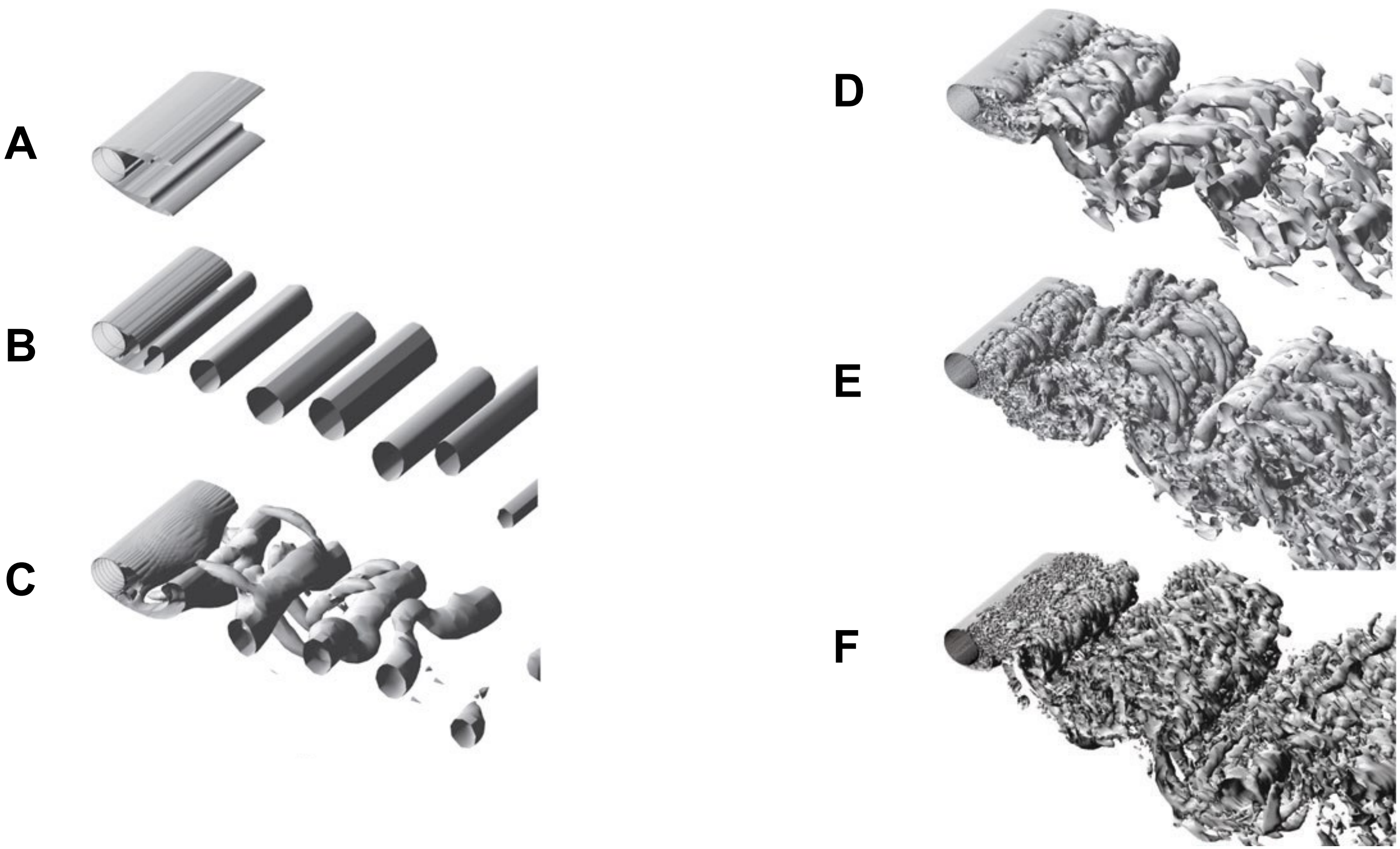


SRS simulations – Scale-resolving simulations

- In LES/DES simulations we aim at resolving a good percentage of the turbulence energy spectrum, something between 50% and 80%.
    - When we resolve 50% of the turbulence energy spectrum, we talk about VLES (very large LES).
    - We should always aim for at least 80% of the turbulence energy spectrum.
- For the small scales, simple models are introduced.
    - As for RANS/URANS, most of these models are based on the Boussinesq hypothesis and the gradient diffusion hypothesis.
- LES/DES simulations are much more costly than RANS/URANS simulations.
- And LES simulations are more costly than DES simulations.
- In general, LES simulations are not very practical for most engineering applications.
    - They require a lot of computational resources.
- LES/DES simulations can be wall resolving or wall modelling.
    - Obviously, wall resolving LES/DES simulations have larger computational requirements.
- Remember, in RANS/URANS simulations all scales are modeled.
    - This is the main difference between SRS simulations and RANS/URANS approaches.

