Introduction to Civil Engineering Profession
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Lecture – 20
An Overview of Computational Science and Engineering

Sitting on that side of the desk myself, so I thought I can run you through some of the things that I have been doing in the past 10 years or so, and give you an overview of Computational Science and Engineering.

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My name is Chandra Annavarapu, I joined the Civil Engineering faculty here just about 10 days ago and let me walk you through some of the paths that I took to get here.

So like I said, I was sitting on the other side of the desk, about 12 years ago. I was I am a B Tech in Civil Engineering from IIT Madras myself, and I remember taking this course back when I think Professor Matthews was coordinating the lecture series. And I also remember being very wide-eyed not knowing what, not just civil engineering, but what engineering is.

You know, I would confuse routinely confuse the engineering with science. I think, you guys are way ahead of me in the game because as I understand this is the internet age you have your phone in your hands, you have Wikipedia, you have Quora, I do not know you have all these avenues of information. So, you must know a lot more than me about civil engineering.

I would have made this lecture a lot more interactive, but I understand that they are recording me. So whatever you say, maybe we cannot get that on the video, but let us have that discussion when we have a q and a sometime later.

So after my B Tech, I liked what I was doing. So, I went ahead and did a Ph.D. in Computational Mechanics which is which sounds very fancy, but you know it is a subfield of mechanical, civil and aerospace engineering.

So, I will talk a lot more about this in the talk. But after doing my Ph.D, I went ahead and worked at a Department of Energy, National Laboratory for 5 years sort of expanding on what I did in my Ph.D. and developing these large-scale simulation platforms to simulate reality. more or less in the geoscience space, I will talk some of that talk about some of that later too.

And I worked at ExxonMobil Corporation, also as a Computational Scientist and now back here I am to maybe make your life easy or difficult, I do not know, we will see.

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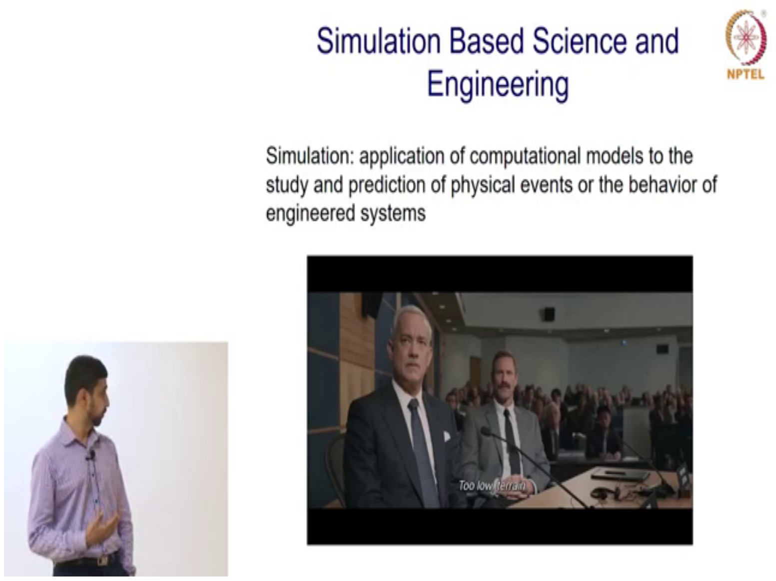

So, before we get into any of what these computational science, is what computational engineering is, a let us start with the basics. So for any of these principles, we need to simulate reality. And when you talk about simulation, the definition is out there for you can see, its essentially defining a computational model that is simple enough for you to study and predict any of the physical events that happen outside in nature.

Well, that is a very drab definition, I do not know how many of you would be able to relate to it. So I thought that I will play a clip of a movie, let us see how to get rid of the laser pointer.

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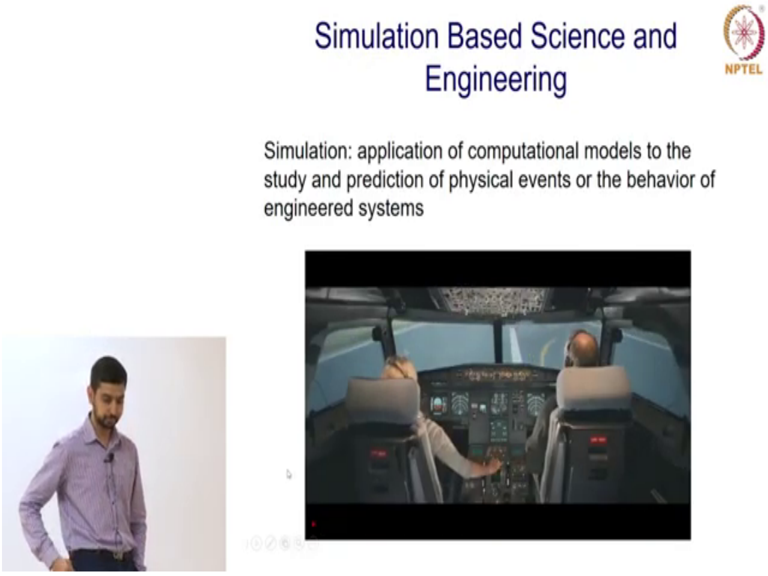

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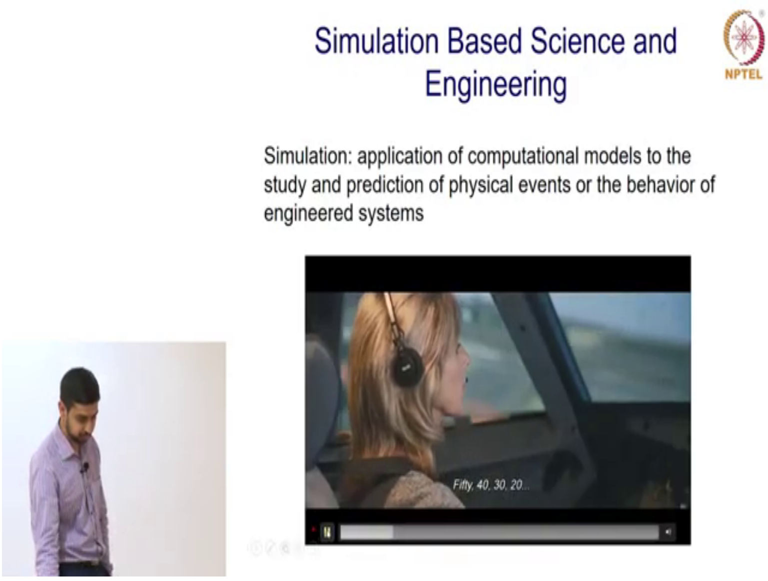

So I do not know how many of you have seen this movie, its a movie called Sully where, basically its about a real event where the pilot tries to land the aircraft or in Hudson river, because he realizes that its going to crash otherwise. So, what they are trying to do here is they are trying to figure out whether that was the best course of action for him to take or whether he should actually have followed the guidance that was given to him by Air Traffic Controllers and go and land it in a nearby airport. So, if you have not seen this movie, I highly recommend it by the way.

Successful landing at Teterboro, runway 1-9.

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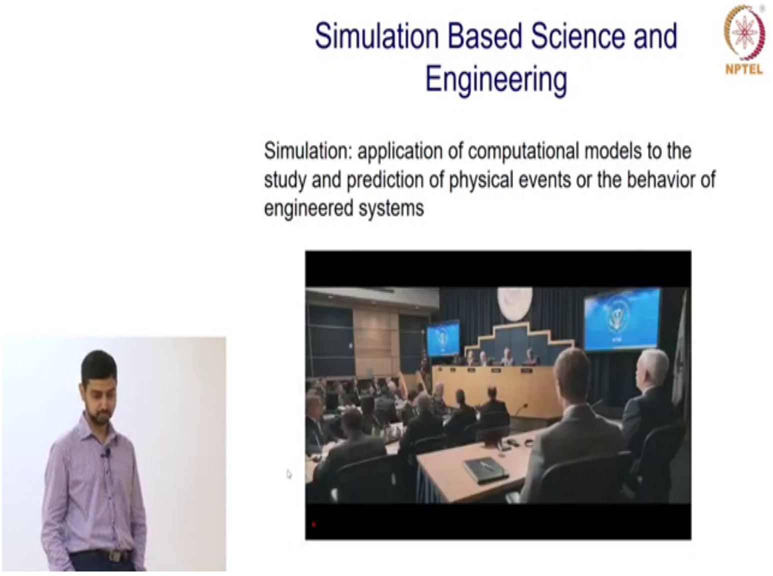

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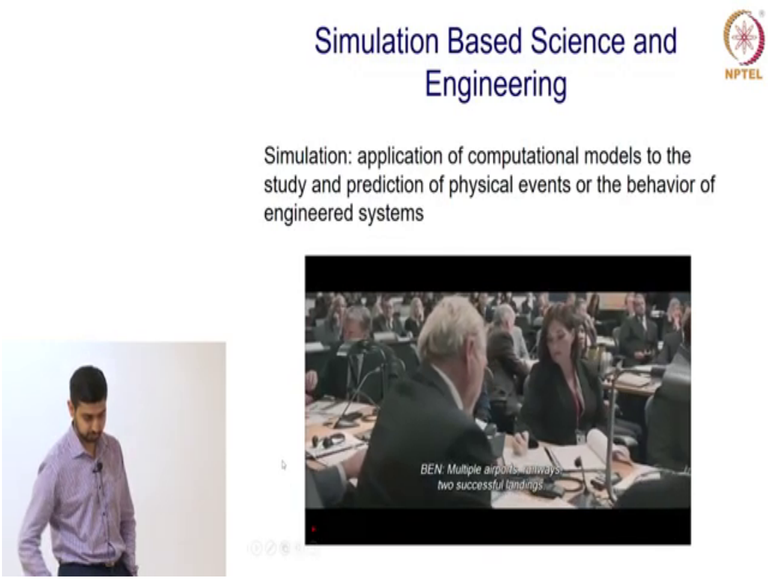

Multiple airports, runways, two successful landings.

We are simply mimicking what the computer already told us.

A lot of toes were stepped on in order to set this up for today and frankly, I really do not know what you gentlemen plan to gain by it.

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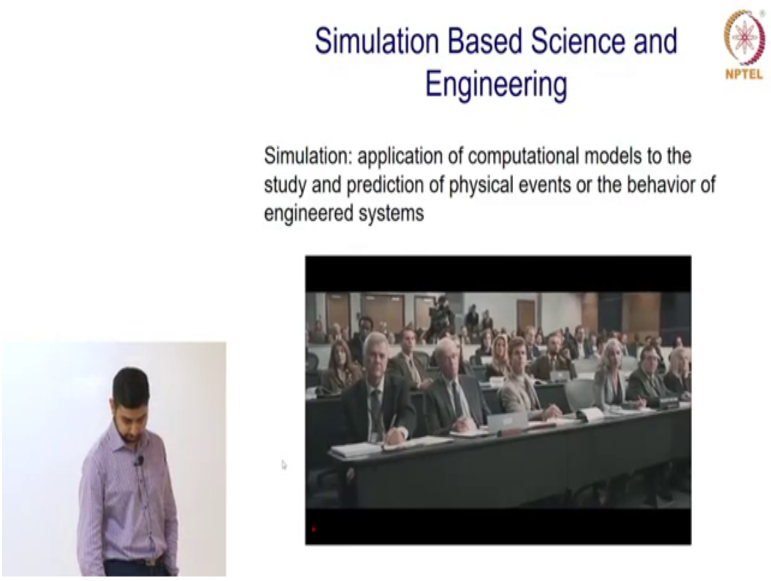

Can we get serious now?

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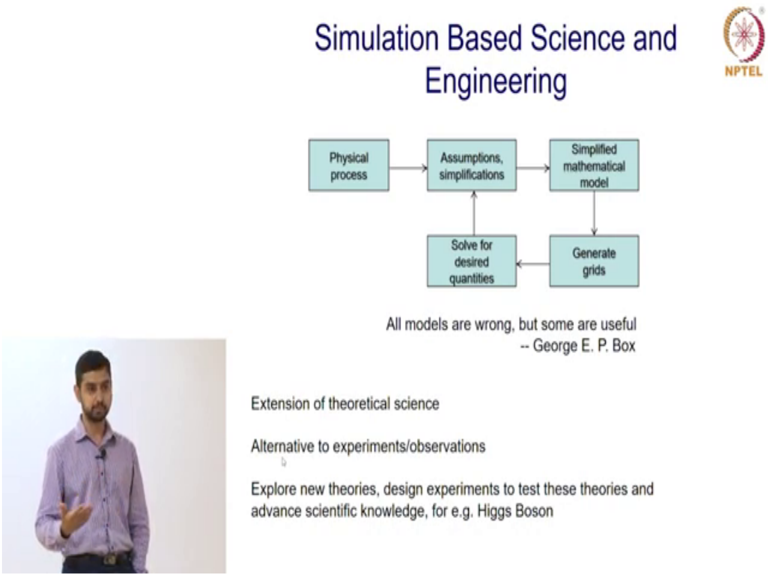

All right, Tom Hanks has asked us to get serious. So, we have to get serious, I guess. So, what he is really trying what they were really trying to do there is essentially run a flight simulator. So, that was a practical example of what simulation is, it tries to mimic reality, you try to model a real event and see what would happen when you cannot really do it as an experiment.

So, just to give you a quick overview you have a physical process and for you to simulate it on the computer, you have to come up with a simple enough model which you can mimic on the computer. And for you to develop this simple model you need to come up with assumptions and simplifications of the physical reality.

So, and once you have the simplified mathematical model, then you have to approximate it on the computer using some sort of discretization. So, you break of a complex geometrical shape into many tiny pieces and you solve this simple mathematical model on those each of those tiny pieces.

