Computational Materials Physics (2023-10-02)
Week 1 : setting the stage

(automated transcription)

Welcome to this first real scientific feedback webinar of the course on Computational Materials Physics. So after the introduction of last week, this time we start for real with the content that you have studied in the past week. And this content was meant in the first place to set the stage, to set the context in which the topic of this course fits. But let's start first with another look on who you are, who are the participants to this course. I asked this question in the live session last week to the people who were present in the room, but meanwhile many of you have signed up to the website and so we can have a different view on who is present. So if I look at the data of the past 30 days, so during the month of September, the state of yesterday was that 44 people made a self-presentation, and I like to read through these self-presentations very much. That's really interesting to see the diversity of people that are present in the course. I see some people with whom I have something in common, I noticed there was somebody who describes him or herself as a runner, so am I. There are also people who come from a totally different background, and it's this combination of diverse profiles that makes an interesting cocktail. As of yesterday, more than 30 people had filled out the Are You On Board forum during the past month, the Are You On Board forum for the first module, so that means that that's about the number of people who have completed that first module in the past month, and there were 28, and I just looked even a bit more, subscribers to the administrative news channel on Zurich, which means that these people are interested to follow the course in sync with the edition at Ghent University. So all together I would say something between 20 and 50 people have started following this course, which is a nice group to work with. In contrast to that number, only very few time reports were submitted for the first week, so I guess I estimate only two people did that for a few modules of the past week, for a few pages in the module of the past week. That's not really much, so I encourage you to spend a bit more attention to that, it's really helpful if you fill out the time report at the bottom of every page. Where do all these people come from geographically? Again data of people who registered in the past 30 days, and there were 71 of them who filled out the geographical information, and that's a nice part of the world, of course quite some participants from Europe, but also Africa, South of Asia, even very remote locations as New Zealand, and North and South America, so all continents are represented, very nice. Age wise, so 178 people who filled out these data in the past 30 days, roughly, well somewhat more than 1 quarter of you is under 25, about half of you is between 25 and 35, then there are a few people 35 to 44, and a few people who are even older than that, that's a very normal distribution, but also here it's good to have people from different ages. And what are your backgrounds in terms of career stage? There is a small fraction of bachelor students, then about 1 quarter of you are master students, 1 third are PhD students, a few postdocs, and then smaller groups of staff scientists, people from industry, or even hobby learners, so that too is a nice and common distribution. I asked you also in that first week what do you expect about the course, and here the data do not show much discrimination, the four suggested topics were all rated to be similarly important, to learn about concepts from materials physics, to learn about concepts of ab initio methods, to learn, to get hands on expertise on using ab initio methods, and to be able to read papers that make use of ab initio methods. So most, the MacKenta peak, which is the indication that you find this very important, is dominant for all of these four situations. If I look at the specific comments that you wrote about this, some people say explicitly I expect that after this course I will be able to use computational codes to study materials properties, or formulated in a different way, I hope I will be able to carry out independent research making use of density functional theory. Somewhat differently, but equally valid, I hope that in this course I can connect with other students working in this field to expand my network of professional contacts, that's a valid justification as well. Some people wrote very specific scientific goals, I want to be able to learn something about magnetism, for instance spin excitations, or I want to be able to simulate thermoelectric devices, that is perhaps a bit too specific, so I can guarantee you that these specific topics will not be dealt with, although the methodology in general for sure can be used to apply it to the situations that are listed here. There were a few questions you raised about the practical organization of the course, so let me go through these. Some people wondered what is meant by reports that have to be submitted, I only see forms and yeah, that's right, I use the word report perhaps in a bit too general way. So if you scroll

