

**Mathematical Modelling and
Simulation of Chemical Engineering Process
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Lecture 10
PDE – integral transforms**

Hello everyone, in this lecture, we are going to study about the different integral transform techniques that is generally used for solution of linear PDEs particularly the analytical solutions.

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So, just getting started all of you are aware of the you know these two popular transform techniques. I am sure you must have studied this in your (you know) undergraduate engineering mathematics that is related to Laplace transform and Fourier transforms. Now, here we are just going to see that how these techniques can be used to transform a PDE and to convert it into an ODE and then how the solution can take place.

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Linear PDE whose solutions are periodic in nature.
An integral transform $F(s)$ of a function $f(t)$
can be described as $F(s) = \int_a^b K(s,t) f(t) dt$
Kernel

So, let us begin today's class as you know that for any PDE which have (you know) this solution is periodic in nature. So, a linear PDE whose solutions are periodic in nature can be essentially solved by this technique of the integral transform. So, an integral transform is nothing but you know this transformation of one of the coordinates or one of the independent variables using a kernel function. So, the integral transform, let us say $F(s)$ of a function $f(t)$ we can describe this as... So, this k is a kernel. So, using this kernel we can essentially transform this function $f(t)$ into the integral domain. Now, these kernels so, this is essentially a kernel and this kernel represents, I mean the functional form of this kernel tells you that what sort of (you know) integral transform are we going to use.

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Type	$k(st)$	a	b
Laplace	e^{-st}	0	∞
Fourier	$\frac{1}{\sqrt{2\pi}} e^{ist}$	$-\infty$	∞
Fourier sine	$\sqrt{\frac{2}{\pi}} \sin(st)$	0	∞
Fourier cosine	$\sqrt{\frac{2}{\pi}} \cos(st)$	0	∞
Hankel	$t J_n(st)$	0	∞
Melline	t^{s-1}	0	∞

So, some of the examples of these kernels are let us say, will list down some of the popular ones and let us look into the kernel functions and also their integral limits. So, for the case of Laplace transform, this is an exponential function, the kernel is an exponential function and this is always in the semi-infinite domain. In the case of Fourier transform, the kernel function is like this in the complex domain and it is in the full infinite domain. There are two subcategories of Fourier transform, the Fourier sine and the Fourier cosine functions based on the trigonometric sine and the cosine functions, both of which are in that semi-infinite domain.

Next is the Hankel transform. This is also sometimes you know popular particularly for cylindrical coordinate systems and involves the use of the Bessel function as the kernel and then also you have to Mellin transform. There are several other such kind of you know transformation techniques, but these are generally the most popular types of transform. So, in this lecture we are going to mainly focus on the Laplace and the Fourier transform. So, let us to begin with the Laplace transform and as you know the Laplace transform involves the use of the exponential function.

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Laplace transform

$$\mathcal{L}[f(t)] = \int_0^{\infty} e^{-st} f(t) dt$$

Inverse transform

$$f(t) = \mathcal{L}^{-1}[F(s)]$$

Properties

1. Associative
$$\mathcal{L}[c_1 f_1(t) + c_2 f_2(t)] = c_1 F_1(s) + c_2 F_2(s)$$
2.
$$\mathcal{L}[e^{at} f(t)] = F(s-a)$$
- 3.

So, let us talk about the Laplace transform. So, \mathcal{L} (say \mathcal{L}) is a Laplace operator. So, if I use this Laplace transform over a function $f(t)$, it essentially means I am going to do this or use this kernel function and will give me the Laplace transformation of the original function in the Laplace domain. Similarly, once we get something in the Laplace domain, you also need to get back to the original time domain.

So, writing something in terms of s is in the Laplace domain and writing something in the in that time domain is like the original domain. So, if you want to get back your you know transformed function into the original fraction you need to do the inverse Laplace transform. So, let us call the inverse Laplace operator as \mathcal{L}^{-1} , we will talk about the inverse Laplace transformation and the end.

So, what are the properties of this Laplace operator is that, first of all it is associative in nature which means that, if I try to operate over two functions, summation of two functions which is equivalent to its individual summation in the Laplace domain. If you have (you know) function which is multiplied with the exponential function. This means that in the Laplace domain it is just the negative of that. Differentiation perhaps this is the important you know property.