You solve for the desired quantities and then you start reiterating your start iterating on the loop. So, you relax any assumptions you think that you that should not have been there in the first place and then you keep solving till you are satisfied with what you obtain as desired quantities. But in this process, what happens is that because of the many assumptions and simplifications, your mathematical model may just be that, its a model it may not necessarily be reality.

And that is why its always good to keep this pithy saying at the back of your mind that is that all models are wrong, but some models can be useful. What that means is that models can be informative, they can within certain application areas the assumptions that you are making may in fact, be reasonable enough.

So, what this framework allows you to do is that its an extension of theoretical science. So, all these pen and paper calculations that you are used to doing they are very good for really simple problems, but when it comes to complicated reality, you may not be able to do those things on pens and papers because it may just take too long for you to do them or you may just have too many variables in place that you cannot necessarily solve any of these.

These are this method for science and engineering is a very good alternative to experiments and observations and the reason for that is maybe alternative is not the right word, I think its a very good complement to experiments and observations.

And the reason for that is that experiments can be really expensive and the same goes for observations, there are many; there are many phenomena that you may not be able to observe either with just your eyes or because of the spatial location, you know like you do not know what is happening in Mars unless you land a Curiosity Rover there, right.

Exploring new theories, designing experiments to test these theories out and advanced scientific knowledge. For example, the Higgs Boson I mean we are going into particle physics right now. But Professor Higgs had come up with this particle way back in the 1960's and then they devised experiments, they went into the I mean you may have heard of the particle accelerator at sun and then they did all these colliding a particle colliding experiments and then they were able to verify his predictions that he made way back in 1960's.

And there are several computational models out there which were able to predict it. So, these computational models are able to help you design these alternate experiments that could eventually advance scientific knowledge.

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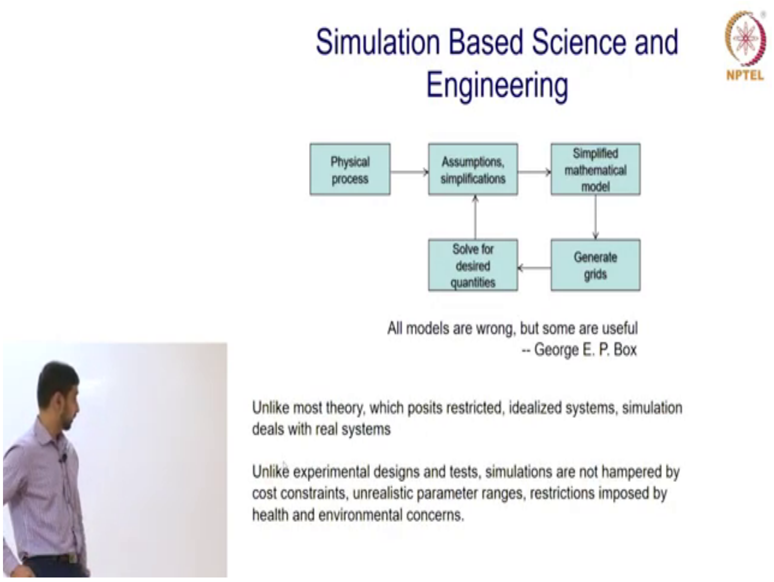

More advantages, so like I said, unlike most theoretical arguments which are always predicated on idealized systems, let us go back to your high school physics. Right, what do you start with? Let us assume things are in vacuum, in a frictionless state or something like that and that has never what happens in the real world.

So, the simulation based science and engineering tries to address those limitations. And you come up with models for real systems, and like I think mentioned in the last slide unlike experiment design experimental designs and tests, we are not necessarily as constrained by cost. I mean, these things will still cost, right.

I mean, you have to basically run these models on a maybe a super computer, you have to have very advanced people who are developing these models and writing these large-scale codes. So, there is a cost to all of it, but that is nothing as compared to the cost of let us say an equipment that is available only for some hundreds of crores of rupees or millions of US dollars, right.

Moreover, you can run any of these models on the computer screen without worrying about what sort of adverse effects its causing on the environment or the health of the person who is running these experiments because, I mean this is a virtual laboratory its not a real laboratory. So, the regulations and restrictions that you need to place on them are also much smaller.

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So, let me set the stage for this video. So, the idea behind this presentation I am giving is to give you some sort of an overview of what application areas are available for these simulations and these computational models that we develop. And one of the areas is energy sector which is where I worked for about 5 and a half years now.

So, I have a very good understanding of and I can sort of relate to it how these computational models are actually addressed in real world challenges, how they are making oil and gas recovery much more efficient and how that translates into real world money and engineering. So, what I have here is a video from this company called Marathon Oil Corporation this operates in Texas in the United States of America and they are very heavily focused on extracting unconventional oil and gas sources.

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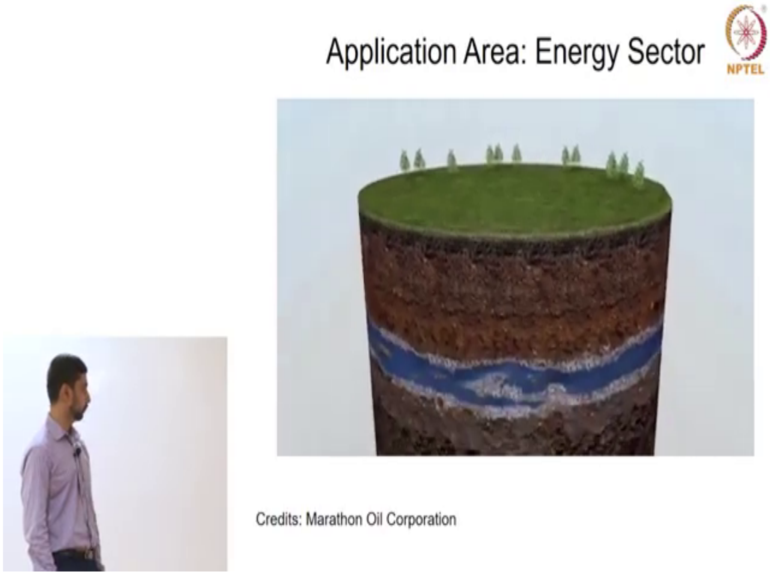

And what unconventional oil and gas sources means is that till not long ago, these sources were considered to be very economically unviable because of where they are and how less permeable the rocks where these oil and gas resources sit.

So, for you to actually extract them you have to spend in so much money and by the time they come out into the market, they are no longer economically profitable. But, because of technological advancements in the past decade or so, these resources have become economically viable.

And simulation has a large part to play in that and here, I think this video will explain what the real world engineering challenges are and then we will go back and look at how simulation can actually address some of those values.

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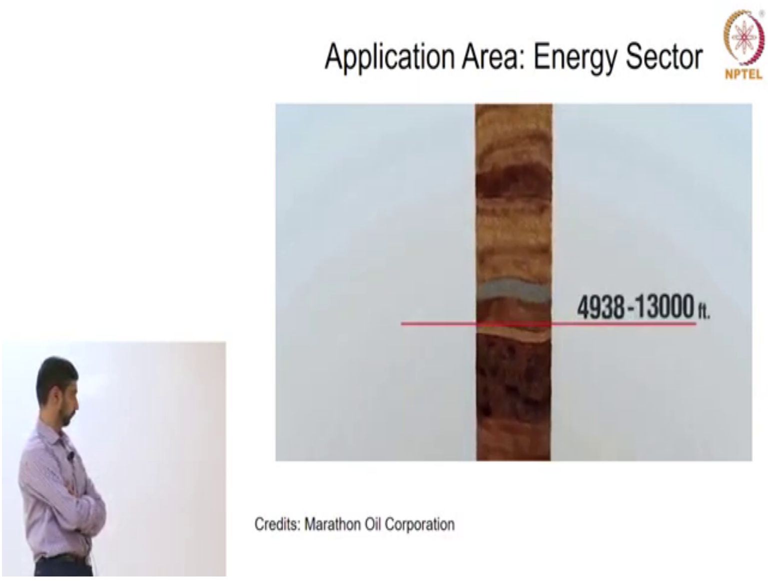

Geologists have known for years that substantial deposits of oil and natural gas are trapped in deep shale formations. These shale reservoirs were creating tens of millions of years ago.

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Around the world today with modern cars all drilling techniques and hydraulic fracturing, the trapped oil and natural gas and the shale reservoirs is being safely and efficiently produced, gathered and distributed to customers.

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Let us look at the drilling and completion process of a typical oil and natural gas well. Shale reservoirs are usually 1 mile or more below the surface or below any underground source of drinking water which is suitably no more than 300 to 1000 feet below the surface.

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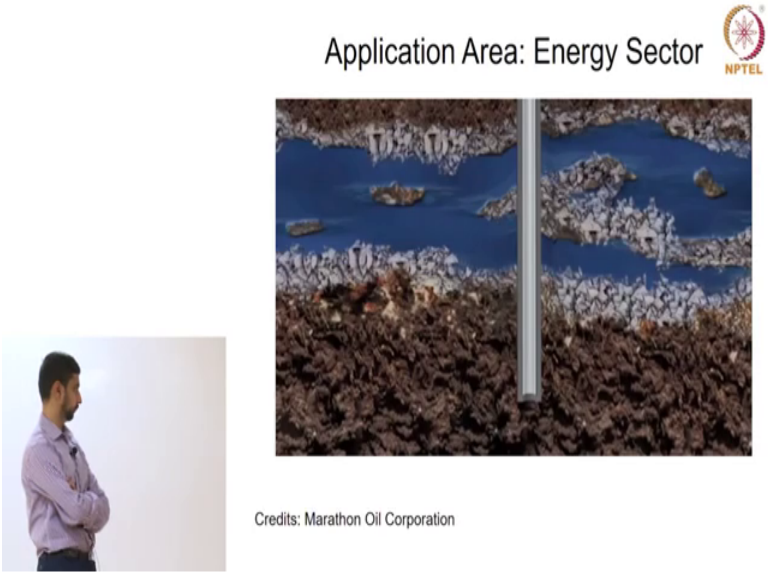

Additionally, steel pipes called casing cemented in place provide a multi-layered barrier to protect freshwater aquifers.

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During the past 60 years, the oil and gas industry has conducted fracture stimulations in over 1,000,000 wells worldwide.

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The initial steps are the same as for any conventional well. A hole is drilled straight down using fresh water based fluids which cools the drill bit, carries the rock cuttings back to the surface and stimulises the wall of the wellbore.

Once the hole extends below the deepest freshwater aquifer, the drill pipe is removed and replaced with steel pipe called surface casing. Next, cement is pumped down the casing. When it reaches the bottom, is pumped down and then back up between the casing and the borehole wall creating an impermeable additional protective barrier between the wellbore and any freshwater sources.

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In some cases, depending on the geology of the area and the depth of the well, additional casing sections may be run. And like surface casing, are then cemented in place to ensure no movement of fluids or gas between those layers and the groundwater sources.

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What makes drilling for hydrocarbons in a shale formation unique, is the necessity to drill horizontal. Vertical drilling continues to a depth called the kick-off point; this is where the well water begins curving to become horizontal.

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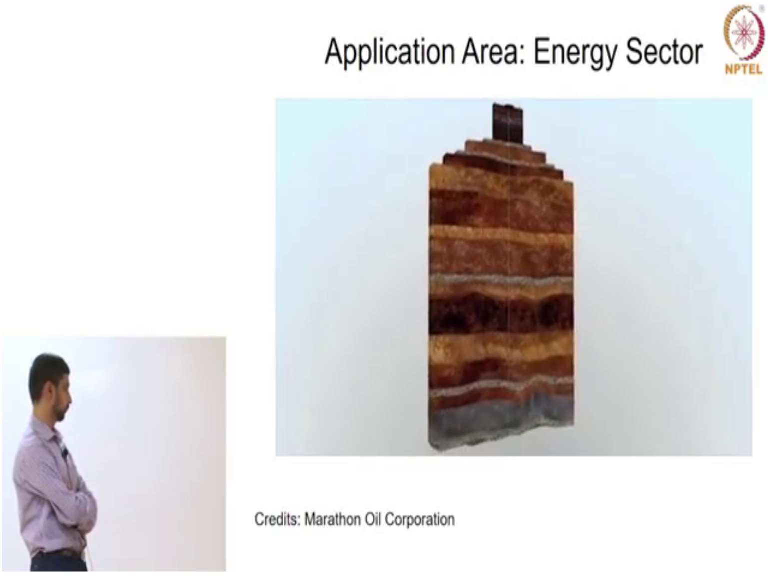

One of the advantages of horizontal drill is that, its possible to drill several wells from only 1 drilling path, minimizing the impact to the surface environment.

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When the targeted distance is reached, the drill pipe is removed and additional steel casing is inserted through the full length of the wellbore. Once again the casing is cemented in place. For some horizontal developments, new technology in the form of sliding sleeves and mechanical isolation devices were place cement in the creation of isolations along the wellbore.

Once the drilling is finished and the final casing has been installed, the drilling rig is removed and preparations are made for the next steps well completion. The first step in completing a well is the creation of a connection between the final casing and the vertical rod. This consists of lowering a specialized tool called a perforating gun which is equipped with shaped explosive charges down to the rock layer containing oil or natural gas.

This perforating gun is on fire which creates holes through the casing, cement and into the target rock. These perforating holes connect a reservoir in the wellbore.

