Turbulence and CFD models: Theory and applications

Roadmap to Lecture 10

1. SRS simulations
2. LES equations – Filtered Navier-Stokes equations
3. Sub-grid scale models for LES
4. DES brief review
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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6. Final remarks on LES/DES turbulence models

SRS simulations – Scale-resolving simulations

- Overview of the main turbulence modeling approaches.

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

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

Increasing computational cost

Increasing modelling and mathematical complexity

- It is time to focus our attention on these approaches
- But remember, the workhorse in CFD is RANS/URANS.
- A next step are RSM, ASM, and EARSM models.

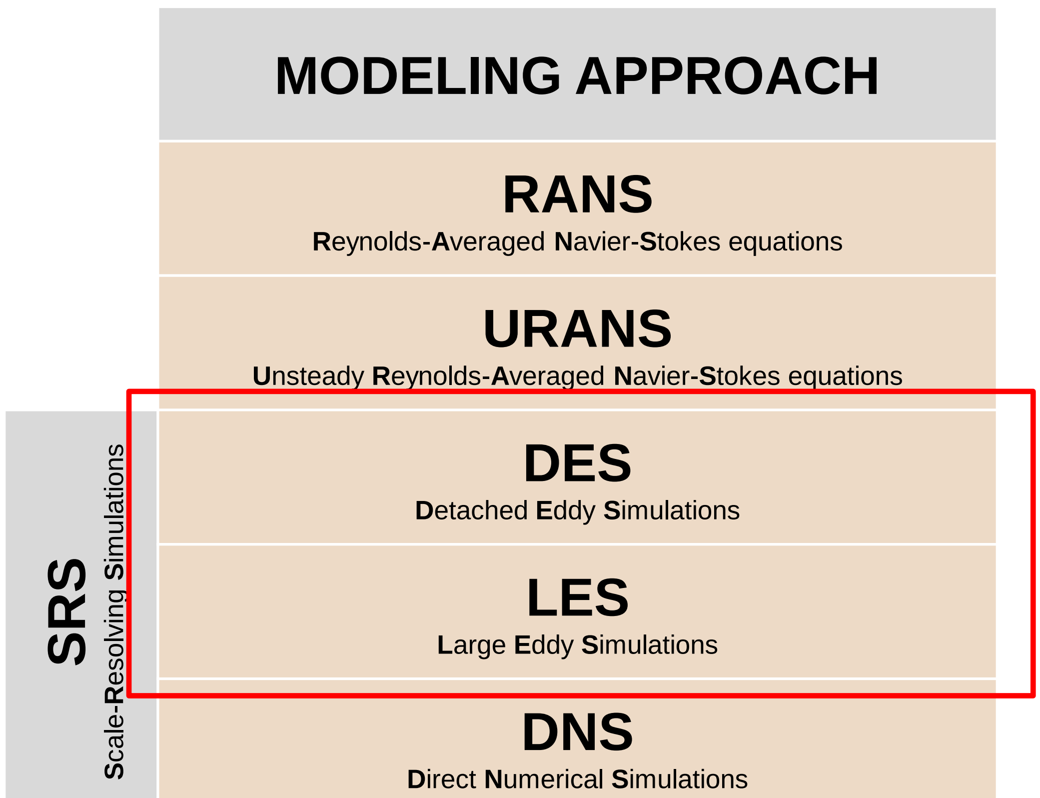
SRS simulations – Scale-resolving simulations

- We have seen so far that DNS requires no mathematical modeling.
- From the theoretical point of view, it is the simplest of the approaches when dealing with turbulence.
- The problem relies in the fact that very fine meshes and small time-steps are required to properly solve all 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/URANS.
- They are much affordable than DNS, but they still 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.

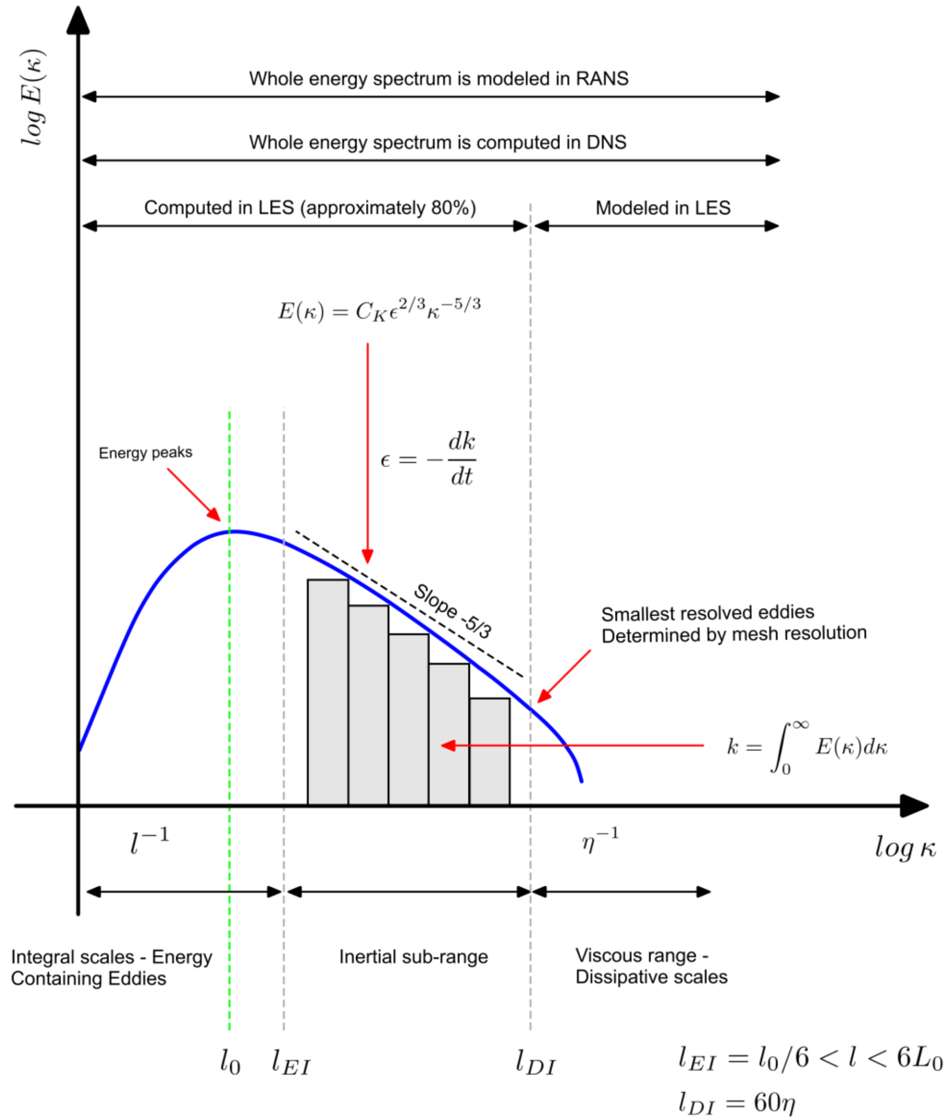
	MODELING APPROACH
	RANS **R**eynolds-**A**veraged **N**avier-**S**tokes equations
	URANS **U**nsteady **R**eynolds-**A**veraged **N**avier-**S**tokes equations
SRS **S**cale-**R**esolving **S**imulations	**DES** **D**etached **E**ddy **S**imulations
	LES **L**arge **E**ddy **S**imulations
	DNS **D**irect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

SRS simulations – Scale-resolving simulations

- 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

Some comments on the resolution of the turbulence energy spectrum

- 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).
  - However, for good accuracy, we should always aim for at least 80% of the turbulence energy spectrum.
- It is not straightforward how to quantify the level of resolution of the turbulence energy spectrum, a lot of metrics need to be measured.
- In a similar way, it is not easy to recognize how much energy is being modeled in LES/DES simulation.
- We must always gather the unsteady statistics of all transported quantities, including those related to the Reynolds stress budget and turbulent kinetic energy budget.
- 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.

