Mathematical Modelling and Simulation of Chemical Engineering Process Professor Dr. Sourav Mondal Department of Chemical Engineering Indian Institute of Technology, Kharagpur Lecture 30 Demonstration of COMSOL Multiphysics

Hello everyone. In this lecture today, we are going to have a demonstration of one of the most popular PDE solver software's known as COMSOL Multiphysics. I mean, I am sure many of you have heard about this tool before. So, this is a general purpose PDE solver tool, that is something which I mean the PDEs that we encounter in heat transfer, fluid flow, mass transfer, reaction, electro kinetics. Most physical systems where you encounter multi dimensional PDEs is something that can be solved by this powerful software tool known as this COMSOL Multiphysics.

This software is based on the idea of the finite element methods, finite elements in a nutshell, to give you an idea that you choose, I mean, you do the meshing similar to the finite difference or the finite volume schemes. But the solution a priori is approximated by a test function between two points and you just do the iterations to improve the accuracy of this test function towards the final solution. That is how the finite element works.

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You can look into several textbooks on finite element methods and understand more about it. So, in this class, of course, we are not going to talk about finite elements but essentially how to handle this PDE software, look into some of its essential details at basics, how we can frame the problem there, how we can set up the model equations and how we can create geometries and essentially, how we can post process results.

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So, we will talk about two example problems, one is relate to heat transfer conduction, thermal conduction problem. Another one is relate to a fluid flow problem both in two dimensional situations. Of course, having said this, I must also say that, there are other similar software's which can handle these similar sort of problems where you encounter PDEs for example, MATLAB has a very nice PDE toolbox as well as PDE library function to solve PDEs.

But there are some limitations and I mean, I leave it to your good sense to understand that which is more user friendly, which is more flexible and what are the capabilities of the different tools available, even you have for fluid flow problems or transport phenomena problems Ansys Fluent is also a good choice.

But one of the biggest advantages that I find with COMSOL Multiphysics is that it is good for learners for somebody who is who wants to do a preliminary model, as the equation framework in this system is very nicely presented, it is user friendly and you can customize or write your own equations or you can understand the background of the equations very nicely without much of complexity or knowledge that is required in other platforms, where you have to introduce your own code for any user customized function.

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So, the first problem, let me talk about the first problem. So, this is a two dimensional heat conduction problem, I suggest all of you to just note it down, so, it will be easier to follow during the COMSOL demonstration. So, what we are going to do is that we define a solid block a two dimensional block of with 0.6 meter, 1 meter as the domain, so, just a rectangular block.

And then we suggest that the bottom boundary is heated, it is heated at 100 degrees or 373 degree Kelvin, and the left boundary wall is Neumann boundary condition and the right and the top boundary walls are like convicting to the ambient, the thermal conductivity is mentioned. And we want to find out what is the steady state temperature distribution in this lab.

So, this is a problem, which actually involves the solution of the Laplace equation, at steady state, it is nothing but the Laplace equation leading to the elliptic PDE in two dimensions,

which is you can easily solve out by separation of variables. So, you know the analytical solution for this problem. So, that is something we can be used to benchmark the solution.

So, I have, so, this is the benchmarking solution, so, T at x is equal to the right boundary. So, that is 0.6 meter and y is equal to 0.2 meter is the right wall these temperature let us say we should try to see how much we are getting from the computational calculations or the from the computation using COMSOL Multiphysics.

So, let me move into the COMSOL Multiphysics platform, before that, I must say that this COMSOL Multiphysics software is available for a free trial for a certain period. And if any one of you find it difficult to get access to this software, please inform us and we can definitely be able to help you with the access for a limited period of time. So, we are now moving to the COMSOL platform. And I will show you from the beginning that how what are the things to set up? And what are the things to choose and what does each of these settings mean before we start for framing or work on this problem.

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So, if you start the software COMSOL Multiphysics, this is the first window that we will be getting. And it will ask that whether you want to go for a Model Wizard or whether you want to go for a model or a blank model? So, it is always advisable to start with the Model Wizard. So, in this case, if I click on this model wizard, it will ask you that what sort of spatial dimension are you looking for whether it is a three dimensional problem, whether it is a two dimensional problem, again two dimensional problems has two versions 2D axisymmetric.

So, this is generally for the case when you have theta and phi symmetry and you are trying to solve only the R and z coordinate problems. And in general, you can also work from the 2D coordinate systems 1D, again, 1D axisymmetric. Please note that the axisymmetric versions significantly reduces the computational load, and then it is the point of the 0D formulation. So, in our case, I mean, it is a two dimensional problem. So, we select these 2D this is the thermal conduction problem, then it will ask that what sort of physics do you want to work in the system.

Now, the available physics in your case may be different from what it is showing here it could be more it could be less. So, the base package has certain physics it will it only includes the mathematics module. So, these are called the modules. So, it only includes the mathematics modules, which is the general purpose PDE there are some classical PDEs you can choose or you can use the general purpose PDE as well as ODE, PDEs, I mean, classical

PDEs are the Laplace poison and those Helzmoltz wave equation and all those things, that is the mathematics module where you can work with them purely from the equational perspective.

But it is always recommended that if the physics of the problem is very well defined, and it is something that even if it is more than one physics, it is multiphysics problems still can be coupled. That is why it is called COMSOL Multiphysics.

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So, if you have, in our case, it is a heat conduction problem. So, there is a particular module known as the heat transfer in solids. So this I mean, why I am choosing this specific module and not the Laplace equation, I can also work with the Laplace equation, there is no harm in that, it will still give me the same answer for this case, but generally in these dedicated modules, the solution algorithm is often optimized and it is developed so that these specific physical issues with the certain types of background can be handled in a smart way as well as in a nice way because the solution algorithms for different types of systems are generally different even though the nature of the PDE is still the same.