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3. Differentiation

$$\mathcal{L}[f^{(n)}(t)] = s^n F(s) - s^{n-1} f(0) - s^{n-2} f'(0) - \dots - s f^{(n-2)}(0) - f^{(n-1)}(0)$$

So, $\mathcal{L}[f''(t)] = s^2 F(s) - s f(0) - f'(0)$

$$\mathcal{L}[f'(t)] = s F(s) - f(0)$$

“Handbook of mathematical functions” by Abramowitz & Stegun



So, in general operating the Laplace transform over nth derivative are you know this nth derivative of a function can be written down in terms of this polynomial expansion. Please note that when I write something as capital F, it is in the Laplace domain and something written down in as small f is in that time domain. So, just to simplify let us say if I want to do the Laplace derivative of a second (you know) second order equation, then I would get something like this, similarly, for the this first order equation and we getting something like this. So, we can look into any math standard mathematics textbook to get more about (you know) these properties of the Laplace transform and its integration properties and all those things.

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Example

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}$$

@ $t=0, u=0$
 @ $x=(0,1), u=1$

Take Laplace transform on both sides,

$$\int_0^{\infty} e^{-st} \frac{\partial u}{\partial t} dt = \int_0^{\infty} e^{-st} \frac{\partial^2 u}{\partial x^2} dt$$

$$\Rightarrow s U(x,s) - u(x,t=0) = \frac{\partial^2 U}{\partial x^2}$$

Since $u(t=0) \rightarrow 0$

$$\Rightarrow \boxed{\frac{d^2 U}{dx^2} - sU = 0}$$

So, now, let us look into an example problem for this (you know) unsteady heat transfer equation is something we have also tried to solve using separation of variables (isn't ?) in the previous lectures you have you know that already so, the boundary conditions are defined as t is equal to 0 u is 0 and that x is equal to both the boundaries you have u is equal to 1.

Now, take Laplace transform on both sides so, please note that in this equation we are going to apply on the time domain. So, the terms where you have the time derivatives will be getting converted into the Laplace domain and part for the spatial derivatives will just that dependent variable will be converted to the Laplace domain. So, if I do this, what do I get... this is the left-hand side and right-hand side.

So, the left-hand side I can easily write down from the differentiation property it is s into $U(x,s)$. So, capital U is in the Laplace domain now, and this is nothing but x and value at t is equal to 0. So, in the Laplace so, the C2 equations of the variables get converted only in the Laplace domain right are the ones that is in the time domain that part gets converted to the Laplace domain and in the right-hand side it is nothing but things that are getting changed in the Laplace domain with respect to the derivative of x . So, this entire thing can be written down as $\frac{d^2 U}{dx^2} - sU = 0$. And this is nothing but my capital $U(s,x)$, is not it?

So, from this one, you know that since u at t is equal to 0 is equal to is nothing but 0 the initial condition so, you get the equation that. So, this is the (you know the) reduced form of the PDE into an ODE in the Laplace domain, is not it? So, in this case you do not have any time derivatives, so the time derivatives are getting transformed in the Laplace domain and essentially you will end up with an ODE.

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Homogeneous linear ODE \rightarrow transformed eqn:
 $u(x,s) = C_1 \exp(\sqrt{s}x) + C_2 \exp(-\sqrt{s}x)$
 @ $x=0, u=1 \Rightarrow u(x=0,s) = 1/s$
 BC also needs to be converted in Laplace domain
 $C_1 + C_2 = 1/s$
 @ $x=1, u=1 \Rightarrow C_1 \exp(\sqrt{s}) + C_2 \exp(-\sqrt{s}) = 1/s$
 $C_1 = \frac{1 + \exp(-\sqrt{s})}{2s \cosh(\sqrt{s})} \quad C_2 = \frac{1 - \exp(\sqrt{s})}{2s \cosh(\sqrt{s})}$

So, this is a second order linear ODE. And equation to this this this equation this ODE is very well known in term of the exponential. So, this is a homogeneous linear ODE. The transformed equation is a homogeneous linear ODE and the solutions to this equation is in the Laplace domain of course, C_1 exponential root over s and x plus sorry, C_2 into exponential minus ... alternatively you can write this in terms of the sine hyperbolic and the cos hyperbolic terms.

So, let us use the boundary condition. So, the first boundary condition is at x is equal to 0 you get you have u is equal to 0. So, what does this mean I do the transformation of this boundary condition sorry it is u is equal to 1 not equal to 0. So, in the Laplace domain u have to be I mean 1 has to be also considered in the Laplace domain. So, these boundary conditions, so, the boundary condition also needs to be converted in the Laplace domain.

