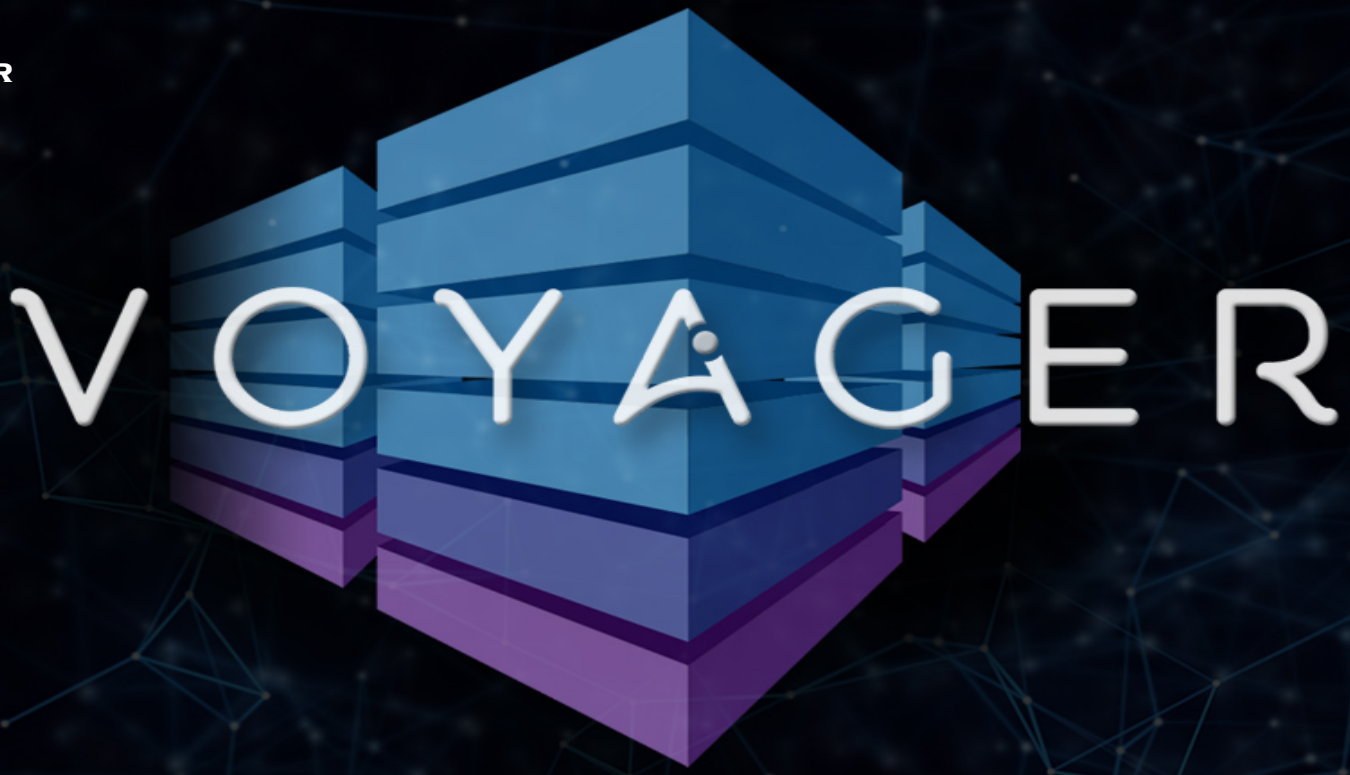
Engineering

August 7, 2020

Amit Majumdar
SDSC



San Diego Supercomputer Center

NSF Award 2005369

Voyager: NSF Category II Award to UCSD

- $5M for hardware acquisition
- $6.25M (anticipated) for 5 years of operations

Amit Majumdar, SDSC, PI
Rommie Amaro, UCSD Chemistry and Biochemistry Department, Co-PI
Javier Duarte, UCSD Physics Department, Co-PI
Mai Nguyen, SDSC, Co-PI
Robert Sinkovits, SDSC, Co-PI
Shawn Strande, SDSC, Project Manager

External Advisory Board
Science Use Case Researchers
Industrial Relations – SDSC AI Technology Lab (AITL), Ron Hawkins

Christopher Irving, SDSC, HPC Systems Manager
- Trevor Cooper, HPC Systems group
- Haisong Cai, HPC Systems group
- Fernando Silva, HPC Systems group
- Scott Sakai, Securities group