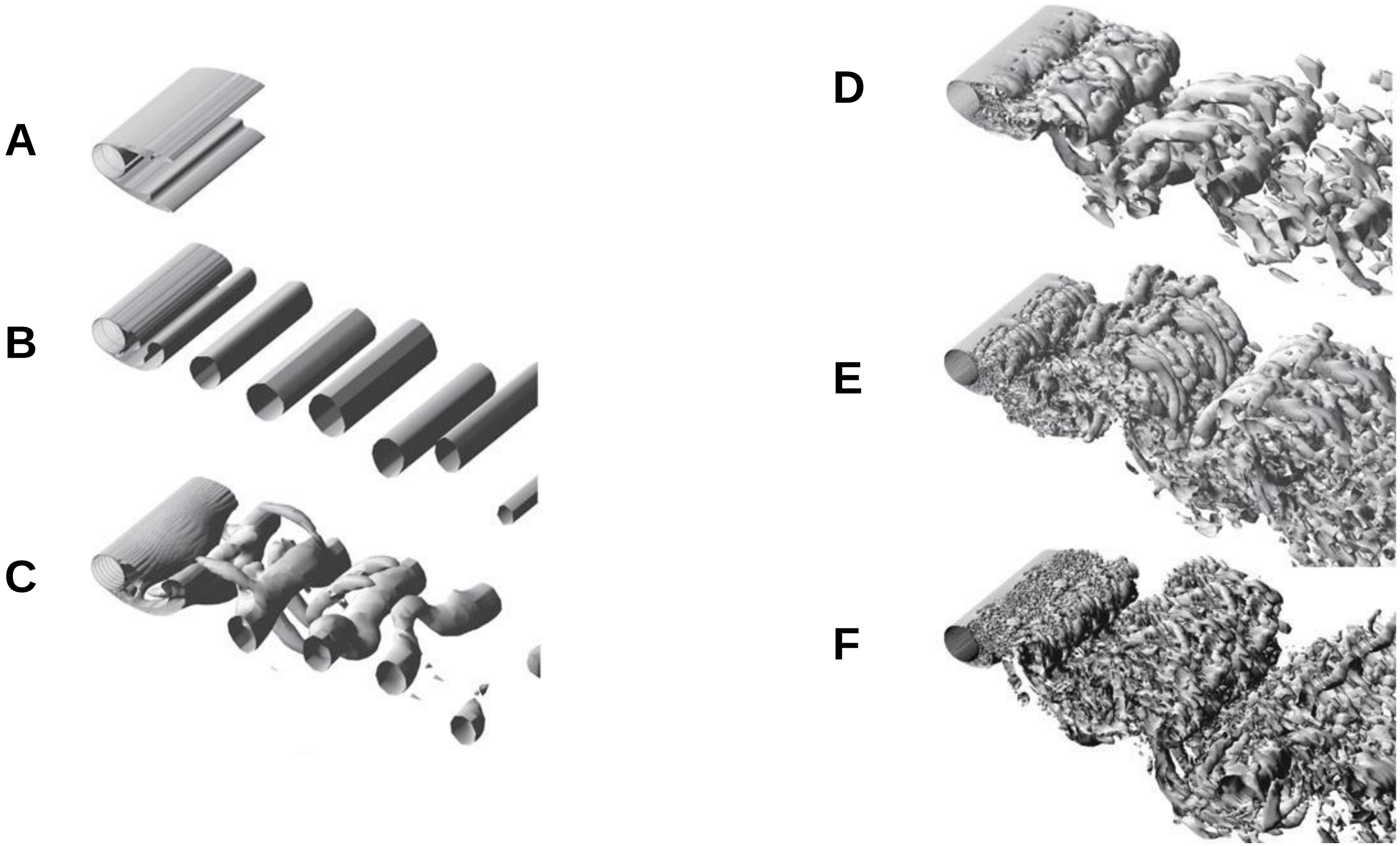
SRS simulations – Scale-resolving simulations

Some final comments on the cost of LES/DES simulations

- 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.
  - And from the practical point of view, it makes no sense conducting wall resolving LES because they are equivalent to DNS.
- 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

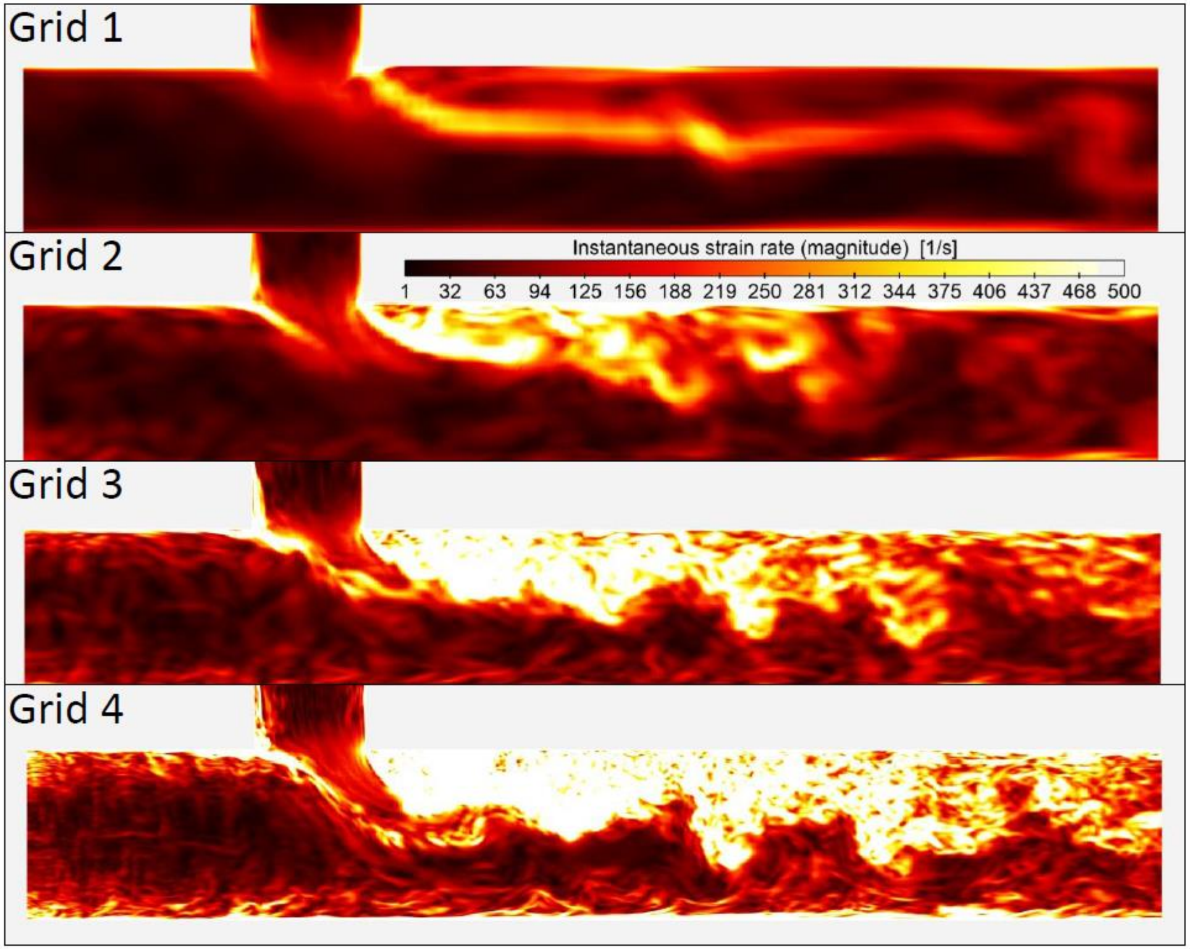
- Simulation results for flow over a cylinder (vorticity isosurfaces).
- Turbulence is modeled as (a) shear-stress-transport (SST) steady RANS. (b) 2D SST URANS. (c) 3D SST URANS. Spalart-Allmaras DES on a (d) coarse grid and a (e) fine grid/ (f) SST DES on a fine grid [1].



References:
[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].

