

**Introduction to CFD**  
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**Lecture - 60**  
**Basics of Turbulence Modeling (continued)**

In this last lecture on turbulence modeling, we very briefly discuss about large eddy simulation and direct numerical simulation.

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Large Eddy Simulation (LES)

Separate out the large eddies from small scale eddies or small scale vortex motions.

Filtering approach  $\rightarrow$  filtered variable will be indicated by an overbar.

$$\bar{f}(x) = \int_D f(x') G(x-x') dx'$$
$$\int G dx' = 1$$

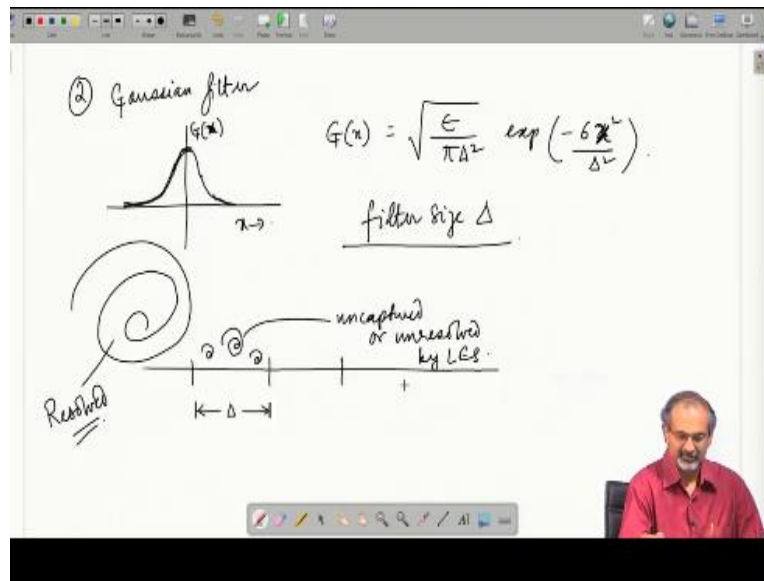
① Box filter

$G(x) = \begin{cases} 1/2 & \dots |x| \leq \Delta/2 \\ 0 & |x| > \Delta/2 \end{cases}$  top hat filter

In this approach which we very briefly discussed in a previous lecture on turbulence modeling, we separate the large eddies from small scale eddies or small scale vortex motions. And how do we do it? We use a so-called filtering approach. The filter variable will be indicated by an over bar. We have used over bar earlier also in the context of Reynolds averaging. So, we have to keep track that where a particular symbol is meaning what.

So, if we are filtering a function  $f$  of  $x$  over a region  $D$ , then that can be achieved to a filtering function  $G$  which can be defined accordingly. So, the filtration is attained. Now, the filter function again over that region should also satisfy this property that when integrated, it should give you a value upon. There are different kinds of filters which you can think of, one of the most common types of filters is what is called as a box filter. If you look at its nature, it is like. This it is often called as a top hat filter also.

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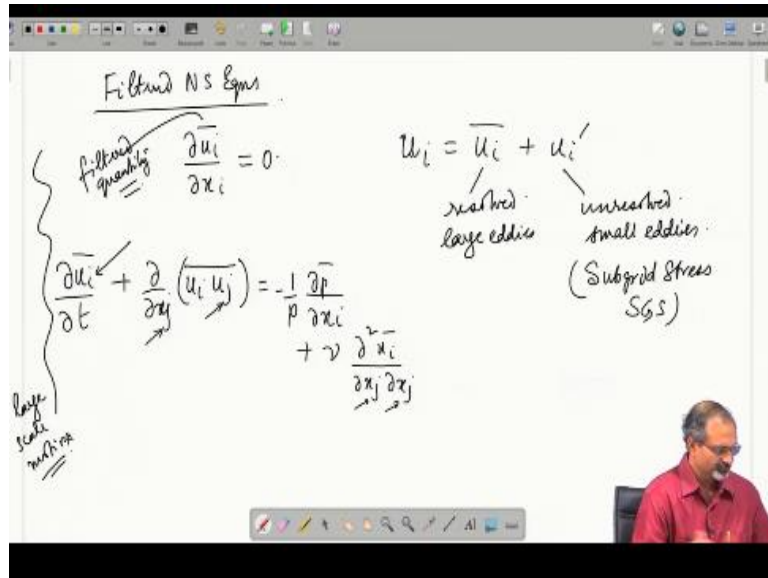


There could be a more smooth filter like a Gaussian filter which looks more like. This should be  $6x$  square by  $\Delta$  square. So, apart from the filter function, very important thing that we need to keep in mind is the filter size  $\Delta$ . That means on what width or what length scale we are applying the effect of the filter. How does it matter? Because depending on the length scale that we are fixing for us ourselves.

