Season 1, Episode 4 transcript
Alicia Magann: Tuning Quantum Chemistry's Dials
Speakers: Sarah Webb, Alicia Magann

Sarah Webb 00:00
Hello, I'm your host Sarah Webb, and this is Science in Parallel, a podcast about people in projects in computational science. In this episode, I'm speaking with Alicia Magann, who recently completed her Ph.D. at Princeton University working with chemistry professor Hershel Rabitz. Her graduate research was supported by a Department of Energy Computational Science Graduate Fellowship, or DOE CSGF, for short. Alicia studies quantum control theory, ideas that could allow chemists to zoom into the atomic and molecular scale to direct reactions. We talk about her work on quantum algorithms, her cross-country road trip from New Jersey to her practicum in California and how her dad is her scientific hero.

Sarah Webb 00:44
Good morning, Alicia.

Alicia Magann 00:46
Good morning, Sarah.

Sarah Webb 00:47
Could you tell me how you first got interested in science? Was there a key person or event that helped shape your interests?

Alicia Magann 00:54
I think growing up, I was always interested in science because my dad was interested in science. My dad's an engineer. He was one of my heroes. And he would, you know, talk about interesting things and the things that he worked with. And I think that's what got me excited about science. And then the more I learned about it, the more the more I enjoyed it. And so when I started my undergraduate degree, I picked chemical engineering. And as I went through the degree, I found certain aspects of it particularly interesting. And I was inspired to, to do a Ph.D. as well.

Sarah Webb 01:33
What was it, do you think, that kind of grabbed you about chemical engineering? What was fascinating to you?

Alicia Magann 01:39

I think when I first started the degree, I really didn't know what I wanted, I knew that I liked math. I knew that I liked science. I knew that I liked solving problems. And as I kind of got started, I liked the more mathy parts kind of the most. And so I became particularly interested in an aspect of chemical engineering, which is control systems engineering, which looks at how we can control chemical processes, like what might happen in chemical plants, where you might want to create some chemical product, and you want to tune the temperature or the pressure or something like that in your chemical reactor to optimize how much product you get, and that sort of thing.

Sarah Webb 02:25
So now I want to talk a bit about your graduate research. You were mentioning that you work on quantum control. First of all, what is quantum control?

Alicia Magann 02:33
What initially drew me to quantum control was its connections to the research that I did in undergrad, or at least the spirit of that research. So in undergrad, I worked on control systems engineering, thinking about how we might modulate things like temperature of a chemical reactor to increase the amount of products that we that we get that we want. I also became interested in quantum mechanics as an undergrad. And in the context of controlling chemical reactions, like what I thought about in my control systems work.

Alicia Magann 03:08
And the idea that kind of hooked me at the beginning is that if you zoom in to a chemical reaction, at the most fundamental level, your molecules are behaving according to the laws of quantum mechanics, right? You just have kind of this lump of atoms and nuclei and electrons. And they're described quantum mechanically, how they move how they respond to each other. And so quantum control thinks about the prospect of going in there and speaking to them at the level of quantum mechanics. And so what you need for that is you need to be able to tune your controls at the timescales of the molecular motion, which is very, very fast. And the exciting thing is that with lasers, we can actually design the light that comes out of lasers, to speak to molecules at those timescales.

Alicia Magann 04:08
So we can actually go in and interact with them at the quantum level. And through that interaction, we can try to control how they behave and hopefully control how they react and have a bit of control over the amount of products that we might get out. For example, it's a different paradigm for thinking about controlling chemistry, it's completely different from what I was used to. But this prospect was just very, very appealing. And so that kind of hooked me in quantum control is more general than that. That's kind of the application that really appealed to me. But quantum control is a field of research just considers how we can control systems that behave quantum mechanically. So usually very small systems, systems like molecules or atoms or spins or electrons-- things like that,

Sarah Webb 05:01
I'd like to learn a little bit more specifically about what you've been working on.

Alicia Magann 05:06

So I remember when I first came to Princeton, and I met my Ph.D. advisor, he was telling me about the different research that our group does. And our group is kind of interesting. We have theorists and we have experimentalists. And I remember being really excited about what the experimentalists were doing. But I didn't think I could be an experimentalist, I didn't think it was the right fit for me. So I said, you know, maybe I can do simulations to support what the experimentalists are doing. Okay, I remember he explained to me, you know, doing simulations, to support quantum control experiments is really difficult. The simulations are really hard. And that's because in order to do the calculations that you need to do the computer memory and the computer time costs just scale terribly with the complexity of the quantum system that that you're thinking about. And so I kind of ended up pointing my research, not doing simulations to support experiments but in developing computational techniques in order to make quantum control simulations easier so that in the future, maybe I could do simulations to support experiments. But my work to date has really focused on computational methods for facilitating simulations of quantum control.