SRS simulations – Scale-resolving simulations

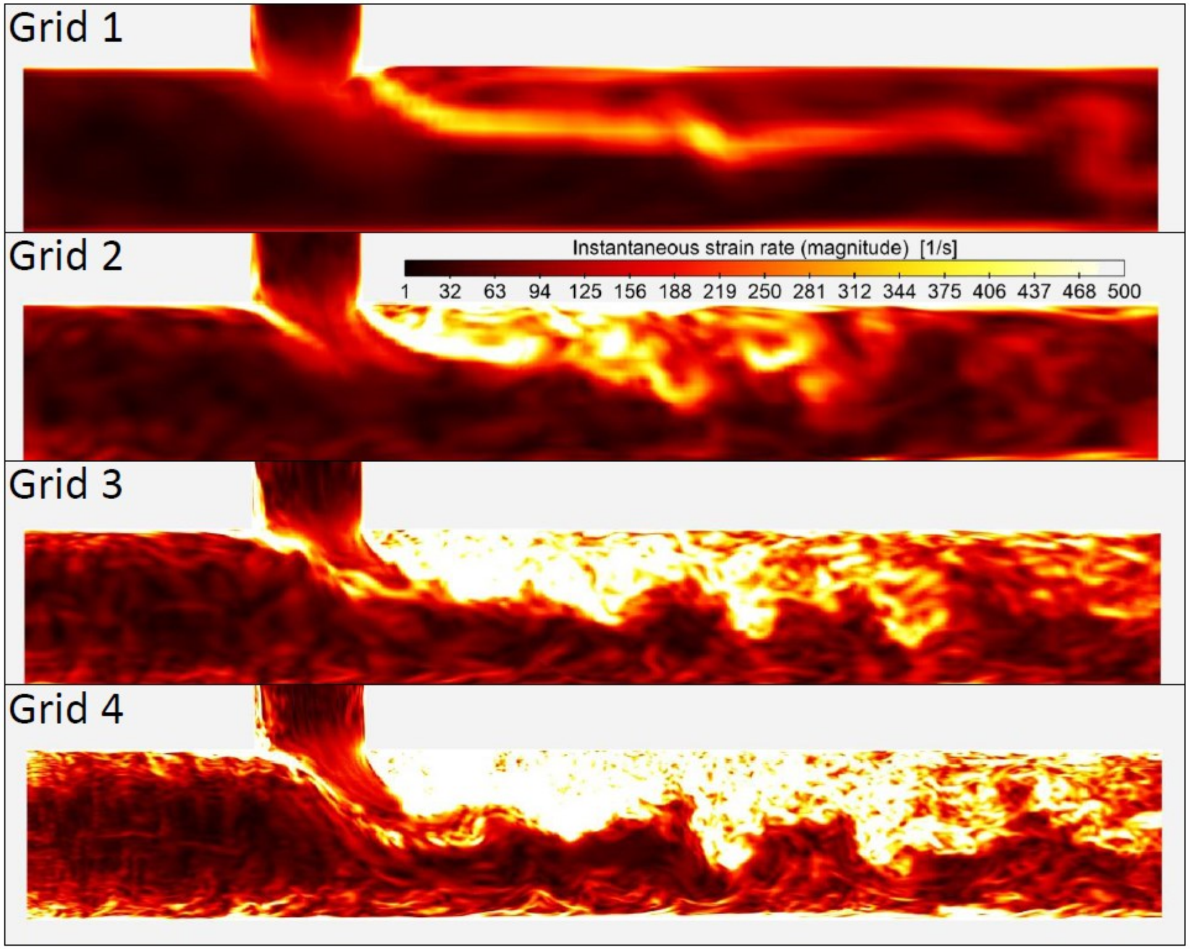
- Simulation results for flow over a cylinder (vorticity isosurfaces).
- Turbulence is modeled as (a) shear-stress-transport (SST) steady RANS. (b) 2D SST URANS. (c) 3D SST URANS. Spalart-Allmaras DES on a (d) coarse grid and a (e) fine grid/ (f) SST DES on a fine grid [1].



[1] P. Spalart. Detached-eddy simulation. Annual Review of Fluid Mechanics, 41:181-202, 2009.

SRS simulations – Scale-resolving simulations

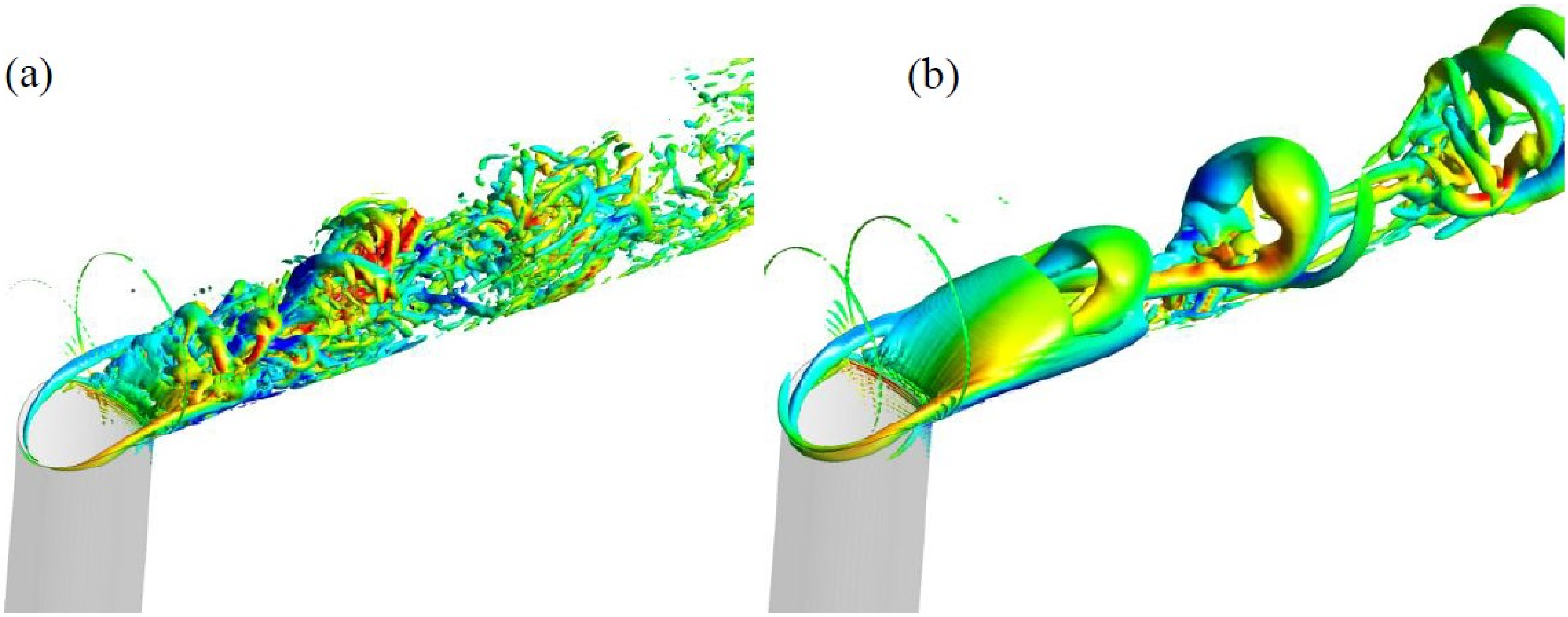
- Influence of mesh density on the turbulent flow structures in SRS LES simulations [1].



