EXPANDING HPC AT UTRGV

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UTRGV

UT RIO GRANDE VALLEY

- The University of Texas Rio Grande Valley is one university spanning four counties and multiple locations (Brownsville, Edingburg, Harlingen, and more).
- Formed in 2013 by the merger of two pre-existing UT campuses: UT Brownsville, UT PanAm
  - Includes a school of medicine
  - Approx. 32,000 students
- Acquiring PhD programs (PhD in Physics starting Sp'22)
- UTRGV's leadership has set a long term target for $100M in external research funding
- Growth in HPC enabled research areas will play a critical role: recognized by UTRGV leadership

HPC CENTER

- We are in the process of acquiring a GPU cluster for the newly established UTRGV HPC Center (*Director:* Mark Chu; *Assoc. Dir.*: Soumya Mohanty)
- Combining 2 back-to-back grants:
  - NSF ($680 K) and DOD ($550k)
  - Interdisciplinary team for both: Electrical and Computer engineering, Computer Science, Physics & Astronomy
- Support for sysadmin from UTRGV EVPR (Dr. Parwinder Grewal)
- Support for facilities expansion from UTRGV
- Cluster to be housed in the existing data center at Edinburg Campus
- Center goals (besides research): train faculty and students in using HPC; ease transition to TACC; Provide HPC information, expertise, and grant writing support

COMPUTATIONAL NEEDS & CLUSTER SPECIFICATIONS

- Grant proposals: strong justifications for on-premise HPC required given national level cloud computing facilities
  - GW: High data throughput stifled by job queue times
  - DL: Long runtimes when training + rapid turnaround required on parameter tuning
- Cluster specs: We looked carefully at the needs of the major projects
  - Two types of computations: Data-parallel & Deep Learning
  - Took availability of TACC resources into account ⇒ Changed from CPU + GPU nodes to all GPU nodes
- Internal discussion to arrive at consensus: split budget between 2 types of compute nodes
- Also scoped size and type of external storage requirements

Gravitational wave (GW) astronomy data analysis

- Data-parallel computation

AI applications

- Several applications in GW data analysis
- Standard Deep Learning cluster architecture

Computational quantum chemistry

- VASP
- Speed up with GPUs for VASP

ACQUISITION PROCESS FOLLOWED

- SDM attended a very timely TACC institute: HPC Leadership
  - Very useful information about building HPC resources on campus
- Formed cluster acquisition team, identified stakeholders, and conducted multiple Request For Information (RFI) meetings with vendors (> 30 meetings in 2 months!)
  - Discussions regarding target research projects and their computing needs
  - Some vendors allowed benchmarking of our codes – very important in guiding the RFP
- Discussions with UTRGV data center and facilities
- Discussions with UTRGV Procurement staff
- Discussions with TAMU and TACC – invaluable!
- RFP was released on Oct 15!

CHALLENGES AND LESSONS (SO FAR)

- Both UTB and UT PanAm had operated clusters in the past but that experience was insufficient: HPC technologies evolve at a rapid pace, people move along with knowledge, etc.
- Prior experience with using TACC resources is a must: provided a framework for RFI discussions with vendors
- UTRGV Data Center & Facilities planners want complete specification of cluster for space/power/cooling but this can be quite variable in the RFI phase as cluster requirements evolve: Established direct connnections with vendors
- ⇒ Surprise: New expenses associated with facilities expansion!
  - We are fortunate to have received tremendous support from UTRGV EVPR in solving these unforeseen problems
- Management of discussions, meetings, etc:
  - TACC HPC Leadership institute guidance proved invaluable: Document everything!
  - Used cloud-based services like MS Teams (or Slack), OneDrive etc.
- Lessons:
  - Be prepared for surprises!
  - Vendors have much to teach -- be open to their advice
  - Use great learning and networking opportunities such as TACC institutes and this conference!