Sarah Webb 06:30
So it sounds like you're doing work that will help to eventually work on the problem that you'd hoped to tackle in the beginning.

Alicia Magann 06:38
Yeah, yeah, that's exactly right. I that's what I will be true. I yeah, I'm still very excited about the experiments that that might be possible. And so I would, I would really, really love to do theory for them in the future. But there's kind of a long way to go in order to build up the computational capabilities to actually do that kind of theory.

Sarah Webb 06:59
Can you describe one piece of this work, one particular challenge that you've worked through and how that went for you?

Alicia Magann 07:06
And one of the challenges associated with doing a quantum control simulation is that if my quantum system has multiple degrees of freedom, so maybe it's, you know, just a molecule with lots of different atoms, or different vibrational modes and rotational modes, and so forth, the amount of computer memory and time that I need to simulate the system, in order to understand how to control it scales exponentially in the number of degrees of freedom that it has. And so this is a huge bottleneck. I mean, exponential scaling, means that you can only consider systems that are very simple with just a few degrees of freedom. And that really prohibits you from thinking about or simulating interesting systems, in the sense of complex systems with important practical value, and so forth. And so what I have done in the last year or two, is explore how we might address this bottleneck, using a quantum computer to do that simulation. And so this is a very appealing prospect. Because quantum computers, being composed of quantum bits, or qubits, are a more natural setting for simulating quantum systems, like the molecule that we might want to control. And so given that they have certain advantages, and the most exciting advantage is that they don't suffer from this exponential scaling when it comes to the memory and time that you would need for quantum control simulations. And so this has been a project that I have worked on, towards the end of my Ph.D., where I focused on designing algorithms for

carrying out these kinds of computations on a quantum computer. It looks very promising. Unfortunately, we don't have the quantum computers available today, in order to actually implement this, but quantum computing technology is advancing constantly. So I'm very hopeful that in the future, we'll be able to use quantum computers for this purpose.

Sarah Webb 09:29
So it sounds like you have an algorithm, but now you need a system to try it out on.

Alicia Magann 09:34
Exactly, exactly. I have the algorithm but I don't have the computer.

Sarah Webb 09:38
Over the course of your research. You've also worked at Sandia National Laboratories. Can you tell me a little bit about that work and how it fits with your Ph.D. research?

Alicia Magann 09:47
So this was an opportunity that I had through the DOE CSGF program, where I had the chance to spend a summer doing research at a DOE lab, and I went to Sandia. And this was a really important kind of turning point in my Ph.D. So what this allowed me to do is, first of all, to become interested in quantum computing and what quantum computers might have to offer, in the context of quantum control simulations, and then going to Sandia to spend a summer there allowed me to actually meet quantum computing experts, and work with them and actually do a project in this area. And so it really had the effect of broadening out my Ph.D. So the work that I had done at Princeton, focused on quantum control simulations, in particular, involving chemical systems. And so going to Sandia allowed me to start thinking about quantum computers, which I hadn't been able to do before. I liked it so much I've continued working in the area of quantum computing, and exploring different aspects of that throughout the rest of my Ph.D. And I hope to continue doing research on quantum computing, even beyond my Ph.D.

Sarah Webb 11:13
Alicia, describe a little bit more what a quantum computer is actually like, and what makes a quantum computer quantum.

Alicia Magann 11:20
So since quantum computers are composed of quantum bits, or qubits, which behave according to the laws of quantum mechanics, they're able to take on kind of exotic properties that conventional bits can't. And so two of these properties are called superposition and entanglement. And what that buys you is that when it comes to the first one, superposition, it means that if I have a quantum bit, it can take on the value zero or the value one like we might conventionally think of a bit doing bit can also be both zero and one at the same time. And that's called being in a superposition. And what entanglement buys you is essentially that if you have multiple qubits that are working together to carry out a computation, that they can be correlated with each other in ways that are not explainable.

Sarah Webb 12:18

What part do you hope to play in this future of quantum control and even quantum computing?

Alicia Magann 12:25
So far, I've been more on the algorithm side, thinking about these current quantum computers, which are error prone. And so they're not able to run the landmark algorithms that we hope to run in the future. A big question is, how can we use them in a profitable way, because they do still behave quantum mechanically? It's just that we don't have complete and perfect control over how the quantum computers behave. And so what's been really exciting in the last few years is there have been a lot of efforts all over the world trying to develop new types of algorithms that are robust to these kinds of errors that we know that we have in our quantum computers today. And so this is something that I've also worked on a little bit in the last year, is trying to think of new ways to get the quantumness out of these devices and use that in order to solve practical useful problems in the near term.