For example, fluid flow is given by, I mean represented by Navier Stokes equation, but solution of Navier Stokes equation in the laminar domain and in the turbulent domain is cannot be done in the same way. For turbulent flow there are several different models including the Navier Stokes equation, which generally helps in finding the solution. So, that is why these dedicated modules are generally preferred or is advised to used, to be used rather than the simple straightforward equation based PDEs.

Because often these in the standard PDEs, the equation is already set up for you and you need to just use those equations in the standard framework and work with the coefficients. Whereas, in the generalized PDE formulation, you can develop your own set of equations in the PDE format, and that may have some issues in optimizing or generalizing the different

term or the flux term or the artificial diffusions and all those things stabilization issues and so, it is always advisable to use the dedicated module as it will also give you a background flavor of the physics of the problem.

So, depending on the licenses available in your case, you can see either all these modules or maybe more or maybe less that is something to realize but please note that in the base package itself, this heat transfer in solids is available.

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Also in the fluid flow case the laminar flow module is available, in the fluid flow case, if you further go you will have this single phase, laminar flow is something which is available in the case of the this base package. So, at least that is available if you have access to COMSOL Multiphysics. Now, trying to work with the heat transfer in solids, you just select this particular physics, click on this Add. So, it will be added to your particular model.

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So, when you go to the study it will ask that whether you want to perform stationary studies or whether you want to perform time dependent studies or transient studies. In this problem, we want to find the steady state so, we choose for the stationary mode. So, I select a stationary mode and then I click done. So, this wizard is completed. Now, we have set up a model for the case of heat transfer and in two dimension, as well as we are going to work in the steady state phenomenon.

Now, in this platform, the left hand side is known as the model builder, I mean there are certain settings I mean there are certain settings that needs to be defined by choosing the different model components, what are the model components, definition, the defining the parameters or the constant in the system.

Then we have the definition of if you want to define any function, any variable then work on the geometry defining the materials or the material properties, but this is something which I do not encourage much and I would suggest that you write any material properties yourself directly into the equations or as a parameter, but of course, there is a wide variety of material library, where you can get information of the different these material characteristics as a function of temperature, function of concentration, it is a good database it has and then it will ask you to go for the components.



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So, I mean this is the heat transferring module where the equation is displayed here you can see this is the generalized form of the steady state heat equation these additional terms q0 dz Qted then dzQ it is all like additional source and sink term time depending on whether you are having line heating or volumetric heating, bulk heating and all those things.

So, this is the equation of course, for the case of solids this u is equal to 0. So, this is a general purpose convective diffusive heat equation. So, this u is 0 so, there is no component of the u it is only grad dot small q is equal to zero and if you insert the heat flux or thermal conductive flux in terms of q it will give you the Fourier equation sorry, this is the Fourier equation which will give you the Laplace equation finally. So, this is the equation and then we will work about the introducing the proper I mean the values of the thermal conductivity and etc. But before that, let us try to create the geometry.

(Refer Slide Time: 14:41)



So, creation of the geometry is very similar to a CAD operation. So, please note that it can import any standard CAD files which is prepared in other software's or in other platforms. And then you can import that geometry here and try to work on that so, that possibility is always there and other option is of course, to have the geometry built yourself. So, it has all

standard geometric CAD operations that is available in most sophisticated CAD software's too.

(Refer Slide Time: 15:16)



For example, all this creation of both 2D and 3D things, it is only listing down all the possible 2D operations, it can also do Boolean operations partitions and other primitive designs, you

can also have a parametric variation of your shapes, any polygons and these shape geometrical features can also be dependent on the parameters that you are defining in this system.

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So, let us say let me define two parameters as the width and the height. So, let us say the box width as 0.6 meter so, this is the parameter I am defining and the box height as 1 meter. So, when I create this rectangle, it will ask for the dimensions. So, instead of specifying the values, I can write the name of the parameters. So, instead of width I write box width. So, it will take that value and later on if I wish I can change them very is easily during the calculations also or as a separate parametric variation of this shape. So, it will ask for the base position let us say I put this to the center, center is 0, 0.

So, if I click on Build Objects, it will create a rectangle of 0.6 width and 1 meter of the height. So, this is our box or the rectangle is created. So, going to the this geometry is done next is to define the rest of the parameters.

For example, thermal conductivity, so, thermal conductivity is in this problem is already given to you, so and the value of the thermal conductivity is 52 it is in watt per meter Kelvin. So, SI unit so, we not worry about the units and the heat transfer coefficient heat transfer coefficient is mentioned as 750 watt per meter square Kelvin.

Temperature of the bottom T bottom is 373 Kelvin and T ambient the atmospheric temperature is 273. So, these are most of the parameter values that we, is given in the problem and it is something we are listing down. So, in the case of their definitions of these

values, we will write the names of the parameters. So, at one place we list down everything and then we just mentioned them in the calculations.



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Like similarly, how you call it up. So, instead of defining the values of different parameters, you generally define them at the beginning and then you refer them with the help of the name

of those parameters or the variables. So, in heat transfer in the solid this is the module which we have which we are utilizing here and you can see the equations as well as at the bottom if you want you can also explore the name of the dependent variable. So, in this case the dependent variable is essentially T temperature. So, the symbol of the dependent variable if you want you can also write instead of T you can also write T1, T2, TT and all.

