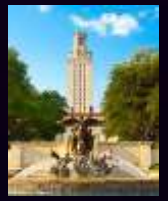
COMPUTING FOR THE ENDLESS FRONTIER

Melyssa Fratkin
Industrial Programs Director
May 2023

TACC AT A GLANCE



Personnel
180 Staff (~70 PhD)

Facilities
12 MW Data center capacity
Two office buildings, Three Datacenters, two visualization facilities, and a chilling plant.

Systems and Services
>Seven Billion compute hours per year
>5 Billion files, >100 Petabytes of Data, NSF Frontera, Stampede2 (XSEDE), Jetstream (Cloud), Chameleon (Cloud Testbed) system

Usage
>15,000 direct users in >4,000 projects, >50,000 web/portal users, User demand 8x available system time. Thousands of training/outreach participants annually

OUR MISSION

- Mission: To enable discoveries that advance science and society through the application of advanced computing technologies.

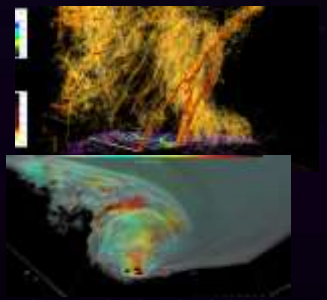


Figure: "World's Most Detailed Tornado Simulation", Leigh Orf, Wisconsin – used more than 200,000 cores on Frontera

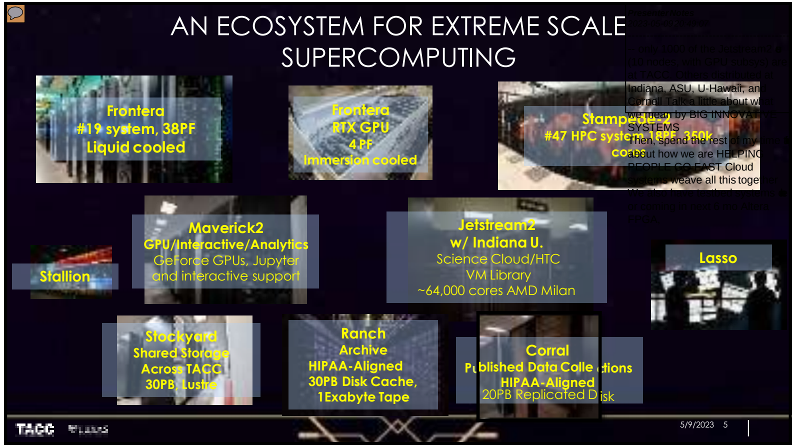
MODERN COMPUTATIONAL SCIENCE

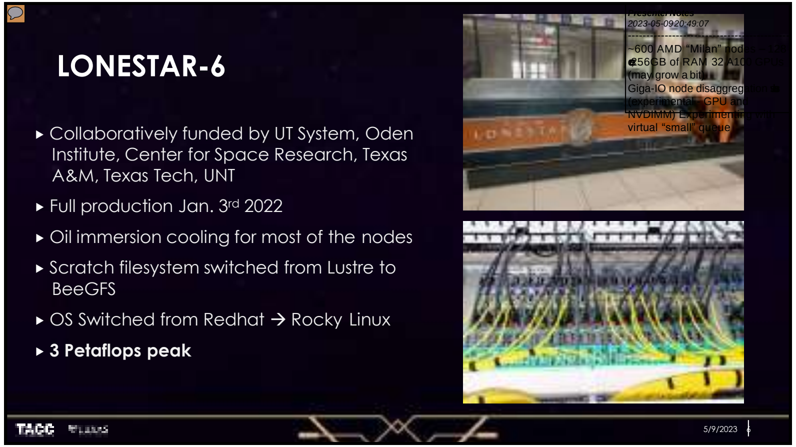
Simulation
Computationally query our
mathematical models of the world