through the pages of the course, then you will see that there are sometimes specific requests, like write something in this form, or fill out this form, or submit a file here, with report I mean any of those actions, and it should be self-explaining if you go through the pages what are the tasks that need to be done. People from universities that are not Ghent, they can ask questions about how to get access to a high-performance computing facility, so for the people from Flanders, and in particular for the people from Antwerp, that is easily realized, I got an email from your HPC administrator and apparently you have, the people from Antwerp have got accounts already. The people from Ghent University, they find in the course site instructions how to set up their HPC account, and part of that, the technical part of the setup is valid for the other Flemish universities as well, it is only the procedure of getting the account that is a bit different. So for people within Flanders, HPC access should be straightforward. A few people asked, well I'm a student in another country, not Belgium, so how do I get HPC access, and do I need that at all for studying in this course? That's the first question I cannot really answer, it will depend on your local situation. If you are working in an institution that wants to grant you HPC access, then you can definitely use it for this course, if that is not the case, there is nothing I can do about that. However, you do not strictly need HPC access. Most of the tasks and exercises in the course can be done on a laptop, and the software instructions that you have found in the first week, they were meant in the first place for using a virtual machine on your laptop. So therefore, if you don't have HPC access, that is not strictly necessary. You could then wonder, if I use my laptop, and someone else uses an HPC system, will that affect the results? If we do calculations on both, will there be a difference? And here the answer is no, you should get the same results. The ones running on the HPC may get their results faster, but the numbers themselves, the results themselves, they should be identical. Somebody asked, the exercises in the course are described with quantum espresso as the DFT code, is it also possible to do the exercises or to participate in the project with a different code? And here the answer is yes, you can do that, only I will not be able to give you specific support with this. But if you have at your site another DFT code that is properly installed and where you are somewhat familiar with, then no problem to use this for the exercises or for the project. In the project it could be even complementary to what other people in your team do with quantum espresso, you can compare the results. If you have any remaining questions on the practical organization of the course, then feel free to put them in the YouTube chat if you are following this webinar live, and then I will look at the chat later in the session and try to answer your question. For now we continue with the scientific part, so feedback on what you did during the first week of the course, the setting the stage. And we started with a video that is already several years old now, but that remains totally valid, a video from Gerbrand Sieder about the idea of creating materials from thought. And the question I asked you about it, the confident statement was, I can explain why this vision of materials design at the quantum level, why this is attractive for a material scientist. And you see this histogram, towards the right means, yes I can explain this, towards the left means, no I cannot explain this, and you see that the distribution is towards the right, so that means that this is something you feel confident about. If I read through the answers to the summaries and comments that you wrote about that video in the forum under the video, I see that only very few of you strongly disagree with that message. And if I compare that with the kind of answers I got on this a few years ago, that's really a difference. It shows that this idea of material science is something you can do at the computational level, directly from quantum physics. This idea is slowly starting to get familiar with the scientific community. People 5 years ago would be very suspicious about that. Is that possible at all, would that be useful? There were a lot of doubts. Now less and less. I quote here a few of the specific answers or comments that you gave, somebody wrote it is in my opinion the most empowering thing that can happen in materials engineering. Absolute respect for resources and environments, because you don't use any materials, you simulate and test at the thought level and only then you bring it into the real world. So that emphasizes some of the possible advantages of this approach. I must say absolute respect for resources, that's maybe not totally true because high performance computing requires a lot of electricity. So it's not, it doesn't come for free, you do use resources. There are however a few people who have some sound reservations, so this answer here tells it is important to note that a simulation isn't always what happens in reality. Therefore if you would exclusively use this single computational tool, that would be a bad idea, because these simulations are only as accurate as they are programmed to be. And that is definitely true, you will always need an experimental verification of what you predict. But the goal is that we have this experimental verification only at the end of the thought process and not at the beginning and throughout the thought process as it is currently the case. Someone else says, I still believe that the real world, that experiments in the real world are indispensable as

only these will truly show how a material behaves. So that's partly the same as the previous comment. A kind of a warning, we do have good tools available, good experiments available, it would be a pity not to use them. And I agree with that, but it only is a matter of how much of these experiments and when in the development cycle will you put them. Somebody made a comment, well, good, nice, but these calculations require supercomputers and not everybody has access to one. So therefore some people may be forced to work at the experimental level. And this is something to which I do not completely agree, because you will see during this course that even with your laptop you can do useful things. So supercomputers are of course helpful and in some cases for some problems necessary, but even without you can do it, or you can do useful things. And somebody pointed out also an alternative route to this fully computational materials design, because also at the experimental side things are changing. Some labs are developing a new style of experimentation, where rather than doing one experiment by one researcher, you have a robotic setup, where many variants of the same