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So, now going into the, so, these three components solid 1, initial values and thermal insulation what these are the by default settings which is associated with this model, so, that the problem is completely defined without any user input. So, by default it assumes that all the wall is having Neumann boundary condition and the solid of course, the solid properties still needs to be defined, but at least the boundary conditions are by default defined as

Neumann boundary condition unless you change them. So, this is just how the software set itself for the calculations.





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So, again you can see the equations here and at the bottom, you see that the heat conduction or this parameter thermal conductivity is mentioned and it is written from material, but you can use them to be as user defined. And in the case of the user defined instead of writing the absolute value, you can also write the thermal conductivity as the name of the parameter just, let me check. So, thermal conductivity. So, I should write the same.

And then there is a choice that whether this thermal conductivity is constant I mean if you want it to be varying with temperature you can just write multiplied with T. So, this will simply make the thermal conductivity varying with temperature or if any spatial function you want to give let us say this heterogeneous media and there are different thermal conductivity of different zones of this system then you can just try this thermal conductivity is multiplied with T or multiplied with 1 plus x or something like that alternatively you can define different thermal conductivities in different dimensions and different directions and you can choose the full matrix of the thermal conductivity and you can define all the anisotropic conditions of this.

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So, let us for the sake of simplicity write this to be only isotropic in the system and we consider it to be constant, but very easily can write that to be you have any other type of functionality which you want for example, most resistances that you see has very strong function of temperature. So, you can write thermal conductivity as a function of temperature too also semiconductor materials are like highly dependent on temperature. About the density and the heat capacity, so, you know that these values are not important.

So, instead we just specify any arbitrary value to these quantities, but the software still ask those values because it is set in a way that this can be needed in the case of the fluid in the heat transfer problem or in the case of the transient problem. But in the case of the stationary problem, these are not at all relevant, but we just put some random values and if you will, if you change them they do not affect the solution of course, because they will not form part of the solution, but you have to define them that cannot be undefined.

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Next is the initial value. So, the initial value to this problem is the initial temperature guess for stationary problem, this is the initial temperature guess of the entire system. In the case of time dependent problem this is the initial condition but for stationary problems initial values represent the starting iterative guess to the solution. So, let us say the guess value we can write them as T ambient, something like this and next come the boundary condition.





So, by default it has chosen this if you click on this equation here, and the boundary conditions or the boundaries are designated as 1, 2, 3, 4. So, if you click on each of these now, you will see that which is 1, which is 2 and which is 3 and which is 4, so, 1 is the left one, 2 is the bottom one, 3 is the top one and fourth is the one, so by default, it has chosen that the conductive heat flux or dt dx is not dx, dt dx or dt dy corresponding to which

boundary we are talking about, because this flux is multiplied with n and n is known as the outward normal vector.

So, in the case of the sidewall, the resultant equation turns out to be dt dy to be 0. For the case of the bottom boundary, it is dt dx to be 0, sorry, it is if you considering this boundary conditions, I mean the Neumann boundary conditions which is generally applicable for adiabatic walls, this more or, this condition of minus n, which is outward normal vector dot the Q which is the heat flux or the conductive heat flux is equal to 0. So, for the right boundary wall, this is dt dx is set to 0, for the top boundary wall it is dt dy set to be 0. Similarly, the left and the boundary conditions are set in appropriate way.





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But here we have a different boundary condition to the problem the bottom is Dirichlet type. So, we have to select that if you choose this temperature, which is equivalent to the Dirichlet condition and you can set a temporary at the particular wall. So, here you have to first choose the wall. So, if you just click on this wall it will just mark in red and if you make a left click, it will select that wall and you will see that the boundary number 2 is selected and the boundary value there is given we have already specified the parameters in bottom so, that is the boundary conditions.

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Once we select if you go back to the previous one that is thermal insulation you will see that boundary number 2 is marked as overridden. So, we have specified a different boundary condition, that is why this is not applicable as thermal insulation you cannot apply two boundary conditions at the same wall.

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And the other boundary condition it is specified is that heatflux. So, for the heatflux the boundary condition is the right wall and the top one, these two are shown I mean are specified to be the heat flux should be equated to the convection. So, the equation instead of heat flux as the general inward heatflux you can choose it to be the convective heat flux. So, if you choose the convective heat flux, you will see that the equation minus n dot q the conductive flux is equal to h into T ext minus T where you have to define h and T external. So, this h is nothing but the heat transfer coefficient which we have already defined as 750 watt per meter square and T external is T ambient. I will just once again check from the parameters whether these names have been written correctly, yes, it is written correctly.

So, this definition is complete. So, I do not need to worry I mean, I do not need to worry about setting the appropriate this boundary condition because it is the by definition this is already available with us. If you want to select the heat transfer coefficient or you want to select a different value of the heat flux you can choose the other instead of defining as convective heat flux, you can choose general inward heat flux and you can define some other types of boundary conditions that is always possible you can also define some heat rate or something else.

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So, this now completes the problem because once the boundary conditions are defined, you will see that the system is completely defined. Now, please note that the default thermal insulation condition you see that boundary 2, 3 and 4 are overridden because we have applied the Dirichlet boundary condition and the heat flux boundary condition on those two sides. So, with this the definition of the boundary condition and the problem setup is complete.

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Next step is the meshing. In general, it has two default modes, one is the user controlled mesh, another is a physics controlled mesh. So, when you choose the physics control mesh, you just have to choose the kind of element refinements you are talking about. This is all written down in terms of subjective nature, that what is coarse normal, extra coarse, fine, extra fine. And then based on the physics of the problem based on the boundary condition, the system or the software automatically does refined meshing at the required boundaries, where there is a likelihood of the formation of the boundary layers. So, if I choose normal, just see what happens.

