Meet Mary Thomas

Dr. Mary Thomas is a computational data scientist in SDSC’s Data Enabled Scientific Computing (DESC) division. Her areas of focus include parallel computing, coastal ocean modeling, and cyberinfrastructure.

During her previous time at SDSC from 1996 to 2001, Thomas focused on developing web portals, leading projects such as the NPACI HotPage and the GridPort toolkit. Since her return to the Center in 2018, she has primarily dedicated her time to her role as the lead for training and education on Comet and Triton Shared Computing Cluster (TSCC). One of her undertakings is Developing Interactive Jupyter Notebooks for SDSC HPC Systems, which her four REHS students helped with this summer.

Q: How did you first come to join SDSC?
I came here in the mid ‘90s. I was doing research in optical physics across the street at General Atomics, which used to manage SDSC, with high-energy laser beam scattering experiments on the fusion reactor there. It was fun, but what I truly loved was computer programming. Merging the two became computational science, which is developing the code and algorithms for scientific computing. I enjoyed it much more than pure physics, so I decided to get a masters in computer science and change my field direction by trying internships at different places, including down at Point Loma and here at SDSC.
Q: After some time away from the Center, what propelled you to return last year?
Originally, I left the Center to start a new supercomputing center at the University of Texas at Austin, but we moved back here once we had our son, Michael. I started teaching at San Diego State University, which I did for quite a while; but after some low funding, I started looking around for what I wanted to do next. When I received an offer to help with education and training on Comet and TSCC, I was definitely ready to come back — I had always liked working here. I finished up what I was doing, and it was just time to move into the next phase of my career.

Q: What are some of the changes you’ve observed at SDSC from your initial time here?
There’s a lot of new people, but also a lot of people I know. It’s still a great place to work, so the primary change to me is the increased diversity of projects, which is very exciting. When I was here in the ‘90s, the main focus was building big supercomputers for the National Science Foundation. Since then, SDSC has been phenomenal in its expansion. They now have data sciences, computational science, computational chemistry, and many more interesting things. There’s a lot more going on here, and it makes it very interesting to be here at the Center.

Q: You’re currently working on the parallelization of the General Curvilinear Coastal Ocean Model (GCCOM). Can you elaborate on its applications?
We use this model to study high-resolution coastal ocean processes. Because it’s a full 3d curvilinear model, there’s no pixelation, or approximation of the surface curvature. You have added accuracy, and it can do meter scale, which is going to be critical for future weather forecasting models. Anywhere that the water, land, and atmosphere interface, you need that higher resolution, especially when looking at issues such as global warming and increased sea level. It’s an exciting opportunity to contribute to that.

Q: What motivated you to join the REHS program as a mentor?
From my experience teaching graduate-level parallel computing classes, I’ve found that students aren’t very well prepared for the rich and challenging world of parallel computing. Most are in a particular area of science or a business application, so they lack a foundation. I think we should be teaching parallel computing in first grade. They really need to have that native grasp of what multiple processes do and how to control them, so the earlier we can reach out, the better.

Q: How would you describe the distinction between mentoring high school, undergraduate, and graduate students?
They’re all smart and capable, but there’s a gap in experience. You have a different expectation level, but I believe in the theory, “Don’t hire somebody for what they know. Hire somebody for what they can learn.” At the end of the day, if you hire somebody for what they know today, it’s outdated in two years. The real question is: in the meantime, what have they been able to learn on their own? I try to feed that capability of self-study in every student I mentor.

Q: Finally, what do you view as the most important qualities of a researcher?
Any researcher needs to be able and willing to explore something entirely unknown. You have to be prepared to assimilate a lot of information, and refactor it down to some small, essential core knowledge. For example, the stack of research papers that I read for my dissertation was about three feet tall. I reduced it to just a couple of inches. You don’t need it all, but at the beginning, you need to go everywhere possibly needed — and without depending on anybody to hold your hand to get there. As I mentioned before, you have to be able to ask for help when you need it, but still maintain an independence. Additionally, be in a field where when you try hard on your own, you’re good at it. If you’re in the wrong field, get out of it. Try something new that comes more naturally.
Q&A with Alisha and Ryan

As two of the four REHS students mentored by SDSC Computational Data Scientist Dr. Mary Thomas, Alisha Chakraborty and Ryan Wei spent this summer working on Developing Interactive Jupyter Notebooks for SDSC HPC Systems. The Jupyter Notebook is a web application for the creation and sharing of documents that contain live code, equations, visualizations, and narrative text. These interactive notebooks will be used for the education and training of Comet and TSCC users.