experiment are done by a robot. And in this way you can do at a much higher rate, you can examine specific properties of combinations of materials. So accelerated materials discovery without calculation, but with automated experimentation. And some groups are even connecting these two ideas, that you do part of the screening computationally, at some point you hit a material that you think is interesting, that's transferred to the robot, who does the experiment, who gives feedback to the computation, yes you were right or no this was wrong, and based on that the computation then changes its path in the search space, that I go in a different direction, or I proceed with more detail in this direction. So experiments and calculation can even work together in this respect. After this long-term vision, we go zooming in on the question, what does it actually mean to do a calculation ab initio, what is an ab initio model. And I asked you, why do we call quantum physics an ab initio model, why do we call classical mechanics an ab initio model, and is classical electromagnetism an ab initio model, and if it is, what are the first principles of classical electromagnetism. Many of you gave a correct answer here, I show one of them. Classical mechanics and quantum mechanics are models that want to explain everything within their field, through some basic equations, the Schrodinger equation for quantum mechanics, Newton's law for classical mechanics, and because they do that, because they use some basic equations, some axioms, and then explain everything in their field based on these axioms, therefore they are ab initio models, ab initio methods. And in the case of electromagnetism, that too is an ab initio model, and the axioms of that model are Maxwell's laws, so you take Maxwell's laws, they fall out of the blue, there is no way to prove them, you accept them as axioms, but from there on you start calculating and all electromagnetic phenomena are predicted, so electromagnetism too is an ab initio model. Then we look at the objects we will study, solids, and in this section I want to convince you that solids really are quantum systems. And the first thing I asked you was to give your definition of a solid, and I show here two definitions that some of you gave, that in a way circumvented the point I tried to make, so I will not read them, they are correct definitions, but they were not addressing the point that I was interested in here. In contrast to the majority of your definitions, and I show only a few of them, but I have highlighted one word, the word atoms, or sometimes particles, which underlines the hypothesis I had, if you ask somebody to describe what a solid is, people will very often answer it's something that is made of atoms, and that is what in this course we will not look at. Atoms in our treatment of solids do not exist, atoms exist in the sense of elements, the elements of the periodic table, that's absolutely a reality, you can take one single item of such an element and put it in a vacuum, and that will be an atom, no doubt about that, but if you condense these atoms into a solid, then it's not so uniquely possible anymore to determine where is that atom now, where does one atom stops and the other atom begins. There are no good physical criteria to determine that boundary, so the concept of an atom somewhat loses its validity once you are in a solid. What remains valid is that in the solid you have positive nuclei and negative electrons, and these are in a way the only objects that really matter. So we will study a solid as a collection of positive nuclei, not atoms, positive nuclei and negative electrons, and these two types of particles, they electromagnetically interact with each other, nuclei with nuclei, electrons with electrons, and electrons with nuclei, and they do that not in a classical way, they move according to the laws of motion of quantum physics. That description, that is our definition of a solid, we will look at a solid that way. You may ask at this point, isn't that same definition applicable to a liquid? So how would we distinguish a liquid from a solid? And I completely agree with that, this description is also applicable to a liquid, and in the computational sense there is not much difference between a solid and a liquid. The only difference is that in a solid the positions of these nuclei do not change very much over time, and are on average static, so you can do one single calculation and you capture already a lot of the information of the solid, whereas in a

liquid there is no average position of the nuclei, they keep moving in every different directions throughout the volume in which they are allowed to move. So therefore doing these type of calculations for liquids will require many subsequent snapshots in time, so many different calculations and that will always be more time consuming and gives you access only to statistically averaged predictions and not to precise predictions as possible for solids. So we will concentrate on solids, but in a way the things we do here will be applicable to liquids as well. Well if that is all so nice, if you can describe solids as a quantum system fully with an ab initio method, what is then the problem? Why does not everybody do it that way? And I asked you exactly that question, why is not yet everyone today using plain quantum physics to talk about solids? And well there was a video about that and I asked you to summarize your understanding of that video, and here are a few examples. Somebody says, it may not be sufficient using quantum physics to define solids, because solids could also go beyond that definition, there could be a variety of layers of characteristics that may not be captured using quantum physics alone. I don't agree with that answer, not at all, yet I find it a very interesting answer, because it may show that what quantum physics means is not fully understood by the one who wrote this answer. If quantum physics really is an ab initio description of a solid, ab initio means that these few fundamental