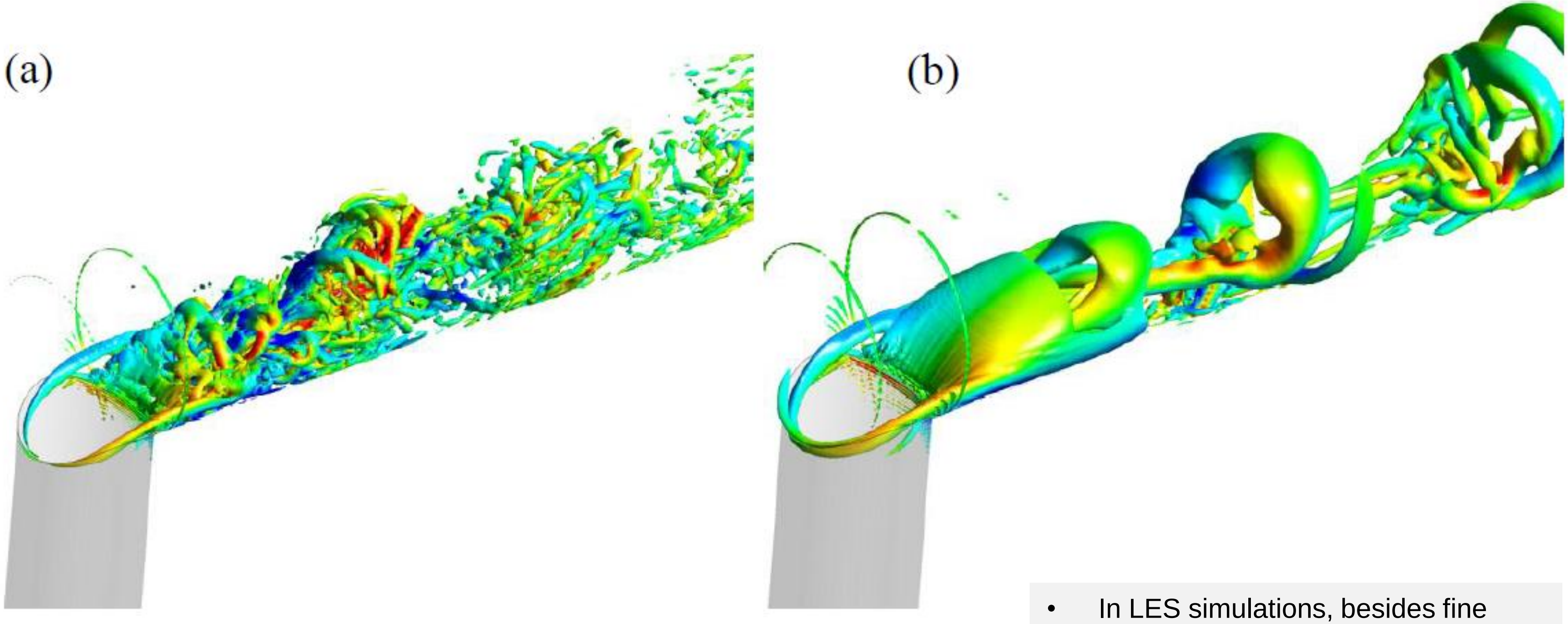


- In LES simulations, as we keep refinement the mesh, we model less and less scales.
- So, in theory, a LES with a very fine mesh is close to a DNS simulation.
- This is not the case with RANS/URANS, even with very fine meshes we always need to model the Reynolds stress tensor.

References:
[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].

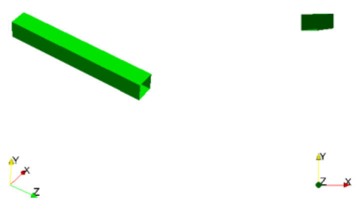


- In LES simulations, besides fine meshes, we need to use low dissipative discretization schemes, in space and time.
- Not every discretization scheme is born with LES in mind.

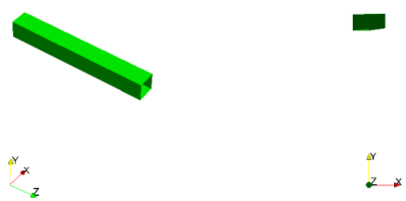
References:
[1] F. Menter. Best Practice: Scale-Resolving Simulations in ANSYS CFD. Version 1.02. Ansys Germany, 2012.

SRS simulations – Scale-resolving simulations

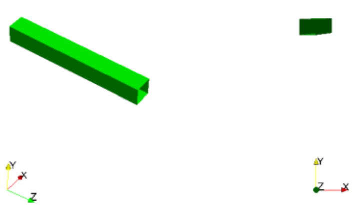
Vortex shedding past square cylinder – Vortices visualized by Q-criterion



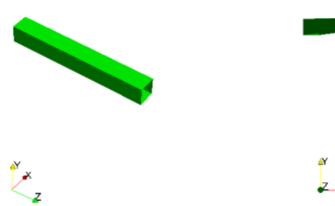
URANS (K-Omega SST with no wall functions)
www.wolfdynamics.com/wiki/squarecil/urans2.gif



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

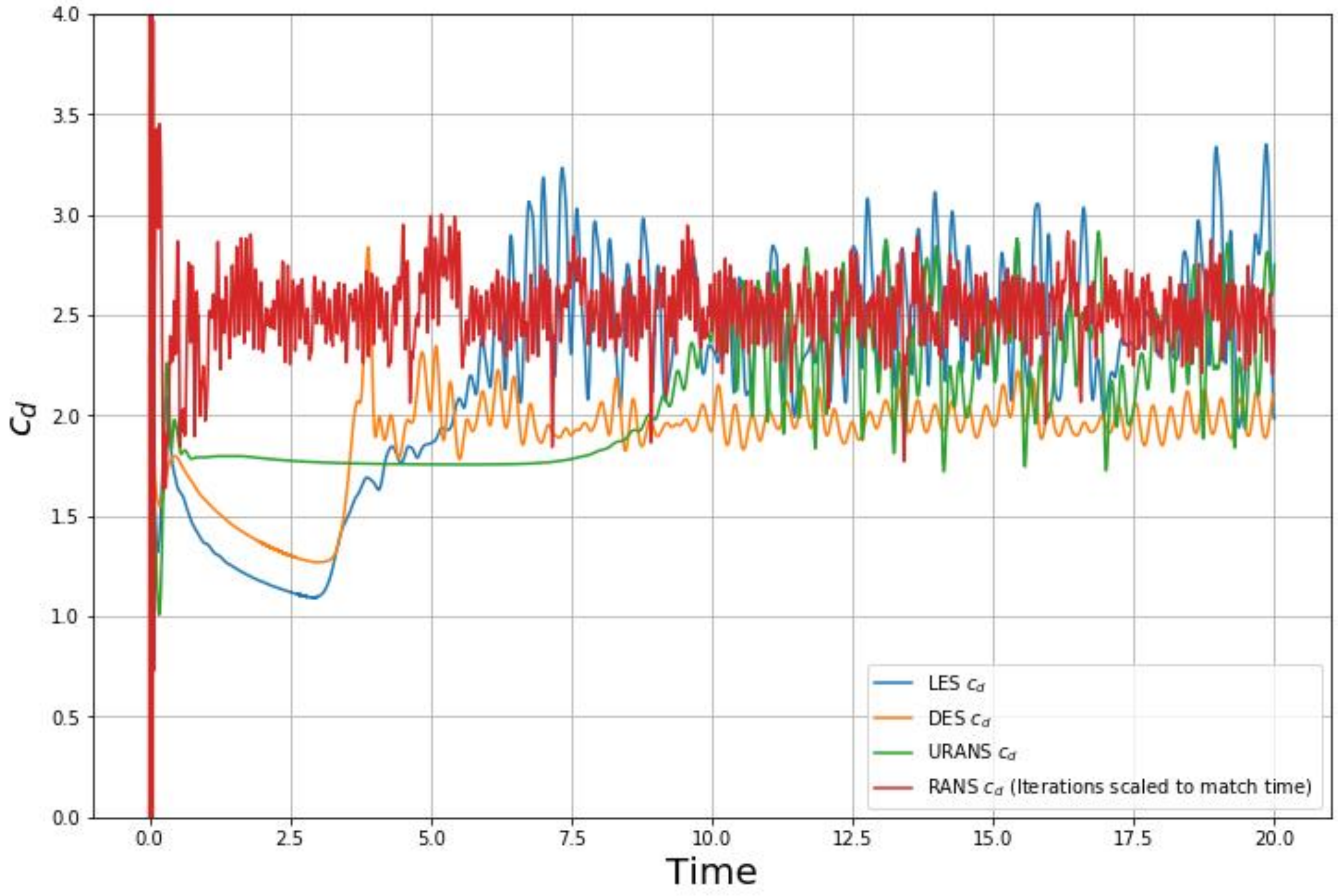


Laminar (no turbulence model or DNS)
www.wolfdynamics.com/wiki/squarecil/laminar.gif