Machine Learning/AI
Computationally query our
data sets
(depending on technique, also called deep learning)

Analytics
Computationally analyze our
experiments
(driven by instruments that produce lots of digital information)

Modern science and engineering combine all three


AN ECOSYSTEM FOR EXTREME SCALE SUPERCOMPUTING
Frontera
#19 system, 38PF
Liquid cooled
Frontera
RTX GPU
4 PF
Immersion cooled
Stampede-2
#47 HPC system
Maverick2
GPU/Interactive/Analytics
GeForce GPUs, Jupyter and interactive support
Jetstream2
w/ Indiana U.
Science Cloud/HTC
VM Library
~64,000 cores AMD Milan
Stallion
Lasso
Stockyard
Shared Storage
Across TACC
30PB, Lustre
Ranch
Archive
HIPAA-Aligned
30PB Disk Cache,
1 Exabyte Tape
Corral
Published Data Collections
HIPAA-Aligned
20PB Replicated Disk
TACC
5/9/2023 5


LONESTAR-6
Collaboratively funded by UT System, Oden Institute, Center for Space Research, Texas A&M, Texas Tech, UNT
Full production Jan. 3rd 2022
Oil immersion cooling for most of the nodes
Scratch filesystem switched from Lustre to BeeGFS
OS Switched from Redhat → Rocky Linux
3 Petaflops peak
TACC
5/9/2023

THE FRONTERA PROJECT

NSF-supported project ($60M) to do 3 things:

- Deploy a system in 2019 for the largest problems scientists and engineers currently face.
- Support and operate this system for 5 years.
- Plan a phase 2 system, with 10x the capabilities, for the future challenges scientists will face.

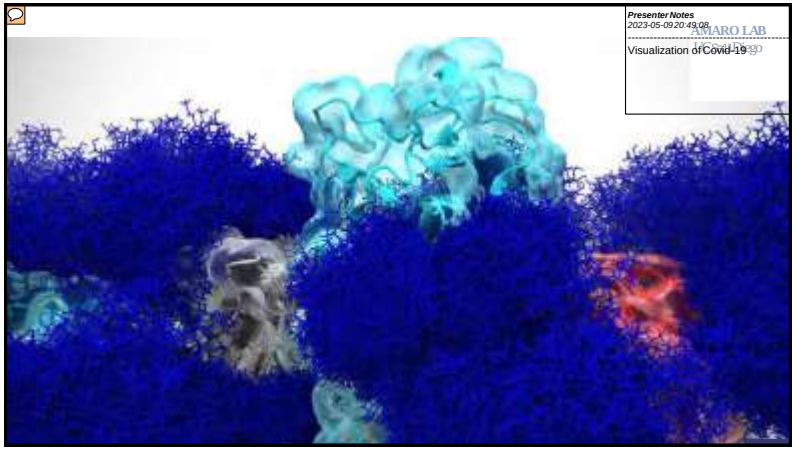
FRONTERA

FRONTERA TODAY

- Frontera is the #19 system in the world – and the fastest at any university in the world.
- Fastest primarily Intel-based system
- Frontera and Stampede2 are #1 and #3 among US Universities
- NSF provided additional funds to add racks to Frontera for future *Urgent Computing* needs

A FEW METRICS (FRONTERA) FOR YEAR 3

- In the last 12 months:
  - Uptime of 99.2%
  - Average Utilization of 95.4%
  - ~72M SUs delivered
  - 1.13M jobs delivered
  - Zero security incidents.
- Very successful compared to other large system deployments.
  - On the bright side, we are always full. On the downside, no way to squeeze anything else in.



TACC'S COVID RESPONSE

- 90+ projects supported. involved with more than 300 researchers, plus NSF, CDC, DOE, DARPA on COVID Response
- People
  - Lauren Meyers
  - Gordon Wells
  - DARPA Contact Tracing
- Structures
  - Rommie Amaro, UCSD
  - Arkansas, North Texas, etc.
- Genomics
  - Argonne, Brookhaven, Illinois, U. Chicago, UVA, George Mason, Johns Hopkins, Rutgers, Penn State.