equations, here the Schrodinger equation, they do describe everything. So if you say there are also layers of characteristics not captured by quantum physics alone, what would that be? Which other physical mechanism would play a role that goes beyond quantum physics? That does not exist, not as far as we know. Maybe what you mean is that there are some characteristics, like say the interaction of two dislocations in a metal, that require so many atoms, that describing that problem with quantum physics will be computationally very hard, but that doesn't mean that fundamentally quantum physics would not be able to describe that. No, quantum physics does describe such phenomena perfectly, only we have to resort to second best methods that just compute a bit faster than doing it with only quantum physics. Another answer, well quantum mechanics is a very hard subject and intuitively not very easy to understand and therefore people will not easily discuss solids via quantum physics. Also here I don't think that this is a correct answer, that this is not what happens in reality. Because even if only a few people would truly understand quantum physics, they could still program this methodology in a computer and everybody else can use it. You don't have to know how the engine of your car works, before you are able to drive your car. That's a very similar situation. A few technical people should be able to know how the car works, but most of the drivers just don't have to. So no, this cannot be the reason why quantum physics is not routinely used for solids. If that would be the reason, then only people who work in a car workshop would be allowed to drive a car. This here is an answer that goes better into the direction of the truth. The computations are incredibly hard and require a lot of assumptions and even then they cannot be perfectly solved. That hints in the right direction, but it's only partially true. Because in principle we do know algorithms to solve the Schrodinger equation exactly. This is no secret, we can write down the recipe how to do it. Why don't we do it then? That is given in this answer, captured by this answer, the computational power that you would need to solve a system that represents a large solid, that computational power becomes unrealistically large. So it's not complexity as such that is the hurdle, it is time. We know how to do it, we know how to solve the Schrodinger equation, but these algorithms, even when executed on the fastest computers, they would just take too much time. And therefore the practical application of this methodology is still to some extent limited. It can do more and more, the faster the computers become, the more it can do, but there will always be, for the time being, some upper limit. For the time being, because there may be on the horizon fundamentally different ways to deal with this, somebody made the suggestion of using quantum computers. Now here in this course and in your project you will use classical computers, chips made from semiconductors, that can be very fast, that can compute orders of magnitude faster than the human brain can do, but maybe not fast enough that is needed to describe a truly quantum system. Maybe in order to describe, to do the calculations for a quantum system, you would need a computer that works in a quantum way, and quantum computers, yes, they are being developed, they are still, they do not have the capabilities that your laptop has, but for some very specific problems they are becoming sufficiently powerful. As that technology proceeds, there will be more and more problems to which quantum computing can be applied, and maybe someday also solving Schrodinger equations for realistic solids, in a time frame that is much much shorter than a classical computer ever would be able to do. We understand now why quantum physics is not yet routinely used to study crystals, and now we take a step back again, and we ponder what would be the advantages if that would be possible, how would materials engineering look like if we can solve this Schrodinger equation routinely, and my point here is that in that

case, materials engineering would look like construction engineering looks today, and we used here the example of developing a superconductor that is superconducting at room temperature, or developing and building a new bridge, how many attempts does the construction engineer need before he or she can deliver a new bridge, and how many samples does the materials engineer has to produce before he or she can deliver a room temperature superconductor. That was the question I asked to you, and it will be very obvious that the bridge is built only once, and you know in advance even before you start building that this bridge will be the good one, whereas for the superconductor you have to generate many samples, and up to today this room temperature superconductor has not yet been found. Why is that? Because in construction engineering they can solve their fundamental equations, while in materials engineering that is not yet possible, at least not for every crystal and every property. And that is basically what this answer here expresses. I used this example already several years, and a few years ago there was one student who came up with a cartoon that really nicely explains this idea, and even applies it to the problem of the bridge, and I like to share that cartoon with you. It's a Calvin and Hobbes cartoon, where Calvin is driving in the car with his parents, and they are crossing a bridge with a sign load limit 10 tons. Calvin asks to his parents how do they know the load limit on these bridges, and the father starts explaining, they drive bigger and bigger trucks over the bridge until it breaks, and then they weigh the last truck and rebuild the bridge and put that 10 ton load limit sign next to it. Which of course is not what happens, that is what would have happened if construction engineering was still at the stage where materials engineering is today. Then we pondered a bit the difference between theory and computation, and I