So, if this is  $\Delta$  the filter width that we are talking about, then any structure which goes below that filter width automatically gets filtered. That means it is un-captured or unresolved by LES. Any larger structure compared to  $\Delta$  would get directly resolved in LES or directly captured because there is no averaging that you are applying which will smooth out the effects.

Unlike, what we did in the runs approach. We did time averaging which would do some kind of a smoothing. Again in terms of the wave number space I hope you recall the idea of the energy spectra.

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When it comes to the filtered Navier Stokes equations, let us see how they look like. So, continuity equation looks like this. Keep in mind that now, this means filtered quantity, not Reynolds averaged. So, typically  $u_i$  would now be written as filtered or resolved and the dash quantity is unresolved. So, this is part of the large eddies. This is part of the small eddies which we are not directly capturing but you are going to capture their effects indirectly.

So, through the so-called sub-grid stress or SGS which will discuss. As far as Navier Stokes equation is concerned, again remember about the repeating indices. Here, the index  $j$  is repeating here again  $j$  is repeating and so on. And this is an equation a conservation for the  $i$ th component of velocity. Now, these equations essentially model the large scale motion. Now, energy is being fed into the turbulent structures from mean flow.

And then they are percolating from the large scales which you are directly computing into the smaller scales which you are modelling. That is the basic strategy in largely simulation.

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Subgrid scale stress tensor

$$\tau_{ij}^R = \overline{u_i u_j} - \overline{u_i} \overline{u_j}$$

Residual kinetic energy

$$k_r = \frac{1}{2} \tau_{ii}^R$$

$$= \frac{1}{2} [\overline{u_i u_i} - \overline{u_i} \cdot \overline{u_i}]$$

entire flow      resolved flow

Reynolds stresses:

$$\overline{u_i' u_j'} = \overline{u_i} \overline{u_j} - \overline{u_i} \overline{u_j}$$

Now, we bring in the concept of the residual stresses through the sub-grid scale stress tensor. R stands for residual. This has a structure very similar to what you saw in the Reynolds stresses. So, this is the mean of the product and this is the product of the means. So, this is somewhat similar to what you see here also in the sub-grid scale stress tensor. So, this is standing for the entire flow. This is standing for the resolved flow.

And then the difference stands for the unresolved flow. That is the concept. Based on that we have a definition for the residual kinetic energy that means the kinetic energy contained in the unresolved scales which comes from the tau i j R tensor by just looking at its diagonal components. So, this evidently is. So, this is again the k e contained by the entire flow, the kinetic energy of the resolved flow.

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Anisotropic residual stress tensor:

$$\tau_{ij} = \tau_{ij}^R - \frac{2}{3} k_r \delta_{ij}$$

$$\overline{p}_{modified} = \overline{p} + \frac{2}{3} k_r$$

This helps us to model the anisotropic part of the residual stress tensor which has a superscript small r which is represented in terms of the sub-grid scales stress tensor. This is SGS part and a portion coming from the turbulent kinetic energy of the residual structures and this is familiar to you, this is the Kronecker delta. So, the contribution from the residual kinetic energy would be absorbed in pressure like we saw even in Reynolds average Navier Stokes equations.

So, the modified pressure will be represented like this. This should be suffix k r suffix. Now; having worked out these things.

