



The O'Donnell Data Science and Research Computing Institute

Faculty Research Acceleration Grant

Neena Imam, Ph.D.
Peter O'Donnell Jr. Director

SMU[®]

The Changing Computing Ecosystem Landscape

Convergence of Data Science, HPC, AI/ML, and Future Technologies

- HPC— exascale here, race towards....
- Rise of hybrid-architecture, AI-centric HPC/supercomputing
- Computing ecosystem becoming more distributed---edge computing
- Artificial Intelligence ---future of AI is generative AI, as well as distributed AI
- Plateauing of *Moore's Law*—Post-Moore Computing—Quantum, Neuromorphic?
- Energy efficiency/sustainability
- Geo-political issues (CHIPS and Science Act)



Accelerated Data Science (Data Science+ AI + HPC)

DATA ANALYTICS

Extracting insights from big data



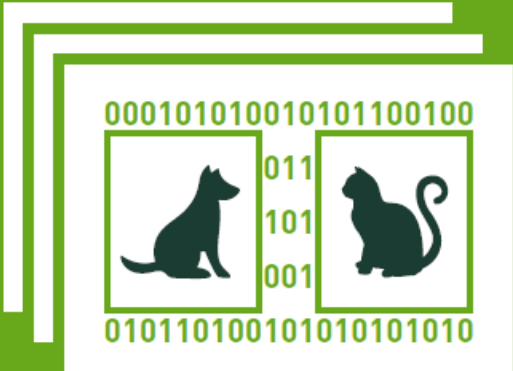
MACHINE LEARNING

Learning from examples in the data



DEEP LEARNING

Automating feature engineering



The O'Donnell Institute Mission

- Research in data science, HPC, AI/ML, and future technologies
 - Launch multi-disciplinary research initiatives
 - Identify funding opportunities from government, industry, and philanthropic organizations
- Education and training
 - Fund internships and other means of support to students at various levels, as well as advising research projects and mentoring
 - Provide workshops and trainings that leverage the unique capabilities of the institute
- Act as a gateway to SMU HPC platforms
 - Engage in enhanced collaboration with researcher using SMU HPC platform
 - Provide domain science expertise to HPC users (e.g., computational chemistry, energy sciences, bioinformatics, etc.)



Data Science Seed Grants for Faculty

Five Data Science seed grants allocated in October 2023

- Data Science for Arts:
PI: Zannie Voss (Meadows)
- Using LLMs for Better Psych Evaluation
Pis: Mehak Gupta (CS) and Joshua Oltmann (Psych)
- Novel Methods for Scalable and Reliable Learning from Spatiotemporally Complex Data
PIs: Marcin Jurek (Statistics and Data Science) and Mohamad Faradonbeh (Math)
- Deep Generative Modelling for Accelerating Scientific Computing
PI: Difeng Cai (Math)
- Improving the Design of Generative AI Applications with Personalized Recommendation
PI: Jane Tan (Cox)