- **15M Node Hours**
- **30% of capacity**
- **50-60 TACC staff**

- Resources:
  - NSF "Dear Colleague Letters" explicitly offering TACC resources.
  - White House/OSTP -driven COVID HPC Consortium
- Outreach
  - Wall St. Journal, NYTimes, Washington Post, Bloomberg TV, Newsweek, many regional/trade.
- Funding
  - $30M in proposals submitted

TACC PROVIDES THE SOFTWARE, HARDWARE, SERVICES AND TEAM FOR END TO END COMPUTATIONAL SCIENCE FOR TENS OF THOUSANDS OF ENGINEERS.

VISUALIZATION LABORATORY

- 2900 Sq Ft (UT Main Campus)
- Stallion tiled display
  - 18 65-inch Samsung 8K QLED monitors, giving it 597 megapixels resolution
- Lasso touch-screen
- Bronco 4xHD projector
- Saddle Collaboration Room

https://www.tacc.utexas.edu/vislab

RECENT SCIENCE RESULTS & PROJECTS SUPPORTED BY TACC

OUTLOOK FOR THE BLUE ECONOMY

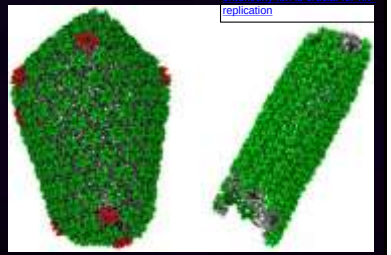
- A new project led by researchers at Texas A&M seeks to understand how changes to the climate and oceans will impact fisheries in the U.S. and around the world.
- The project aims to develop medium to long-term fishery forecasts, driven by some of the highest-resolution coupled climate forecasts ever run.
- The scientists want to know how climate change is going to alter upwelling in coastal regions, and how the sustainability of the future fisheries will be impacted.
- "TACC is unique in providing resources for researchers like us to tackle the fundamental questions of science," Chang said. "… We want [to get] a better understanding of the Earth system dynamics that are missing in current climate models to make our model and our methods better.

STOPPING HIV REPLICATION

GREG VOTH, U CHICAGO

- A study by chemists at the University of Chicago has uncovered a new key step in the process that HIV uses to replicate itself.
- HIV carries its genetic material inside a little capsule known as a capsid.
- The study focused on how the IP6 ion helps form the capsid – and what happens without IP6.
- The team is interested in finding out whether this process is occurs in viruses beyond HIV.

https://www.tacc.utexas.edu/latest-news/-/asset_publisher/zTY3I77CjSZq/content/hiv-ion-is-crucial-for-hiv-replication

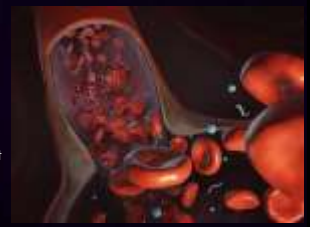


On the left is a simulation of a normal capsule; on the right is a simulation of a capsule formed without the IP6 ions. Without the ions, the capsule cannot close and the virus cannot replicate. Image by Gupta, Pak, and Voth.

TARGETING TUMORS WITH NANOWORMS

YING LI, UCONN

- Researcher seeks to understand the complicated behaviors of these materials and the biological systems down to the nanoscale.
- Nanoworms are long, thin, engineered encapsulations of drug contents.
- Modeled how these structures move in blood vessels of different geometries mimicking the constricted microvasculature.
  - Nanoworms can travel more efficiently through the bloodstream, passing through blockages where spherical or flat shapes get stuck.
  - Can use magnetic fields to influence flow.
- Can increase percentage of (highly toxic) drugs delivered directly to tumor.
- Published in *Soft Matter*, 2021.