(Refer Slide Time: 28:13)





So, it creates almost like uniform mesh sizes. So, if you want more refinements, and you see that at the bottom, the message comes, and it tells you that the mesh contains almost 346 domain elements. So, if you select fine, extra fine, it will refine the mesh. And the number of mesh elements increases to almost like three thousand, three and half thousand.

But please note that in this case, since it is a conduction problem, it is a conduction problem. And this, this mesh works, fine. That is why there is no different type of mesh or what should I say, mesh size variations are not present. If we if you have worked on if we work on the problem of fluid flow, where there is a strong gradient near the no slip walls, generally the mesh can be more refined there. So, by default, it will, the software will be able to generate that.

But even if you are not happy with the software generated mesh, you can go for the user controlled mesh. But for beginners, this is slightly more complicated because you have to select a lot of mesh parameters. And then of course, you can have boundary layer mesh, you can have different refinements at different zones of the mesh.

But this needs a very clear understanding of the let us say approximate idea on the thickness of the boundary layer. That is why mostly these things play a big role. And whether the mesh size in those boundary layers is sufficiently small, like what is the degree of resolution in the far field you are talking about and all those settings. But for this problem this level of refinements is good enough. I mean, from experience I am saying this, but you can also work out yourself then we go to the study.



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So, and there is one more thing I wanted to say, but that is probably for the case of time dependent problems, but there is something known as the damping factor. So, if you select this method of the solution to be automatic or constant, it will ask for the initial damping factor. So, if you set constant Newton process the damping factor can be constant in each iteration. So, what is this damping factor?

So, this damping factor is essentially a scale if the solution, the change in solution in each time step is too much or in each iteration is too much, then it will try to take a smaller time step based on the idea of this damping factor but these things are generally quite relevant for time dependent problems, for stationary problem, it does not really matter that much.

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So, now, if I click the button called compute, it will do the calculations and it will generate the results, but we have to make the results calculate the results the way we want it will show some default results, but let us see what happens when we click on this calculation button. So, all calculation activities can be seen in this log. So, if I click on this, it will start the software will start calculation and during this time, you cannot actually change anything in this problem.

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So, calculation is done. And if you see in the log, it will tell you that how much memory is utilized, what is the start time end time, how many degrees of freedom to the problem has been done, and in one intervention step only solution was converged. So, once the solution is done, by default, it will show some of the plots depending on the kind of physics we are trying to solve. So, in this case, it is the temperature. So, the temperature profile, you can see it here it is very nicely displayed as a contour with the color bar. So, let us try to see the boundary condition on the left hand side we had the Neumann boundary condition.

So, if I try to plot the profile of dt dx on the left boundary, this should be equal to zero with that is something we will do just wait. The bottom boundary condition is fixed temperature that is 373 and you can see almost it is hitting that part that is 373 and the right and the top wall are the heat flux boundary condition.

(Refer Slide Time: 33:32)

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So, before trying to calculate what is the value at 0.2 meters above the right hand boundary, let us just try to get an understanding of let us say, if you want to calculate the dt dx value at a particular y point. So, these are very important post processing things. So, what you need to do is that in their results, that is the post processing actually I find the most complicated or most I mean the harder bit. So, you have to click on this derived values and then before that you have to make a cut line because at what y value you want to do this dt dx let us say if you want to do that.

(Refer Slide Time: 34:15)

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So, first we have to make a cut line and let us see I do this cut line value I have to define my x and the y points. So, the first one is at y value of minus 0.3 for example or maybe slightly more minus 0.1 at this point let us do that and this is x1. So, if you just see I tried to locate two points.

(Refer Slide Time: 35:02)

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And if I, just tried to define the two points on the right side and the left hand side and then that creates a line. So, along this line I want to evaluate what would be my dt dx. So, for that, I have to select another line plot.

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So, 1D plot plus it is in one dimensional plot and farther again I have to make line graph. So, in the line graph in the data set, I have to select the cut line 2D and then it will ask for the expression that what function I want to evaluate or want to compute. So, if I write T then x it means dt dx. If I write Ty that means dt dy, if I write 2x it means double derivative of temperature.

(Refer Slide Time: 35:52)



So, if I then click on the plot, this one I should write as x so it will be clear to you. So, this is the x coordinate value and with that the temperature this dt dx is plotted and you see that at x is called the left wall dt dx is 0. So, this is the gradient that I have plotted. If I just plot the

temperature profile along this point, you will see that it will, it will be constant close to the left boundary.

(Refer Slide Time: 36:30)

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You see that gradient which is the temperature profile now the gradient close to the left boundary is getting zero.

(Refer Slide Time: 36:42)



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So, if I just show the legends I think it will just tell you that what does this different locations tell you, so I can write expression, expression is y, kindly bear with me, so, these are the different y locations I mean, this is theoretically close to zero only just showing in a different way. So, these are different y locations over which I have plotted the temperature profile.

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I hope this is visible to everyone all of you. So, this is how you can get the temperature profiles in this slab and you can also do a similar exercise for the vertical dimensions, let us try to benchmark our results that yT is equal to that particular value T is equal to I mean on the right wall it is 0.2 meters above the base, what is the temperature value.

(Refer Slide Time: 38:58)



So, to do that, there is option called derived values you can go to this point evaluation and you can essentially select the temperature corresponding to that point but unfortunately that point is cannot be selected you can get the temperature value across the whole y that is one option or here you can only get the four corner points whatever vertex is already defined in

this problem. So, or you can define a vertex at that particular point during the geometry and then now you can evaluate the point temperature at that point that is a possibility. So, let us try to do that.



(Refer Slide Time: 39:38)

So, in the geometry, you can mark a point. Let us see where is that point option or I can also do in the definitions, a probe. So, I can put a point probe a particular location I can relate.