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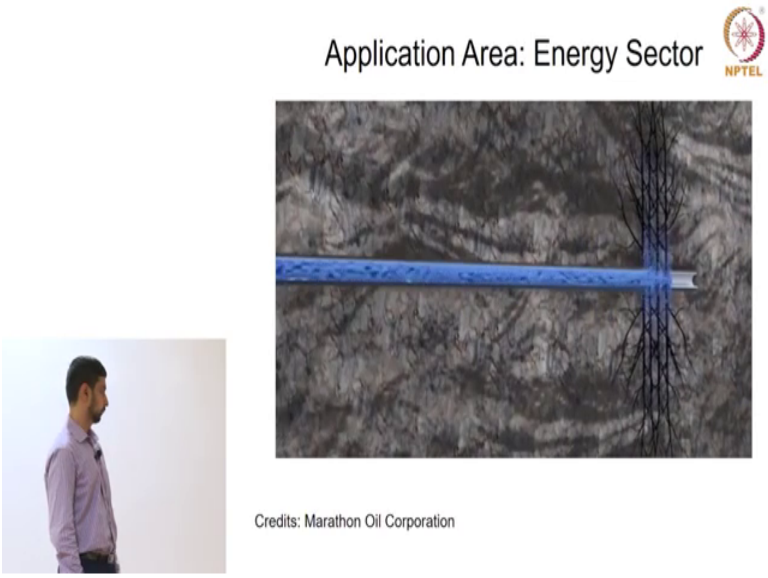

Since these perforations (Refer Time: 15:13) inches long and have performed more than a mile underground, the entire process is imperceptible on the surface. The perforation gun is then removed in preparation for the next step; hydraulic fracturing.

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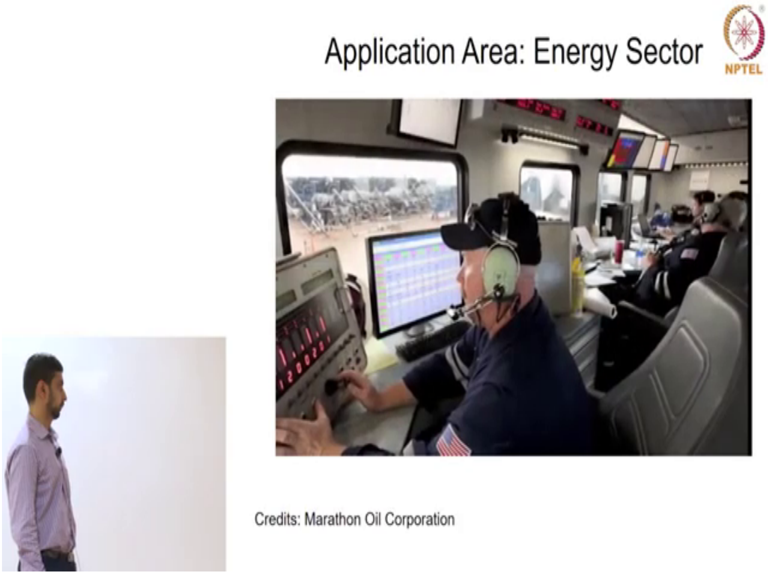

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The process consists of coming a mixture of mostly water and sand plus a few chemicals under controlled conditions into deep underground west water formations.

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The chemicals are generally for lubrication that keep bacteria performing and help carry the sand. These chemicals typically range of concentrations from 0.1 to 0.5 percent by volume and have to improve the performance of the simulation.

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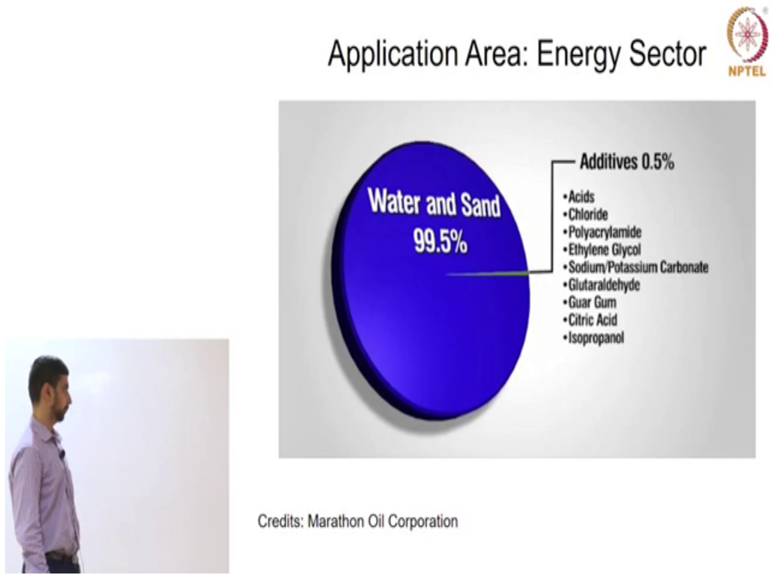

This simulation fluid is sent to trucks that pumps the fluid into the wellbore and out through the perforations that we noted earlier.

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This process creates fractures in the oil and gas reservoir rock. As sand in a black fluid remains in these fractures in the rock and keeps them open when the top pressure is relieved. This allows the previously trapped oil or natural gas to flow to the wellbore more easily.

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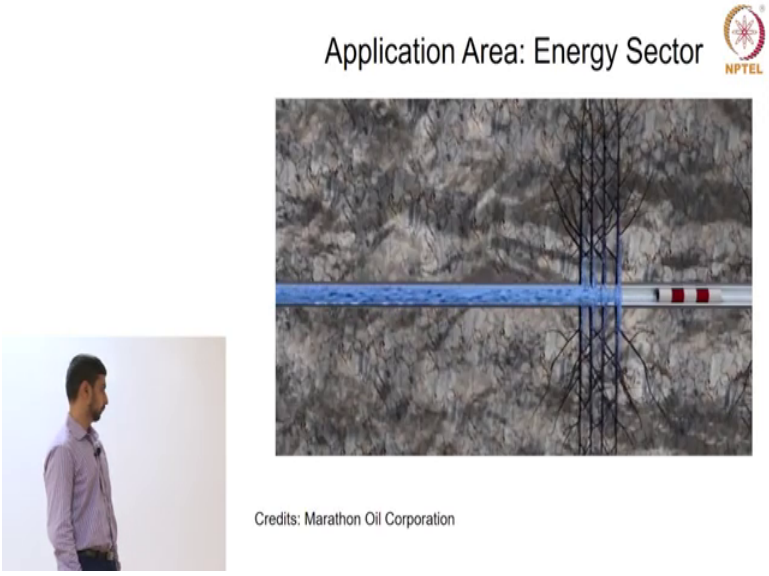

This initial stimulation segment is then isolated with a specially designed plot and appropriating guns are used to perforate the next stage. This stage is then hydraulically fractured in the same manner.

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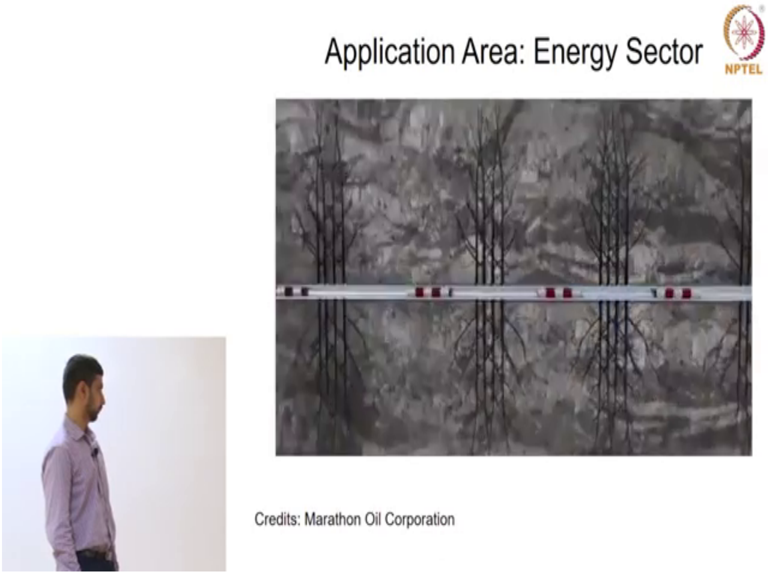

This process is repeated along the entire horizontal section of the well which can extend several miles. Once the simulation is complete, the isolation plugs are drilled out and production begins.

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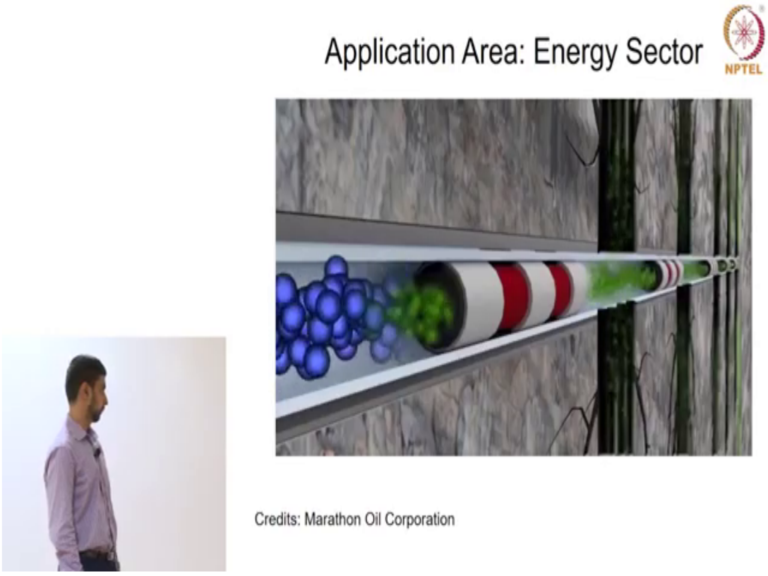

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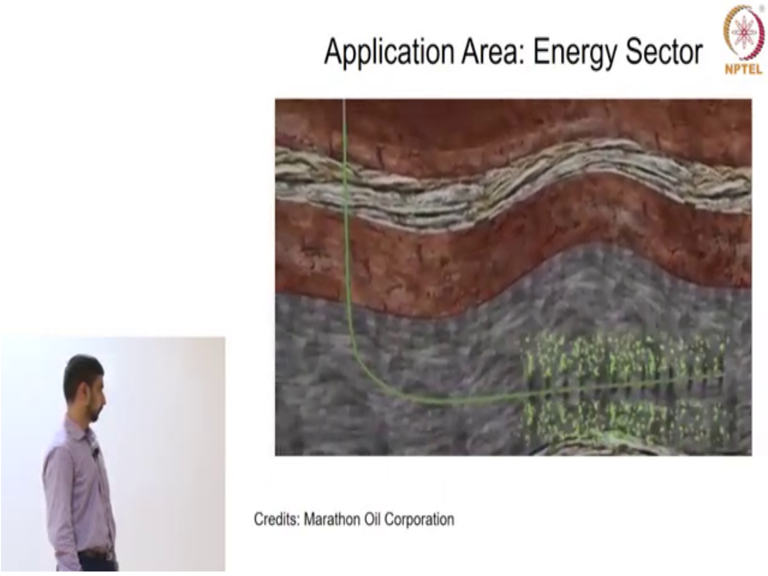

Initially, water and then natural gas or oil flows into the horizontal casing and of the wellbore. In the course of initial production of the well, approximately 15 to 50 percent of the fracturing fluid is recovered. This fluid is either recycled to be used on other fracturing operations or simply disposed off according to government regulations.

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The whole process of developing a well typically takes from 3 to 5 months.

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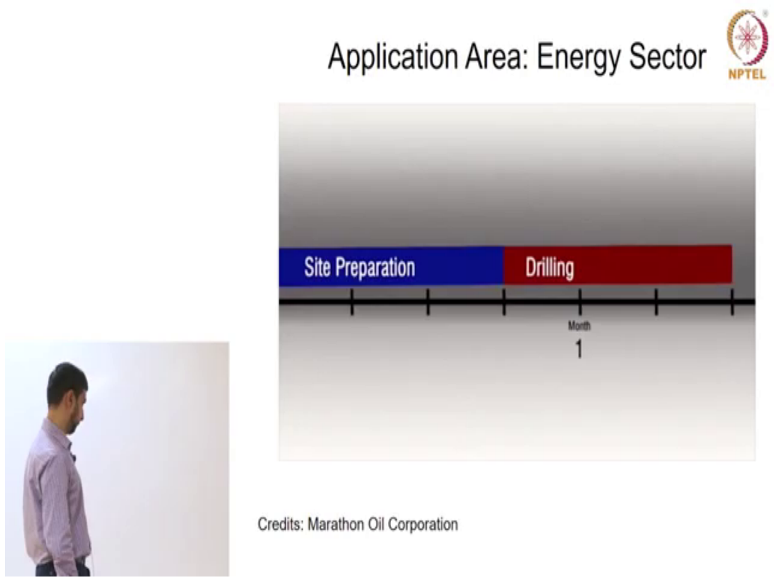

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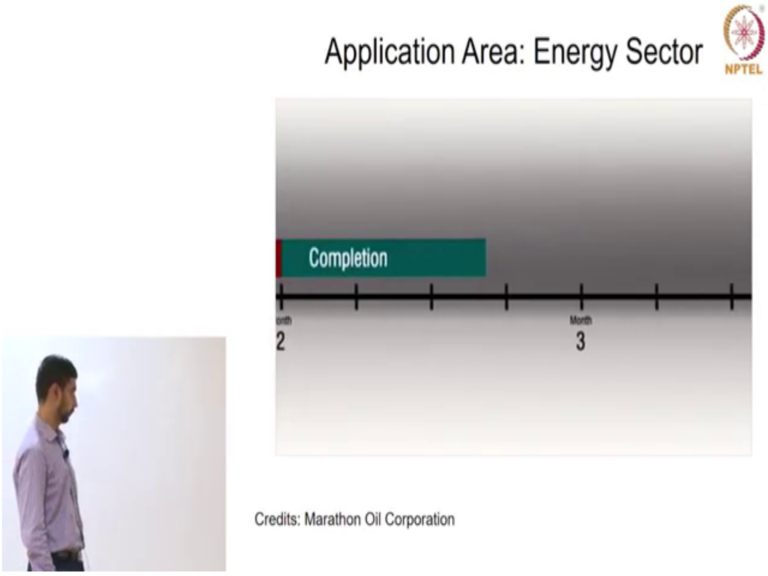

A few weeks to prepare the site, for the 6 weeks to drill the well and then 1 to 3 months of completion activities; which includes 1 to 7 days of stimulation, but this 3 to 5 month investment can result in a well that will produce oil or natural gas for 20 to 40 years or more.