[1] J. Lavedrine. Impact of grid refinement on SRS LES calculation. Version 1.1. Ansys France, 08/2009.

SRS simulations – Scale-resolving simulations

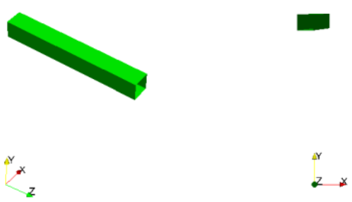
- Influence of the numerical discretization scheme on the turbulent flow structures in SRS LES simulations. (a) Central differences schemes. (b) Bounded central differences scheme [1].



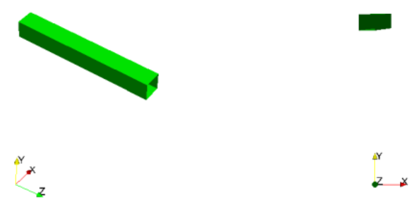
[1] F. Menter. Best Practice: Scale-Resolving Simulations in ANSYS CFD. Version 1.02. Ansys Germany, 2012.

SRS simulations – Scale-resolving simulations

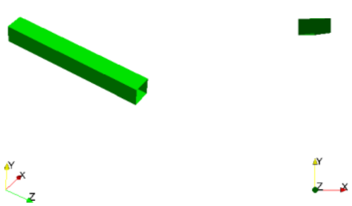
Vortex shedding past square cylinder – Vortices visualized by Q-criterion



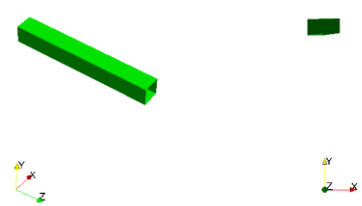
URANS (K-Omega SST with no wall functions)
www.wolfdynamics.com/wiki/squarecil/urans2.gif



LES (Smagorinsky)
www.wolfdynamics.com/wiki/squarecil/les.gif



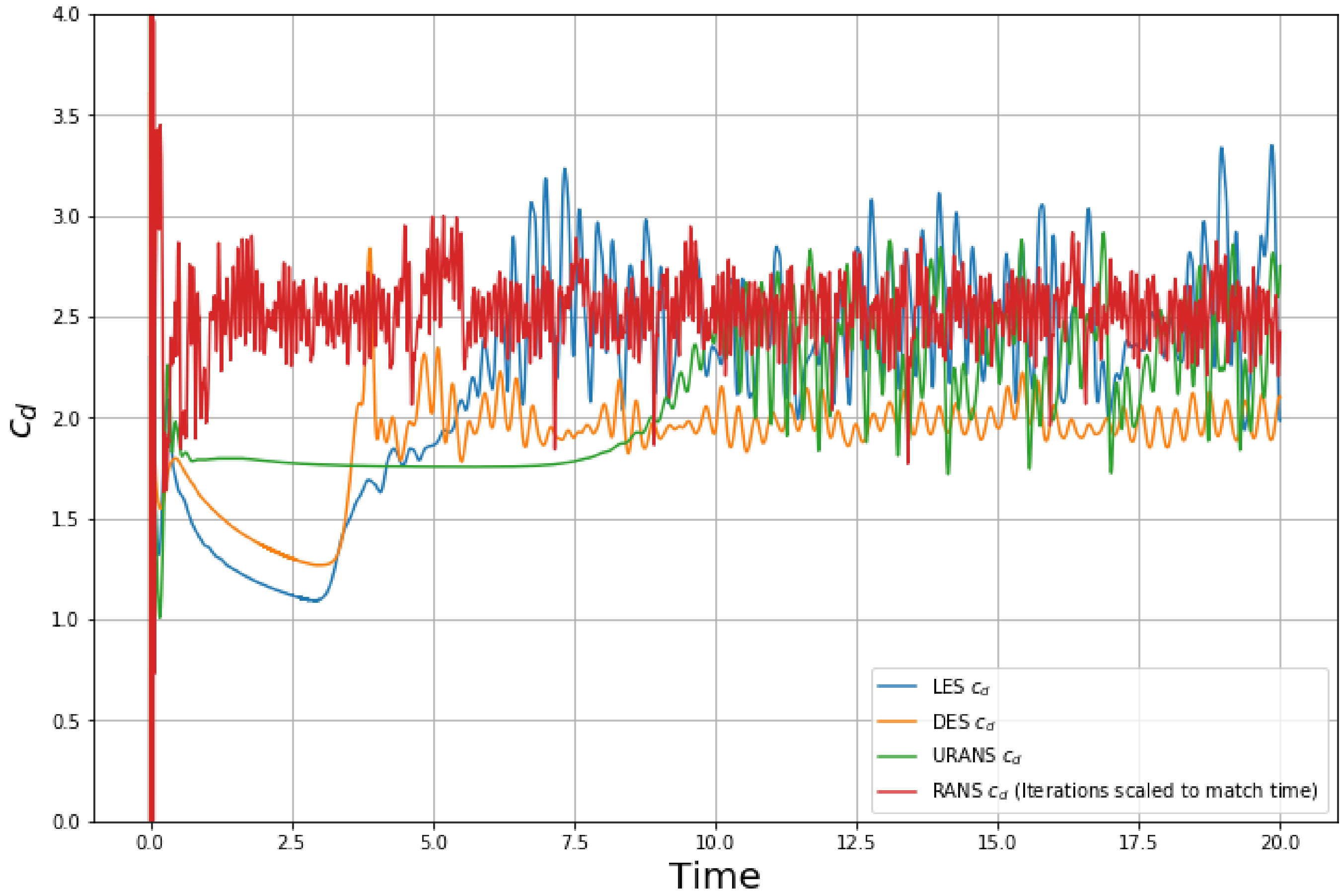
Laminar (no turbulence model or DNS)
www.wolfdynamics.com/wiki/squarecil/laminar.gif