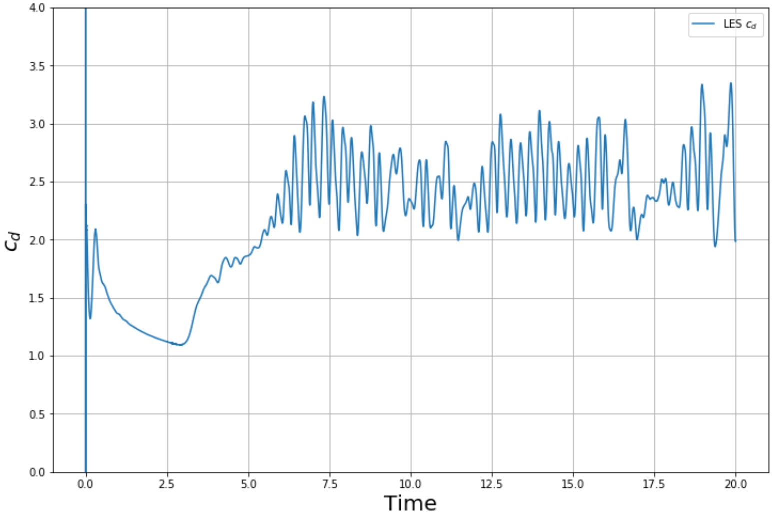
DES (Spalart-Allmaras DDES)
www.wolfdynamics.com/wiki/squarecil/des.gif

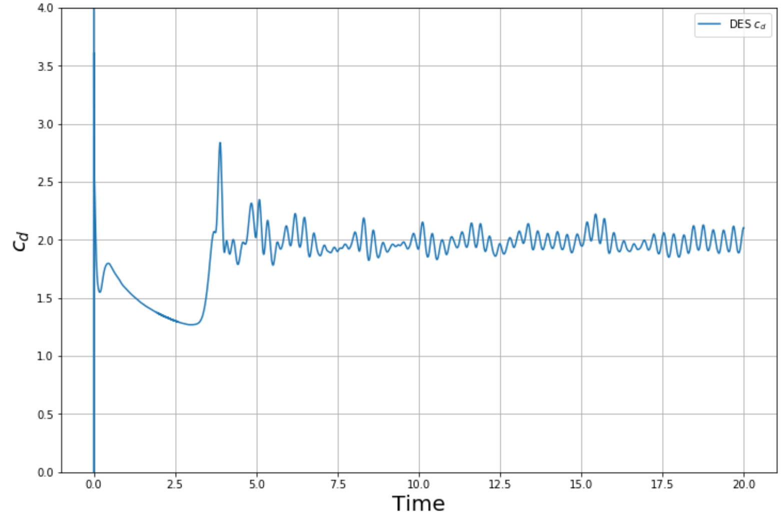
Vortex shedding past square cylinder – Drag coefficient signal

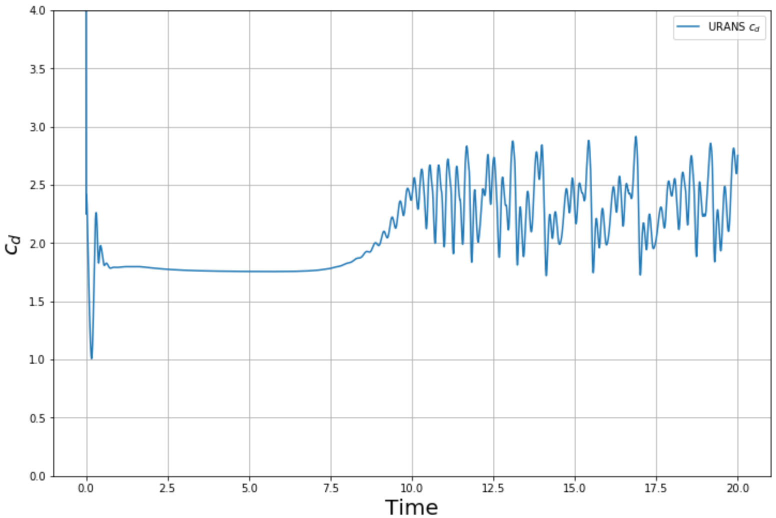


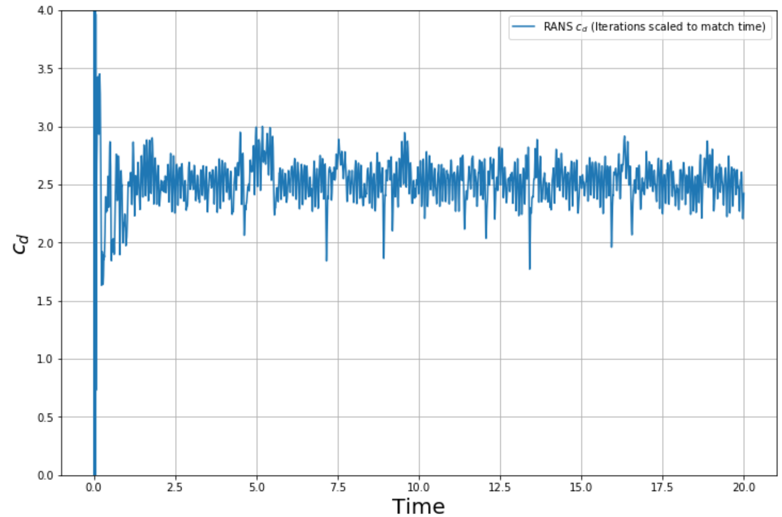
SRS simulations – Scale-resolving simulations

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 simulations, in order to remove the small scales, we use a **filter operation in space**.
- This filter operation in space is very different from the time average used in RANS/URANS.
- We can see the space filtering operation as a rolling average (in physical space).
- The filtered quantities represent the resolved scales or what we can resolve with the mesh (grid scales).
- The main difference between the techniques used to remove the fluctuations contained in the small scales are,
  - LES is filtered in **space**.
  - RANS/URANS is average in **time**.
- These two concepts (filtering and time average) might appear to be similar, but they are not.
- In fact, the averaging/filtering rules used are different.

LES equations – Filtered Navier-Stokes equations

- 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

Instantaneous value

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

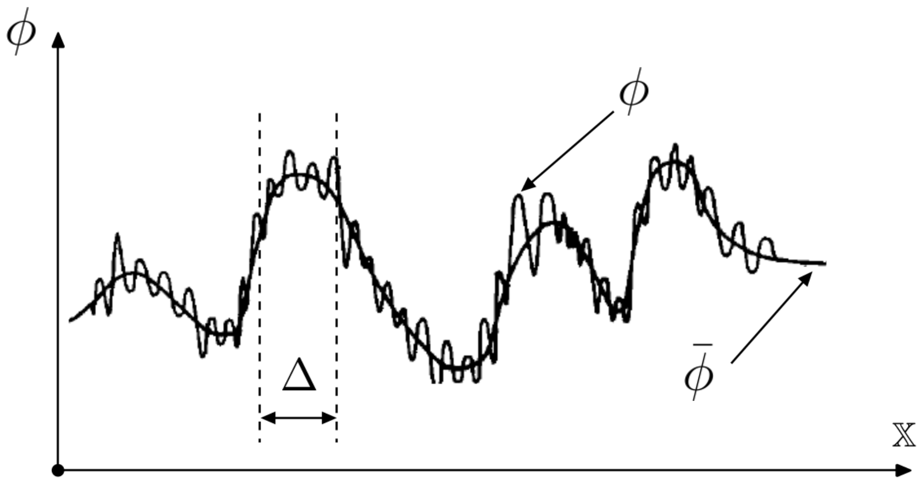
Filtered quantity or resolved field
Grid scales GS

- Note that the whole decomposition is time variant and three-dimensional.
- The filtered quantity already contains fluctuations. That is, the mesh or filter is able to solve the fluctuations.
- And the primed quantity represents the unresolved fields, that is, what is modelled.
- The unresolved fields are related to fluctuations that cannot be resolved with the filter.

LES equations – Filtered Navier-Stokes equations

Representation of the filtering operation in space.

- Representation of the filtering operation in space.
- In the figure below, ϕ represents any field quantity, Δ the filtering operation, and $\mathbb{X}$ is the physical space (x,y,z).
- The filter Δ can be any mathematical operator able to remove the small scales.
- When conducting LES simulations, we use **low-pass filters**.
- Earlier we made the analogy to a rolling average. However, rolling average (which is easy to implement) is not used because it shift the signal after the filtering operation is done.
- As can be seen, the amount of filtering is directly related to the cell size and the filter width, which not necessarily have the same dimension.