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Probe, this is not a possibility, I cannot define a particular point here, so, the other option is of course, to make this cut point. So, in the two dimension you can choose a particular point by using this dataset cut point. So, if I do this cut point 2D I can just try the coordinate of that particular point and so, this x coordinate is 0.3 and the right wall coordinate is minus 0.3 that

is like 0.2 meters above the bottom of that point. So, this is the point. So, at this point, I can go to derived values.



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And I can do a point evaluation I can choose this cut point and the temperature expression is already there. So, if I click on evaluate, it will tell me what is the value and you see the temperature value is 291.25 which is same as the value that we can obtain from the theoretical calculations. So, I hope all of you liked this demonstration, we may have another demonstration. So, the last demonstration on the COMSOL software was related to a heat transfer problem on conduction.

(Refer Slide Time: 41:42)



This second problem demonstration which we are going to do is regarding a fluid flow problem where we are going to study or investigate the von-karman vortex streets formation and these are, this fluid flow, nice fluid flow patterns is also observed in oceanic flows, in atmospheric flows, that is on a much bigger scale, in a small scale also. The sort of instabilities in the flow or flow vortex are formed whenever there is a flow past a particular cylinder at substantially high flow rate and near this region there is formation of this vortex and sort of this instability initiates and there is these zones of high and low pressure zones are created along this channel, the inclusion of any obstruction in the flow path.

So, let us try to observe these phenomena and see that how numerically the von-karman vortex formations are realized. So, let us try to consider the problem of a rectangular channel, the dimensions are already mentioned, you place a small circular intrusion essentially since the two dimensional problem. So, the circular intrusion is ideally a cylindrical intrusion in the three dimensional perspective, you consider the density close to 1 and viscosity 10 to the

power minus 3. And walls of the channel is no slip boundary condition and the same the surface also have no slip condition.

So, there is a strong boundary layer separation from the as the flow past this particular inclusion. Outlet has no-shear condition and inlet is having condition, is having the mean velocity is 6 meters per second, that is substantially high. So, you can also evaluate the Reynolds number for the problem. So, now let us start the COMSOL platform. So, we will move to the COMSOL Multiphysics software platform now. And we will start take it forward from there.

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So, this is something that you get in the beginning, like this previous case. So, here it asks for the choice of the different conditions for your model. So, this is again, a two dimensional system. So, we select 2D. And now here we will try to select the fluid flow profile because it is a fluid flow problem. So, we will go, so all the Navier Stokes equation is already embedded in this particular module. So, you select the single flow phase flow system because it is only

one phase flow and select laminar flow for these problems not turbulent essentially. So, we add on that and then we go to the study.

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And next it asks for whether it is stationary or time dependent. Please note that this is a time dependent problem. So, it is transient problem so we cannot select stationary mode. So, it is a time dependent problem.

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Often time dependent problems are also helpful in studying scenarios where you have the steady state solution is very difficult to achieve or to find even though theoretically it is possible to have a steady state solution or the theoretically the equation satisfy the steady state condition, but you can solve the temporal the transient condition and evolve and do the evolution of the process towards a steady state that is why the steady state problem is useful.

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Now, let us once again write in the parameters the problem dimensions. So, let us say the channel width sorry the channel I would say the length is 2.2 meters please note that you have also the flexibility of changing the dimensions or the units of the problem, but I strongly advise not to do that keep everything in SI units and if you want to change a working or use different units, you just change the values like if something is in millimeters you just convert it in terms of equivalent meter and write it here instead of changing the units. There is also a possibility I mean there is option to change the units here for example, if you go to this component sorry in this definitions, I think units there is there is an option same as. So, you can choose SI units, FPS units and all.

So, there is a possibility of changing the units you can also use your own user defined units system, but I strongly suggest that instead of changing the units you work with the this standard units and then convert those values and put it here, so, here is the value that you can scale the values while changing units you are I mean by the software or you can do it yourself, which is the preferred mode and length units can mean different ways that you want to write but again as I say that it is better to always write it in meters so that not to confuse yourself in the process.

Then the channel height is marked as 0.4 meters as per the problem, and the radius of the or the diameter of the cylinder dia of cylinder that is inserted is 0.1 meters it is mentioned in the

problem. The density rho is 1 and viscosity mu is 10 to the power minus 3 and that is something also you mean inlet velocity is going to 6 meters per second.



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So, now, let us create the geometry the geometry slightly exciting in this problem. So, we go to geometry first create a rectangle. So, with this CH length, height, build all objects this is the geometry which is built I can align the center instead of because it says aligning the center I mean the position is based on the corner value as 0, 0 I can also mark instead of 0, 0 as the corner I can mark as yh, so, this is just making it uniform height by 2 sorry, it is minus

that will go down. This is how x is equal to zero point is the center line. So, now we have to create a circular inclusion here.

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So, first let us create that circle. So, circle x is equal to 0 sorry y is equal to 0 and the x position as mentioned in the problem is 0.2 and the circle radius is given by this parameter, I made a mistake, this dia circle I have to write dia of the cylinder by 2 to make it the radius. So, this is this circular intrusion that is shown here. And please note that this region or this

circle has to extracted out, this should be a cavity in this body and at the moment it is appearing as a solid.











So, to do that what do you mean you need to do is this geometric Boolean operation of the difference. So, Boolean difference, select the objects to add. So, if you take the mouse over that object, if you click it, it will be selected. So, from r1 or this from this channel, I want to select the circular cylinder. So, if you take over the mouse to that circular region, it will select that.

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And now if you create build objects, you will see that this is a cavity in this problem instead of another solid in this problem it is an our cavity and the interior surface is defined now.