Tom Hutton, SDSC HPC Networking

Mahidhar Tatineni, SDSC, User Services Manager
- Manu Shantharam, User Services
- Marty Kandes, User Services
- Nicole Wolter, User Services
- Paul Rodriguez, Scientific Computing Applications

VOYAGER

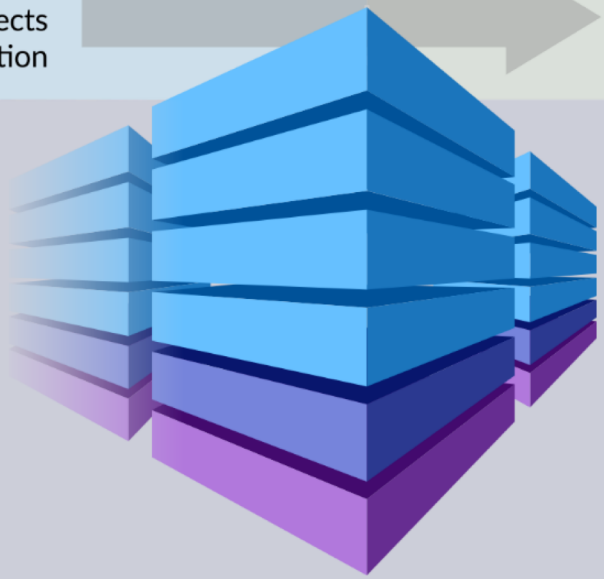
EXPLORING AI PROCESSORS in SCIENCE and ENGINEERING

3-YEAR TESTBED PHASE
Focused Select Projects
Workshops, Industry Interaction

2-YEAR ALLOCATIONS PHASE
NSF Allocations to the Broader Community
User Workshops

INNOVATIVE AI RESOURCE
Specialized Training Processors
Specialized Inference Processors
High-Performance Interconnect
X86 Standard Compute nodes
Rich Storage Hierarchy

OPTIMIZED AI SOFTWARE
Community Frameworks
Custom user-developed AI Applications
PyTorch, MXNet, Tensorflow



IMPACT & ENGAGEMENT
Large-Scale Models
AI Architecture Advancement
Improved Performance of AI Applications
External Advisory Board of AI & HPC Experts
Wide Science & Engineering Community
Advanced Project Support & Training
Accelerating Scientific Discovery
Industrial Engagement

Voyager system and software

- Supermicro Inc and SDSC jointly will deploy Supermicro-integrated AI focused hardware solution at SDSC
  - Further details about architecture coming in the future
- Specialized Voyager Training Nodes
- Specialized Voyager Inference Nodes
- Training and Inference nodes attached to standard X86 compute nodes
- Additional X86 compute nodes
- Storage system – potential to experiment with various parallel file systems (Ceph, Lustre)
- DL frameworks TensorFlow, PyTorch etc.
- Users will be able to develop their own AI techniques using software tools and libraries built specifically for Voyager's innovative AI architecture.