DES (Spalart-Allmaras DDES)
www.wolfdynamics.com/wiki/squarecil/des.gif

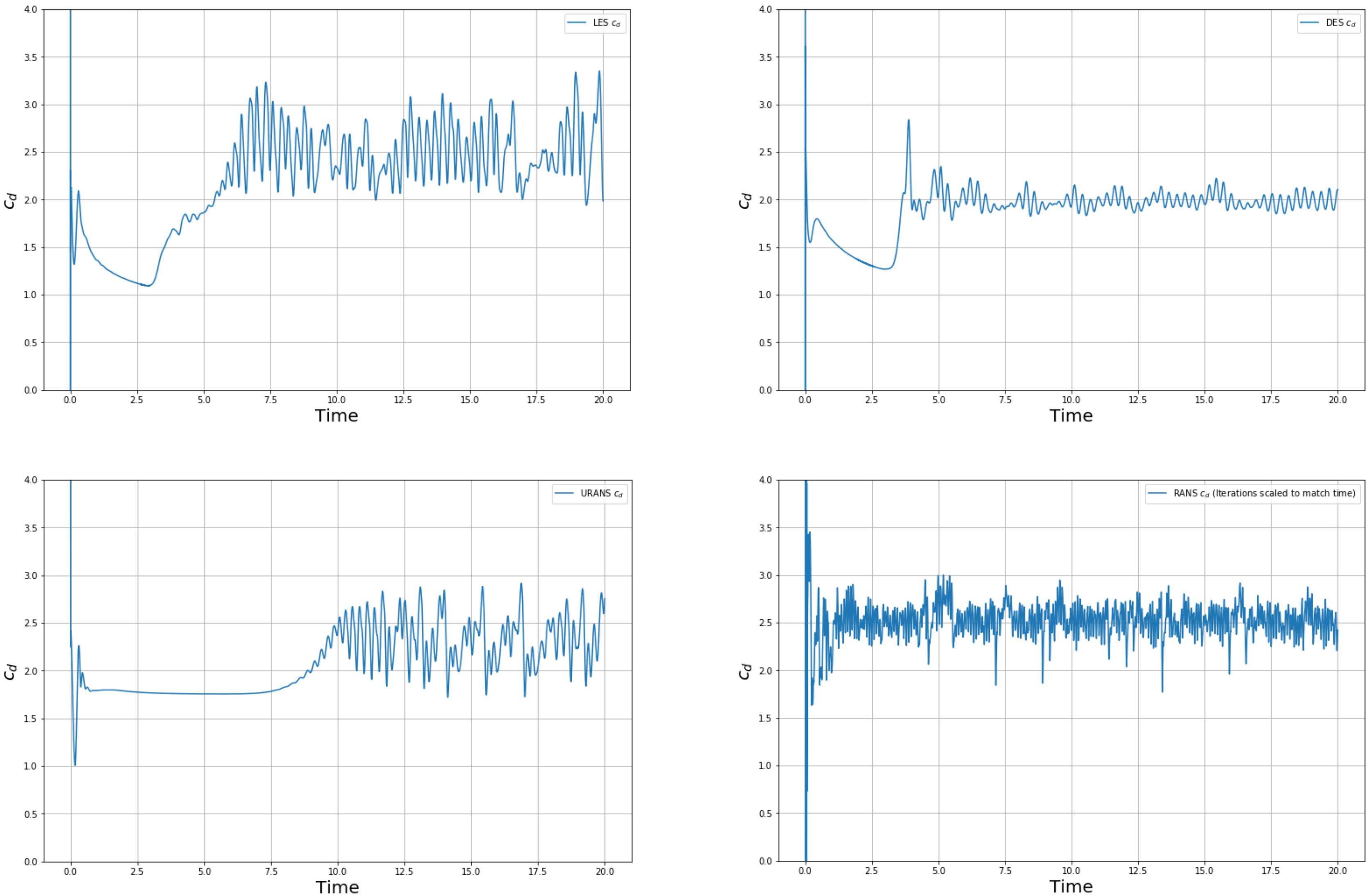
SRS simulations – Scale-resolving simulations

Vortex shedding past square cylinder – Drag coefficient signal



SRS simulations – Scale-resolving simulations

Vortex shedding past square cylinder – Drag coefficient signal



SRS simulations – Scale-resolving simulations

- LES simulations are about:
  - Resolving the turbulent motion in space and time by using fine meshes and small time-steps.
  - Where we aim at modeling only a small portion of the turbulent spectrum, about 20% or less.
  - We also need to use low dissipative discretization schemes (in space and time).
  - LES simulations are also about computing your unsteady statistics and analyzing time series.

