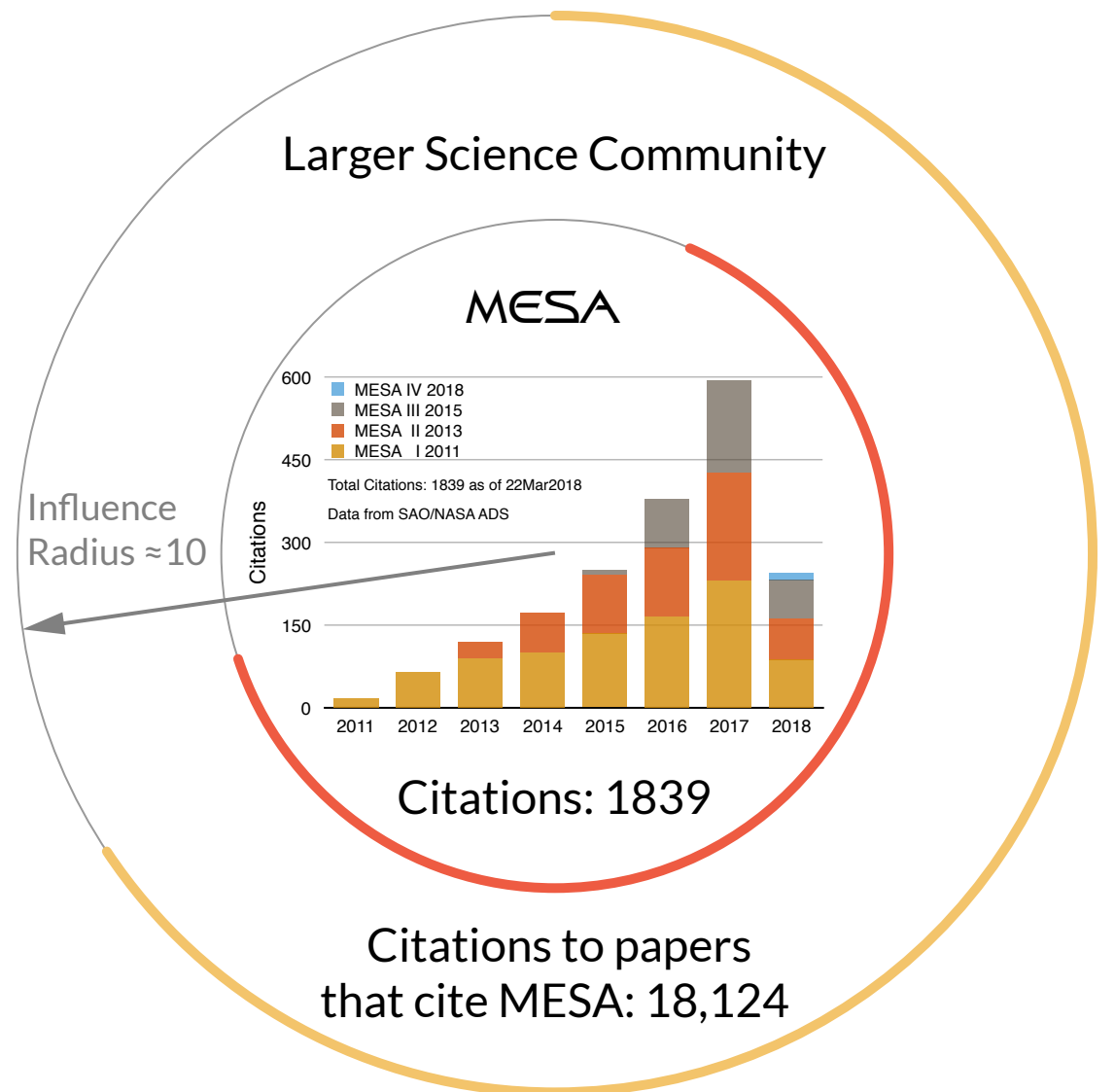