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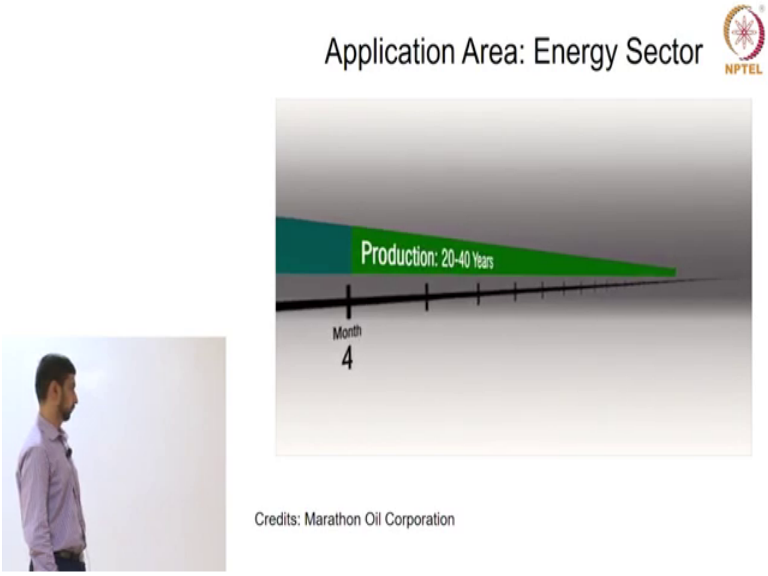

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When all of the oil or natural gas that can be recovered economically from a reservoir has been produced, work begins to return the land to the way it was before the drilling operations commence.

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Well will be filled with cement and pipes cut off 3 to 6 feet below ground level. All surface equipment will be removed and all pads will be filled in with dirt or replanted. The land can then be used again by the landowner for other activities and there will be virtually no visual signs that well was once there.

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Today, hydraulic fracturing has become an increasingly important technique for producing oil and natural gas.

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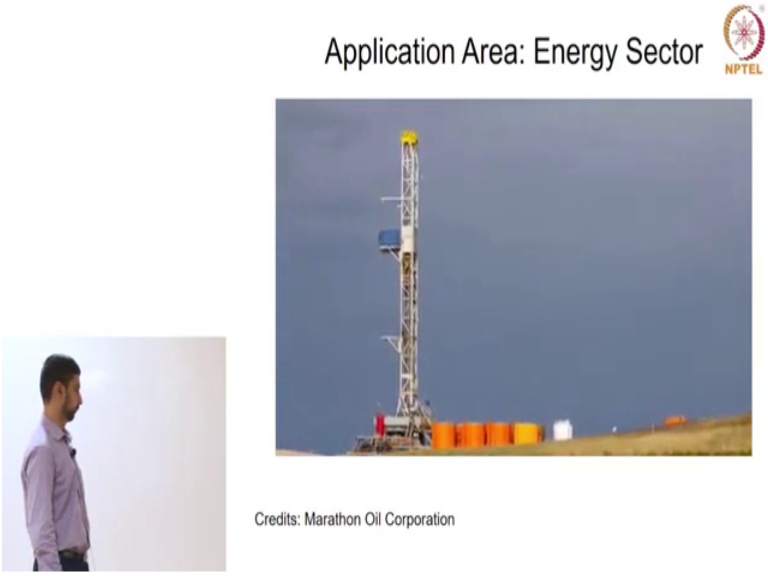

In places where the hydrocarbons work previously inaccessible, technology will continue to be developed to improve this same and economical development of oil and gas resources.

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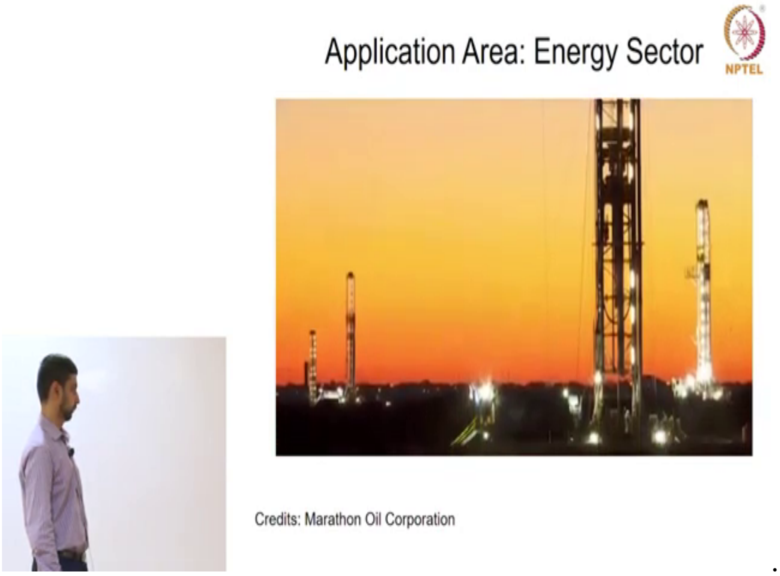

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So, there is a lot to process in that video. I mean, its essentially describing the entire process from the time when they actually drill the well to the time when they close the well and the production is completed. But, routinely many engineering decisions are being made there, right. How do you drill under the ground? See, so one thing to remember is that there is nothing that you can see under the subsurface, right.

So, its all essentially a black box and you have to make these decisions which have real world implications. So, you either do it based on a trial and error approach, right. So, you drill one well you look at the performance of this well and then you go back and then you learn from this whatever you learned from this drilling this well and go ahead and maybe you use those learnings to drill another well.

But, one thing to remember is that geology of the terrain there will change based on the location where you are drilling the well. So, the learnings from one well may not necessarily translate into another one. If you look at the process there is fluid flowing through the porous medium which is the rock, right.

Then you are pumping in pressurized fluid into the well so that you can fracture the rocks which you need to so that you can enhance the permeability of these shale formations. So, that natural gas can be extracted in an economically viable manner. Then you are also injecting sand particles so that the fractures remain open once you create them. Because otherwise, the earth is so compressed that you may create a fracture.

But as soon as you stop pumping the fluid they will all shut and that basically makes this entire process futile. So like I said, since its a black box, you have no idea what is happening under the subsurface and a lot of the engineering practices are empirical, they have been doing things in the past; in the past 10 or 20 years and they just keep following the same processes. But there is a lot of room for improvement by applying science and technology and that is where simulations come in.

You can actually model this entire process on a computer through first principles where you. So, each of these processes can be represented by a computational model. How does fluid flow through a porous medium? That is a computational model. How does the rock break when you inject a pressurized fluid into the rock? That is a computational model.

And when you inject sand particles then how does this mix in with water? How do these sand particles mix in with water? How do the additives and the chemicals mix in with water? And how do they prop up in this fractures? This is a computational model.

And the all these computational models are linked together. So, you have to essentially solve them in a coupled manner to obtain what you think may be happening under the surface and then translate those results back to the engineers who are trying to make decisions real time. And just to set the context, each of these wells costs in tens of millions of dollars.

So, if you are able to recommend that you are not drilling one well that results in a lot of cost savings. And the kind of decisions that they are trying to make is, how are these wells spaced? Are they spaced in a uniform manner or are they spaced in certain patterns so that you are able to extract let us say this piece of land to its maximum capacity?

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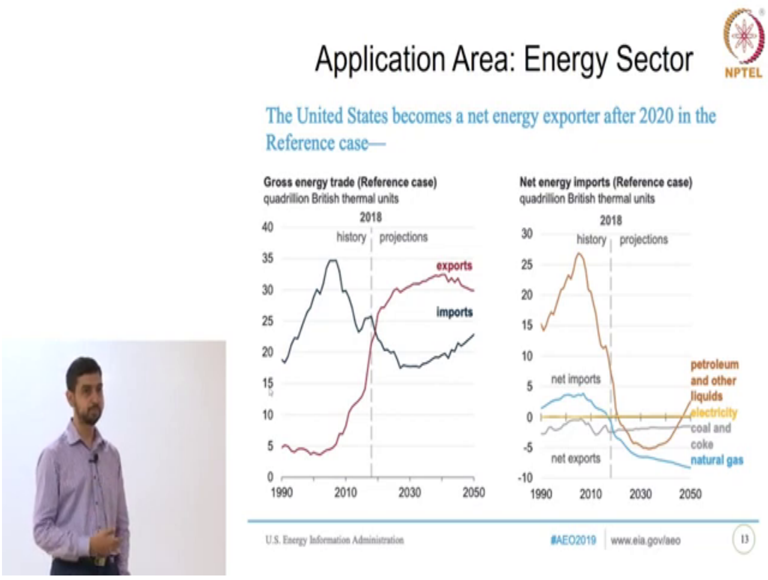

And the results are for all to see. I mean United States used to be a net importer of energy or in very much like our own country which imports to meet imports oil and natural gas to meet most of its energy demands.

But since they have uncovered a lot of these shale deposits, they are now becoming a net exporter of energy. So, and this has huge implications for a country's economy. For example, you may notice every time oil price goes up our the rupee depreciates and we go our country goes into a lot of debt because we have to purchase these.

Our energy demands are not going down our energy demands are only going up with the number of people increasing, right. So, as oil prices go up it has a huge cost on our country. So, science and technology can actually have a huge impact on how to actually meet our energy demands and also improve our economy.

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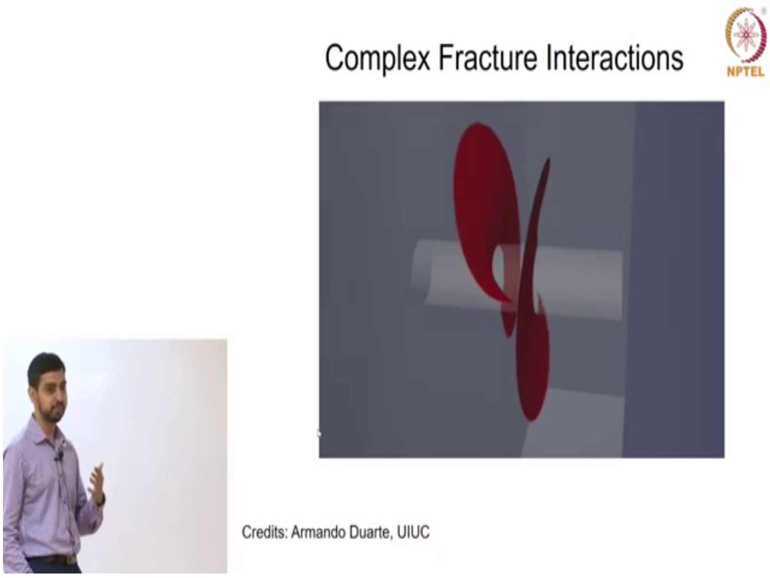

So, here is an example of how this can be simulated in a computer. And this I am pulling from one of my collaborators at the University of Illinois. So, they are modeling hydraulic fracturing process that you just saw as a fully coupled multiphysics process on the computer.

So, the cylindrical object that you see on the screen is actually a well and you have two perforations that are created and now you are trying to drive those fractures by injecting pressurized fluid. Now, let us see what happens.

So, you see the fracture starts growing with increasing pressure. So, the pressure exceeds the failure stress of the rock and that essentially results in a growing fracture. And what you do notice is that, as one fracture interacts with the other, you have a fully three-dimensional shape of the fracture that does not necessarily is not necessarily obvious to us in a mental picture, right.

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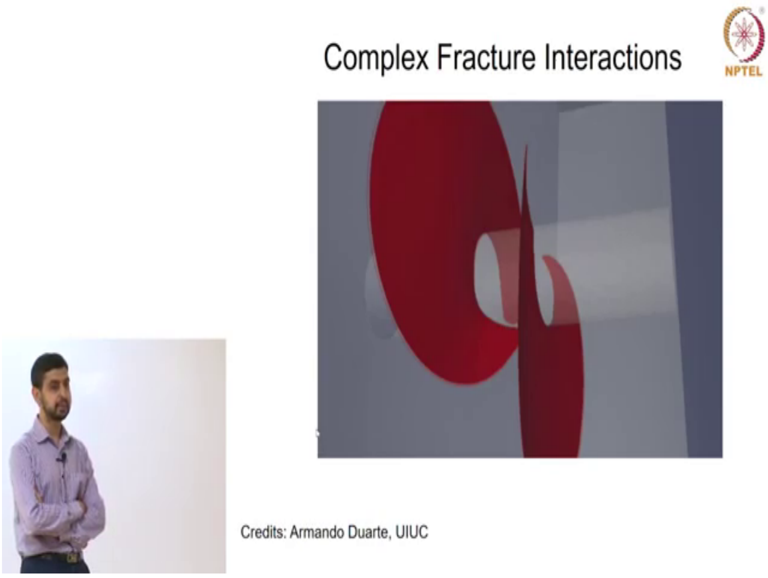

We would think that the fractures are probably growing straight because they have been initiated in the same location. But, you have a tortuosity there in the near wellbore region. And this essentially has an impact on what the how the engineer should essentially tailor their perforations. Maybe having 2 perforations really close to one another is not such a good idea. Right, this is a recommendation that can be made.

Maybe, if you have one stage of hydraulic fracturing operations having multiple clusters may or may not be economically profitable.

