ANNA MORALES MELGARES: Hi. My name is Anna. I'm from Barcelona, although I'm starting an EPFL, which is in Switzerland. It's the Polytechnical Federal School of Lausanne. And today, I wanted to show you potential energy surfaces. But I thought that might be a bit boring, and since it's my video, and I do what I want, I'm going to show you theme parks and slides, because why not? Going to make myself smaller here.

OK. What do we have here? Well, this is the Water World. The Water World is this theme park which is in Lloret de Mar, a city next to Barcelona, kind of. And as you can see, they have these amazing slides that end up in a funnel, like you can see this guy at the bottom of the funnel just fall through this hole.

But what if I want to simulate this? I would need a software that enables me to do this, right? There is some software that can do something like this, but I chose to use Wolfram Mathematica. And now I will show you my little funnel. Here it is. My humans are these black particles here. Now, what if I let some time pass? What happens to my humans? They get closer to the center of the funnel.

That makes sense, because gravity pulls them to the lowest height, right? This height is actually related to gravitational energy, since gravitational energy is proportional to height. Therefore, this is just exactly the shape that the potential energy surface for the gravitational energy looks like. So we have constructed actually a potential energy surface.

But these kind of surfaces can represent many other types of energy, not only gravitational energy, and can be plotted with other coordinates rather than space. Here, we have x and y, which only defined the space where these humans and funnels sit, but I could use other coordinates. Like for example, the distance between two items, or the state of the system, or things like this. Things in which energy, the energy that employing depends on.

In order to simulate these things-- to simulate the funnel that I did or what I'm going to show you after, I need statistics. But don't run away, they're easy to understand. So what I'm going to do in order to simulate this is the following. Imagine that I have this blue line, which will be like a slide, and imagine that the bottom of this blue line will represent the floor-- the ground. We'll call it ground state. And the upper part is like something which is higher in energy. Now, I'm going to separate this slide into some finer parts. This is going to be the discretization of

the system. I'm going to discretize my system. Here, I discretized it in five steps. You can see these red steps.

What I'm going to tell my particles, which will represent the state of the system, is the following. So my particle will be in the initial state. I will tell my particle the following. It will attempt to go either down or either up. It will have 50% probabilities of trying to go up and trying to go down. Now, there is something we have to differentiate. One thing is the attempt. One thing is to try to go somewhere, and another different thing is actually going somewhere. So my particle is going to try to go up and down with equal probability.

Now, if it chooses to go down, it will have probability equal to one to go down. This means that if it tries to go down, it will actually go down. Now, if it chooses to go up, it's not that clear that it's going to go up because-- and I'm going to make my screen bigger so I can show you-- probability of going up will be equal to this term here. This term depends on energy two, which is the energy of the upper state, and energy one, which is the energy of the initial state. The more separated they are, this means the bigger this barrier is. This is actually called energy barrier. The bigger this step is, the more difficult it will be for my particle to actually go up.

There is another term I didn't talk about yet, which is this one. This is temperature. Temperature, here, will-- if temperature increases, the probability of my particle to go up will also increase. This means that the more energy we give-- the more thermal energy we give the system, the more temperature we give the system, it will be more probable for my particle to be able to go up. In a system where my temperature is close to zero, in a system where my temperature is super low, my particle will tend to go to the ground state, which is the bottom of my curve. If I give energy enough, then particle will be able to go anywhere.

Now, what I'm talking about here is not a system with only one coordinate. I'm talking about a system with two coordinates, therefore I'm not talking about lines. I'm not talking about curves. I'm talking about surfaces. Then, the example I showed before was basically a particle that can go up and can go down, as you can see here with this blue row. But now, I'm going to have a surface, so my particle will be able to go many other places. Therefore, my particle will attempt-- the attempts that it can do are not two. There are going to be eight which will describe this surface.