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 (probably 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 (which contains fluctuations).
- The prime symbol represents the unresolved quantity (or residual). The fluctuations that cannot be resolved, therefore, the fluctuations that need to be modelled, are contained in this term.
- The LES decomposition uses local low-pass spatial filter (or in the simplest case, spatial average).
- This is the main difference between the LES and Reynolds decomposition (which uses time averaging).

References:
[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.

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

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

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

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

The operator is linear

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

The differentiation operator commutes in time

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

- The differentiation operator commutes.
- Which strictly is not true when filtering.
- It holds when the filter function is homogenous in space. That is, when the cell size is uniform or very close to a uniform distribution.

- Remember, the overbar represents a spatial filter.
- Notice that the filtering properties in the left column are very different from the averaging rules used in RANS/URANS.

LES equations – Filtered Navier-Stokes equations

- Let us derive the filtered Navier-Stokes equations or FNS.
- The first step is to apply the filtering operator directly to the primitive variables.
- By doing so, we obtain the following set of equations,

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

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

Note that the overbar indicates filtering

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

This is a property of the filtering operator

- In this set of equations, we cannot solve the system for both $\bar{\mathbf{u}}$ and $\overline{\mathbf{u}\mathbf{u}}$.
- Therefore, we need to manipulate this set of equations to get a new set of equations expressed only in function of $\bar{\mathbf{u}}$.
- Remember, the overbar indicates filtering.

LES equations – Filtered Navier-Stokes equations

- To express the non-linear term $\overline{\mathbf{u}\mathbf{u}}$ in function of $\bar{\mathbf{u}}$, we can add and subtract the term $\bar{\mathbf{u}}\bar{\mathbf{u}}$ to the left-hand side of the filtered NSE equations.
- By doing so, we obtain the following set of equations,

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

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

- After some algebra, we arrive to the exact filtered Navier-Stokes equations (FNS),

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

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

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

LES equations – Filtered Navier-Stokes equations

- At the end of the day, the FNS equations are written as follows (using vector notation),

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

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

- Where the sub-grid scale stress tensor τ^{SGS} is an apparent stress that arises from the filtering operation and is equivalent to,

$$\tau^{SGS} = -\left(\overline{\mathbf{u}\mathbf{u}} - \bar{\mathbf{u}}\bar{\mathbf{u}}\right)$$

or

$$\tau^{SGS} = \bar{\mathbf{u}}\bar{\mathbf{u}} - \overline{\mathbf{u}\mathbf{u}}$$

LES equations – Filtered Navier-Stokes equations

- The sub-grid scale stress tensor τ^{SGS} arising from the filtering operation, namely,

$$\tau^{SGS} = -\left(\overline{\mathbf{uu}} - \bar{\mathbf{u}}\bar{\mathbf{u}}\right) \qquad \text{or} \qquad \tau^{SGS} = \bar{\mathbf{u}}\bar{\mathbf{u}} - \overline{\mathbf{uu}}$$

- Represents the effect of filtered scales.
- And similar to the the RANS/URANS equations, the sub-grid scale stress tensor τ^{SGS} requires modeling.
- However, in LES simulations, the finer the mesh, the less modeling is involved.
- So, if you have a fine enough mesh, no modeling is involved.
  - Therefore, finer meshes resolve more coherent structures.
  - However, truncation errors may be present.
- Instead, in RANS/URANS, the integral length scales are pretty much grid independent (revisit tutorial 1 or any RANS tutorial).
  - That is, you are not going to resolve more coherent structures using finer and finer meshes.

LES equations – Filtered Navier-Stokes equations

- Notice that the FNS and the URANS equations are very similar,

FNS equations
The overbar denotes filtering

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

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

$$\tau^{SGS} = -\left(\overline{\mathbf{u}\mathbf{u}} - \bar{\mathbf{u}}\bar{\mathbf{u}}\right)$$

URANS equations
The overbar denotes time averaging

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

$$\frac{\partial \bar{\mathbf{u}}}{\partial t} + \nabla \cdot (\bar{\mathbf{u}}\bar{\mathbf{u}}) = -\frac{1}{\rho}(\nabla \overline{p}) + \nu \nabla^2 \overline{\mathbf{u}} + \nabla \cdot \boldsymbol{\tau}^R$$

$$\tau^R = -\overline{\mathbf{u}'\mathbf{u}'}$$

- The main differences are,
  - The FNS equations are filtered in space.
  - Whereas the URANS equations are time averaged.
  - Also, the apparent stress appearing in both the FNS and URANS equations is different.
  - Nevertheless, they both represent the smallest scales and they both need to be modelled.

LES equations – Filtered Navier-Stokes equations

- The sub-grid scale stress tensor τ^{SGS} is given by,

$$\tau^{SGS} = -\left(\overline{\mathbf{u}\mathbf{u}} - \bar{\mathbf{u}}\bar{\mathbf{u}}\right) \qquad \text{or} \qquad \tau^{SGS} = \bar{\mathbf{u}}\bar{\mathbf{u}} - \overline{\mathbf{u}\mathbf{u}}$$

- This term is analogous to the Reynolds stress tensor in the URANS/RANS equations.
- Let us expand this tensor by substituting the following decomposition (LES decomposition),

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

Instantaneous field

$$\mathbf{u} = \overline{\mathbf{u}} + \mathbf{u}'$$

Filtered quantity or resolved field
Grid scales GS

LES equations – Filtered Navier-Stokes equations

- After some algebra and by grouping some terms, we obtain the following equation (an expansion of the sub-grid scale tensor),

$$\tau^{SGS} = \left(\overline{\bar{\mathbf{u}}\bar{\mathbf{u}}} - \bar{\mathbf{u}}\bar{\mathbf{u}}\right) + \left(\overline{\bar{\mathbf{u}}\mathbf{u}'} + \overline{\mathbf{u}'\bar{\mathbf{u}}}\right) + \overline{\mathbf{u}'\mathbf{u}'}$$

- This decomposition is known as the triple decomposition (or Leonard decomposition) [1].
- Note that according to the filtering properties, the filtered sub-grid scale is not equal to zero, that is,

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

- Recall that in RANS/URANS simulations the product of the fluctuating quantities vanishes.
- This is not the case in LES simulations. This effect needs to be modeled (or resolved).

References:
[1] A. Leonard. Energy cascade in large-eddy simulations of turbulent fluid flows. Proceedings of Turbulent Diffusion in Environmental Pollution, vol. 18, 1974.

LES equations – Filtered Navier-Stokes equations

- The LES triple decomposition, that is,

$$\tau^{SGS} = (\overline{\bar{\mathbf{u}}\bar{\mathbf{u}}} - \bar{\mathbf{u}}\bar{\mathbf{u}}) + \left(\overline{\bar{\mathbf{u}}\mathbf{u}'} + \overline{\mathbf{u}'\bar{\mathbf{u}}}\right) + \overline{\mathbf{u}'\mathbf{u}'}$$

- Is a little bit more complex than the definition of sub-grid scale stress tensor arising from the filtering operation, namely,

$$\tau^{SGS} = -\left(\overline{\mathbf{u}\mathbf{u}} - \bar{\mathbf{u}}\bar{\mathbf{u}}\right) \qquad \text{or} \qquad \tau^{SGS} = \bar{\mathbf{u}}\bar{\mathbf{u}} - \overline{\mathbf{u}\mathbf{u}}$$

- As it takes into account interactions between all scales, that is, resolved (grid scales) and unresolved (sub-grid scales).
- Remember, the overbar represents a spatial filter.

LES equations – Filtered Navier-Stokes equations

- The sub-grid scale stress tensor τ^{SGS} arising from the triple decomposition represents the effect of filtered scales and small scales, and can be written as,

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

- In the previous sub-grid scale stress tensor,
  - **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).
- It is important to mention that this decomposition is not unique.
- In this case we used the triple decomposition (or Leonard decomposition) [1], which is often used with scale similarity models.

References:
[1] A. Leonard. Energy cascade in large-eddy simulations of turbulent fluid flows. Proceedings of Turbulent Diffusion in Environmental Pollution, vol. 18, 1974.