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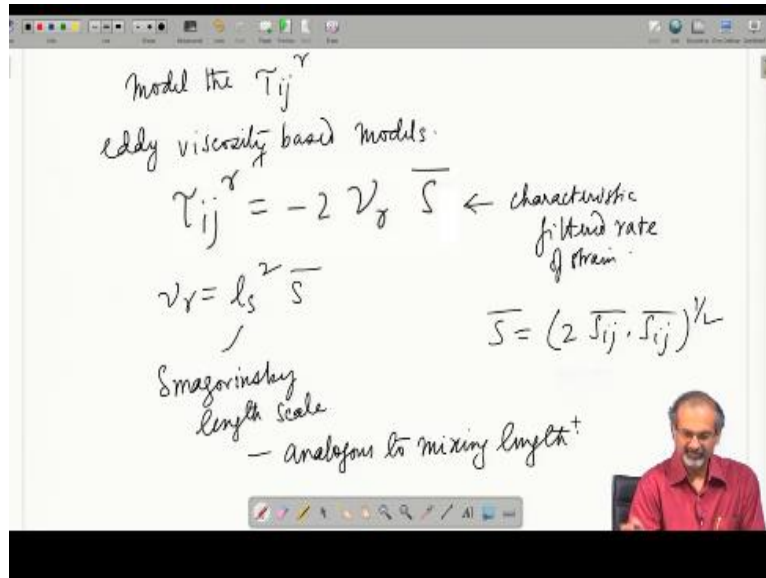
$$\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial}{\partial x_j} (\overline{u_i u_j}) = -\frac{1}{\rho} \frac{\partial \bar{p}}{\partial x_i} + \nu \frac{\partial^2 \bar{u}_i}{\partial x_j \partial x_j}$$

$\tau_{ij}^R$  &  $\tau_{ij}^r$

$$\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial}{\partial x_j} (\overline{u_i u_j}) = -\frac{1}{\rho} \frac{\partial (\bar{p})}{\partial x_i} - \frac{\partial \tau_{ij}^r}{\partial x_j} + \nu \frac{\partial^2 \bar{u}_i}{\partial x_j \partial x_j}$$

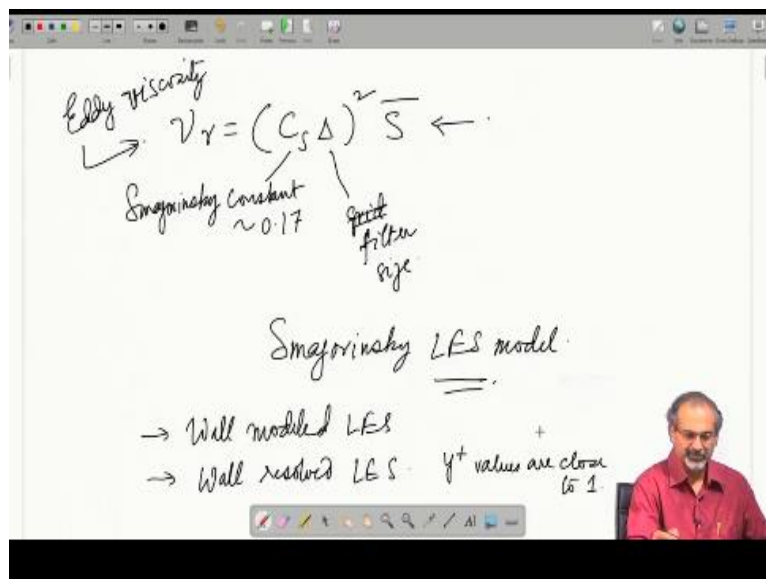
Now, you can go back to the filtered Navier Stokes equations and you can rewrite them slightly in terms of tau i j R and tau i j small r. So, you will be finally able to show that the equation can be represented like this. This is p modified which will still be represented by p bar only and then comes the anisotropic part of the stress tensor and the viscous contribution. Now, in order to solve this equation we model the anisotropic residual stress tensor, model the tau i j small r.

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So, usually we use eddy viscosity based models which we have discussed in the context of k epsilon model for example and make use of a characteristic filtered rate of strain. And how do we define that? That may be defined by doing a scalar product of the filtered rate of strain or rate of deformation tensor. And then the eddy viscosity is again expressed in terms of Smagorinsky length scale which is analogous to mixing length.

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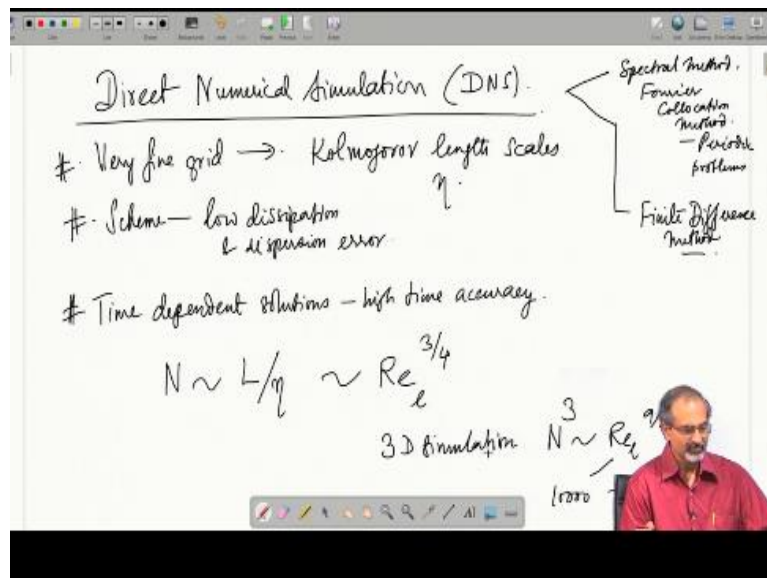