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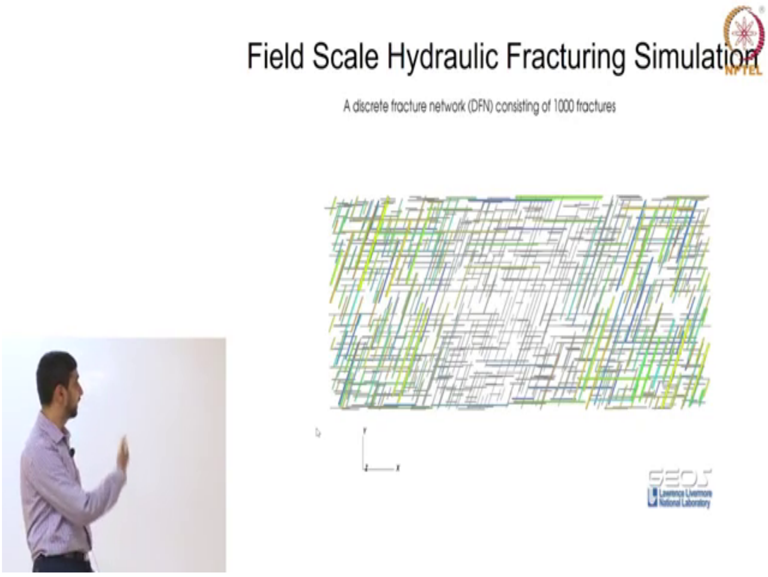

Here is another example where you have several natural fractures which is essentially when you have that earths geology, in addition to the fractures that you are creating by injecting pressurized fluid. There is already many many fractures that exist because of a tectonic activity and geologic folding. And here, we are trying to mimic those natural fractures based on certain data which are oriented in certain directions.

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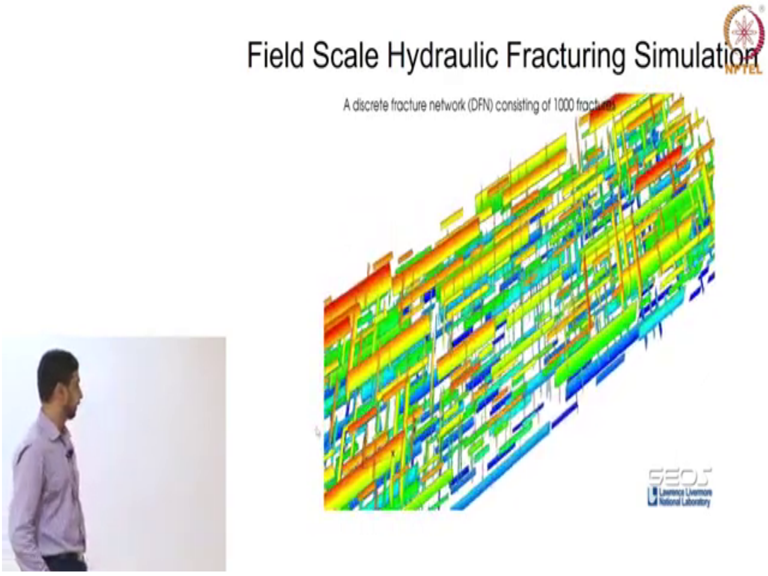

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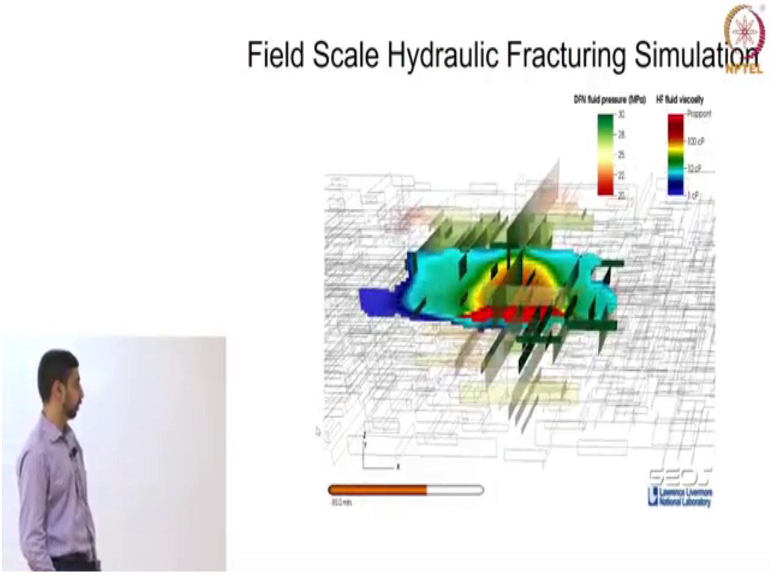

And, if you look at a hydraulic fracture that is being driven in somewhere in the middle of those fractures, we try to look at how that hydraulic fracture interacts with the natural fractures around it.

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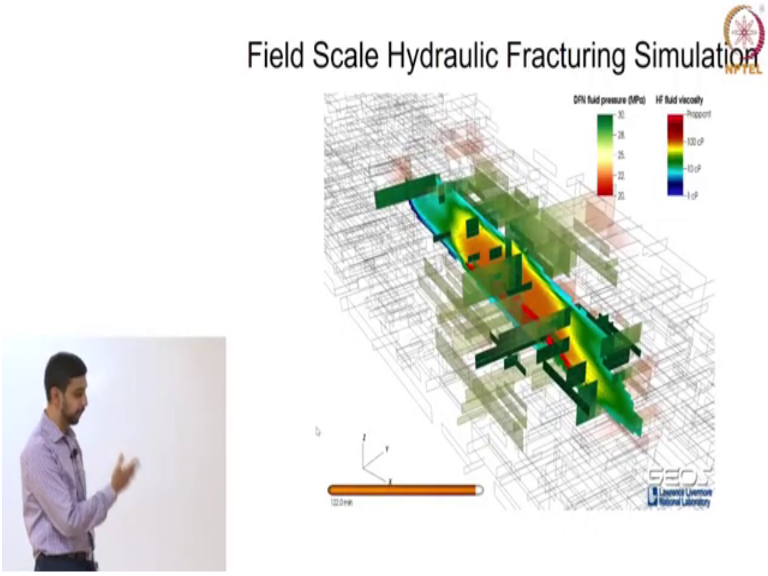

So, the colours that you are seeing are essentially the concentration of the proppant that you are injecting and how the fluid flows from the main hydraulic fracture that you see here into the surrounding natural fractures.

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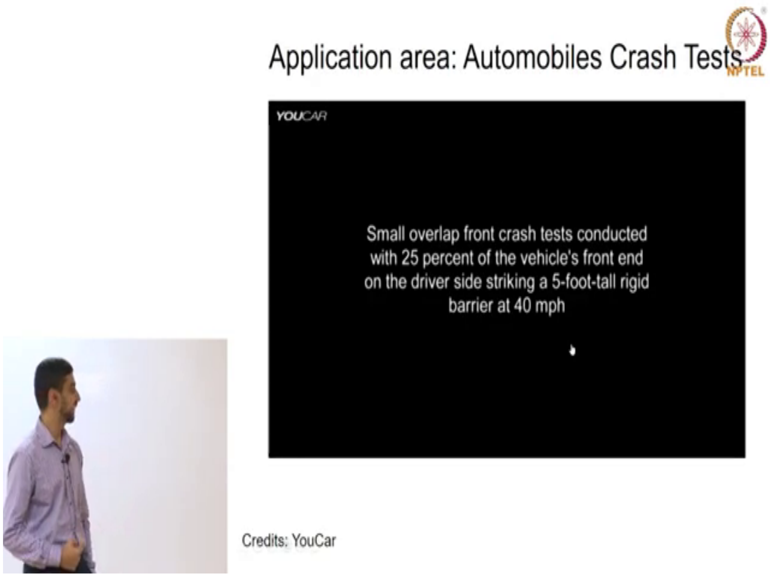

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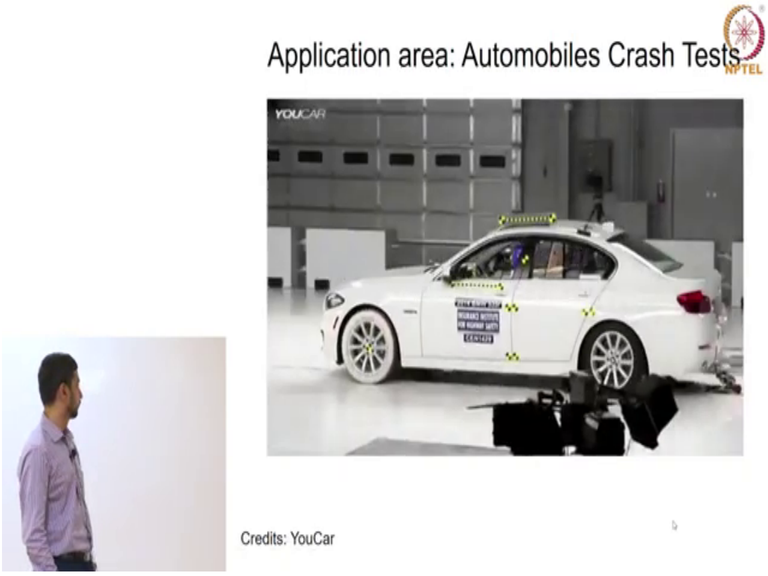

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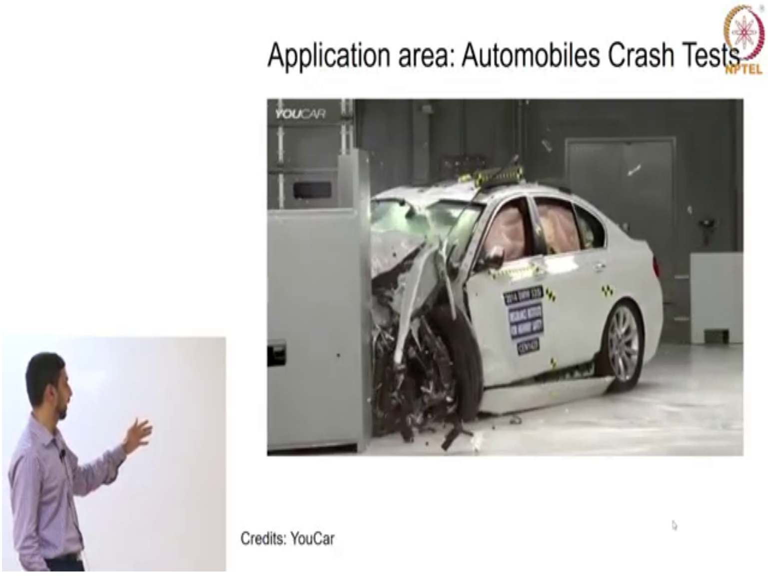

So moving on to the next example area, its not just geosciences where these simulation based technologies are useful; automobile crashes crash tests have been one of the signature used cases for this simulation based science and engineering approaches.

And what I am showing here is actually a real crash test. So, this is you can go to YouTube and look at if you are interested in how impacts affect crack cars then you can look at several videos and here a BMW is being driven at 40 miles per hour into a rigid barrier. And you look at what that impact does to the car and also to a driver who is sitting in that.

So, this essentially makes us based on these impact tests, we can design safety features in a car and they also make sure that we meet any safety requirements that are set forward by the government. So, you see what happens there and this is why you should always drive safely. So, this is a real crash test.

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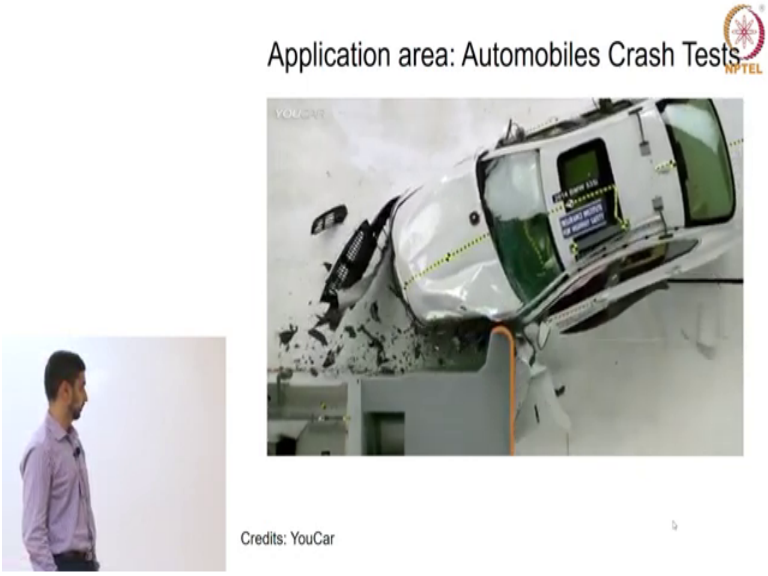

So, you see the car crashing into the barrier getting smashed in the front and the airbags deploying.