LES equations – Filtered Navier-Stokes equations

- The sub-grid scale stress tensor τ^{SGS} arising from the triple decomposition represents the effect of filtered scales and small scales, and can be written as,

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

- 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**), 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

- At the end of the day, these are the exact incompressible filtered Navier-Stokes equations to be used with LES models,

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

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

- Where we can use any of the following definitions of the sub-grid scale stress tensor τ^{SGS},

$$\tau^{SGS} = \bar{\mathbf{u}}\bar{\mathbf{u}} - \overline{\mathbf{u}\mathbf{u}}$$

$$\tau^{SGS} = (\overline{\bar{\mathbf{u}}\bar{\mathbf{u}}} - \bar{\mathbf{u}}\bar{\mathbf{u}}) + \left(\overline{\bar{\mathbf{u}}\mathbf{u}'} + \overline{\mathbf{u}'\bar{\mathbf{u}}}\right) + \overline{\mathbf{u}'\mathbf{u}'}$$

- At this point, we need to introduce models to approximate τ^{SGS} (similar to RANS).

LES equations – Filtered Navier-Stokes equations

- From this point on, let us assume that we want to model the whole sub-grid scale stress tensor τ^{SGS} , such as,

$$\tau^{SGS} = \bar{\mathbf{u}}\bar{\mathbf{u}} - \overline{\mathbf{u}\mathbf{u}} = -2\nu_{SGS}\overline{\mathbf{S}}$$

$$\tau^{SGS} = \left(\overline{\bar{\mathbf{u}}\bar{\mathbf{u}}} - \bar{\mathbf{u}}\bar{\mathbf{u}}\right) + \left(\overline{\bar{\mathbf{u}}\mathbf{u}'} + \overline{\mathbf{u}'\bar{\mathbf{u}}}\right) + \overline{\mathbf{u}'\mathbf{u}'} = -2\nu_{SGS}\overline{\mathbf{S}}$$

- Notice that we are using the Boussinesq hypothesis, and that we are lumping all terms into this approximation.
- That is, we are not modeling individual effects (which is possible).

LES equations – Filtered Navier-Stokes equations

- The sub-grid scale stress tensor τ^{SGS} can be decomposed into a deviatoric part (anisotropic part) and a spherical part (isotropic part), as follows,

Index notation

$$\operatorname{dev}\left(\tau_{ij}^{SGS}\right) = \tau_{ij}^{SGS} - \frac{1}{3}\tau_{kk}^{SGS}\delta_{ij}$$

$$\operatorname{sph}\left(\tau_{ij}^{SGS}\right) = \frac{1}{3}\tau_{kk}^{SGS}\delta_{ij}$$

$$\tau_{ij}^{SGS} = \operatorname{dev}\left(\tau_{ij}^{SGS}\right) + \operatorname{sph}\left(\tau_{ij}^{SGS}\right)$$

Vector notation

$$\operatorname{dev}\left(\tau^{SGS}\right) = \tau^{SGS} - \frac{1}{3}\operatorname{tr}\left(\tau^{SGS}\right)\mathbf{I}$$

$$\operatorname{sph}\left(\tau^{SGS}\right) = \frac{1}{3}\operatorname{tr}\left(\tau^{SGS}\right)\mathbf{I}$$

$$\tau^{SGS} = \operatorname{dev}\left(\tau^{SGS}\right) + \operatorname{sph}\left(\tau^{SGS}\right)$$

- This procedure is known as additive decomposition of a second rank tensor.
- Notice that the deviatoric part (dev) is traceless.
- This kind of decomposition is often used in continuous mechanics.

LES equations – Filtered Navier-Stokes equations

- Using the additive decomposition of the sub-grid scale stress tensor, the exact FNS equations can be rewritten as follows,

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

$$\frac{\partial \bar{\mathbf{u}}}{\partial t} + \nabla \cdot (\bar{\mathbf{u}}\bar{\mathbf{u}}) = \frac{-1}{\rho} \nabla \overline{P} + \nu \nabla^2 \bar{\mathbf{u}} + \nabla \cdot \mathrm{dev}\left(\tau^{SGS}\right)$$

- Where,

$$\mathrm{dev}\left(\tau^{SGS}\right) = \tau^{SGS} - \frac{1}{3} \mathrm{tr}\left(\tau^{SGS}\right) \mathbf{I}$$

$$\overline{P} = \bar{p} + \mathrm{sph}\left(\tau^{SGS}\right) = \bar{p} + \frac{1}{3} \mathrm{tr}\left(\tau^{SGS}\right) \mathbf{I}$$

LES equations – Filtered Navier-Stokes equations

- In the previous equations, the deviatoric part of the sub-grid scale stress tensor is often modeled using the Boussinesq hypothesis,

$$\operatorname{dev}\left(\tau^{SGS}\right) = -2\nu_{SGS}\overline{\mathbf{S}}$$

- Expanding and rearranging this equation, we obtain the following relationship,

$$\tau^{SGS} = -2\nu_{SGS}\overline{\mathbf{S}} + \frac{1}{3}\operatorname{tr}\left(\tau^{SGS}\right)\mathbf{I}$$

- The second term in the right-hand side performs a similar function as the equivalent term added in the RANS/URANS equation ($2/3\rho k\mathbf{I}$).
- It guarantees that the trace of the right-hand side is equal to the trace of the left-hand side.
- For an incompressible flow, the trace of the strain rate is zero; therefore, the identity holds.

LES equations – Filtered Navier-Stokes equations

- Notice that the spherical part of the sub-grid scale stress tensor τ^{SGS} ,

$$\mathrm{sph}\left(\tau^{SGS}\right) = \frac{1}{3}\mathrm{tr}\left(\tau^{SGS}\right)\mathbf{I}$$

- Can be written as,

$$\mathrm{sph}\left(\tau^{SGS}\right) = \frac{1}{3}\mathrm{tr}\left(\tau^{SGS}\right)\mathbf{I} = \frac{2}{3}k^{SGS}\mathbf{I}$$

- Where,

$$\mathrm{tr}\left(\tau^{SGS}\right) = 2k^{SGS}$$

- Usually, the sub-grid scale kinetic energy k^{SGS} is omitted because there is no model for it (same for the deviatoric part of the sub-grid scale stress tensor).
- Therefore, its contribution is usually absorbed into the pressure (as we will show in the next slide).

LES equations – Filtered Navier-Stokes equations

- In the previous equations, the deviatoric part of the sub-grid scale stress tensor is often modeled using the Boussinesq hypothesis,

$$\operatorname{dev}\left(\tau^{SGS}\right) = -2\nu_{SGS}\overline{\mathbf{S}}$$

- The spherical part of the sub-grid scale stress tensor can be added to the filtered pressure $\bar{p}$.
- Forming in this way the modified filtered pressure $\overline{P}$.

$$\overline{P} = \bar{p} + \operatorname{sph}\left(\tau^{SGS}\right) = \bar{p} + \frac{1}{3}\operatorname{tr}\left(\tau^{SGS}\right)\mathbf{I}$$

Notice that we need to multiply the second term by the density, so we get the same pressure units

- The isotropic contribution (or the spherical part of the additive decomposition) in the modified filtered pressure $\overline{P}$ can be resolved, modeled, or neglected [1,2].
- By using the additive decomposition of the sub-grid scale stress tensor τ^{SGS}, and substituting the Bousinessq hypothesis in the exact incompressible FNS equations, we can derive the solvable incompressible FNS equations.

References:
[1] R. Rogallo, P. Moin. Numerical simulation of turbulent flows. Annu. Rev. Fluid Mech., 16:99-137, 1984.
[2] A Vreman. Direct and large eddy simulation of the compressible turbulent mixing layer. PhD Thesis. University of Twente Enschede, Dept. of Applied Mathematics, 1995.

LES equations – Filtered Navier-Stokes equations

- The incompressible solvable FNS equations can be written as,

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

$$\frac{\partial \bar{\mathbf{u}}}{\partial t} + \nabla \cdot (\bar{\mathbf{u}}\bar{\mathbf{u}}) = -\frac{1}{\rho}\nabla \overline{P} + \nabla \cdot \left[\left(\nu + \nu^{SGS}\right)\nabla \bar{\mathbf{u}}\right]$$

- Where,

We need to multiply this term by the density, so we get the same pressure units

$$\overline{P} = \bar{p} + \mathrm{sph}\left(\tau^{SGS}\right) = \bar{p} + \frac{1}{3}\mathrm{tr}\left(\tau^{SGS}\right)\mathbf{I}$$

- At this point and similar to RANS/URANS turbulence modeling, the problem reduces to finding closure relations for the sub-grid scale viscosity ν^{SGS}.