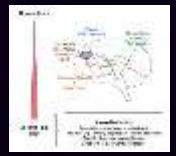
THE OPIOID CRISIS

A2CPS: Acute to Chronic Pain Signatures Program

- Identify biosignatures (sets of biomarkers) that predict addiction to medicines.
- Catalyze development of new drugs that won't trigger addiction.
- Data Integration and Resource Center (DIRC) for Common Fund Acute to Chronic Pain Signatures Program

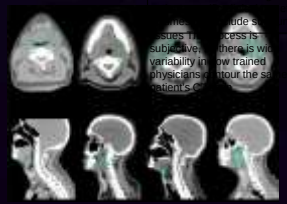
Goal of DIRC: Integrate the efforts of all components of the A2CPS and serve as a community-wide nexus for protocols, data, assay and data standards, and other resources generated by the A2CPS Program.

Datasets: Electronic health records, patient reported outcomes, accelerometer data, sensory testing, CNS imaging, 'omics assays (proteomic, metabolomic, lipidomic, extracellular RNA, transcriptome, array-based gene variants).



AI FOR DETECTION OF HEAD AND NECK CANCERS

- Researchers from MD Anderson Cancer Center developed a new method for automating the contouring of high-risk clinical target volumes using AI and supercomputers
- Carlos Cardenas used Maverick to analyze data from 52 oropharyngeal cancer patients who had been treated at MD Anderson between January 2006 and August 2010
- He developed a deep learning algorithm using auto-encoders — neural networks that can learn how to represent datasets — to identify and recreate physician contouring patterns
- This method offers speed and efficiency: ***While an oncologist might take 2 to 4 hours to evaluate the scans, the supercomputer did the job in under a minute.***



Comparison between computer-predicted ground-truth clinical target volume (CTV1) (blue) and physician manual contours (red)

- https://www.tacc.utexas.edu/-/an-ai-oncologist-to-help-cancer-patients-worldwide

TOOLS FOR EARTHQUAKE FORECASTS

- UT Austin's Thorsten Becker and Laura Wallace are collaborating with researchers around the world to develop tools, software, and instructional materials, and train students.
- The ultimate goal is to forecast the chances of an earthquake happening, like weather prediction
- Focusing on three of the world's earthquake hotspots: the Pacific NW (USA), New Zealand, and Japan.
- 5-year project, funded by NSF

GPS site in New Zealand - continuously monitors changes in the Earth's surface near earthquake hotspots.

https://news.utexas.edu/2021/08/09/earthquake-forecasts-move-a-step-closer-to-reality/

LEGACY OF ARECIBO OBSERVATORY

- TACC partnered with UCF, the University of Puerto Rico, EPOC at Indiana University, Globus, and CICoE (Cyberinfrastructure Center of Excellence at USC) to safely preserve 3PB of data from the collapsed Arecibo radio telescope
- Data is copied to hard drives and transferred to the University of Puerto Rico
- Globus enables the team to securely and reliably move 12 terabytes of data per day
- The goal is to expand access to over 50 years of astronomy data

https://www.tacc.utexas.edu/-/continuing-arecibo-s-legacy

DEEP LEARNING FOR TRAFFIC CAMERA VIDEO ANALYSIS

- Traffic Camera Video Analysis Project (City of Austin & CTR)
  - Use deep learning methods to automatically recognize moving objects from video stream, e.g. car, pedestrian, cyclist, bus
  - Covert video into indexed objects that can be searched / analyzed later
  - Traffic volume estimation, location based safety study.