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Now, let us go to the laminar flow part where we have to define all the fluid flow parameters and please note that in the laminar flow, if you click on this equation, you will see that the Navier Stokes equation is written now. What is this k? k if you recall is the shear rate tensor which is dependent on the I mean the viscosity and everything. So, this is what k represents and f is the body force term sorry k presents the shear stress and the shear stress is related to the shear rate by the rheological model, rho is the density and in the second case you see that it is written down that it is continuity equation.

So, there are two equations and these since we are dealing with the incompressible fluid, rho is outside of these derivatives or the equation is written down in the non-conservative form. I think if we choose compressible flow, yes, so, if you choose compressible flow, you see that the continuity equation is changed.

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So, in this problem it is an incompressible flow so, we do not change that setting. And if you go down at the bottom you can see what are the dependent variables. So, dependent variables the vector field is represented by u at the velocity field components u, v, w, w is for the z direction which is not applicable here and pressure is p.

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If you want to consider its as to be a Stokes flow or a very low Reynolds number flow you can select this component as neglect industrial terms, but in this case, inertia is irrelevant. It is a laminar flow not Stokes flow.



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Problem 2: Flow past cylinder: von-karman vortex



Now, going to the fluid properties it will ask you to define the fluid density and the viscosity. So, we will write user defined and fluid density, we will take the name of the variable as rho, so, we will write this fluid density as rho and viscosity as mu, already the default units are mentioned here. So, you can cross check your values with respect to the defined units. So, I just need to I think I should look into the value of the viscosity as for the problem statement, so please excuse me for that. So, it is 10 to the power minus 3. So, I think we are all good. So, a mu is defined as 10 to the power minus 3 and the default units mentioned here is 10 to the power minus 3 Pascal second.



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The fluid properties are considered to be Newtonian, if you want any non Newtonian model, you can also choose one of the popular non Newtonian models, power law, Carreau fluids and others. Alternatively, you can also write down your own rheological model here for the viscosity part.

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So, please note that K is the stress tensor, K in mu into this is for the case of the Newtonian fluid.

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Now, if I change this Newtonian relation to non Newtonian, you see that this formula changes and it is written down for the generalized power law formulation where shear rate is given by this expression S.



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Anyway, so, we revert back to Newtonian case and initial value, I mean initial values to the problem, let us define it 0, 0. This is the starting case there is no flow.



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So, important is the I mean the boundary condition by default, it has selected wall boundary condition, wall boundary condition means no slip So, u is equal to zero or the corresponding velocity components is 0, but we know that we have to specify an inlet and outlet. So, we first we choose the select the inlet then we select the boundary the leftmost boundary, so, that is the inlet condition and there the velocity instead of selecting the inflow velocity, it is better

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to select the velocity field. So, there is no y component velocity but there is x component of velocity.

So, the x component velocity entering the system I think we want to instead of providing a constant velocity we it is better or it is recommended that we insert a parabolic flow profile or a positive flow profile assuming that the flow is fully developed in this as it enters the channel, why is because we want to study the von-karman effects or the flow instabilities in a fully developed flow. So, if you do not, if you consider that the flow is still developing at the entry if you cons, if you put in fixed velocities then the flow will be or there will be hydrodynamic boundary layer and the flow will be developing.

So, it will be distorted or it will interact with the boundary layer, separation or formation due to these obstruction in the flow. So, if we consider a fully developed flow I assume that they are previously there is a pipe where the flow gets fully developed before it enters the region of the obstruction.



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The fully developed flow can be written down as like this I hope it satisfies the boundary conditions so, no it does not satisfy the boundary condition. So, we have to choose a slightly different form of the parabolic flow profile so, that the boundary conditions are chosen appropriately.

So, this is can be written down something like this. So, U mean is the centerline velocity and then at the two boundary conditions it satisfies 0. So, the value of y at the top boundary and the bottom boundary divided by half height of the channel will give you 1 and this will give you a parabolic profile. So, this is the way to write down the velocity field and so, we are all set with the problem.

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The next step is to define the mesh sorry, we have also defined the outlet condition I forgot that that is asking that there is some error so, I think we missed some brackets bracket mismatch issue, it is done and we have to also define the outlet condition. So, we select outlet condition and by default we have considered that the outlet shear is 0. So, if I select the total shear is set to zero so, if I select this p0 to be 0, then there is total shear is set to be zero as the default outlet condition and we have also selected the case that backflow is suppressed so means which means that this criteria of the pressure is also satisfied the outside pressure is less than the pressure inside so, there will be no backflow. So, now it is let us verify the boundary conditions.

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So, apart from the inlet and outlet rest everywhere there is no slip boundary condition including the surface of the cylinder or this obstruction.

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Next is the mesh if I click build mesh. Now, please note by default, the software is able to detect the Dirichlet or the no slip boundary condition where there is a strong formation of the boundary layer. So, without any subsequent settings, this is like different from the case of the heat transfer where there was almost uniform structured mesh here you will see that there is a

size dependent machine our machine is different at different locations in the problem because of the no slip boundary conditions in the channel.



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I can further refine a little bit more to have these refinements close to the wall in a better way and accordingly the number of elements in the physics of the system is changed.

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Before we run since this is time dependent process, so it will not be solved in a second or so it will take a minute or a couple of minutes. So, it is better to save it before running. But we have to define the time here, in the previous problem on the heat transfer it was a stationary problem. So, time was not a factor but here time is important.

So, the time that we and please note, this a very interesting part I must highlight here is that a time that you mentioned here or the times where the solution will be reported or stored, it need not to be the case that these are the times where the software will take as the time steps are the problem, it will take its own time steps such that all the stability criteria is satisfied, if you recall that stability criteria, we talked about numerical simulation a couple of weeks before.