LES equations – Filtered Navier-Stokes equations

- It is difficult to associate the sub-grid scale stress tensor τ^{SGS} directly with a physical process involving fluid motion because it is based on filtering rather than averaging.
- It is thus not surprising that the sub-grid scale stress tensor τ^{SGS} tends to be modeled formally without a detailed physical picture in mind.
- In fact, sub-grid scales models often use the Boussinesq hypothesis and the gradient diffusion hypothesis to model the sub-grid scale stress tensor τ^{SGS} and related terms.
- But instead of using the average velocities, the filtered velocities are used,

$$\tau^{SGS} - \frac{1}{3}\mathrm{tr}\left(\tau^{SGS}\right)\mathbf{I} = -2\nu_{SGS}\overline{\mathbf{S}}$$

- Where,

$$\overline{\mathbf{S}} = \frac{1}{2}\left(\nabla\overline{\mathbf{u}} + \nabla\overline{\mathbf{u}}^{\mathrm{T}}\right) \qquad \mathbf{I} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

- Remember, in the context of LES simulations the overbar denotes filtering.

LES equations – Filtered Navier-Stokes equations

- In the previous explanation, we assumed that the Leonard stress term **L**, the cross-stress term **C**, and the sub-grid scale Reynolds stress term **R**, appearing in the triple decomposition, they were all modeled using the Boussinesq hypothesis, as follows,

$$\tau^{SGS} = \underbrace{(\overline{\bar{\mathbf{u}}\bar{\mathbf{u}}} - \bar{\mathbf{u}}\bar{\mathbf{u}})}_{\mathbf{L}} + \underbrace{(\overline{\bar{\mathbf{u}}\mathbf{u}'} + \overline{\mathbf{u}'\bar{\mathbf{u}}})}_{\mathbf{C}} + \underbrace{\overline{\mathbf{u}'\mathbf{u}'}}_{\mathbf{R}} = -2\nu_{SGS}\overline{\mathbf{S}}$$

- It is also possible to only model the sub-grid scale Reynolds stress term **R**, and use approximate forms of the Leonard stress term **L** [1,2,3,4,5] and the cross-stress term **C** [3,4,5].
- This approach is known as scale similarity models [6,7], and it can account for backscatter effects.
- It is important to mention that different formulations of the approximate forms of the Leonard stress term **L** and the cross-stress term **C** exist depending on the particular filtering function used.

References:
[1] A. Leonard. Energy cascade in large eddy simulations of turbulent fluid flow. Advances in Geophysics, 18, 237, 1974.
[2] N. Mansour, P. Moin, W. Reynolds, J. Ferziger. Improved Methods for Large Eddy Simulations of Turbulence. In:Turbulent Shear Flows I. Springer, 1979.
[3] R. Clark, J. Ferziger, W. Reynolds. Evaluation of subgrid scale models using an accurately simulated turbulent flow. Journal of Fluid Mechanics, 91, 1, 1979.
[4] R. Peyret, E. Krause. Advanced Turbulent Flow Computations. CISM Courses and Lecture No.395, International Centre for Mechanical Sciences, Vienna, 2000.
[5] S. Shaanan, J. Ferziger, W. Reynolds. Numerical simulation of turbulence in the presence of shear. Report No. TF-6, Dept. Mech. Eng., Stanford University, 1975.
[6] M. Germano. A proposal for a redefinition of the turbulent stresses in the filtered Navier-Stokes equations. Phys. Fluids, 29(7). 1986.
[7] 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

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

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

- In this case we used the triple decomposition or Leonard decomposition [1].
- Another way to decompose τ^{SGS} is by double decomposition but with a sharp cut off filter [2,3].

$$\tau^{SGS} = \bar{\mathbf{u}}\bar{\mathbf{u}} - \overline{\bar{\mathbf{u}}\bar{\mathbf{u}}} = \underbrace{\overline{\bar{\mathbf{u}}\mathbf{u}'} + \overline{\mathbf{u}'\bar{\mathbf{u}}}}_{\mathbf{C}} + \underbrace{\overline{\mathbf{u}'\mathbf{u}'}}_{\mathbf{R}}$$

References:
[1] A. Leonard. Energy cascade in large-eddy simulations of turbulent fluid flows. Proceedings of Turbulent Diffusion in Environmental Pollution, vol. 18, 1974.
[2] P. Sagaut. Large Eddy Simulation for Incompressible Flows: An Introduction. Springer, 2006.
[3] F.F. Grinstein, L.G. Margolin, W.J. Rider. Implicit Large Eddy Simulation: Computing Turbulent Fluid Dynamics. Cambridge University Press, 2007.

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.

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

- Note that the triple 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.

References:
[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,

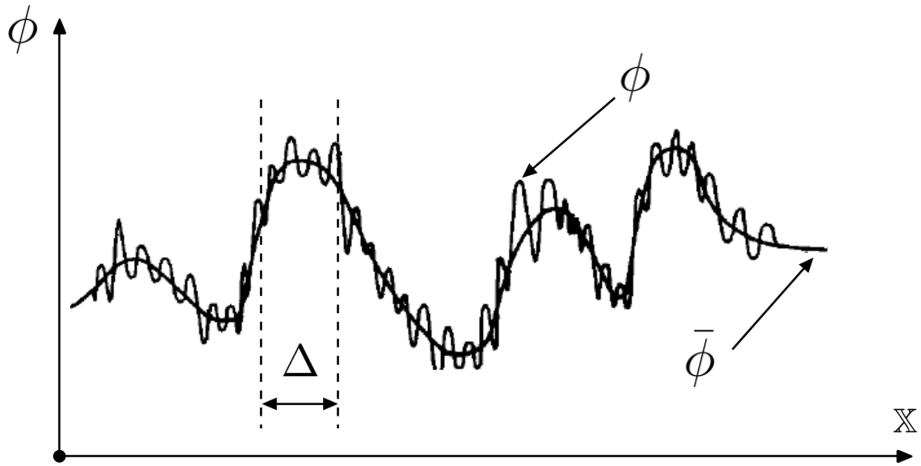
$$B_{ij} = L_{ij}^m - L_{ij} = \bar{u}_i \bar{u}_j - \bar{\bar{u}}_i \bar{\bar{u}}_j$$

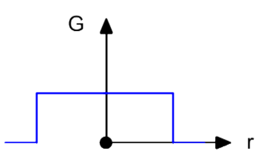
- This term is known as the scale-similarity term [1] and is used in scale-similarity models, such as the one we just introduced.

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

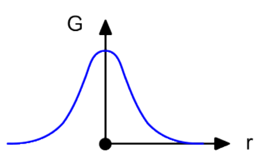
LES equations – Filtered Navier-Stokes equations

- In LES models, the governing equations need to be filtered (low-pass local spatial filter).
- You can see these filters as a rolling average (not strictly true).
- 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.