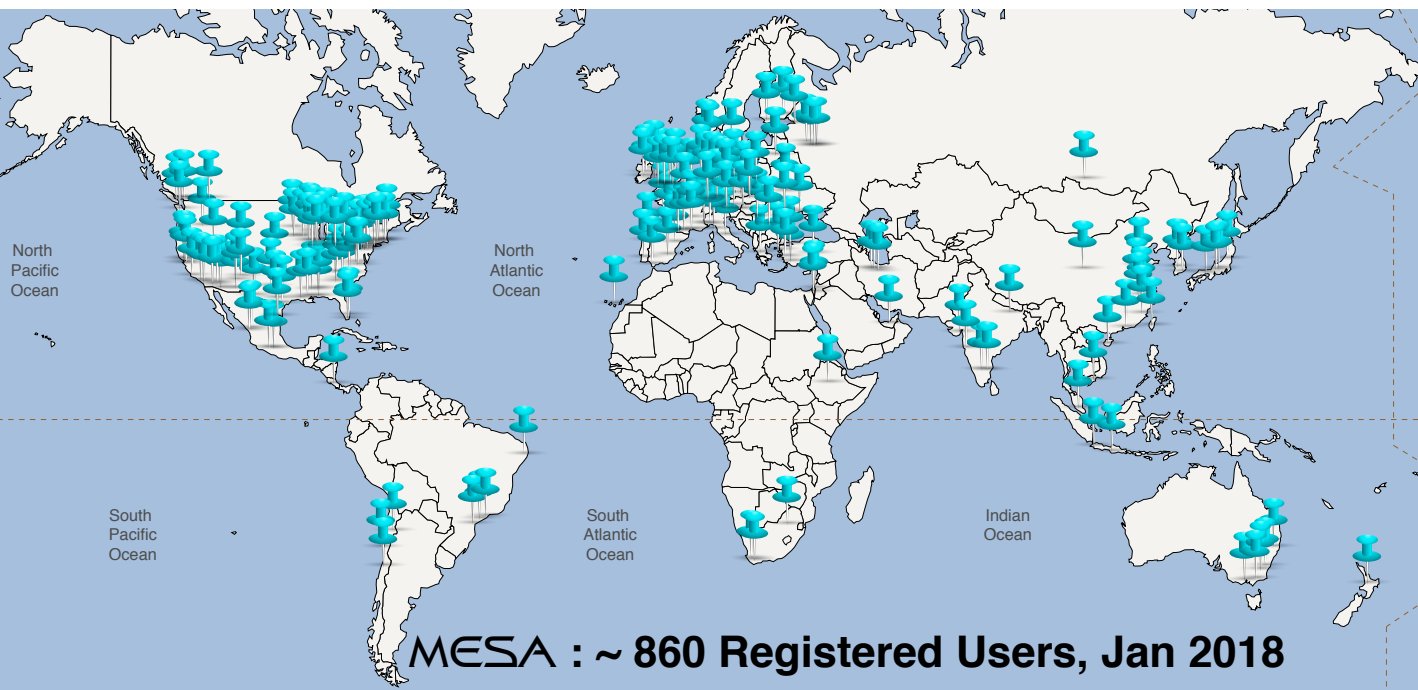
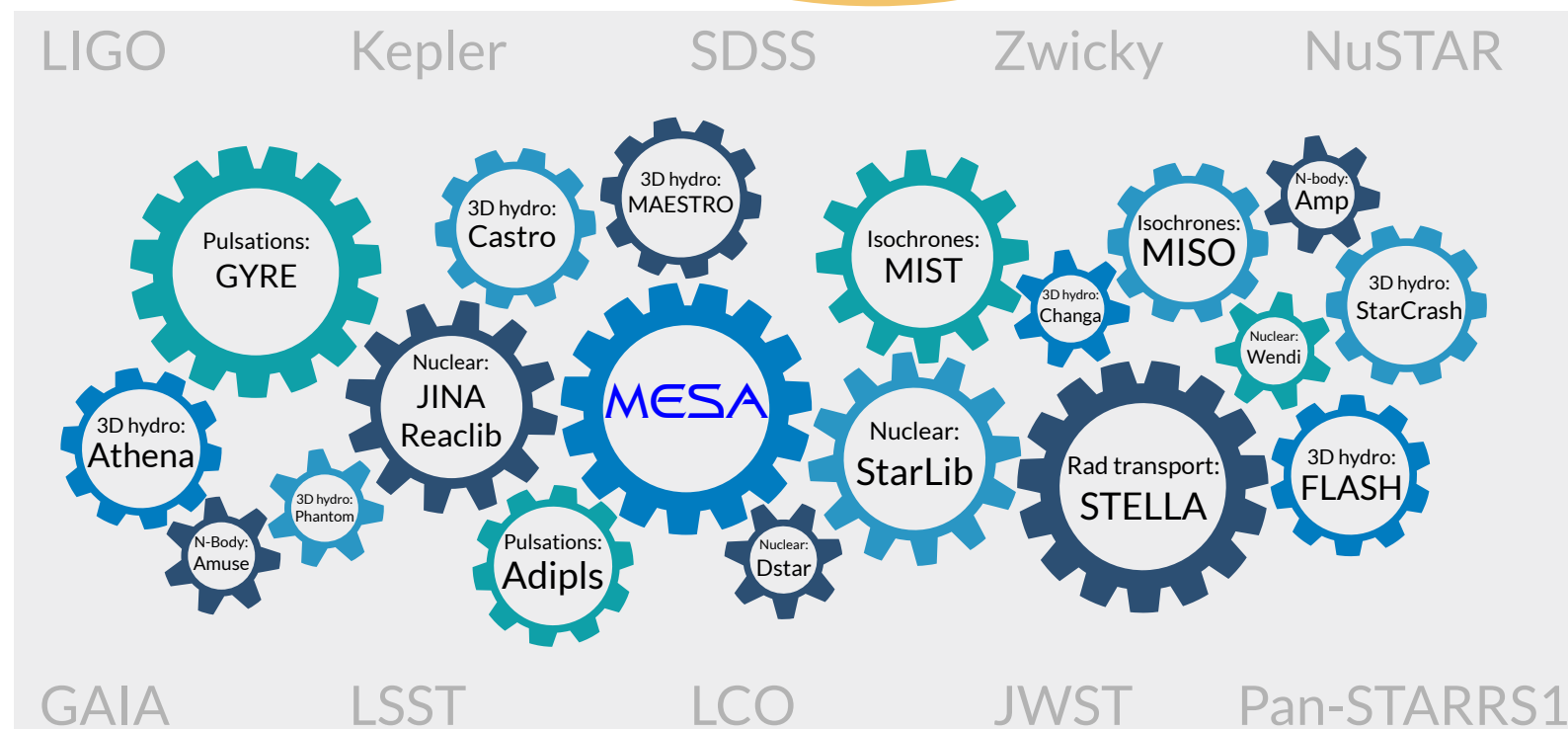