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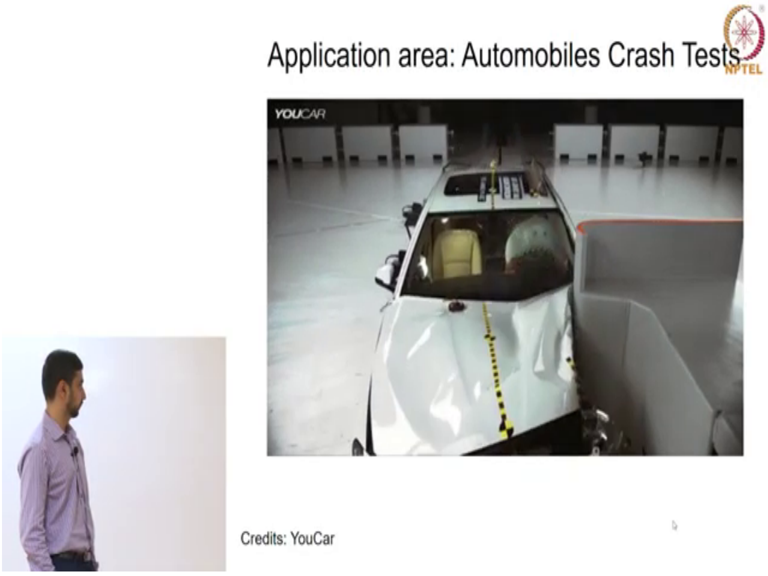

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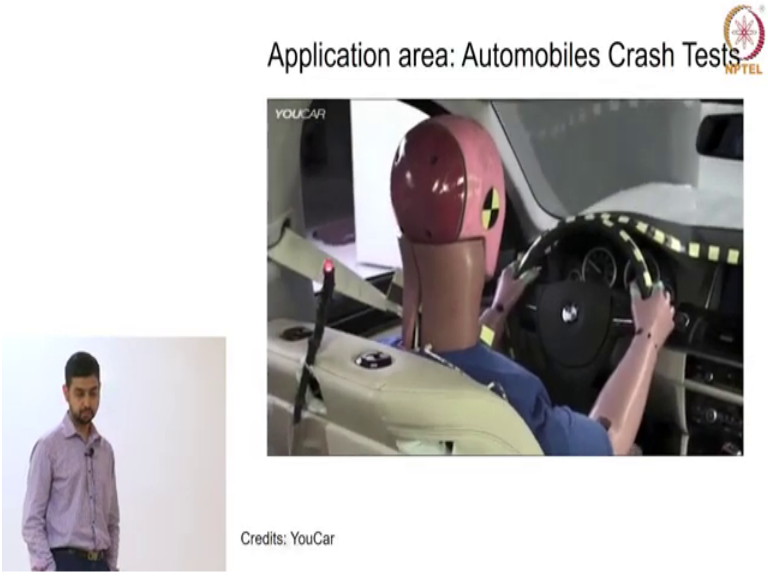

I do not need we I do not think we need the music over there, but.

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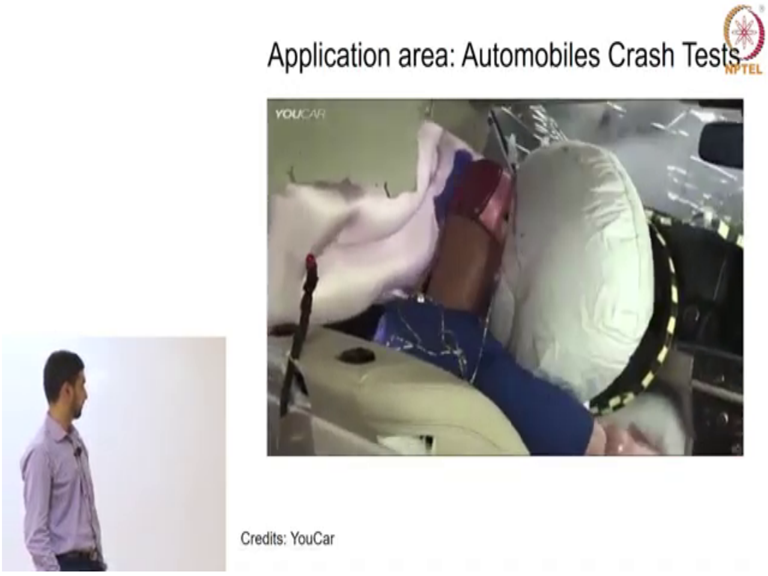

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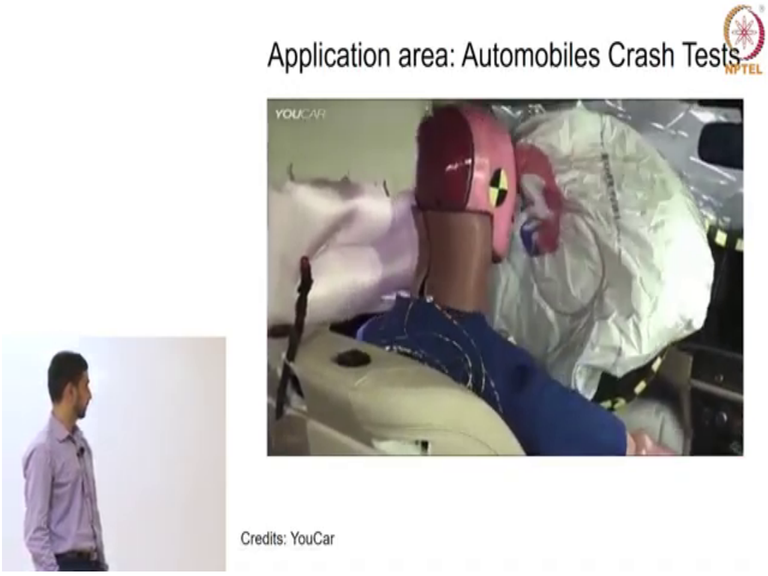

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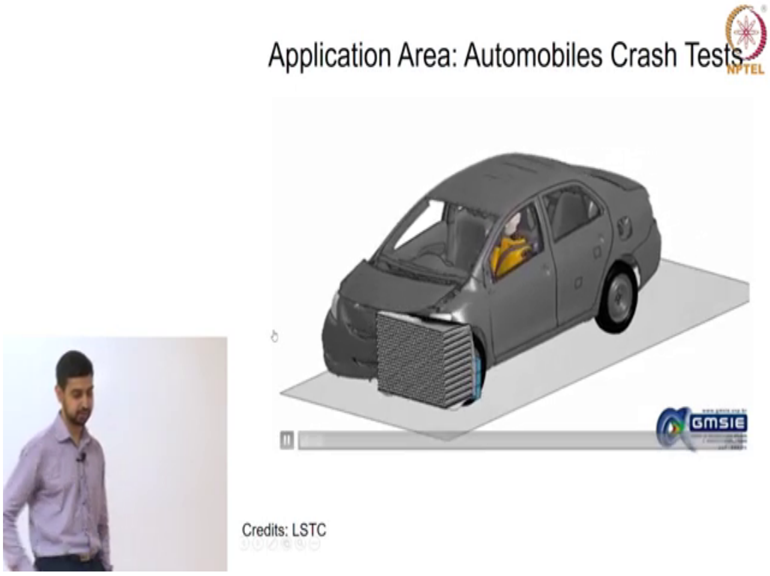

But we can actually simulate this process on a computer, we do not need to crash several of these BMW's, right. every time we want to test a new safety feature and if you look at this model of the exact same scenario, you notice how similar the pattern is.

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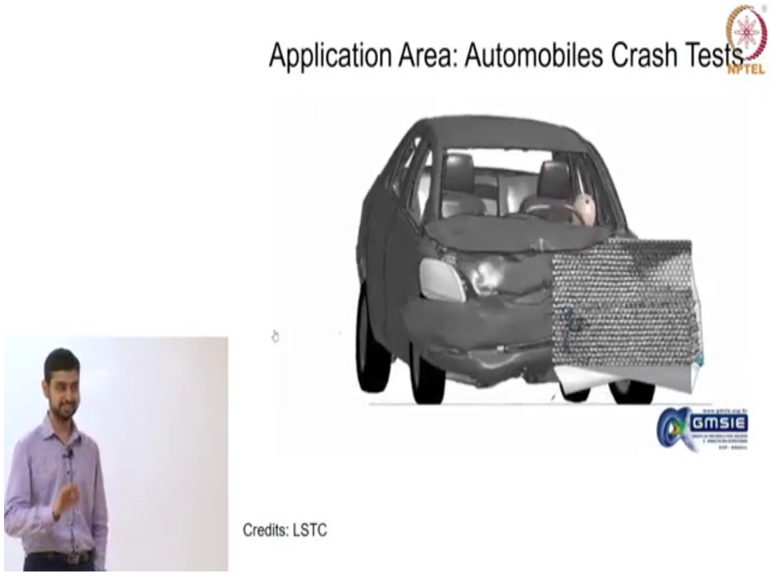

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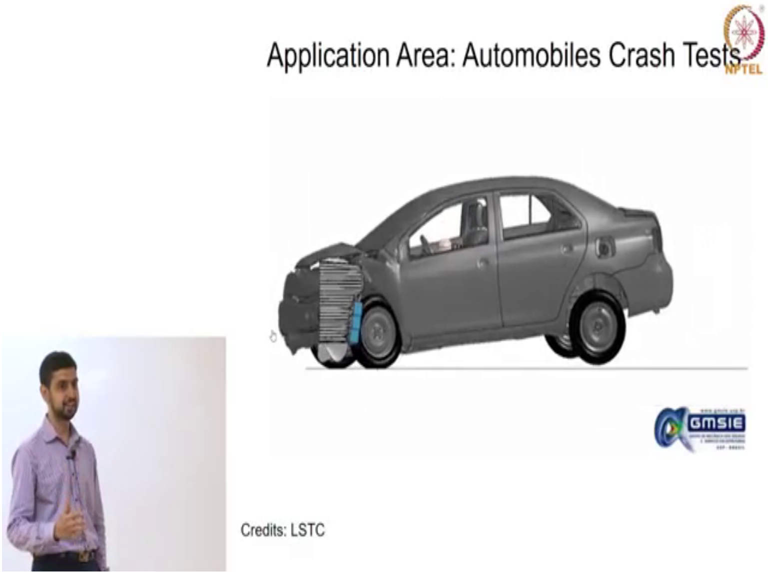

And this is not a video game by the way, this is this is simulating the equations of physics which are close to what happens in real life and there are assumptions, but this is nowhere near as bad as a video game.

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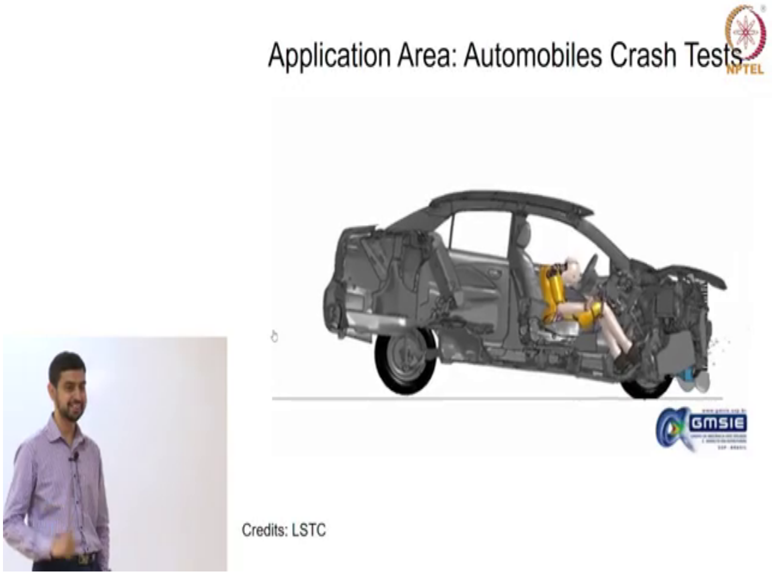

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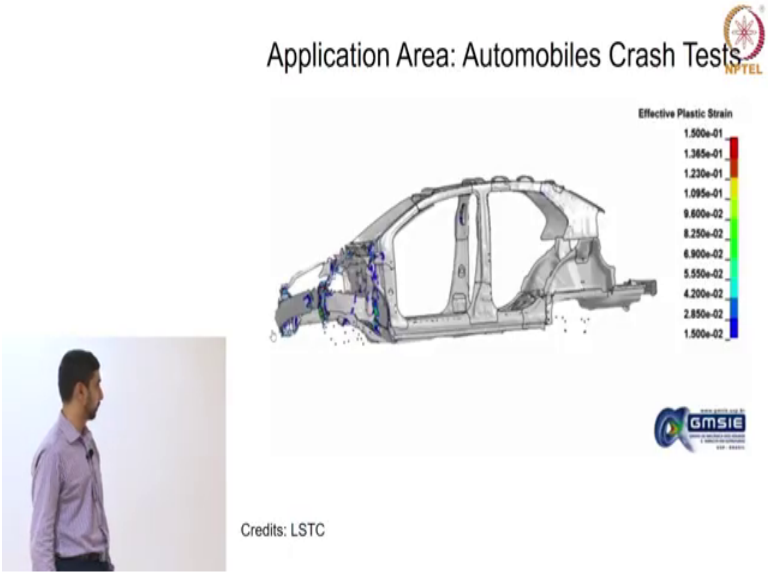

So now you notice, in the structure of the car where the maximum deformation is.

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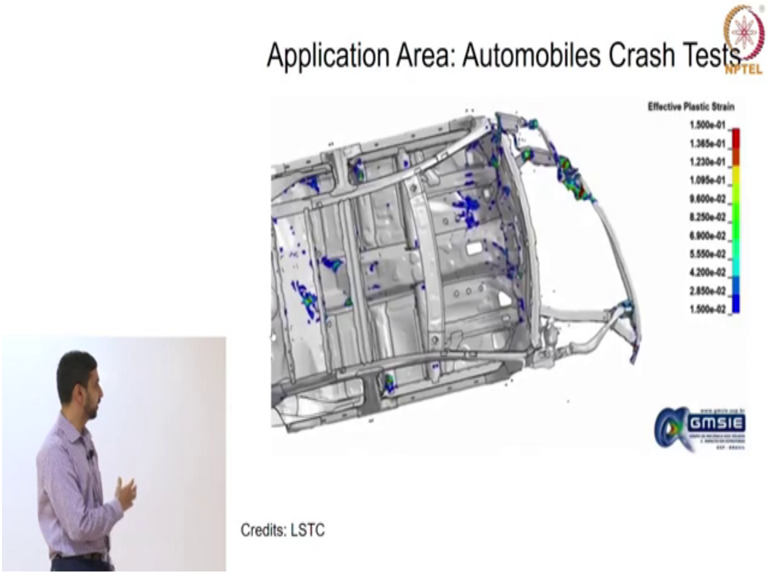

And where would you need to put in any augmentations or any safety augmentations that you would require.