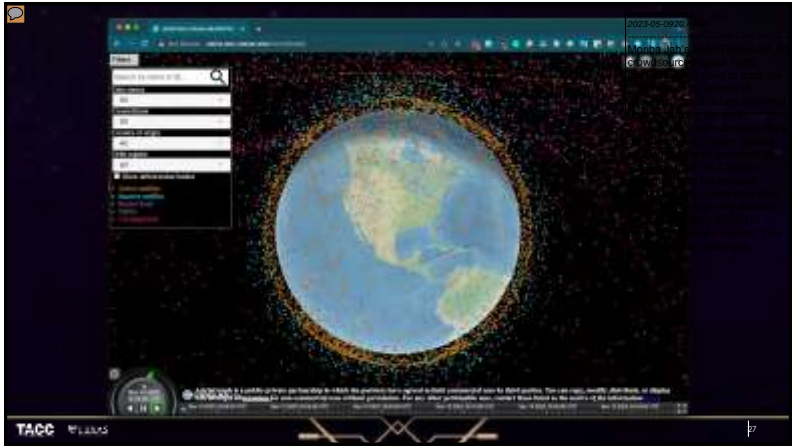
TACC

DETECT THE UNEXPECTED

TACC

THE ANSWER WAS…

TACC



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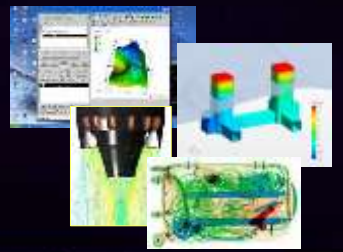
INDUSTRY COLLABORATION

SCIENCE & TECHNOLOGY AFFILIATES FOR RESEARCH (STAR) PROGRAM

- 25+ Members
  - Fortune 500 to local start-ups
- Annual Meeting
  - Includes meet & greet with UT students
- Quarterly webinars
- Workforce Development & Internships
- Hardware/Software testing & benchmarks
- Access to TACC systems & expertise

- https://bit.ly/TACCindustry




CURRENT STAR PARTNERS
Chevron
CAT
Technip
ExxonMobil
LOCKHEED MARTIN
FIREFLY
Raytheon
sandbox
SYNTHETIK
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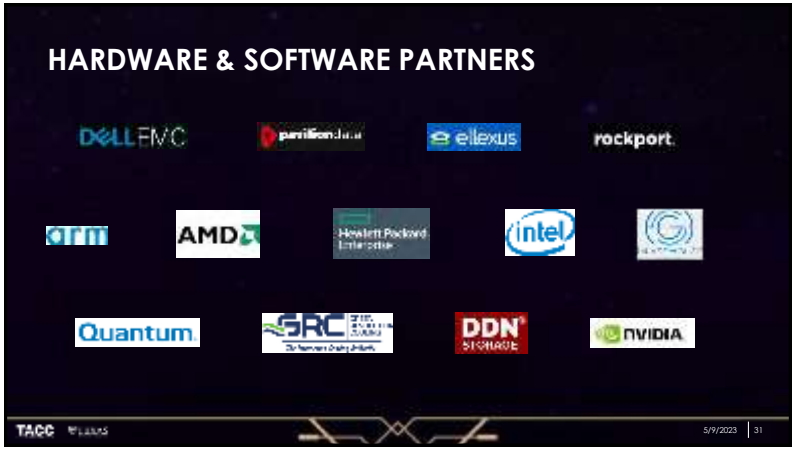
HARDWARE & SOFTWARE PARTNERS
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Hewlett Packard Enterprise
intel
Quantum
DDN STORAGE
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Firefly Aerospace

Presenter Notes

Firefly Academy, a nonprofit run by Austin-based firm Firefly Aerospace, has partnered with UT to establish Firefly@UT — a $1 million, multi-year program aimed at the first time will offer UT students the opportunity to design, develop, assemble and test a rocket engine capable of launching to the edge of space.

Firefly, a TACC industrial partner, designed their 'Reaver' rocket engines using Stampede.