want to emphasize here that these are two different activities, and I asked you then, quantum based materials calculations, these are a simulation activity, a computational activity, and not a theoretical activity, that's the statement. How would you convince someone about that statement in a few sentences? I read here one of your answers, theory, that is a process where we are trying to come up with a mathematical formulation to describe a system, and once we know that this mathematical formulation agrees with the experimental work, with the experimental results, then the theoretical work is done. Simulation enters this stage now, because simulation, that is the process to apply that theoretical model to different situations, and to solve the model for the specific situations in order to predict what will happen in these situations, and that can then be tested experimentally. That is a completely correct answer. The same answer but much shorter formulated, theoreticians will try to develop new science, computational scientists will try to optimize that science for practical use. I agree with that statement. Both have their own version of creativity, it's not that one is more creative than the other, but it's a different kind of creativity. And the next part in the question was, why do you think that many people intuitively have the opposite opinion, and think that simulation activity is theory? Here the answer at the left hand side is the shortest way I think how you can answer this. Many people have as general attitude, if there is no laboratory instrument involved, then it means that this is theoretical work, which I claim is not the case. If you are doing simulations, that's not experiment, and that's not theory, that's something in its own right. Somebody asked here, how is machine learning going to affect all of this? So you have your density functional theory, we'll deal with that method in the coming modules. You have your density functional theory to make predictions for quantum systems, but will developments in machine learning perhaps replace density functional theory in the long run? And that is to some extent happening nowadays, we are today witnessing a transformation where people move from solving the Schrödinger equation by explicit algorithms as density functional theory, to a more data science approach, where you will train some machine learning algorithm to predict what the DFT answer would be. So rather than solving the equations that are the start of DFT, you give the machine learning algorithm many examples of the answer in this situation is that, in another situation is that, you give a billion of these situations, and then the algorithm learns, well apparently in that situation the answer will be this, without solving the equation itself, but just by comparing it to many other similar situations and doing a kind of smart interpolation. If you succeed to train an algorithm up to that level, that's of course much faster than solving the actual DFT equation, and that activity is now really taking off and will be used in computational material science more and more. So I would say that our triangle of experiment, theory and simulation will get a fourth item, you will have experiment, theory, simulation and data science, that will be the new paradigm in which computational material science will work. A few words about hardware, we already touched it in the very beginning. Explain in which direction the development of faster computers is heading, now that video is really a bit old now, there has been a time when the clock speed of a single processor was always increasing, limits have been reached there, and now computers become faster because they are just combining many, many, many

CPUs. The overall result is that we are still in a time when every two years computers become twice as fast as two years before, which is for a computational field a very unique situation. It effectively means that we have a lab, a computational lab, that every two years is twice as powerful as two years before. That's a comparison that is often made by Nicola Marzari, a computational scientist from EPFL in Switzerland, and it may sound as a trivial statement, but it is extremely powerful. Imagine that that would be the case in your experimental lab. Imagine you are running a lab with an electron microscope, as there are several in Ghent, and without doing anything, two years later you enter your lab and your microscope is twice as good as two years before, and two years later again, and again. In twenty years you have a microscope that can do incredible things, only in experimental research that does not happen. Yes, your microscope will improve, better and better microscopes will be developed, but by far not a doubling in specifications every two years. With the speed of computers, that is still happening. And that means, the result of that is, that this field of computational material science is still in full development. If we look ten years back, what we could do ten years back compared to what we can do now, that is, there is a fundamental scale difference there. This here is a view on the fastest computer of today, a computer in Oak Ridge in the US. It's of course, if you look at the specifications of such a machine, you can dream and you can compare it with your laptop, and you can say, well, if I would have access to that machine, imagine how quickly I could do the calculations that I need for my master's thesis. That's of course true, but even the people who work there at Oak Ridge, they rarely have access to the entire machine, and this machine, just as any other HPC system, will work most of its time for much smaller projects, and then many of them together, so it's not that one researcher has access to the entire machine at once. That may happen for very specific applications, but then only a fraction of the time of a year. Hardware, okay, software is the other thing, you need codes to run on that hardware, and in this page we have a quick first view on the software that is available to