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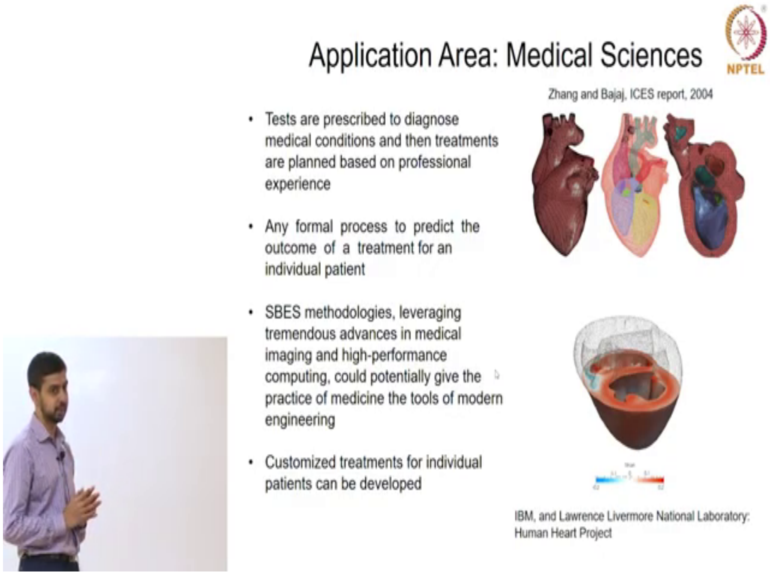

Going forward, there is also medical sciences where simulations are making their foray and there is a lot of similarity between medical sciences and engineering, right. So but, there is no concept of predictions in medical sciences. In engineering, we try to predict a lot we try to predict the future in yes, we are assuming that our world, the world view we have is deterministic and we try to basically assume that the inputs are given to us and they are known. But, we can probably translate a lot of that into medical sciences as well.

Although there is no formal process to predict the outcome of a treatment for any individual patient, we may be able to it. Based on the simulation based engineering sciences and methodologies.

So, what I am showing here is essentially a full model of a full grown human heart and it is an extremely complicated thing to model because, again you have blood flow flowing through the arteries, you have this complicated geometrical shape and you have tissues which are deforming under pressure from the blood which flows in the arteries, right.

So, all these processes need to be accounted for when you are trying to simulate this. But if you can actually develop this kind of a model, you can have customized treatments for individual patients based on the data that you get from that patient. Because you know, you can run you can take that data, you can give that as an input to your computational model and you can run the model and you can see what happens: let us say to drug delivery or what are the hot spots where there is any artery cloggage, etcetera.

And this model was developed in collaboration with IBM at the Lawrence Livermore National Laboratory and it uses high performance computing as well to model the entire process.

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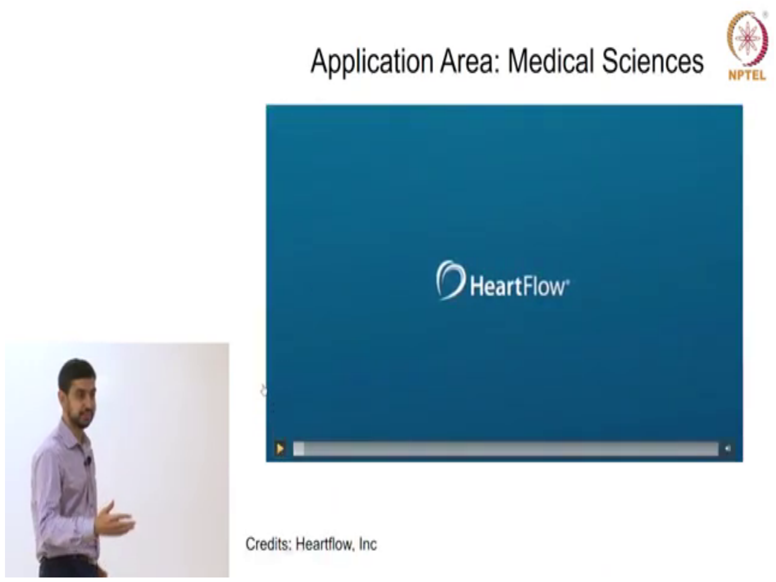

There is also another company.

Heart flow is a personalised.

Another company which tries to take forward these ideas that I just presented and its trying to sell these softwares to hospitals right now and let us see what happens over.

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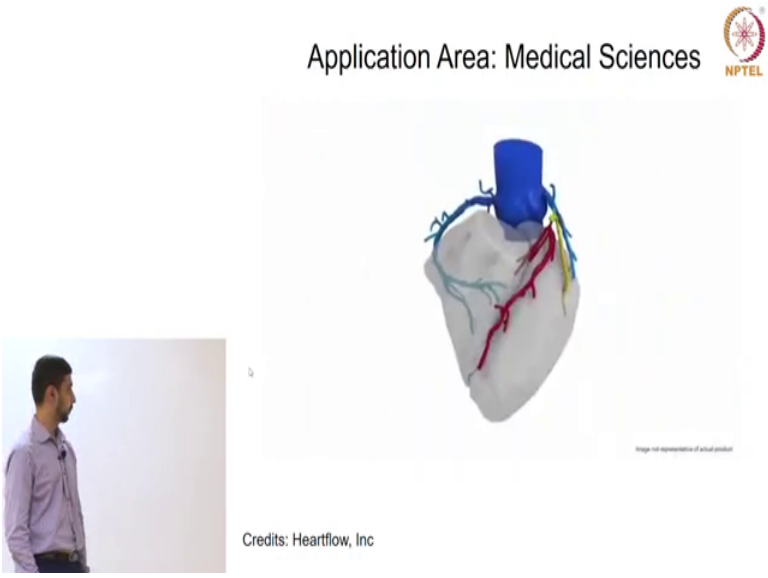

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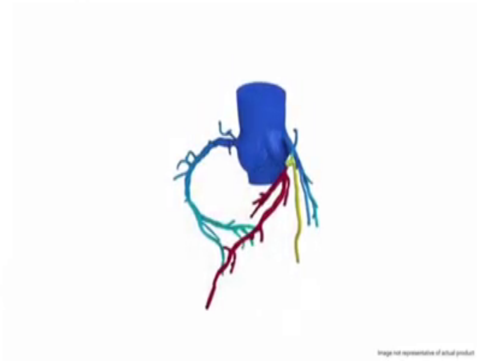
Application Area: Medical Sciences



Credits: Heartflow, Inc

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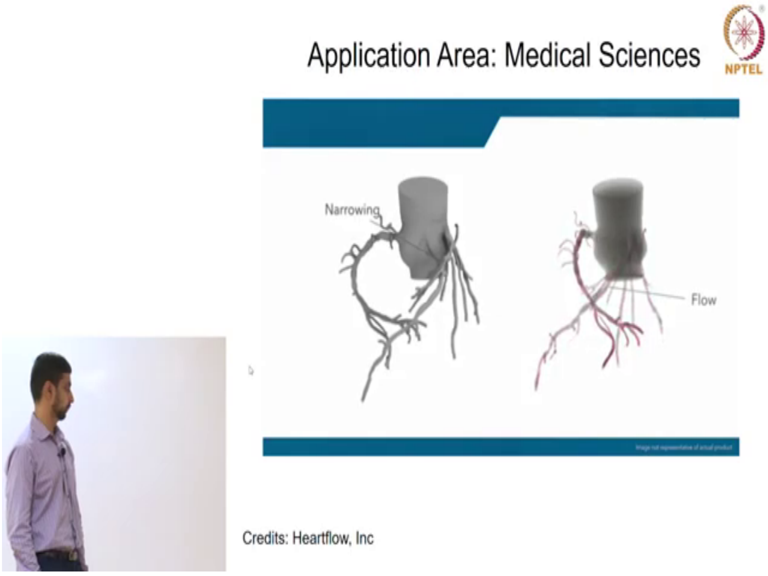

There managed its extraction product the harmful FFRDC analysis is the first and only non-invasive technology for coronary artery disease that offers inside and opiates and a coronary artery now and one critic impacting workflow. Heartflow provides 2 pieces of information based on standard coronary CT scan.

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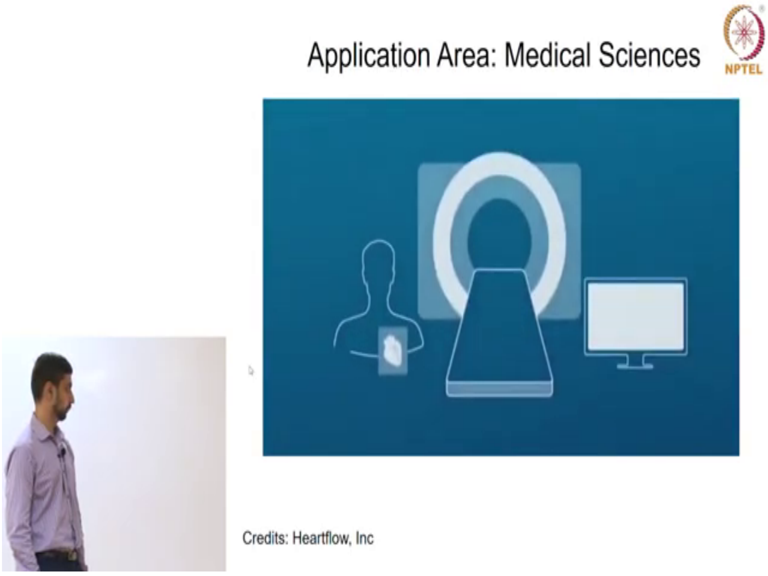

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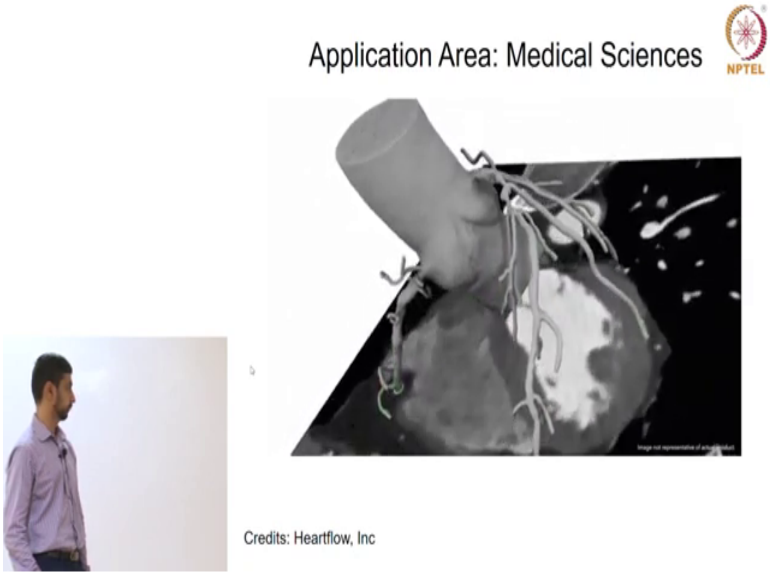

From the CT images, heartflow creates a complete geometric and physiologic model of the patients unique coronary inanimate.

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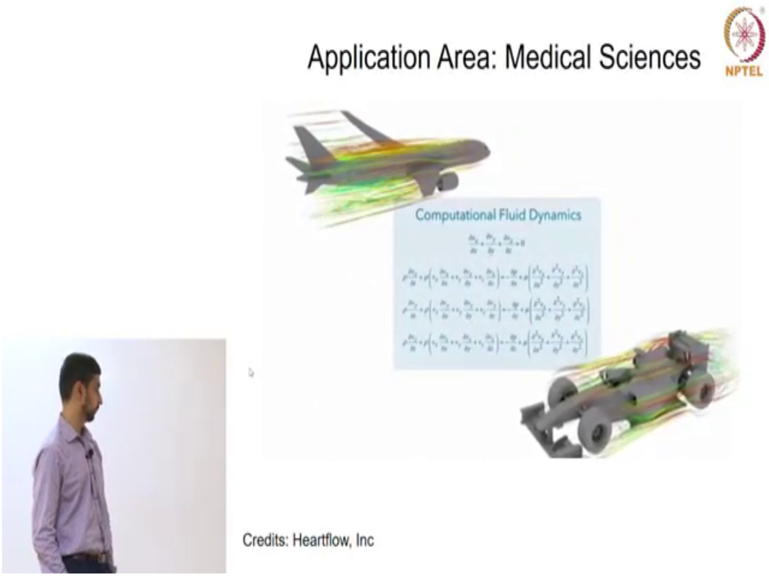

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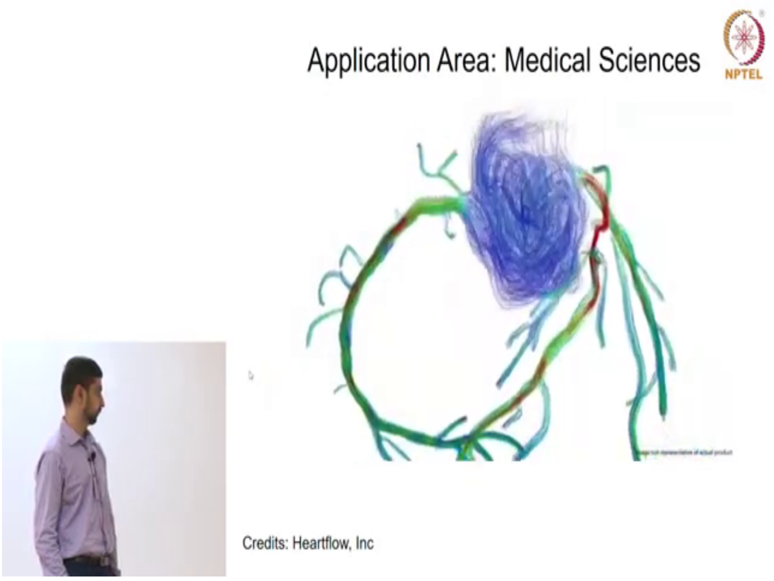

