

Hi welcome to video 2.2 in our series on building a simple electronic structure programme in MATLAB. In this video we're going to show how to implement a Gaussian basis set of Gaussian basis functions in your computer programme. So this is the one where you have the least get very little programming experience. We're going to walkthrough every step of the way on this one. Time sort of outline exactly how we're going to convert information from the idea of these functions into what we need to put onto a computer so we can access that and do all the things we need to do with them. So hopefully this should be pretty easy to follow. We're going to do is we're going to programming or Gaussian functions in your computer set. So we think about a Gaussian function or Gaussian basis that we need to know what information do we. The store for each. Basis function. Sorry. Hi each calcium function were going to only confirmed for eBay said we're only going to consider escort girls in this version of the programme and so for each individual orbital we really only need find you information we need to know the amplitude of our Gaussian function are exponent were going to call outlook. UZ locations of this three-dimensional Gaussian. Next Lexie and fix this form. We have X not why not xenon? That said, those five numbers, the normalisation or exponent and our locations. But it turns out that if we stopping for a second. Is a value, is its capital AR normalisation, constant? Snot inhabited. It only depends on alpha. Are you looking for numbers? So additional second SIM and figured out for yourself? Video. Okay, if you got your number of the normalisation person, you should have gotten through alpha over pinder's quarter to power. So what we're going to do is we need to first try to programme. They can build these individual Gaussian function on. Then we're going to write a second programme that's going to build our faces folders. Your number from the previous video are basis functions are going to be. Song of Gaussian with different export values or different contraction coefficient. And So what we're going to do is we're going to make one. Cellular array. Friend called basis bringing users revels, programme and faces is going to have in elements in each element. In basis will be a set of basis VA school basis function which we had cut him if he came from different counties. There will see how we put that all together on one night in contact. But this is not by any stretch of the fastest way to programme this. It is however a very useful in your way to programme it. Up in the way of my writing, this programme is executed. Maps. Stop. Where? Problem. Finally, once we have know how to write an S orbital computer, then we need to be able to build our basis function or basis function to dependency on two sets of numbers. First the list of atomic numbers or which nuclei were included. We're gonna call that Lizzie event for Z for atomic number, and then we also need a 3/2 full set of atomic workmen. So L is going to be an invite me over a where the first column is going to BS component of each atom in, the second column is going to be the wind component, and the third column is going to be the Z component. And then for each Z for each type of atom, we're going to get the appropriate combination of Gaussians to make up our basis functions. We're just going to get this from the literature. Um. And so for each Gaussian basis function were going to use our function build S orbital to build that that individual Gaussian basis function. I got the number for hydrogen, which is what we're going to do with the first from the basis set exchange. If you go and look at the basis that exchange for 6-31 jeans are. Common, not great, basis said. Just simple. You'll get three. We got a couple different numbers. The first column here your list of fraction coefficients, your outpost. In your second set of numbers is your population. So how much of each normalised? Now scan. It should be said posed off and then we have two bases functions with these hydrogen atom both as orbitals one that three galaxies movement has a single Gaussian super every hundred anatomy added to our we used in our programme are going to basis functions. There's a little bit of a confusion here basis that