solve Schrodinger equations, and you have this picture with logos, and that has just one message, there are a lot of codes available to solve the Schrodinger equation. This was a snapshot from Wikipedia, where you have a table with codes, and then with a few columns that indicate whether or not, green or red, a particular code has a particular feature, and you see that in this variety of codes, there are different combinations of features. There may be some codes that are really mirrors of each other, that both have exactly the same functionalities, and the same advantages and disadvantages, but more often than not, it may depend on the problem you want to solve, and the material you want to study in that problem, which code will be your selected one. You try to find the optimal code for a particular application. Learning to use such a code, that will be an explicit part of this course, and in the past week you have set the first step for this, that was in the let's play tile, the task prepare your environment, and in that task I have asked you to install a virtual machine on your laptop, a virtual machine that contains the DFT code that we will use in this course. So I hope that that has succeeded for all of you, in case it did not succeed, then please report about this, either via the question form, or via the Zulip channel, to point out what exactly was your problem, and maybe there is a way how we can help you. This applies to everybody, if on the other hand you have also access to an HPC system, I said this in the beginning, then you can work with Quantum Espresso or with another DFT code also on your HPC system. For Ghent University there are instructions available how to do that, for Antwerp the technical part of these instructions, they are the same, but they have to ask for their accounts with the admins in Antwerp. That's the content for this week, and I'm a little bit worried that I don't see any YouTube activity, so I wonder whether everything went fine with the stream. It's being recorded, there is no problem about that, so I will definitely be able to put the video online, but maybe there is something wrong with the live access. What will we do in the coming week? We have set the stage, and now we can dive into the methodology that we need to solve the Schrodinger equation, and that will be density functional theory. We will need two weeks for that, so in the coming week density functional theory part one, and these are the items that you see here described in the menu on the screen. In the let's play tile, there we will look at what I call a basic calculation, you will use the Quantum Espresso DFT code to solve the Schrodinger equation for the silicon crystal. I tell you in advance, at this stage you will not fully understand what you are doing. It is more a recipe to go through the different steps, to verify that everything is working on your laptop, to get a feeling with what you should do, and understanding what exactly you do that will come gradually throughout the course. In this week you also can read the project proposal, so the suggestion I gave you this year to work on with a team, if you are interested in that, remember, Flemish 4 credit students, they can choose the project work as their assessment option, or they can alternatively don't do the project and do a final exam, volunteering students, they can participate in project work if they want, but they do not need to. The choice

whether you will participate in the project or not, that is something you have to make in the coming week. There is a forum foreseen in the project tile, where you can sign up for the project if you want so. I should give one warning here, somebody in Zulup noticed that, that is if you have installed the latest version of Quantum Mobile, and you start to run that basic calculation, then it will fail, and the reason is technical, there is somewhere a bug in setting up Quantum Mobile, and by giving the comment that you see here on the screen, you can solve that. This is only a temporary fix, and you have to do this whenever you start your Quantum Mobile, but I have reported that bug, and I hope that the people from Quantum Mobile will soon make a new version with that bug fixed. Okay, at this stage I would ask you, well I will ask you your questions, that will come, but I will ask you first something else. So you find here a link or a QR code to a forum, and I will ask you in this forum two things, first write here on the spot in the 5 minutes that are available for this, write a summary of a few lines about the topic of the past week, so if you have to tell to somebody what did I learn here, what are the important things, well here in this paragraph there you have it. So do that, and secondly formulate an exam question about this material, what would be a fair exam question that probes the understanding of somebody about the topic of the past week. You can put both answers in the forum for which you see the link and the QR code here, and next week I will collect all these results and I will put them under the video of this webinar. And that is meant as a study help, if you read through the summaries that all your colleagues have written, you can test yourself, is that really what I understood about this chapter, or do they point to different aspects that I didn't notice so well, and you can try to answer all these suggested exam questions as a way to train yourself to familiarize yourself with the material. As I just said I noticed that there seems to be something wrong with the stream, so there will no people hear this live, so therefore I will just let this play these 5 minutes and after that the video terminates. I will not come back to answer questions that you may have put in the chat, because there seems to be nobody around to put questions in the chat, but please if you watch this video later, then I still want to ask you, fill out this forum, it's material that will help all your colleagues in studying this course. So with this I see you next week with the feedback webinar on the DFT topic.