First rocket launched at Vandenberg SFB on Sept 2, 2021 (exploded after launch)

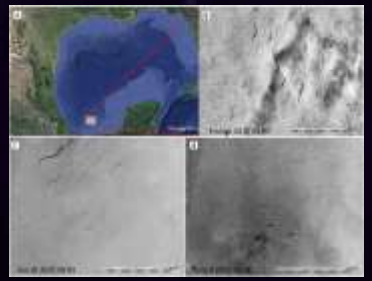
Selected by NASA in March to build the far-side moon lander for 2026

MAKING AIRPORT VISITS FASTER & SAFER

- Synthetik Applied Technologies, another STAR partner, received a grant from the DHS Apex program that will improve the speed and accuracy of passenger screening at airports.
- In Machine learning, a computing system can learn from the data it ingests, identify patterns, and make decisions, with little or no human intervention. This requires large volumes of training data.
- Using TACC systems, Synthetik is developing a new platform to generate this artificial data, to train ML systems to recognize weapons in screened luggage.

DETECTING OIL SEEPAGE ON THE WATER'S SURFACE WITH FRONTERA

- Seepage — slow leaks of hydrocarbons escaping from small holes — is a common problem for geoscientists.
- It's important to distinguish this natural phenomenon from possible leakage from pipelines or oil tankers.
- TotalEnergies worked with researchers at TACC to develop and train a deep learning system that could automate the detection of surface oil.
- The collaboration focused specifically on making the identification process faster, while preserving the accuracy of the predictions.



SHELL & TECHNIP: PRELUDE FLNG FACILITY

- The world's largest floating structure – 500+ yds long – off the coast of Australia
- Liquify natural gas on ship before transport
- Modeled using Frontera: the wave impacts, the water intake pipes, and the rotation of the structure
- Also modeled area 500 sq meters around pipe at sea floor – Multiphysics calculations with mudslides

https://texascale.org/2020/people-programs/platform-discovery/

INTERNATIONAL COLLABORATIONS

- **Portugal:**
  - **CoLab (2007):** Program to support multidisciplinary research in space and science technology, medical physics and nuclear medicine, nano-science and technologies, high performance computing and related themes of data analytics, visualization and artificial intelligence
  - **BigHPC (2020):** A Management Framework for Consolidated Big Data and HPC —includes $2 million in funding over the next three years
- **South Africa/Region**
  - TACC donated portions of the Ranger supercomputer to South Africa (20 racks), Tanzania (16), and Botswana (4).
  - Hosted a training workshop for sysadmins from new university HPC centers in Botswana, South Africa, Lesotho, Tanzania, Zambia, and Zimbabwe.
  - CHPC-South Africa sent an engineer to shadow staff at TACC for 6 months

AND WE AREN'T DONE YET.

LEADERSHIP-CLASS COMPUTING FACILITY

COMING IN 2025

LEADERSHIP CLASS COMPUTING FACILITY

- 10x follow-on to Frontera
- 15MW more datacenter
- Technologies (chips, network, storage) TBA
- Schedule depends on FY2024 Budget passing Congress…
  - Construction starts next March!

TEXASCALE: THE TACC MAGAZINE

- Read online at https://texascale.org/
- Or sign up to get a copy mailed to you!

WOMEN IN HPC

TEXAS WOMEN IN HIGH PERFORMANCE COMPUTING

https://www.txwomeninhpc.org/

WOMEN IN HIGH PERFORMANCE COMPUTING

https://womeninhpc.org

Humphry Davy

Fortunately science, like that nature to which it belongs, is neither limited by time nor by space. It belongs to the world, and is of no country and no age. The more we know, the more we feel our ignorance; the more we feel how much remains unknown.

AZ QUOTES

THANKS

- **The National Science Foundation**
- The University of Texas
- Peter and Edith O'Donnell
- Dell, Intel, and our many vendor partners
- Cal Tech, Chicago, Cornell, Georgia Tech, Ohio State, Princeton, Texas A&M, Stanford, UC-Davis, Utah
- **Our Users – the thousands of scientists who use TACC to make the world better**
- All the people of TACC

THANKS!

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