Next, the scientific principles of computational fluid dynamics are applauded. The model the complexities of fluid will be any results of the heart flow analysis is a color coded map of the coronary arteries

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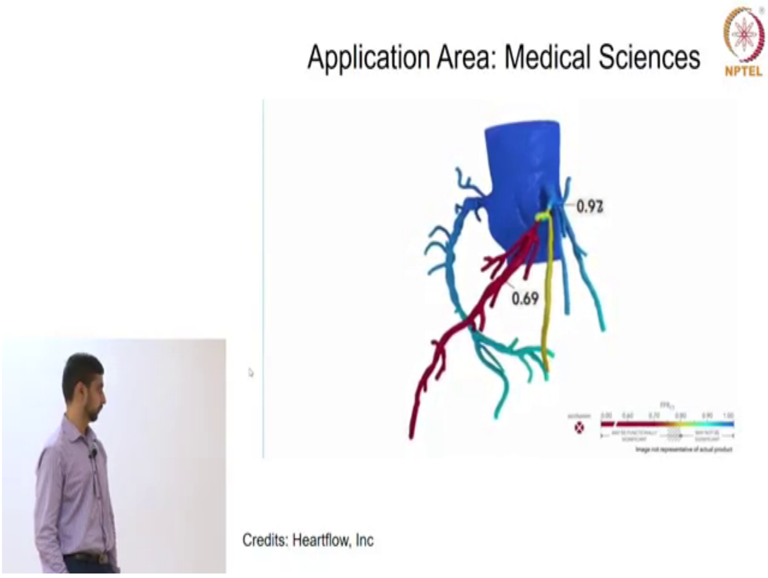

Showing the extent to which any narrowing or disrupting blood flow, a physician can use this information to develop a treatment plan that is right for that patient.

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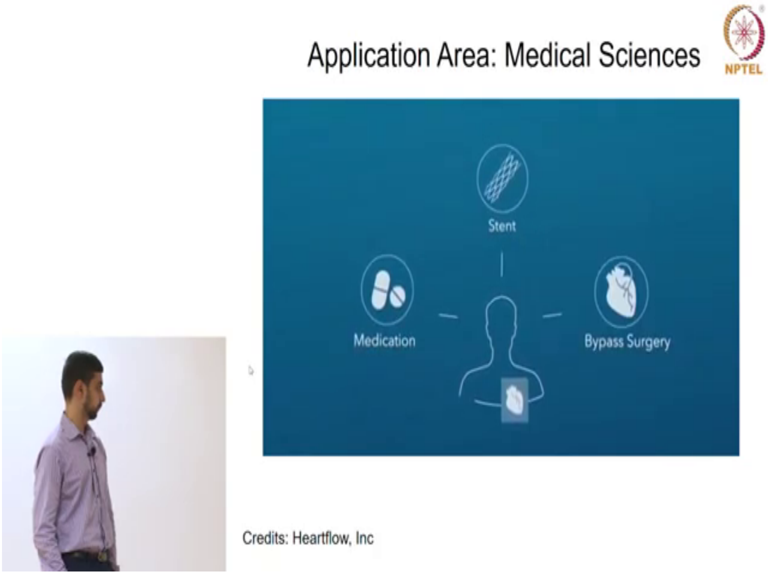

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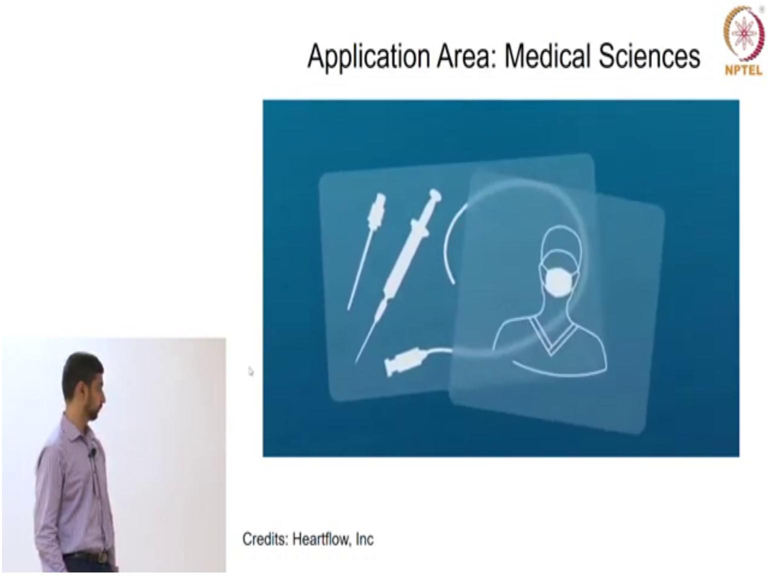

Previously, only through an invasive procedure could physician verify that if a narrowing in the arteries is impacting heartflow.

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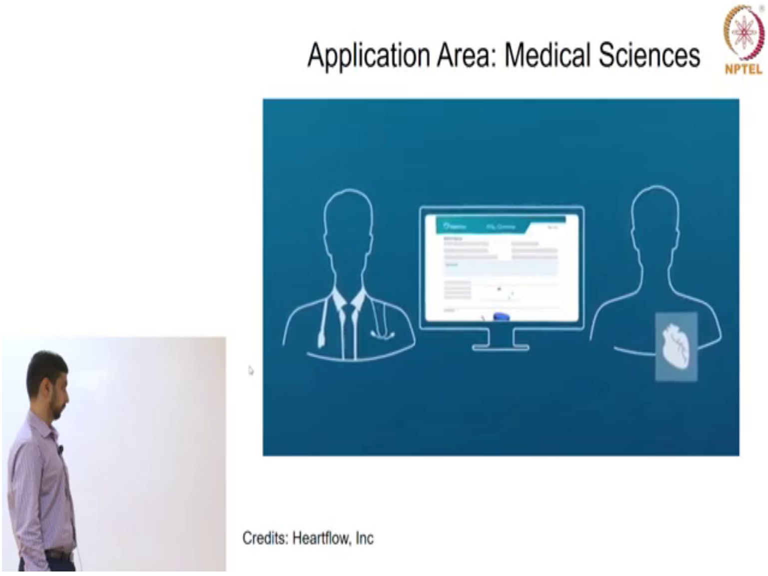

Now not with heartflow, this functional information can be simulated non-invasively. Actively in commercial, use the heartflow FFRDC analysis. How does the potential to help physicians redefine without notice the management of coronary heart disease?

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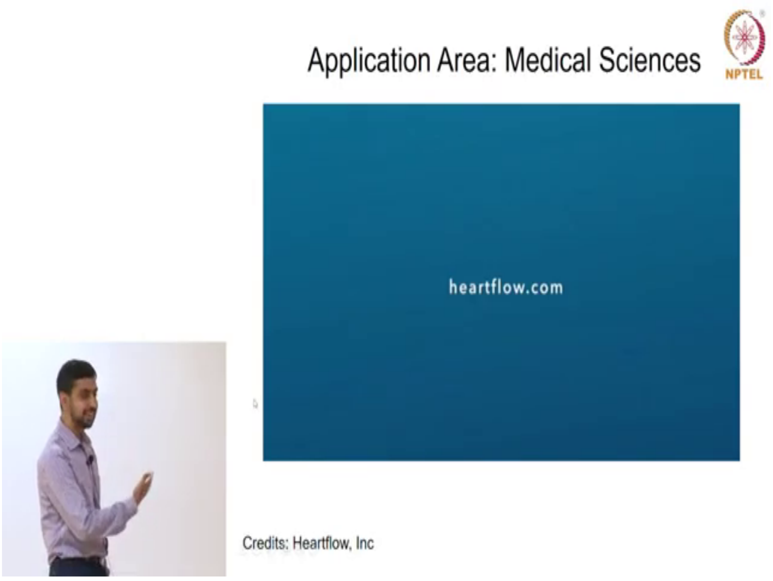

So, you see the advantages there instead of going for an invasive procedure you can take a CT Scan, develop a full blown computational model, run the tests, look at the various treatments even because you can look at whether you know if you are prescribing a medicine, what the drug delivery does? does it narrow any blockages you have or does is it ineffective? And based on that you can come up with an customized treatment for every patient.

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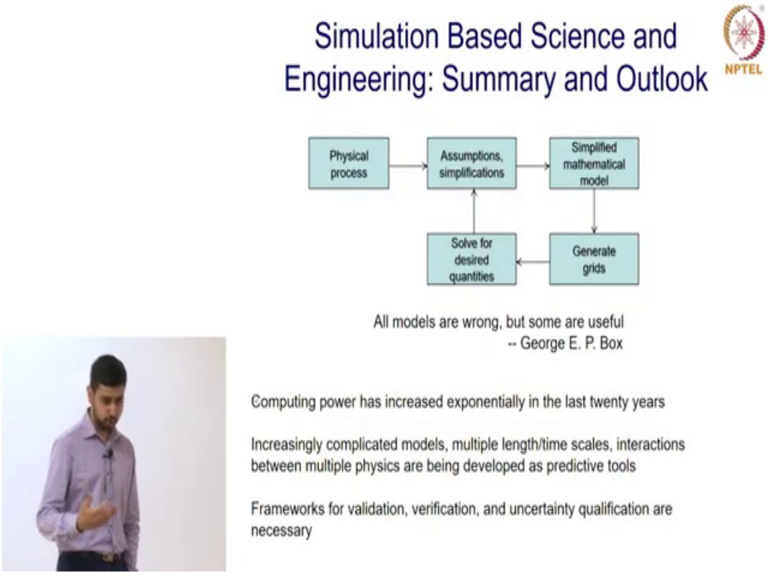

So in conclusion, I would say that these methodologies, the simulation based science and engineering approaches are extremely powerful and they have only been possible because our computing power has increased exponentially in the past 20 years.

However, there is a downside to what I just mentioned. Since, the computational power is increasing exponentially, we also want to use increasingly complicated models to model simple things. And as you may have heard this course from Albert Einstein, your model should be the simplest possible it can be, but no simpler right.

So, if you are trying to use a full a multiphysics approach to model something simple, you are not only wasting computational resources, but you are also making it hard for you to interpret what the results themselves mean. Again, since these are predictive capabilities, we have to be careful in interpreting the results and there have to be rigorous frameworks for validating and verifying these models.

And moreover, like I said, we have a deterministic worldview, but the world is not a deterministic right. I mean, there is a lot of uncertainty in the world. So, there have to be rigorous approaches to quantify this uncertainty so that we can use these computational models in a truly predictive sense.

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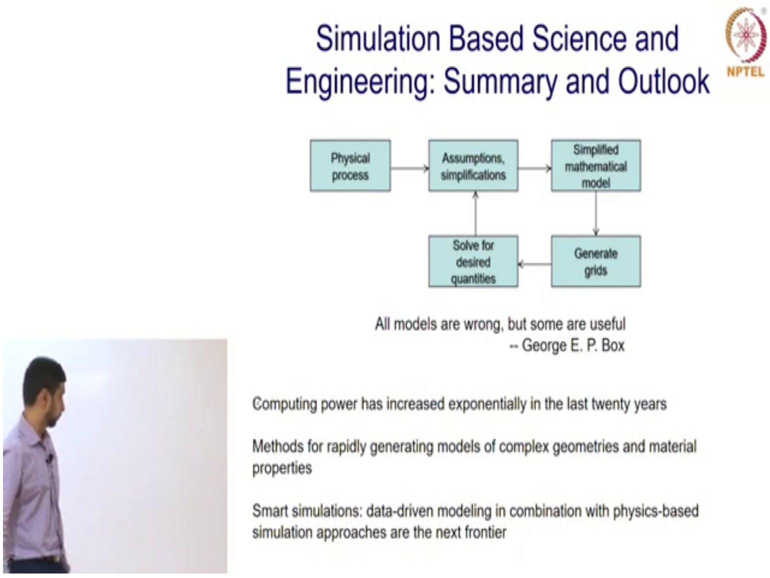

As you saw, most of the real world has complex geometries. So, we do need methods for rapidly generating these models on really complicated geometries and varying spatially and temporally varying material properties.

And in the current in the current world, where increasingly we have more and more data available, we can couple these physics based simulations with data driven remodeling approaches. And you may have smart simulations where your gridding may not be done manually, it can be done through some sort of a machine learning or a neural net approach.

Your constitutive models which can be which may not necessarily be prescribed by you, but it can be developed using some sort of a deep neural network et cetera.

So, this is I think the future of where engineering and science is headed. And I would be open to any questions that you may have. Hopefully, this piqued your interest into what civil engineering. You know, I mean civil engineering seems very far away from computational science and engineering. But to make the connection, all the equations that I all the models that simulate these processes are based on engineering mechanics.

So, you guys are in first semester. So, you may not have done any mechanics of deformable bodies yet. But you have looked at mechanics of statics, rigid bodies and dynamics of rigid bodies, right. So essentially, the same principle apply to deformable bodies. So, when you say rigid bodies, you are making an assumption in your model, right. Its essentially it says that your body does not deform at all.

So, same principles accelerate or deformable bodies can do all these things and more, right. I mean, it makes human flight possible, it makes the possibility of us landing on the moon or on the mars, right. So there is a lot we can achieve through these approaches.

So, hopefully this generates some interest on what you can do with your civil engineering degree.

Thank you.