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LES equations – Filtered Navier-Stokes equations

- In LES simulations, the smallest scales need to be modeled (as in RANS/URANS).
- Therefore, we need to somehow remove or filter the smallest scales of the instantaneous field variables.
- In LES, we use a similar approach to the Reynolds decomposition, but we call it LES decomposition (or filtering decomposition),

$$\phi(\mathbf{x},t) = \tilde{\phi}(\mathbf{x},t) + \phi'(\mathbf{x},t)$$

- Where the tilde represents the filtered quantity, and the prime represents the unresolved field.
- In the literature, most of the times the tilde is used to denote the filtered quantity.
- Hereafter, and just to simplify the typesetting and avoid confusion with the Favre average, we will use an overbar to denote the filtered quantity in the context of LES/DES simulations,

$$\phi(\mathbf{x},t) = \bar{\phi}(\mathbf{x},t) + \phi'(\mathbf{x},t)$$

LES equations – Filtered Navier-Stokes equations

- In LES, to remove the small scales we use a filter in space.
- You can see this operation as a rolling average.
- This filtered quantity represents the resolved scales (grid scales).
- Whereas, in RANS/URANS we use a time averaging to remove the fluctuations.
- This is the main difference between the techniques used to remove the fluctuations of small scales.
- By the way, these two concepts (filtering and time average) appear to be similar, but they are not. In fact, the rules used are different.
- At the end of the day, the instantaneous field can be decomposed as follows (LES decomposition),

Small scales, residual quantity, or unresolved fields
Sub-grid scales SGS

$$\phi(\mathbf{x},t) = \bar{\phi}(\mathbf{x},t) + \phi'(\mathbf{x},t)$$

Filtered quantity or resolved field
Grid scales GS

LES equations – Filtered Navier-Stokes equations

- The derivation of the filtered incompressible Navier-Stokes equations (FNS) is somehow similar to the derivation of the incompressible RANS equations.
- The main difference is that instead of using the Reynolds decomposition, we use the LES decomposition (first introduced by Deardoff [1]),

$$\mathbf{u}(\mathbf{x},t) = \bar{\mathbf{u}}(\mathbf{x},t) + \mathbf{u}'(\mathbf{x},t)$$

$$p(\mathbf{x},t) = \bar{p}(\mathbf{x},t) + p'(\mathbf{x},t)$$

- Remember, the overbar represents the filtered quantity.
- The prime symbol represents the unresolved quantity (or residual).
- The LES decomposition uses local spatial filter (or in the simplest case, spatial average).
- This is the main difference between the LES and Reynolds decomposition (which uses time averaging).

[1] J. W. Deardoff. A numerical study of three-dimensional turbulent channel flow at large Reynolds number, J. Fluid Mech., 41, 453, 1970.

LES equations – Filtered Navier-Stokes equations

- As for the derivation of the RANS equations, we should be aware of a few filtering properties used when deriving the FNS.

$$\bar{\bar{\phi}} \neq \bar{\phi}$$

$$\overline{\phi'} \neq 0$$

$$\overline{\phi\psi} \neq \bar{\phi}\bar{\psi}$$

$$\overline{\phi + \psi} = \bar{\phi} + \bar{\psi}$$

The operator is linear

$$\overline{\frac{\partial \phi}{\partial t}} = \frac{\partial \bar{\phi}}{\partial t}$$

$$\overline{\frac{\partial \phi}{\partial x}} = \frac{\partial \bar{\phi}}{\partial x}$$

The differentiation operator commutes

- Remember, the overbar represents a spatial filter.

LES equations – Filtered Navier-Stokes equations

- To derive the filtered incompressible Navier-Stokes equations (FNS), we apply the filtering operator directly to the primitive variables.
- After some algebra, we arrive to the FNS equations,

$$\nabla \cdot (\bar{\mathbf{u}}) = 0$$

$$\frac{\partial \bar{\mathbf{u}}}{\partial t} + \nabla \cdot (\bar{\mathbf{u}}\bar{\mathbf{u}}) = \frac{-\nabla \bar{p}}{\rho} + \nu \nabla^2 \bar{\mathbf{u}} + \nabla \cdot \tau^{SGS}$$

$$\bar{\mathbf{u}}\bar{\mathbf{u}} - \overline{\mathbf{u}\mathbf{u}}$$

- As you can see, the FNS equations are very similar to the RANS equations.
- The main different is that all variables are filtered in space and the appearance of the sub-grid scale stress tensor τ^{SGS}.
- And as for the RANS/URANS equations, this apparent stress tensor requires modeling.
- To derive the compressible LES equations, we proceed in a similar way, but we use mass-weighted averaging.
- Unfortunately, we cannot say that the derivation is straightforward.