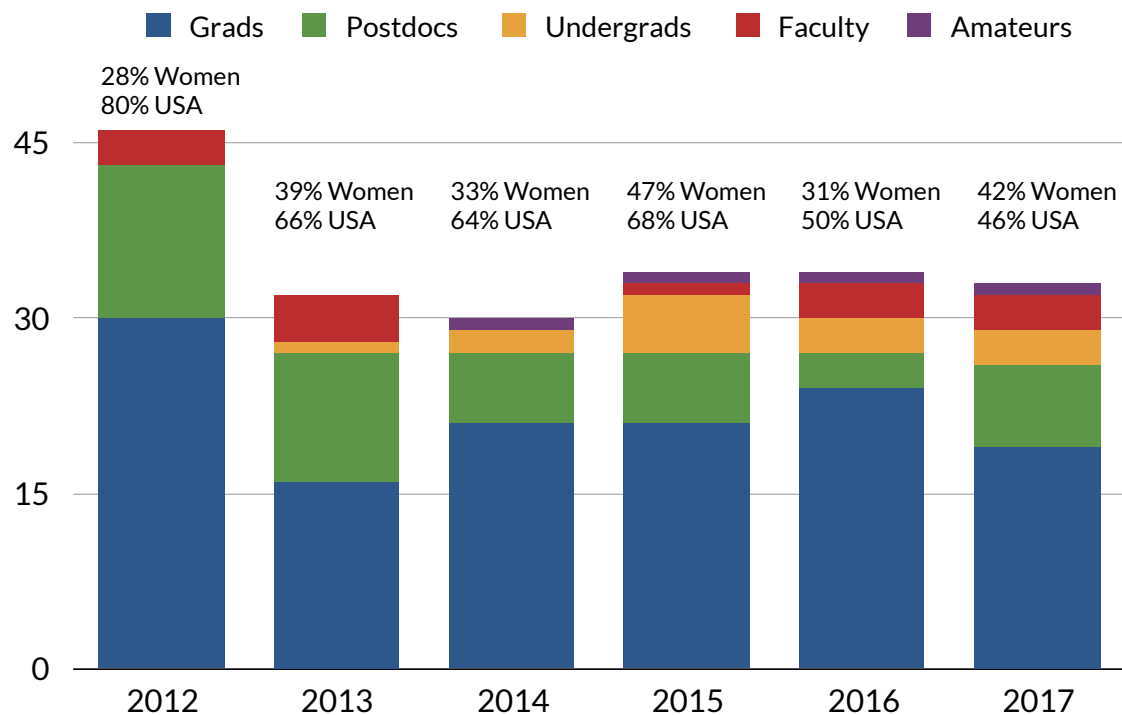