Now, what I wanted to show you is actually a real case where these surfaces can be really useful to understand the system, and these are the transition states. But in order to do this, I'm

going to talk to you about the Lennard-Jones potential first. The Lennard-Jones potential is a very well known potential energy curve that describes the interaction-- describes the behavior of energy of the system as two atoms get closer, and closer, and closer together. Imagine, here, two atoms, which could be two hydrogen atoms and are teared apart. They're super far from each other, and then the energy is zero.

When they are getting closer, and closer, and closer, there is a point where energy will be at its minimum. This minimum energy is the most stable state of the system. This distance will be the optimal distance-- will be the equilibrium state. Now, if we put these atoms even closer, and closer, and closer, the energy of the system will increase. An increase in energy means that the state is less happy. The state is less stable. Therefore, the most stable part of the system will be the minimum. The state will always try to be at it's minimum. Here, this minimum would be in a distance between these two atoms.

What I wanted to talk to you about, actually, is triatomic hypothetic molecules. This molecule, especially HHF. HHF is a molecule which is-- it cannot be isolated. There are some experiments that show its existence for nano or femtoseconds. This exists for a super, super short amount of time. We could even say they are virtual, but it's a state where the system has to pass through in order to change. I'll explain after.

The thing that we have here is one hydrogen atom which has-- we will plot. One of the coordinates will be-- the distance between this hydrogen atom, and the other hydrogen atom, and the other coordinate that we will be plotting is the distance between this hydrogen atom and fluorine. This means that we will have two Lennard-Jones potentials. One between HH and one between HF. This will describe a surface.

First of all, I'm going to explain you what this transition state means. We will have different states of our system. First of all, we will have a molecule which is H2, and some fluorine somewhere. This particles-- the molecule and fluorine-- will collide, and we will end up with an HF molecule and a hydrogen atom somewhere else. In order for this to happen, the system has to undergo through another state, which is called a transition state, which is actually our HHF virtual or hypothetic molecule. If a system wants to go from H2 plus F to HF plus H or visa versa, it will preferentially go through this transition state.

How can we actually see this in a potential energy surface? Here, I show you how the potential energy surface of HHF system is. [INAUDIBLE] described by the HF distance, where this

minimum represents the state of the system where the molecule HF exists, and the other hydrogen atom is somewhere else. Here, we have another Lennard-Jones potential, described by the HH distance. So in this minimum, the state of the system is an H2 molecule and some fluorine somewhere else.

Now, the preferential path for this change to happen from HH to HF, or vise versa, will be through the transition state, which is a subtle point. What is a subtle point? A subtle point is somewhere in the surface where the derivative of energy is zero, but it's not a minimum, and it's not a maximum. It's actually a minimum in one direction, and a maximum in another direction, and this will be the HHF state of the system, as you can see in this contour plot on the left.

To illustrate this, I'm going to show you. Now, my particles-- I'm going to show some particles in the surface. Now, this particle means it represents the system, not atoms. It's the system. Here, I have an HF molecule because the system is in this minimum. Now, if the particle for some reason, when given enough temperature, it goes through this state-- this is the transition state. The system is HHF, but if this particle falls into this minimum, then the system is HH-- this hydrogen molecule and the fluorine somewhere else.

Knowing this, I'm going to show you what happens when I have lots of particles which are lots of representations of the same system because I want to see the probability of the system to be in one state or the other. I'm going to give [INAUDIBLE]. This is an histogram. An histogram is this plot with bars that shows me the population. As you can see here, the particles are just running all over the place because I gave energy enough for them to overcome any energy barriers. But if I decrease temperature, [INAUDIBLE].

OK, now, here you can see that we actually have some preferential places for these particles-- these states of the system to be. They are in the minimums because they cannot jump in the minimum because they cannot jump over the energy barriers.

Now, as you can see, they are also pretty-- like, in the histogram, you can see that if I increase temperature a little bit, the preferential path they take, more or less, is the transition state, which is done at this point. This is one of the things that we can use Mathematica for, but it's much more powerful. It can actually do many other things, and it can solve many other science related problems. And not even science related, you can even do art with Mathematica.