So, that stability criteria has to be satisfied the software will inherently take intermediate time steps, so that those stability criteria are satisfied. So, these time steps are the steps where that the solutions will be stored or it will be reported. So, in this case, at least 7 to 10 seconds of simulation needs to be done to get a realistic view of this von- karman formation.

So, instead of defining that discrete time intervals, you can just write as a range function, start time, end time defined by the interval. So, let us say start from 0, every 0.02 second interval, it will store the value and it will go up to 10 second, so almost this same, so, in each second, it will store 50 points and over 10 seconds, it will store 500 points.

Of course, the first initial few seconds, it will take time to develop the von-karman vortex streets but let us have a uniform time stepping for this problem. So, that maybe if you want to optimize the memory of the system, you may not need to save so much of the problem. So, it is always better to save it before running it because it is a time dependent problem, it may happen the software is crashed, or there is some issues during the running. So, we recommend I recommend you always save your file before running.

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Let us also look into the default solver here and this is a time dependent problem. So, there will be additional settings for a time dependent problem, tolerance time stepping is an important part. So, time stepping, I want to highlight this point here what is the method that you want to specify.

BDF is sort of the free method. So, sorry, this time steps taken by solver there are three, four different types, one is free, intermediate, strict, so free means the software will choose its own time steps irrespective of whatever the user has set, but it will report the solution as those user defined time steps.

So, and that is by interpolation. So, if the software do not take those intermediate, I mean those exact values, it will take some other values, let us say it is able to do a higher time step. So, the calculations will be faster. So, in that case, the user time steps will be ignored, but by interoperate will solve I will store those results.

Intermediate means it will choose its own settings or time steppings initially but later on the other way round, initially it will choose its own settings. But later on it will at here to the user defined time steps and strict is it will whatever internal time, intermediate time steps it chooses, it selects it will select, but when the solutions at which it has to be stored, it will take that time step and it will not be by interpolation.

So, depending on the choice you can make free, strict or intermediate, free generally works faster because as the software is free to take its own time step as long as it can get a converse solution for that problem, anyway, so for this problem free is sufficient and good enough.

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Compile Equations: Time Depende		[Mar 2b, 2022, 3:43 PM] Complete mesh consists of 11728 domain elements and 4/8 boundary elements. [Mar 2b, 2022, 5:45 PM] Saved file: D:Dropbox/working-folder-shared-with-all-devices/NPTEL_course/PMS-course/lecture_ppt_before_recordings/
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So, we just do the calculations here we click on this compute. So, please note that almost 11,000 elements are there. I also click on this log there are several other solutions settings of the solver. Of course, that is beyond the scope of this class, but please look into them. There are several tutorials with the COMSOL website with which you can get a fair idea of the process, but please note, so we just click the compute button. So, now you cannot change any other settings everything will be frozen and the computer will, software will try to work on the calculations.

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You will see there is also a convergence plot. So, this convergence plot tells you that what is the reciprocal of the time steps and it tells you that it has failed in this case to find a reasonable solution.

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So, often, when you when you get a failure instead of worrying about the software solver settings are the process first try to look into the physics of the problem is there is something which you are making a mistake. So, that is something which needs to be fast introspected before you start thinking about the software issues.

So, since the software has an issue the first thing that comes to the mind is the definition of the initial values that is where things may go wrong. So, we have selected the initial value to the problem to be 0 everywhere. So, that is something that the software may find it difficult to initialize. So, that may not be the scenario in this problem as the initial fluid velocity may not be zero everywhere that is one condition or there could be an issue with the boundary conditions.

So, in the boundary conditions, we are defined the inlet velocity in this way and I hope it satisfies the boundary condition, because if the inlet does not satisfy the boundary condition or the wall conditions of no slip then there could be an issue, but I think this is fine. Let me check it once.

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So, this is fine, and initial value let us instead of zero let us give some initial values to the problem and so, that it will slowly get the software will try to calculate the velocity profile but still we see that, so, this convergence plot is a plot with respect to the time steps versus the step size reciprocal of the step size. The reciprocal of the step size suggests that what is

the time step, time step size the software is taking and what is the inverse of that. So, high a smaller is the time step, size of the time step the higher would be its reciprocal.

So, in a way is just to give you an idea that as this curve moves upwards, it means the software is unable to converge for a larger time step or there are so much of variability in the temporal dynamics of the problem such that the system is not able to converge or the stability issues that are coming in the picture that is why it is taking smaller time step and as a result the reciprocal increases.

And x axis is the number of time step or the number of iterations that it is calculating and slowly you will see that in the log there are some printouts I mean the displays that messages you are getting as written as out, out. So, you can just freeze the this thing here by clicking on the clock. So, it will continue to log other results, but it will store it will stay at that point and see that these are the points 0.32, these are the points where the software is saving the result since it is a user defined time interval. Accordingly the calculations are proceeding and we have given time step up to 10 seconds.

So, the adequate vortex formations or vortex formation transitions can also be explored at the right bottom you see this progress bar that is going on. So, since, this is a slightly sophisticated calculation, it is solving the U profile, solving the V profile, solving the pressure profiles, so three dependent variables are getting solved. The number of degrees of freedom for this problem is also large. And initially there was a significant issue with the computation regarding the startup or the initialization of the problem. And now, you see that the time step is almost 0.001.

So, it takes some time to reach possibly to reach up to 10 seconds maybe, but eventually you will realize I mean now it has almost the software is set to this value of 0.001 which means that this is the time step which satisfies all the stability criteria. And further increasing the time stepping is not possible considering the dynamics of the process. And that is why this is the time step that we can achieve in this problem. And that is how the software automatically sets it. Of course it is reporting the value that the user defined functionalities.

