

Statement of Purpose

Mit Kotak, GTech CSE PhD applicant

Motivation: How do we design scientific codes that can leverage next generation supercomputing infrastructure? How do we balance research *productivity* with *portability* and *performance*? Motivated by these questions, I am interested in pursuing graduate studies in scientific computing and solving these problems through the integration of (a) state-of-the-art theoretical approaches, (b) advanced computational algorithms, (c) large-scale computational platforms and (d) collaboration with domain experts.

My education and research experiences have given me a strong basis to rise to this challenge. I have been involved with high performance computing (HPC) since my sophomore year. This involvement includes visualizing black hole (BH) and neutron star (NS) simulations on supercomputers, developing relativistic numerical simulation codes, optimizing numerical libraries for GPU computing, and broadening access to HPC infrastructure through middlewares.

Scientific Visualization with Professor Stuart Shapiro: My research journey began in the summer after my sophomore year when I joined the Center for Theoretical Astrophysics led by Professor Stuart Shapiro where I created 3D visualizations of the numerical simulation data in close collaboration with the theoretical team using VisIt (open-source visualization software package). Given the large dataset sizes, 3D visualizations were crucial to formulate, test and eventually communicate scientific hypotheses. *My visualization work has been featured in two Phys. Rev. Journal articles, has won the first prize in the UIUC Image of Research Competition, has been published in the Coalition for Academic and Scientific Computation (CASC) 2023 brochure and has been funded by the Office of Undergraduate Research through independent summer grants (RSG 2022, RSG 2023).*

Numerical Simulations with Professor Antonios Tsokaros: After taking courses in *Numerical Analysis*, *Numerical Fluid Dynamics* and *Numerical Methods for Partial Differential Equations*, I wanted to dive deeper into the different computational techniques for solving the equations that I had been visualizing with Professor Shapiro. Therefore, in Fall 2022 under the supervision of Professor Antonios Tsokaros, I started working on integrating the Compact Object Calculator (COCAL)—an elliptic solver for single and binary compact systems (like BHs and NSs)—within the EinsteinToolkit—an open source hyperbolic solver for relativistic astrophysics. This integration is essential to help find stable solutions for equations governing the simulation of magnetized NSs. This project is particularly important to me because it extends my first research project (visualizing magnetized NSs) by allowing me to participate in the full simulation pipeline, including developing the code that evolves equations in general relativity and magnetohydrodynamics, modeling physical systems on 3D mesh refinement grids, and analyzing large-scale evolution data to test new hypotheses. Also, given the lack of open source documentation for doing VisIt-based 3D rendering for astrophysics simulations, I am working with Professor Tsokaros on releasing a manual that can serve as a reference for future astrophysics projects.

GPU Computing with Professor Andreas Klöckner: A couple of weeks into my work with the Center for Theoretical Astrophysics, I was completely awestruck by supercomputers and wanted to learn about other ways of speeding up scientific code. This led me to work with Kaushik Kulkarni (advised by Professor Andreas Klöckner) on efficiently executing dataflow graphs on GPUs via NVIDIA's CUDAGraph API. Given the limited work on exploring data flow graphs on GPUs via a *lazy evaluation* framework, we integrated and extended different scientific code bases. This project was both exciting and challenging since it involved working very close to the hardware. As part of an in-progress undergraduate senior thesis with Professor Klöckner, I am currently working on developing a performance model for the runtime scheduling algorithm with the hope of influencing future hardware directions. *I was able to present this work at the annual UIUC research symposium (URS 2022) and at the Center for Exascale-Enabled Scramjet Design annual review meeting (CEESD AST Review 2022), where we were able to demonstrate a speedup of up to 5x for Finite-Element Discontinuous Galerkin*

Operators. This experience made me see how we can access architecture specific features—on-chip parallelism in this case—through the power of tools and abstractions.

HPC Middlewares with Professor Anand Padmanabhan: This year I decided to put my systems building knowledge into action and joined the Algorithms and Systems team led by Professor Anand Padmanabhan at the CyberGIS Center. My overall role was to help drive the development of CyberGIS-Compute, an HPC middleware tool that democratizes access to HPC resources through an easy-to-use Jupyter interface. Along with serving as the point person for CyberGIS-Compute backend support, I developed a self-contained Dockerized framework that can independently run the full CyberGIS-Compute stack on local machines which streamlined the development process for model contributors and developers in the CyberGIS-Compute community. Currently I am working on integrating software distributed through the CernVM Filesystem (CVMFS) into the compute environments on CyberGIS-Compute in order to simplify container management. Despite the work being technical, it was a product for non-technical domain experts in the geospatial community which provided interesting challenges in how we designed, communicated, and interacted with the community.

STEM Outreach: To address the shortage of guidance for undergraduates seeking research opportunities, since my sophomore year, I've been working as a research ambassador and symposium organizer where I have had the pleasure of offering one-to-one mentoring sessions to 40+ undergraduates. In my junior year, wanting to automate my role as a research ambassador, I created a chatbot that could answer commonly asked questions regarding finding research opportunities. I have also been involved in organizing and leading undergraduate research workshops for freshmen/sophomores and planning the annual undergraduate research symposiums (the latest one had 500 presenters). At GTech CSE, given the opportunity, I would like to create an application mentorship program where college seniors can get feedback on their application material through current doctoral students, possibly as an extension to the FOCUS program.

Why GTech CSE: As a FOCUS 2022 scholar, I had the opportunity of interacting with Professor Vivek Sarkar and learning about GTech's close collaborations with national laboratories and supercomputing centers. At GTech CSE, I am interested in exploring quantum algorithms for fluid dynamics with **Professor Spencer Bryngelson** and the Georgia Tech Quantum Alliance. As we enter the exascale computing era, quantum algorithms are likely to play an important role in addressing some of the challenges faced by classical CFD and I would like to contribute to this trend by helping build effective and supportable tools. Along with simulation software, there is a need for fast and scalable numerical infrastructure that I am also interested in investigating. Given the opportunity, I would like to continue my work on *array-based* frameworks with **Professor Richard Vuduc**. In addition to the technical challenge, I enjoy working closely with domain experts and would like to continue to do so in the future by pursuing a career as a researcher at national laboratories. GTech CSE is a top destination for my aspirations given its reputation for interdisciplinary research and while I have mentioned several faculty whose work is particularly interesting, I look forward to getting a closer look at several other research teams in which to potentially pursue Ph.D.