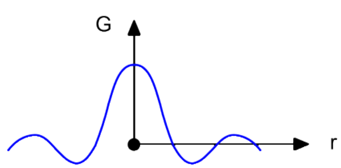




Box filter



Gaussian filter

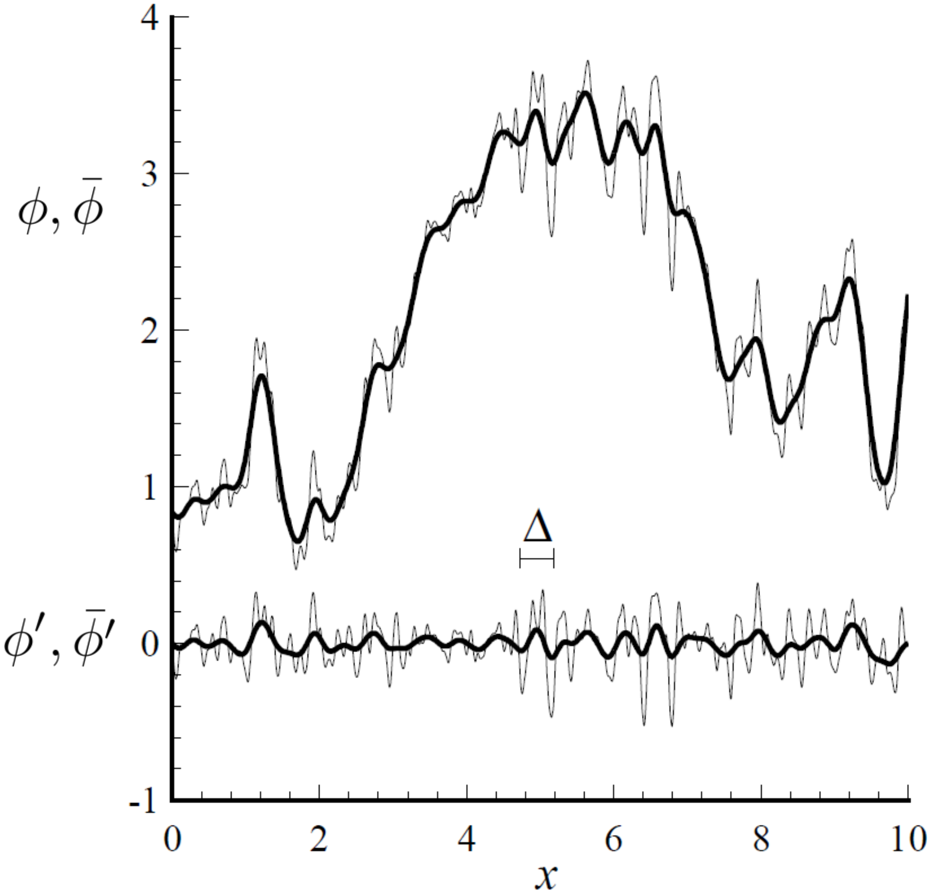


Sharp spectral filter

- At this point, if you want to understand better the theory behind low-pass filter, I invite you to review the literature on signal processing..

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 (unresolved fluctuations) and the bold line the filtered field residual.

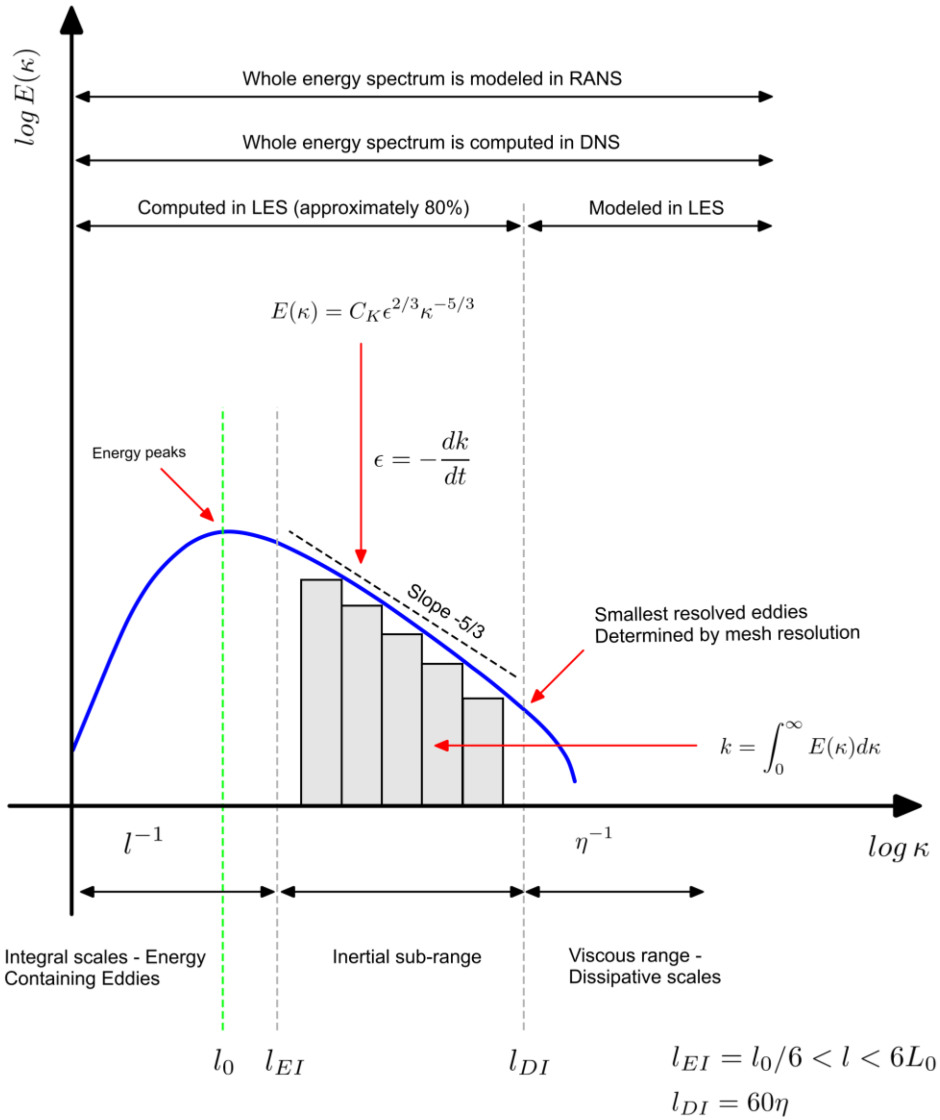
$$\phi'(\mathbf{x},t) = \phi(\mathbf{x},t) - \bar{\phi}(\mathbf{x},t)$$

- <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.

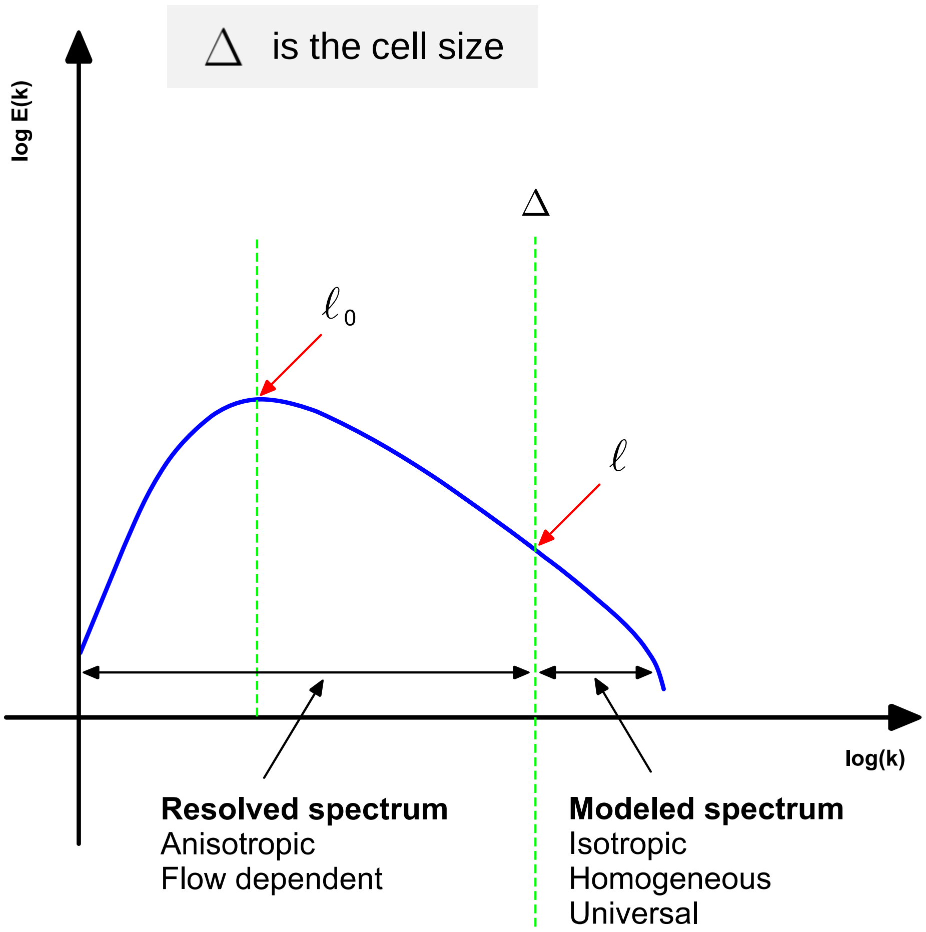
LES equations – Filtered Navier-Stokes equations

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.
- This kind of plots apply only for SRS simulations (unsteady and 3D).
- This plot is local, and sometimes is the only way to know the quality of a SRS simulation.

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.