And finally that length scale is expressed in terms of a product of a constant which is often called Smagorinsky key constant and is of the order of 0.17 and the grid or rather the filter size and the characteristic filtered rate of strain which we already defined. Therefore, you have a definition eddy viscosity to use in modeling the anisotropic residual stress tensor. So, this is how this Smagorinsky LES model is formulated.

Remember that in large eddy simulation could go for a wall modelled, large eddy simulation where near to the wall instead of resolving very close to the wall. You try to use the law of the wall kind of relations and then try to impose the large eddy filtered approach beyond that level when you go into the core part of the flow. In certain more accurate methods, we do a wall resolved LES where you go very close to the wall.

And so, the y plus values are close to 1. So, this is a very brief overview of the large eddy simulation approach where as we mentioned earlier that we are capturing or resolving part of the flow which exists in the form of large scale structures and we are filtering the rest. And modeling that part through the so called sub-grid scales stresses. And we had a brief overview of how the sub-grid scale stresses are modelled through an eddy viscosity kind of approach.

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Let us have a brief look at direct numerical simulation. So, here since we are not modeling any part of the eddy structure, we are expected to have very fine grid because we are ideally supposed to capture the Kolmogorov length scales and traditionally two approaches have been followed in direct numerical simulations; one is the spectral method often in the form of Fourier collocation method.

But very often we have the constant of applying them only to periodic problems. That means problems where periodic boundary conditions have to be imposed and accurate finite difference or finite volume calculations. Again apart from the very fine grid that we need to have, we need to use numerical schemes with low dissipation and dispersion error. Again we need to generate time dependent solutions with high time accuracy.



So, that events which are occurring at very high frequencies can also be properly captured and in order to resolve all the scales of motion right up to the Kolmogorov levels. If you want to estimate the number of grid points that you need for a certain length scale say  $L$ . You need to take a ratio between  $L$  and  $\eta$  the Kolmogorov scale and that is usually of the order of the Reynolds number for the large scales raised to the power of  $3/4$ .

And therefore in the 3D simulation, you can easily estimate that this grid number will scale with  $N^3$  and therefore  $Re^{3/4}$  to the power of 3 which is a huge number usually. So, if  $Re$  is of the order of say 10000, then that basically means that  $N^3$  will be of the order of  $10^9$  which is an enormous number and therefore direct numerical simulations are extremely expensive.

And therefore cannot be used on a routine basis in industry. In fact, it can be very rarely used for industrially relevant problems at all in the current scenario. For industrial problems, runs is the best choice and then if we need more details of the flow, it is absolutely essential then LES is the next choice. As far as the different numerical schemes which would be suitable for carrying direct numerical simulations.

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Spatial discretization

- Compact schemes.
  - centered/upwind form
- Higher order explicit scheme

Higher order time discretization

Runge-Kutta Schemes

$$\frac{\partial Q}{\partial t} + \frac{\partial E}{\partial x} = 0$$

2nd order Crank-Nicolson Adams-Bashforth

Pressure-Velocity

$$\begin{cases} Q_i^{(1)} = Q_i^n \\ Q_i^{(2)} = Q_i^n - \frac{\Delta t}{4} \left( \frac{\partial E}{\partial x} \right)_i^{(1)} \\ Q_i^{(3)} = Q_i^n - \frac{\Delta t}{3} \left( \frac{\partial E}{\partial x} \right)_i^{(2)} \\ Q_i^{(4)} = Q_i^n - \frac{\Delta t}{2} \left( \frac{\partial E}{\partial x} \right)_i^{(3)} \\ Q_i^{n+1} = Q_i^n - \Delta t \left( \frac{\partial E}{\partial x} \right)_i^{(4)} \end{cases}$$

As far as spatial discretization is concerned, you can think of compact schemes which we have seen from our earlier exposure that they have very good spectral resolution or in the wave number space there they have extremely good behaviour numerical behaviour. So, they



are often used in centered or upwinded form. If we are not using compact schemes then we could go for higher order explicit schemes.