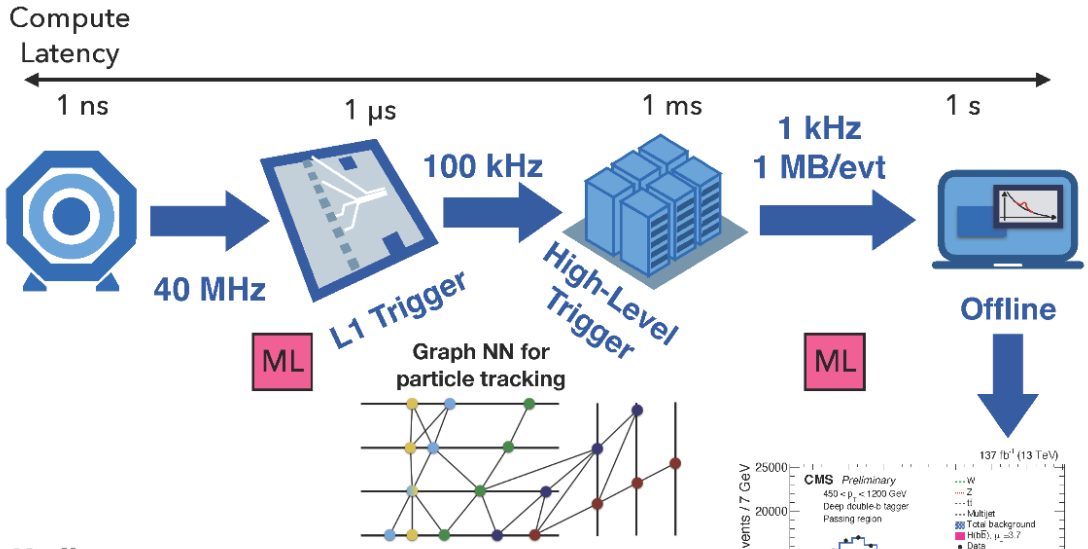
Project Plan

- Available October, 2021
- First 3 years - Testbed Phase
  - Work closely with select research groups – deep user engagement
  - Evaluate Voyager's innovative DL hardware, software, libraries, ML application porting/performance
  - Semiannual workshops, user forums to share lessons learned, bring researchers together
  - Develop knowledge base, best use cases for future users, allocation policies
  - External Advisory Board to help recruit research groups, provide guidance to project
- Year 4 and 5 - Allocations Phase
  - Allocate via XRAC or NSF approved follow-on program
  - Lessons learned from Testbed phase will lead to documentation, training
  - Regular and advanced user support
  - Semiannual workshops continue
  - Industry engagement for similar technology evaluation

Representative Science Use Cases – Testbed phase

- **Astronomy**: multi-object telescope data pipeline
- **Atmospheric sciences**: analyze effect of anthropogenic aerosols on cloud
- **Chemistry, biophysics**, **materials:** use of ML models trained with QM data
- **High Energy physics**: use of ML for LHC data at various stages coming out of detectors
- **Human microbiome:** understanding the role of the microbiome in age-related diseases such as cardiovascular disease, cancer, and Alzheimer's
- **Population genetics**: understanding demographic histories based on genome-sequence data
- **Satellite image analysis**: features applied in social science, wild fire etc.
- **Systems biology**: analysis of functional genomic data to decode regulatory elements and pathways
- **Computer Science**: data deluge from complex HPC (exascale) systems; prediction of system behavior and application performance
- And more…

High Energy Physics – J. Duarte, UCSD Physics



arXiv:1810.06111

Challenges:

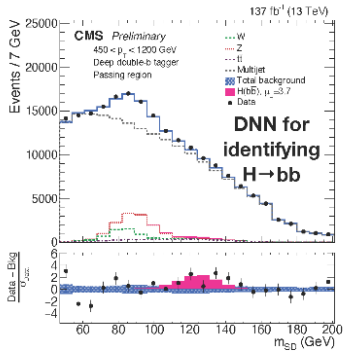
Each collision produces O(10^3) particles

Detectors have O(10^8) sensors

Extreme data rates of O(100 TB/s)