Alisha is a rising senior at Torrey Pines High School, while Ryan recently graduated from Del Norte High School and will be majoring in Computer Science at USC in the fall.

Q: How did you come to apply for the REHS program?
Alisha: I started my computer science journey with my AP Computer Science class. My dad is a software engineer, so I was always aware of the field; but I never thought that I was interested in it until I took that course. After that, I found the REHS program through my mom, who works at UCSD, and I thought that this was really cool opportunity to explore the computer science field.
Ryan: I actually started in REHS last year. I wanted something local and centered around computer science, so the program fit both criteria.

Q: With the final weeks of REHS winding down, in what ways do you feel you’ve grown since the beginning of the program?
Alisha: At the start, I was so overwhelmed with learning all of the unfamiliar material, but with help from my mentor and other students, I learned how to grow these new skills that I’d never known before. As I mentioned, I wasn’t really involved with computer science before REHS. When I began, I thought, “I don’t know how I’m going to do this. I don’t know how I’m going to deal with all of this new stuff.” But now, I feel a lot more confident about learning new aspects of computer science.
Ryan: I learned a lot about new technologies, such as Jupyter Notebooks and Python. In general, I got to explore a realm of computer science that I never really knew much about. In terms of soft skills, I improved on a lot of the essentials, including communication and teamwork.

Q: How has your experience at SDSC compared to your original expectations?
Alisha: I was worried about being in over my head in terms of programming. In fact, it’s not the 24 hours per day coding that I expected. Exploring Jupyter Notebooks and other programs has been great, and this summer has made me super interested in computer science as a college major.
Ryan: REHS has definitely been more open-ended than traditional high school classes, which surprised me the first time. It’s more similar to college: more self-study, self-sufficiency, and less of “Do this assignment” and fill in the blank.
REHS in Review: 10th Annual Poster Session

Although UCSD students still have over a month of sunny freedom to enjoy, yet another summer has flown by for REHSers. This week, as the program comes to a close and local high schools one by one start up a new academic year, REHS interns transition back into the classroom, leaving their offices and the labs of SDSC behind.

In its 10th annual poster session, the program once again celebrated the culmination of all of its participants' hard work over the last eight weeks. With most interns spending well over 160 hours at SDSC this past summer, the poster session serves as a marker of their tremendous work and growth. Friends, family, and SDSC staff were invited to learn about the diverse range of projects students had been working on all summer. As attendees wandered the room, they learned about research on the molecular mechanisms of various neurodegenerative diseases, such as Parkinson’s and Alzheimer’s; the visualization of ultradian sleep rhythms from neuroimaging technologies; multiscale simulation software development and optimization in chemistry and biophysics; and the use of machine learning for improving Comet user support — among many other topics.

While the complexity of many projects appeared daunting and for a high school level, SDSC Director Dr. Michael Norman best summed it up in his speech to the attendees: “What the REHS program proves is you’re never too young to start doing research. Let this be a preview of what you should seek in college. Continue down this path, and by the time you graduate from college, you’ll be ready to not only take on the world, but change it.”

Looking ahead to next year, the world will head into a new decade of the 2020s, and the REHS program will likewise embrace the beginning of its second decade of success, as it enters into its 11th year.

Shayda Moezzi, a rising senior from Carlsbad High School, chats with SDSC Director Dr. Michael Norman. Under the direction of Dr. Mary Thomas, Moezzi worked with three other REHS students on Developing Interactive Jupyter Notebooks for SDSC HPC Systems.

Justin Wang, a rising senior from Canyon Crest Academy, explains his research on Mapping PRC2 — A Widespread Epigenetic Inhibitor with Untapped Potential. Wang was mentored by Dr. Valentina Kouznetsova and Dr. Igor Tsigelny.