So, please note that if you increase the mesh size there is a possibility that the time steps can be increased. So, that is a trade-off between the memory requirement and the computational time if you recall the Von Neumann stability criteria or the CFL stability criteria you will see that if you reduce I mean at least the Von Neumann stability criteria tells you that for smaller step sizes it is possible that you can have larger time steps that that sort of things is possible. But, anyway I think the slowly the problem will come to a closure almost one second is over for this problem.

Please note that during the calculation it is not possible to change any one of the parameter values it can only be done before the start or after the end and do a recalculation. So, I think we will wait for some more time before the calculation is over and almost 20 or 20 percent of the calculation is done and we are almost two seconds of the physical time for this problem. And couple of more things I should highlight about the software use is that as you try to work on complicated problems involving complicated geometries more than one physics for example, if you have fluid flow along with heat transfer for example, natural convection you will have this problem of multiple physics getting coupled.

So, in that case you have to choose two physics from the beginning or you can also add it later on, but then in one of the physics where you try to incorporate the let us say in the thermal convection problem or the natural convection problem, the temperature equation or the energy equation will have the velocity field in the problem. So, the velocity field which is solved from the laminar flow module or from the Navier Stokes equation, those independent, so those dependent variables u, v, w can directly be written down as the velocity field components in the heat transfer equation, that is the beauty and the power of the flexibility that is present in the software that you can directly couple the multiple physics present in the system in this case.

So, there is a nice tutorial problem related to this Rayleigh-Benard convection, which is something you have studied in your heat transfer class and there is something you can simulate using this software in the COMSOL website you can go and check out the tutorial there.

There are also some exciting tutorials related to this free surface flows, mass transport problem, species transport convection, adsorption is something that you can also model it out because if you just include the advection sorry the adsorption equilibrium, the adsorption phenomena or that absorption process can also be simulated in this case. So, any user defined function can easily be incorporated.

Additionally, if you want to change any material properties as a function of time or a function of space as it to be in anisotropic case or something like that, then you can use those functional forms of the material properties with which you can show the results, sorry which you can do the calculations. Mesh generation is a very interesting and exciting topic and often depending on the generation of the mesh, the solution characteristics change, there is something known as the mesh independency check, which is that as you refine your mesh, the mesh size becomes smaller.

So, during the discretization the error in the, this Taylor series expansion or the error due to the higher order terms when you try to linearize the function, the error due to the higher error terms is less. The solution becomes more accurate as you reduce the size of the mesh. But even if you reduce the mesh size further, the solution accuracy may not improve significantly. I mean, how much significant the results should be. I mean that is relative context whether you want accuracy of the third decimal place or accuracy of fifth decimal place is something for you to decide, but you will always see that with the decrease in the mesh size or increasing the number of mesh elements, the relative change of the solution will be less.

So, you have to decide that what is the maximum resolution of the mesh or what is the optimum resolution of the mesh that you want to work for your problem. So, the mesh as you increase the mesh size, the accuracy will increase and then it will kind of plateau. So, beyond increasing the number of mesh elements or the resolution of the mesh and decreasing the mesh size will not affect the solution accuracy. And that is something we say as the independency or the machine dependency check.

And whatever the solution parameter you are talking about, whether it is the mass conservation, the outlet flow or the total enthalpy, balance conservation, whatever property that you are talking about, that has to be calculated for different mesh size, and then you try to make a comparison that what is the level of accuracy that you are obtaining for this problem and that should be the mesh size with which you should work further in the problem. So, that optimum mesh size should be used and your mesh size should be such that the solution parameters are the solution accuracy is unaffected by the choice of the mesh, that is the mesh or the minimum mesh variation that is needed for the problem. So, I think the solution results are available with us and I can show that.

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So, this is a plot of the total velocity magnitude, not the U or the V component, but the total velocity magnitude that is root over a square plus b square.

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So, if I try to see that after some point you will see that at the top the times are written and just I am moving forward in time that how the velocity field is changing and how you can see that the flow is getting distorted and finally, we will see that how the vortex von-karman vortex are formed.

So, you see that, these vortex whichever is found is alternate zones of high and low magnitudes and accordingly there is pressure fluctuations so, you can clearly see that how the vortices are formed in this case and how it is propagating due to this I mean this vortex is whatever the vortex are form is because of the presence of this obstruction in this system and how it is propagating with respect to time.

And slowly this zone of vertexes will actually diffuse out further downstream if the length of this pipe is more, but there is a certain range of the pipe beyond or certain length of the pipe beyond the after the cylinder where these vortices are actually quite prominent. And that is what we are observing here that with time how the fluctuations or instability in the system is actually present and it is changing temporarily that is why a steady state solution is impossible in this case. You can also look the respective U and the V profiles, where you so, this is the U profile and this is the V profile.

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So, there is alternate upward and downward velocity. So, the red is upward velocity and the blue zones is the downward velocity. So, this shows that there is the formation of the vortices, you can also have a plot of the streamlines, let us try that out.

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So, I can also get a streamline plot there is a direct function to get the streamline plot, so, I have to select uniform density.

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So, if you look into the streamline plots also you will see that how the vortices are formed and how the streamlines are getting affected in this. So, this is also the streamline plot where the circular vortex can also be observed immediately after the circular obstruction and how this vortex is getting transported along the channel.

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So, I hope all of you liked this simulation of the von-karman vortex street formation. And I also encourage all of you to try out some of the other tutorials that is available online. Thank you. I hope you found this demonstration of the COMSOL Multiphysics software useful.