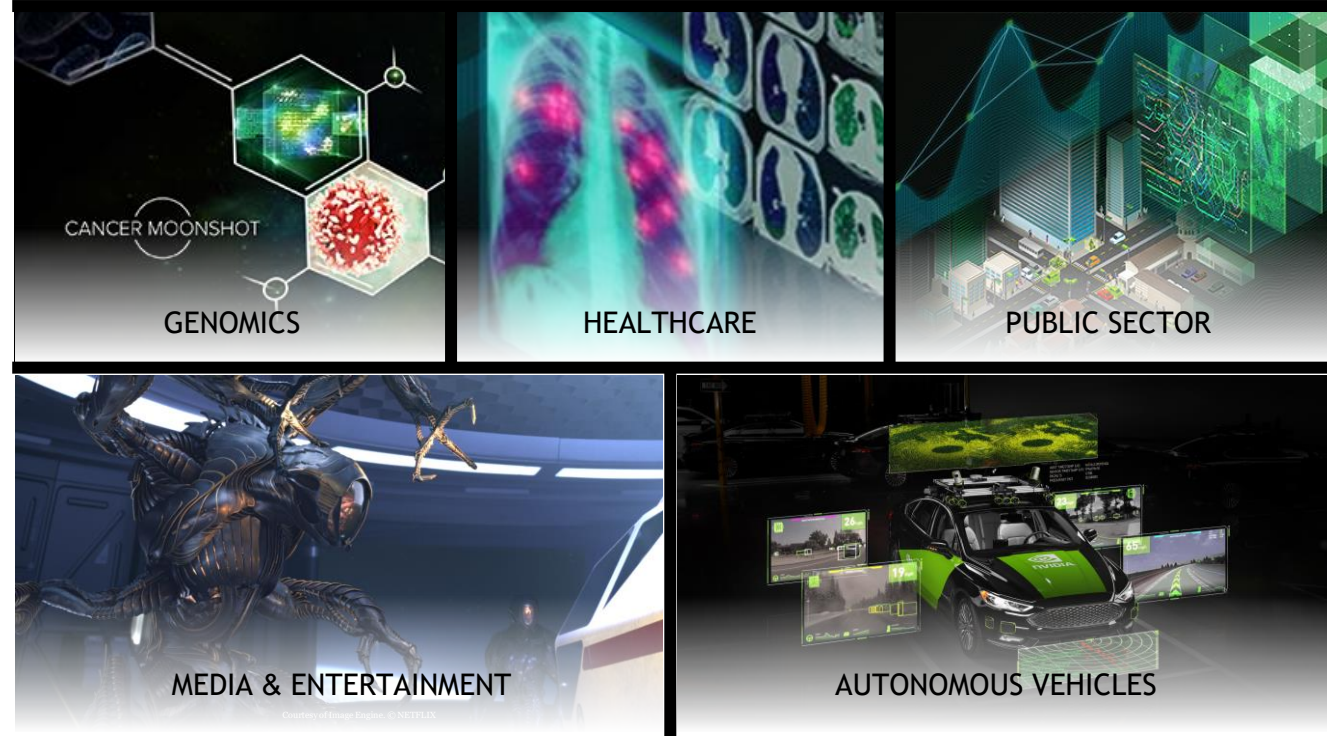
Student Support

CS/DS is becoming a team sport. It's no longer about building a model; it's about what you do with the model.

- Performant and scaled-up implementation

O'Donnell Institute Graduate Student Fellowship:

- Four graduate students
 - Using Deep Learning for energy grid load forecasting: Han Guo (ECE)
 - Predicting properties of proteins relevant to drug discovery using ML: Elyssa Sliheet (Math)
 - Essays on peer effects estimation with partial network data: Shuo Qi (Econ)
 - Study of protein dynamics with molecular dynamics simulations and ML techniques: Sian Xiao (Chemistry)



Faculty Research Acceleration Grant

- Source of funds: The O'Donnell Endowment
- \$100K per year (total)
 - Floor \$50K, Ceiling \$100K
- Eligibility: Lead PI must be faculty at SMU (not restricted to STEM fields)
- Research thrusts:
 - Large-scale data science
 - Multimodal data
 - AI/ML technologies
 - Implementation on SMU HPC platforms

Proposal Submission Details

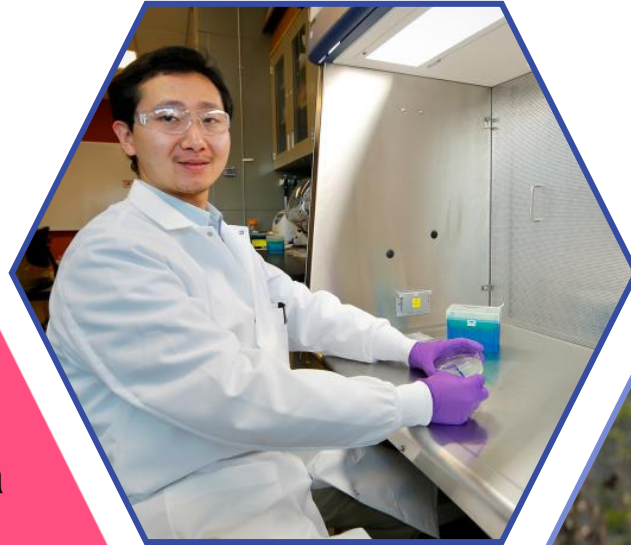
- Full proposal submission deadline: May 3, 2024 COB
- Funding decision made and notification to PIs: May 17, 2024
- How to submit: email to: nimam@smu.edu
- The PI(s) should arrange for confidential letter(s) of support to be written by the appropriate Department Chair(s) and emailed to nimam@smu.edu by deadline
- Proposal format
 - 6 pages maximum, not including references
 - Adhere to the template to be mailed out COB today

Proposal Submission Details

- Restrictions/Conditions:
 - Funding is not available for computer equipment and/or accessories, unless they are essential for the research
 - Funds must be expended within 12 months of the award
 - Summer salary is disallowed
- Proposals that include more than one faculty member will receive higher consideration.
- Post-Award Requirements
 - A report summarizing how the funds were spent and what products were generated and what external funding will be sought must be reported (as detailed in the original award letter)

We encourage multidisciplinary teams

- Large-scale multimodal data
- AI/ML incorporated
- HPC implementation



Any faculty can
be the PI

Postdocs/students can
participate, but not as PI

Proposal requirements

Postdocs/students should be identified in proposals
Faculty collaborating at no-cost should be identified

Selection Criteria

Technical Merit Criteria

- **Significance:** How important is the proposed activity to advancing knowledge and understanding within its own field and across different fields?
- **Innovation:** To what extent does the proposed activity explore original concepts?
- **Qualifications:** How well qualified are the proposers to conduct the project? Is there sufficient expertise to address all the technical requirements of the proposed research plan.
- **Organization:** How well conceived and organized is the proposed activity? Are the estimates of time and effort reasonable? Is the requested level of funding appropriate?
- **Access:** Is there sufficient access to resources?

Strategic Merit Criteria

- **Enduring Capability:** Will the proposed new capabilities bring enduring benefit to SMU?
- **Potential to attract external funding:** Will the proposed research be able to attract external funding?

Heilmeier catechism

George H. Heilmeier, a former DARPA director (1975-1977), crafted a set of questions known as the "Heilmeier Catechism" to help evaluate research proposals

- What are you trying to do? Articulate your objectives clearly
- How is it done today, and what are the limits of current practice?
- What is new in your approach and why do you think it will be successful?
- Who cares? If you are successful, what difference will it make?
- What are the risks?
- How much will it cost?
- How long will it take?
- What are the mid-term and final “exams” to check for success?