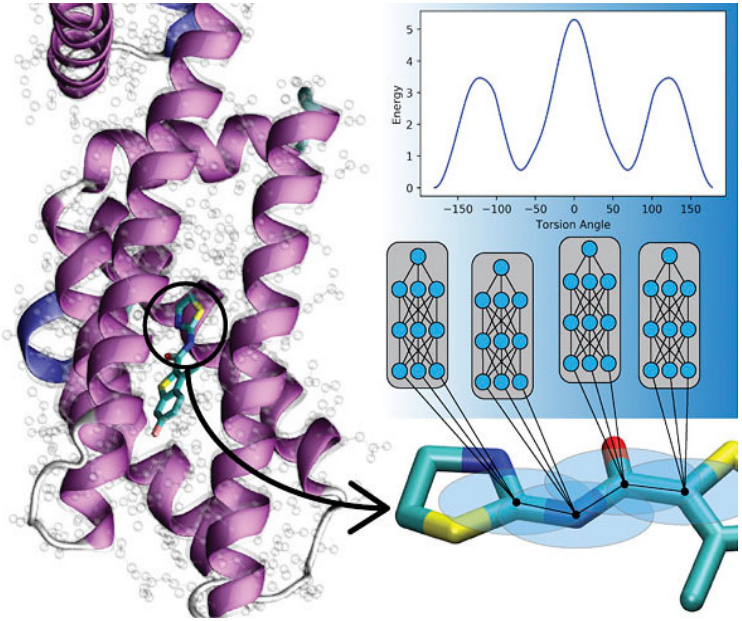
1 in 10^{10} events contains H→bb

ML to improve trigger, event reconstruction, and signal-to-background ratio

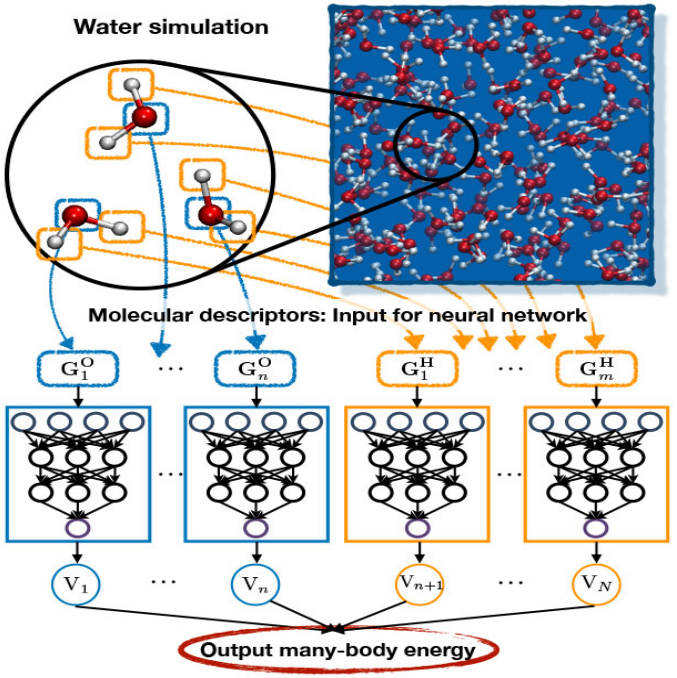


CMS-PAS-HIG-19-003

ML for Molecular Simulations in Chemistry, Biophysics, Materials Science – A. Roitberg, UFL, and collaborators LANL, UNC; A. Goetz, F. Paesani, UCSD

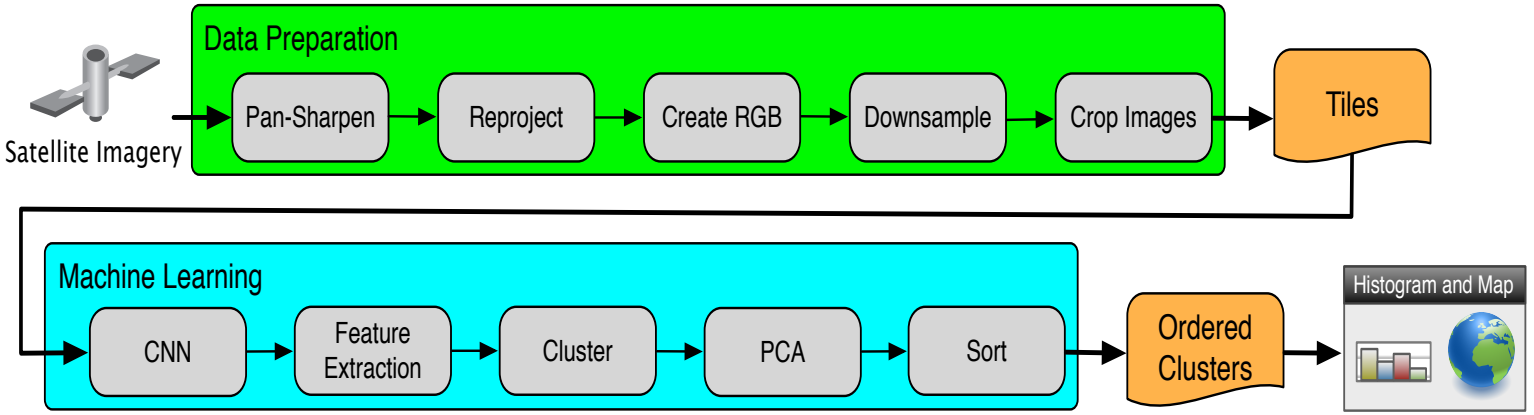


ANI type neural networks enable simulations of molecules and materials with QM quality at fraction of cost.



MB-pol type ML models enable transferable molecular simulations at unprecedented accuracy.

Satellite Image analysis – I. Altintas, M. Nguyen SDSC



Satellite image processing pipeline, showing data preparation and machine learning steps. Training of ML model will be accomplished using Voyager training nodes.

Thank you to our collaborators, partners, users, and the SDSC team!