exchange says. Numbers come from this paper. I went and read this paper. I couldn't find this number where he worked in there or this paper is all about. Now, 2nd row element so. Um. It's a little bit misleading and I apologise for that, but these are at least consistent with also with the programme Galaxy Music. OK, that little can't get out of the way. Let's hop over the Matlab. And start the work of actually writing these up. This is the HF driver programme that we built last time, and now let's go ahead and start implementing them. The first thing we wanted we need to build a single Gaussian functions were going to. And it still us. Right, that file. Alright, so we're going to make this function in a function in that lab is going to return about a set of values. So we're going to say for middle can return orbital equals billed as. Orbital. We're going to need to get this 4th for things. The next location Adams Wine, location Z, location Annan. I said that each Gaussian, each primitive Gaussian is going to be structured in the way that we make a structure in MATLAB will use the dot operator. So I'm going to say temp X not equals AX. Temp not why not? Have dot Z naughty today. Semi colon. Coming out temp dot alpha. Alpha. And then temp dot N normalisation constant. Two times alpha divided by 5. Care. Drink water. Power. Orbital. I'm going to say this, but we're going to show how that actually makes an escort. They will fill us folder. 00 minus one exponent of stuff. You see how it returned an orbital with an excellent why not Z not component, an exponent alpha in a normalisation constant, and if I write F the alpha. I will access the number 7. Rap dot X Nan should get 0F dot end means. You can see I can use the not operator to access individual. Pieces of my plan worked. Now that we know how to build an orbital, we need to go ahead and build our basis function. Edit. Phil. File. Again, we can function. At this time is going to return two things. It's going to turn the total number of electrons in R. Cell array of basis functions, so the return to think we're going to bracket. Basis comma in. Fulfil visa sponsor input arguments going to be. List of atomic nuclei. Tom Ford. OK. Alright, so firstly knows how many atoms we had an Adam equal. Size of the. The size is it? And welcome in total number of electrons. Whole number basis from to this game start at 0. And now even the little look out for me. Or index. One through and out. X not people al. Index. What you doing in the active Mormon? For each one the Y component. Owner. And now we need to not only have the atomic locations for each more bill. Reach out. Now we need to. If the right set of exponent. So we're going to do something called a switch case. Switch. X. He's won, so it's basically we're saying we're going to take the. Number that contained in Z of indexes E1 and E2 and E3 of his former progressive. And we're going to do different things for different values, so case one. A swift SZ in next equals one. It's typing now. The number one. Any plan plus water. And one electron. And now, yeah, it faces. We're gonna get these numbers. Sub zero. Get these numbers directly from the website.

We're going to look through each out today with for me. For index. One threw em out. X not people al. Index. One entering in the ice cream for men. Reach won the Y component. And now we need to. Now that we have the atomic locations for each more battle. Read out. Now we need to get the right set of exponent, so we're going to do something called a switch case. Switch. Please one so it's basically were saying going to take the. Number that contained in Z of index of Z1 and then Z2 and Z3 is poorly progressive. And we're going to do different things for different values, so case one. USwitch is E index equals 1. As hydrogen atom. She's number one. An event was sponsored. We had one electron. And now we have two bases, funk. We're going to get these numbers. 3.11370. We're gonna get these numbers directly from the website. 0.946. Now we had two basis function. Now we're going to get these numbers. 3.11370. We're gonna get these numbers directly from the website 0.0.9. There are a couple of different ways you can get these numbers. Can get these words numbers by

fitting several Gaussians to us later. Orbital will want us leader orbital. You can give them by minimising the energy of the atoms. We need to. 5. Spectre the exponent. Professions. Point. Horse. 9. This could point to watch. I apologise for that. 40. 7. 8137. Some 57. OK. Alright, so now we have those exponent. Plus one to one basis function. Basis. Access to celebrating with currently does not exist in the final few things. First gonna find. It has three calcium functions in it, so dot N tools 3. Pieces. See. \*\*\*. So the coefficients here are just these three value for the call on the second column vector of our matrix S. And then basis? Indeed. Maps. Having a rave of Gaussian structures near to the first one is billed. Ask. Why not? It's not. Why not Z not? \*\*\*. 1. Basis. Nike. Same thing, just. With the 2nd. Traction or second opponent? What? An basis? 1.

An basis? Dodge. Free. Pass. War. Orbital X not why not? See. Not \*\*\*. So we've added those. And now we can add the next basis boxer ever doing two basis functions for each hydrogen atom. That completely defines our basic function or our first Gaussian. So let's do in the  $N + 1$ . The second one. Only have one Gaussian dinner. Faces. Pass. 1. Basis in D. Not. Bill asked. Time. Why not Z not? Look at this number 0.16177. Spacious functions for each half of the hydrogen atom. Is 2. Battle. So you can. Go to the basic exchange basis that exchange yourself and see what the orbital for helium atom would be. Lisa is an exercise you want to watch Mickey typing here. Then that should be. So we now have our function. Basis. Anne. Spell basis. Haha, yeah. To get four hours. So I did. There was Z is 200 Adams. AL located three extra department and so family do the. One and AL. 1.003.6.

6. And there we go, where the. Read. Dot. Right, so we're getting can access each element of our fellow Ryan. So now we know how to make our basis functions on the computer and store all of the information we needed. Sort of complex, the compact place where we know how to access it programmatically. In the next video, will start trying to figure out how to evaluate different matrix elements. Will look at the overlap matrix, the kinetic energy matrix. And see how we can build those matrices starting from these Gaussian basis function. I hope you soon. Bye.