So, this equation tells you that capital $U(x$ is equal to $0, s)$ is equal to so , Laplace transform of 1 is 1 by s . So, this translates to the condition that x is equal to 0 you have $C1$ plus $C2$ is equal to 1 by s . Similarly, at x is equal to 1 you also have u is equal to 1 which implies $C1$ root over sorry $C1$... Again, this has to be converted into the Laplace domain and Laplace transformation of 1 is 1 by s .

So, these are the two equations using the two-boundary condition that you get and you can easily (you know) resolve these equations and you will be getting if you work out the steps $C1$ is equal to 1 plus exponential minus root over s divided by $2s$ cosh root s , this is $C1$ and $C2$, would be 1 minus exponential root over s divide by $2s$ cosh root s . So, with this knowledge of the $C1$ and $C2$ you get the complete solution of this transformed variable u in the Laplace domain.

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Inverse Laplace $u(x,t) = \mathcal{L}^{-1} [U(x,s)]$

$$f(t) = \mathcal{L}^{-1} [F(s)](t) = \frac{1}{2\pi i} \lim_{T \rightarrow \infty} \int_{\gamma - iT}^{\gamma + iT} e^{st} F(s) ds$$

where the integration is done along the vertical line $\text{Re}(s) = \gamma$ in the complex plane such that $\gamma >$ real part of all the singularities of $F(s)$ & $F(s)$ is bounded on the line.

Now, to obtain the final solution, you need to do the inverse Laplace transform. So, inverse Laplace transform once you do over this equation, you will get back the solution back in I mean in the original time domain. So, please note that here the spatial components are not getting transformed, it is essentially the time components that we have tried to transform in the Laplace domain. So, whether you consider a time domain or a space domain, let us say if you have a multi-dimensional steady state problem, then you do not have the time domain it is like 2 spatial

variables. So, you got take choose any one of the spatial variables and convert it into the Laplace domain and then additionally at the end you do the inverse Laplace. So, at least one of the (you know) this dependent (sorry) independent coordinates are in terms of the independent variable you can do the Laplace transform. So, now, if you have (you know) more than two independent variables in the system.

If the PDE does have three or four independent variables. So, in that case, we have to repeatedly do the Laplace transform to reduce it final to bring it down to the ODE. So, if you do Laplace transform over one of the independent coordinates, it will remove that coordinate and but still you will be getting another PDE let us say that it is a three-dimensional unsteady state problem.

So, you have almost four you have four independent variables, time and the three you know the dimensional coordinates. So, if we apply the... this Laplace transform once it will remove one of the coordinates but still it is a PDE, so, you use it again then you use it again and ultimately when you get an ode you get the solution then you continue to do the inverse Laplace transform.

So, the formula for the inverse Laplace transform stands slightly complicated and let me just try to explain you, but please note that there are standard available (you know) charts for this you know most functions or mathematical functions. One of the good books to follow for this you know this mathematical function is Handbook of mathematical functions by Stegun and Abramowitz and you will find several list of the mathematical functions based on Laplace transform and inverse Laplace transform.

So, this integration is done along the vertical line after real part of the Laplace variable s in the complex plane such that this gamma is greater than the real part of all the singularities present in $F(s)$ and $F(s)$ is bounded in the time domain. So, now with this we complete this part of the Laplace domain let us move next to the Fourier transform.

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Fourier transform:
$$U(\omega, t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} u(x, t) e^{i\omega x} dx$$

Inverse transform:
$$u(x, t) = \int_{-\infty}^{\infty} U(\omega, t) e^{-i\omega x} d\omega$$

Properties:

- Linear operator
$$f [c_1 f_1(x) + c_2 f_2(x)] = c_1 f [f_1(x)] + c_2 f [f_2(x)]$$

The slide features a background with technical icons like gears, a circuit board, and an atom symbol. A small video inset in the bottom right shows a man in a light blue shirt. The NPTEL logo is visible in the bottom left corner.

As you know the Fourier transform is also a very powerful technique and often Fourier transform is used to decompose the function into its different frequency domain a frequency components. So, using the same idea, Fourier decomposition of a variable can be written down as something like this... Let us not confuse you with So, let us say I have you know variable u as a function of space and time. So, if I want to get it converted in I mean do a Fourier transform and get it converted into the frequency domain and multiply with this $i\omega x$ and this will get it converted into the frequency domain.