LES equations – Filtered Navier-Stokes equations

- The sub-grid scale stress tensor τ^{SGS} can be further decomposed as follows,

$$\tau^{SGS} = \underbrace{\left(\overline{\bar{\mathbf{u}}\bar{\mathbf{u}}} - \bar{\mathbf{u}}\bar{\mathbf{u}}\right)}_{\mathbf{L}} + \underbrace{\left(\overline{\bar{\mathbf{u}}\mathbf{u}'} + \overline{\mathbf{u}'\bar{\mathbf{u}}}\right)}_{\mathbf{C}} + \underbrace{\overline{\mathbf{u}'\mathbf{u}'}}_{\mathbf{R}} = \mathbf{L} + \mathbf{C} + \mathbf{R}$$

- This is known as the triple decomposition, and it accounts for the interaction of the resolved scales and the small scales.
- In this definition, **L** is called the Leonard stresses, **C** is the called the cross-stress term, and **R** is called the sub-grid scale Reynolds stress (equivalent to the Reynolds stress tensor).
- The Leonard stresses (**L**) involves only the resolved quantities, and therefore it can be computed.
- The cross-term stresses (**C**) and SGS Reynolds stresses (**R**), they both involve unresolved scales and must be modeled.
- The cross-term stress represents the interaction of resolved and unresolved scales, whereas the SGS Reynolds stress represents the interaction of unresolved scales.
- At this point, the problem is how to model the cross-term stress and the sub-grid scale Reynolds stress.

LES equations – Filtered Navier-Stokes equations

- It is important to mention that the decomposition of the sub-grid scale stress tensor τ^{SGS} is not unique.

$$\tau^{SGS} = \underbrace{(\overline{\bar{\mathbf{u}}\bar{\mathbf{u}}} - \bar{\mathbf{u}}\bar{\mathbf{u}})}_{\mathbf{L}} + \underbrace{\left(\overline{\bar{\mathbf{u}}\mathbf{u}'} + \overline{\mathbf{u}'\bar{\mathbf{u}}}\right)}_{\mathbf{C}} + \underbrace{\overline{\mathbf{u}'\mathbf{u}'}}_{\mathbf{R}} = \mathbf{L} + \mathbf{C} + \mathbf{R}$$

- In this case we used the triple decomposition or Leonard decomposition.
- Also, this decomposition is not Galilean invariant (i.e., the solution is not the same in every inertial frame).
- Germano [1], proposed a modification to make this decomposition Galilean invariant,

$$\tau^{SGS} = L_{ij}^{m} + C_{ij}^{m} + R_{ij}^{m}$$

- Where the superscript m indicates the modified stresses.

[1] M. Germano. A proposal for a redefinition of the turbulent stresses in the filtered Navier-Stokes equations. Phys. Fluids, 29(7). 1986.

LES equations – Filtered Navier-Stokes equations

- The modified stresses can be written as follows,

$$L_{ij}^m = \overline{\bar{u}_i \bar{u}_j} - \bar{\bar{u}}_i \bar{\bar{u}}_j$$

$$C_{ij}^m = \overline{\bar{u}_i u_j'} + \overline{u_i' \bar{u}_j} - \left(\bar{\bar{u}}_i \bar{u}_j' + \bar{u}_i' \bar{\bar{u}}_j \right)$$

$$R_{ij}^m = \overline{u_i' u_j'} - \bar{u}_i' \bar{u}_j'$$

- The modified Leonard stress L_{ij}^m is determined with the filtered grid-scale velocity, but the evaluation of the modified cross-term stresses C_{ij}^m and modified SGS stresses R_{ij}^m requires the use of models.
- The difference between L_{ij} and L_{ij}^m is,

$$B_{ij} = L_{ij}^m - L_{ij} = \bar{u}_i \bar{u}_j - \bar{\bar{u}}_i \bar{\bar{u}}_j$$

- This term is known as the scale-similarity term [1] and is used in scale-similarity models, such as the one we just introduced.

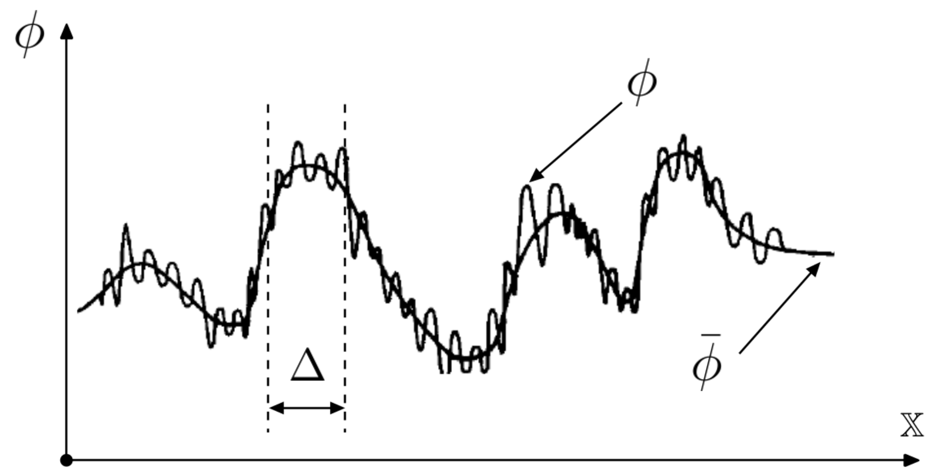
[1] J. Bardina, J. Ferziger, W. Reynolds. Improved subgrid scale models for large eddy simulations. AIAA Paper 80-1357. 1980.

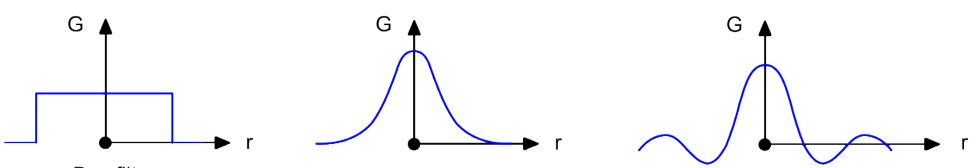
LES equations – Filtered Navier-Stokes equations

- In the appendix, you will find an extended derivation of the filtered Navier-Stokes equations and the expansion of the non-linear term $\overline{\mathbf{uu}}$ using the triple decomposition (or Leonard decomposition).