But then the problem would be that the stencils will become extremely large and maintaining high accuracy at the boundaries is a big challenge. We also need higher order time discretization for which the best candidates could be Runge-Kutta type of schemes and then you would have superior accuracy as well as enhanced numerical stability if you are using Runge-Kutta schemes.

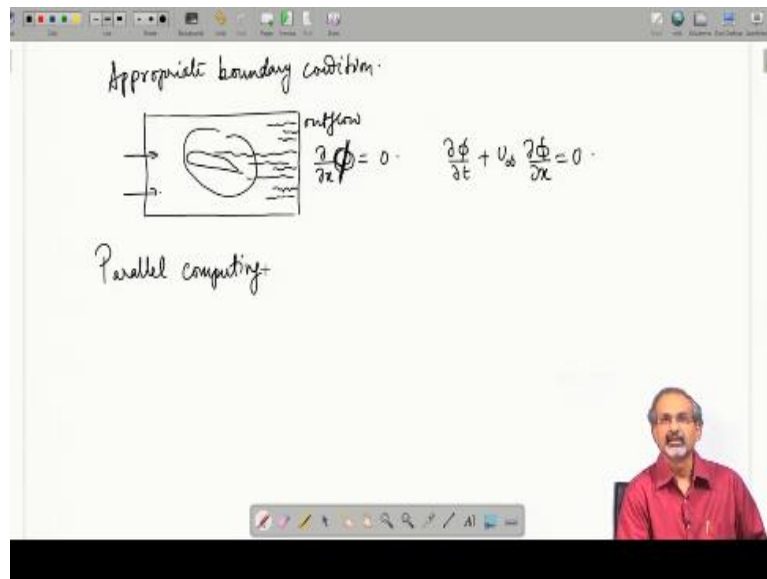
But typically for primitive variable approach in incompressible flows that would mean that you would have to carry out the pressure velocity corrections number of times within a given time step because Runge-Kutta schemes split up one time step into several sub steps. So, just having a brief look at Runge-Kutta schemes because they are extremely good in enhancing accuracy and stability and therefore are good candidates for direct numerical simulations.

So, if you are writing your equations in flux vector form in an R-K (Runge-Kutta) scheme you would actually do the sub-step calculations in this manner where you start from the  $n$ th time step calculations and then take it forward by doing a number of sequential calculations of this kind. We are showing a modified R-K scheme here of fourth order which means that you also have an enhanced formal accuracy.

So, as we mentioned that because there are so many sub-step calculations while you reach the  $n + 1$ th time step value from the  $n$ th value. Therefore, in all these sub-steps you have to keep the pressure and velocity fields at bar. So, that divergence free field is assured. So, that remains a challenge. So, if implementation becomes extremely expensive this way, you may need to look at other schemes which are usually second order.

For example, you can think about Crank Nicolson or Adams Bashforth schemes and these schemes are multi-time step schemes and therefore no sub-step calculations are involved.

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Also, you need to have appropriate boundary conditions in order to enhance accuracy of the simulations. Just as an example say if you are solving flow past a certain body which is immersed flow if you look at the flow moving past the body and creating vortex structures which reach the outflow region in an incompressible flow.

If the outflow boundary condition is not well posed then there could be disturbances numerical disturbances propagating upstream from the outflow boundary which may affect the formation of these structures. So, sometimes we tend to set the Neumann boundary condition that the gradient of the dependent variable is equal to 0 but a still better way of modelling, it could be that you try to model linear advection equation for the variable.

So, that would mean that you try to set an equation of this kind for the variable and solve it. So, this is often a better boundary condition in order to suppress such numerical errors accruing from the boundary. So, we have to think about appropriate boundary conditions and they are very accurate implementation numerically. So, that they do not become a source of numerical errors and corrupt the solution.

Another very important point that we have to keep in mind is that because of the enormous computing load, we have to use parallel computing where we try to compute by sharing the load or distributing the load across several nodes; sometimes hundreds or even thousands of nodes. So, that the calculations can progress at a reasonable speed without which it may turn take months to finish a single computation with this we come to our to the end of the module on turbulence modelling. Thank you.