Sarah Webb 13:30
To shift gears a little bit, I want to learn a little bit about what life is like for you when you're not thinking about your research and quantum control. What are your hobbies? What do you like to do to unwind?

Alicia Magann 13:44
I like to go outside, and I like to go hiking. I like to go for road trips, that kind of thing. So when I spent the summer at Sandia, I drove there so that I would have my car for the summer, but I was coming from New Jersey, so it was kind of a trek to get across the country. And then at the end of the summer to get back. And that was fantastic. It was very fun to get to see kind of the whole country, I really, really enjoyed that I have kind of a mattress in the back of my Subaru. And so I can kind of sleep there and so on the way to California from New Jersey and then on the way back, I stopped at lot of campsites. And that was really a memorable and really a fantastic trip.

Sarah Webb 14:29
Back at the beginning of the interview, you mentioned your father, and you mentioned that he was your scientific hero. Could you tell me a little bit more about your dad and why he's your scientific hero?

Alicia Magann 14:41
So I mean, I think as a kid, I always looked up to him. He got his degree in chemical engineering, which that's also what I ended up pursuing. And he's had a really great career. He's worked on a lot of different things over the years. I remember when I was a lot younger. He was a propellant engineer. And he moved our family to Germany for a few years when I was a little kid, and then he shifted and he worked on radar systems. And then he shifted again, and he worked on unmanned aircrafts. And he's been very successful. So I always imagined that I would try to be something like him. And I ended up diverging-- when I decided that I would pursue my Ph.D., that was kind of the moment that I was stepping in my in my own direction, but I still very much look up to him. And I still hope that I can have a career that's successful, like his has been.

Sarah Webb 15:55
And just for fun, what's your favorite subatomic particle?

Alicia Magann 16:01
I this is a fun question. I don't know that I've ever thought about this before. Probably right now, I'm really interested in electrons, because of the fact that we're getting these new technologies to, to go and speak to them using these add a second laser pulses, I would say that electrons right now or are at the front of my mind.

Sarah Webb 16:23
And remind people how short is an attosecond laser pulse?

Alicia Magann 16:30
Sorry, I would have to look that. Sorry, it's very short.

Sarah Webb 16:36
I couldn't remember exactly how short it was.

Alicia Magann 16:42
No, I got it. I got it. An attosecond is one quintillionth of a second. So it's 10^{-18} seconds. It's very, very short.

Sarah Webb 16:51
Definitely very, very short.

What key advice would you give to new Ph.D. student or to people getting their start in computational science research?

Alicia Magann 17:07
Something that I did, which had a big impact on the PhD research that I ended up pursuing, is that I spent a lot of time exploring different possibilities, different research areas. This was something that I did at the end of my undergraduate degree, when I had decided that I would pursue a Ph.D. I would just spend hours just scrolling around on the internet reading about different research that was happening. I made meetings with a bunch of professors, some that I knew some that I'd never met at my undergrad university, Arizona State. I just talked to a lot of people. And my hope was that, at some point through this exploration, that I would find something that was just really, really interesting. And if I could find that, then, you know, hopefully, I could somehow weasel my way into working on that. And that would be the ideal outcome.

Alicia Magann 18:06
And so at some point, I did discover that there was a field of research called quantum control. And I learned a little bit about what that meant. And that was extremely appealing to me. And that's what motivated me to apply to Princeton to begin with, because the research in the in the group that I work in, is something that is really, really exciting in the area of quantum control. And so what I encourage young scientists, you know, early Ph.D .students or people who are considering doing a Ph.D., what I encourage them to do is to really take the time to do that kind of exploration. I mean, for me, what it meant is I really switched fields. I went from doing kind of classical control systems engineering, to

doing quantum control, which they both have the word control, but they're completely different. And so it was a whole new world for me, but it's been very rewarding. It's been a great fit. But if I hadn't done that kind of exploration, I, I wouldn't have even known about it.

Sarah Webb 19:11
Alicia, thank you so much for your time today. It's been such a pleasure learning more about you and your work.

Alicia Magann 19:17
Yeah, thank you so much for having me.

Sarah Webb 19:20
To learn more about Alicia and her work, check out our show notes at scienceinparallel.org. That's also where you can send us feedback or suggestions. If you liked this episode, please share it with a friend or colleague and subscribe wherever you listen to podcasts. Science in Parallel is produced by the Krell Institute and highlights computational science with a particular focus on work by fellows and alumni of the Department of Energy Computational Science Graduate Fellowship program. The fellowship is celebrating its 30th anniversary in 2021. Krell administers this program for the U.S. Department of Energy. Our music was written by Steve O'Reilly. This episode was produced and edited by me, Sarah Webb.