LES equations – Filtered Navier-Stokes equations

- In LES models, the governing equations need to be filtered (local spatial filter).
- You can see these filters as a rolling average used to filter fluctuations.
- In the figure below, you can see the effect of filtering a signal and three commons filter kernels.
- The local spatial filtering operation simple consist in removing the very small fluctuations.
- Different filters have different properties.





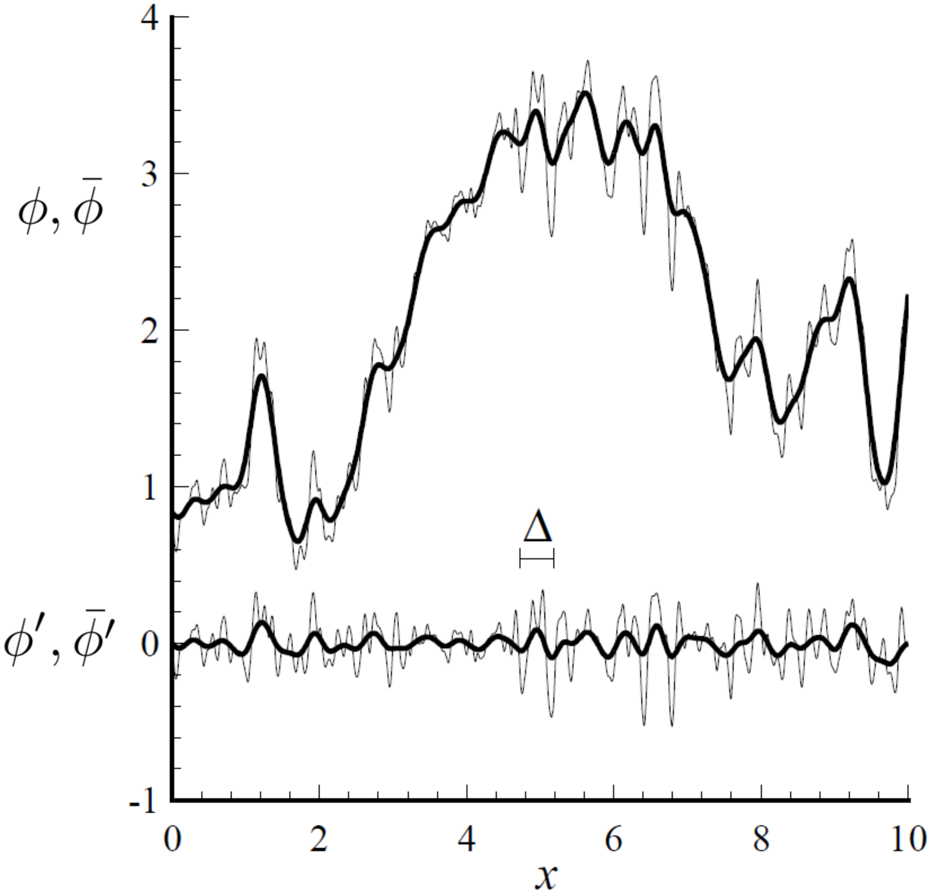
Box filter

Gaussian filter

Sharp spectral filter

References:
S. Pope. Turbulent Flows. Cambridge University Press. 2014.

LES equations – Filtered Navier-Stokes equations



- In the figure, the upper thin line represents the sampled velocity and the bold line the filtered velocity using a Gaussian filter.

Filter function

$$\bar{\phi}(\mathbf{x}, t) = \int G(r, \mathbf{x})\mathbf{u}(\mathbf{x} - r, t)dr$$

- In the figure, the lower thin line represents the field residual (fluctuations) and the bold line the filtered field residual.

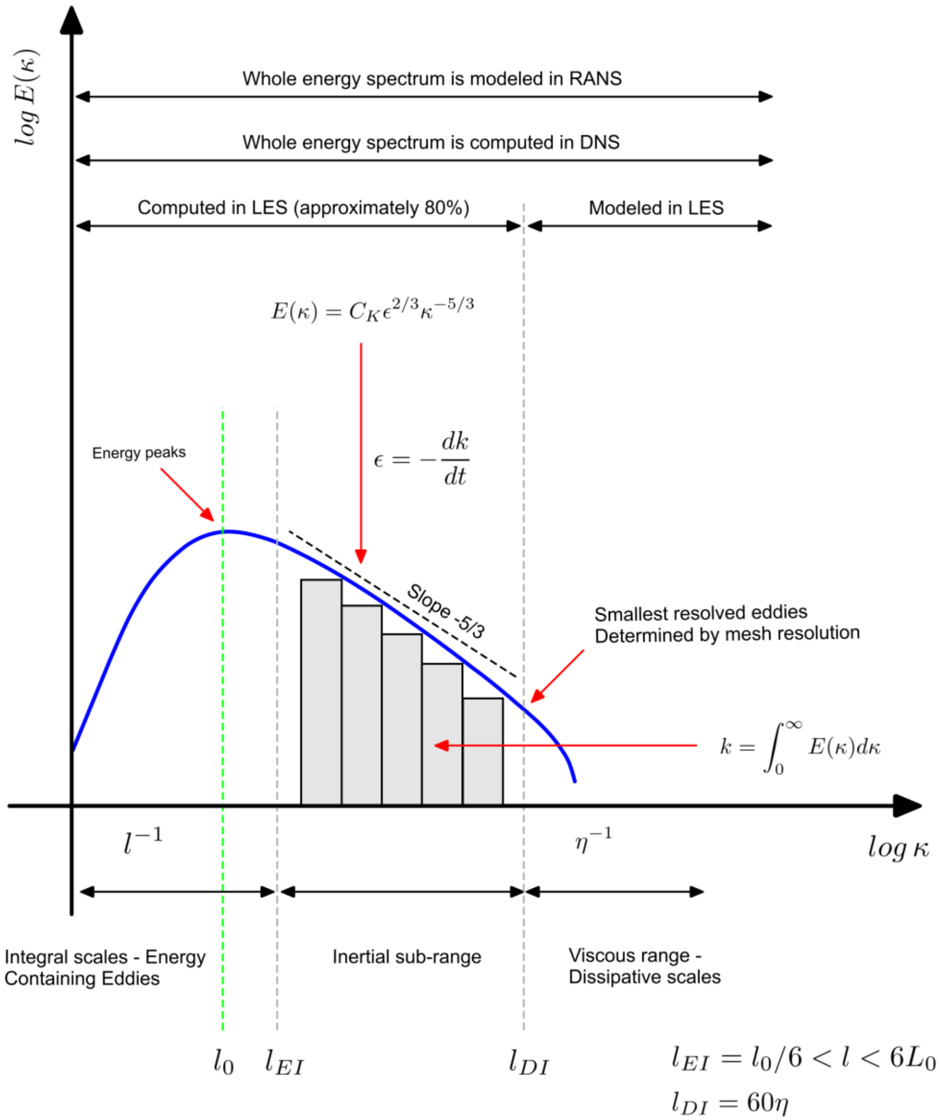
$$\phi'(\mathbf{x}, t) = \phi(\mathbf{x}, t) - \bar{\phi}(\mathbf{x}, t)$$