Interestingly the inverse transform Fourier technique is quite straightforward instead of just e to the power $i\omega x$, you can do minus $i\omega x$. So, here also we follow the same variable description something which is written capital is the transformed variable, and small is the original variable. Now, what are the properties, so, some of the important properties of Fourier transform are it is a linear operator. So, it has the same associative property, if I apply a Fourier transform over to linearly independent function then it is equivalent to the Fourier transform of each of the individual functions.

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• If $f(x)$ is odd/even then $F(\omega)$ is also odd/even

• Derivative

$$F\left[\frac{\partial^n u}{\partial x^n}\right] = (-i\omega)^n U(\omega, t)$$

So $\Rightarrow F\left[\frac{\partial^2 u}{\partial x^2}\right] = -\omega^2 U(\omega, t)$

So, if $f(x)$ is the original variable is odd or even function then the transformed equation, the transfer function is also odd or even. Important part is the derivative property or the differentiation so, for n th order differentiation, this is the (you know) transformed this is the formula and so, it means that for second order equations (sorry) so, this is for n th order equation. So, from this you can also easily write out what happens to the second order equation or the second order component and this is what is most relevant for our case.

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Heat $u_t = k u_{xx}$ BC $u(-\infty, t) = u(\infty, t) = 0$
IC $u(x, 0) = f(x)$

Taking FT on both sides.
 $\frac{\partial}{\partial t} v(\omega, t) = -k \omega^2 v(\omega, t)$

Generic solution: $v(\omega, t) = C(\omega) e^{-\omega^2 k t}$

IC @ $u(x, 0) = f(x) \Rightarrow v(x, 0) = \frac{1}{2\pi} \int_{-\infty}^{\infty} f(x) e^{i\omega x} dx$
for $t=0$, $v(x, 0) = C(\omega)$

So, let us see an example, let us consider the same heat equation conductive heat equation, 1 dimensional transient time dependent heat equation and the boundary condition at plus and minus infinity, so, it is in the full infinite domain is equal to 0, and the initial condition is a function $f(x)$. So, now taking the Fourier transform on both sides, you get the left-hand side gets converted to the Fourier transform variable and the right-hand side is the double derivative terms. So, we write that as minus k omega square in the transformed variable.

Now, please note here that we apply the Fourier transform generally over the space variable whereas, in the case for the Laplace equation, we apply the Laplace transform in the time domain. This is generally the normal, I mean the case but again of course, if you do not have time in your system, then you will be applying into one of the space domains. But generally, Fourier transform is applied over the space domain.

Now, in this case, you can easily see that the equation in this case is just a first order linear ODE and the (general) generic solution to this equation can be written down as in the (you know) frequency domain as C omega, C omega e to the power minus omega kt . Now, using the initial condition at u is equal to 0 you have this $f(x)$.

So, which means, if I just want to convert this into the you know transformed coordinates capital U, I would need to convert the boundary condition same as the Laplace transform. So, this means that if for time t is equal to 0, I have from this equation u capital U(x, 0) is equal to C omega. So, this is how you are going to get your constant of the integration C taking the Fourier transform of f(x).

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Now, the inverse transform

$$u(x,t) = \int_{-\infty}^{\infty} c(\omega) e^{-i\omega x} e^{-\omega^2 kt} d\omega$$

$$u(x,t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} f(\bar{x}) \left[\int_{-\infty}^{\infty} e^{-\omega^2 kt} e^{-i\omega(x-\bar{x})} d\omega \right] d\bar{x}$$

Now, doing the inverse transform, now, the inverse transform. So, inverse transform will take us back from the frequency domain to the space domain. And multiply with minus i omega x. Now since, C is also a function, it is also integration so, this equation will ultimately get converted with 2 integrals. This will give you the complete solution by doing the inverse Fourier transform in this case.

So, couple of things let us just quickly conclude here, couple of things that we have realized or done today is the Laplace transform and Fourier transform and some of the important differences is that in the Laplace domain you generally take the transformation in the time domain, whereas in the Fourier transform, you generally take this transformation over the space domain. And in both cases, the solution has to be periodic. The operational limits for the Fourier and Laplace domain is that Laplace domain can be applied over finite domains, whereas, Fourier transform

has to be in the infinite domain. So, this is one of the constraints, in case you have if you have your problem on the semi-infinite domain, then you can alternatively use the Fourier sine or the Fourier cosine transforms.

So, these are the ways to reduce the PDE to and or simplify the PDE to and ODE. And that is how you solve the ODE and do the inverse transform to get back your original solution. So, I hope you have liked today's class. In the next week, we are going to start the different numerical techniques for the solution of PDEs. See you in the next week. Thank you.