- <u>Remember, the filtering operation is done in space and in every single time-step.</u>

References:
S. Pope. Turbulent Flows. Cambridge University Press. 2014.

LES equations – Filtered Navier-Stokes equations

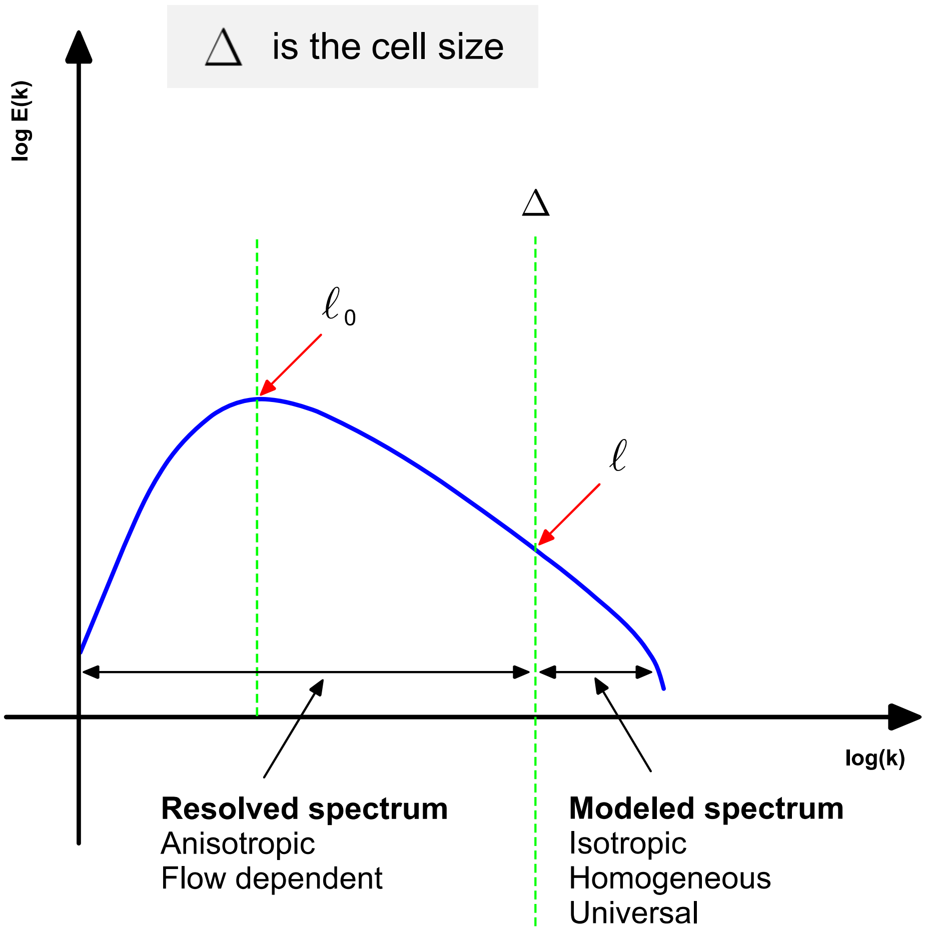
Turbulence energy spectrum



- In LES simulations, we aim at resolving 80% of the turbulence energy spectrum.
- Recall that the turbulent power spectrum represents the distribution of the turbulent kinetic energy across the various length scales.
- It is a direct indication of how energy is dissipated with eddies size.
- The mesh resolution determines the fraction of the energy spectrum directly resolved.
- Remember, the turbulent kinetic energy peaks at integral length scale l_0.
- In SRS simulations, this scale must be sufficiently resolved.

LES equations – Filtered Navier-Stokes equations

Turbulence energy spectrum



- The finer the mesh the less energy that is being modeled.
- The width of the filter function is determined by the local mesh size.
- Many of the filtering functions are designed for uniform hexahedral meshes.
- Therefore, in LES simulations it is highly recommended to use hexahedral meshes with a low growth rate factor (preferably less than 1.1).
- Your goal is to have a mesh fine enough so that it will resolve 80% of the turbulence energy spectrum.