# SI2-SSI : Modules for Experiments in Stellar Astrophysics (MESA)

Frank Timmes (PI), Rich Townsend (Co-PI), Lars Bildsten (Co-PI), Bill Paxton (MESA's First Author), Josiah Schwab (Collaborator), Pablo Marchant (Collaborator), Rob Farmer (Collaborator)



## MESA Summer School





# Gunrock

GPU Graph Analytics

[gunrock.github.io](https://gunrock.github.io)

- Performance  
State-of-the-art graph processing library
- Generality  
Covers a broad range of graph algorithms
- Programmability  
Makes it easy to implement and extend graph algorithms from 1-GPU to multi-GPUs
- Scalability  
Fits in (very) limited GPU memory space  
performance scales when using more GPUs
- Continuous Integration  
Continuous delivery powered by [jenkins.io](https://jenkins.io)



Jenkins





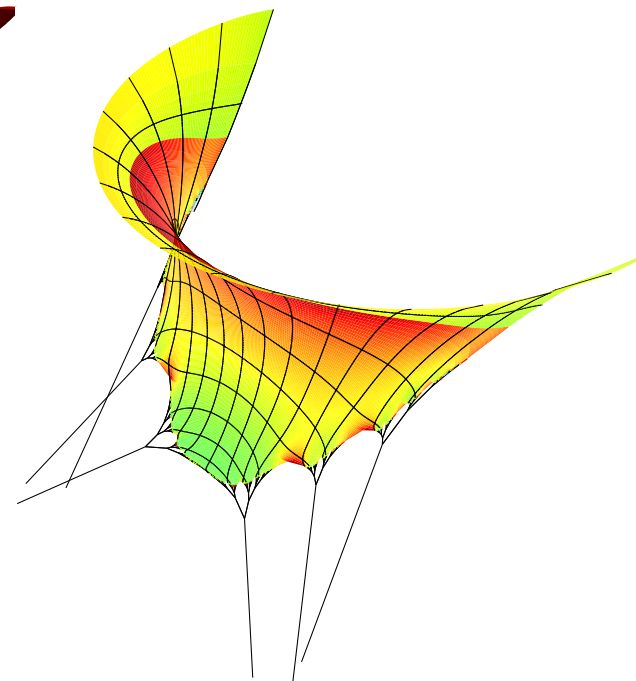
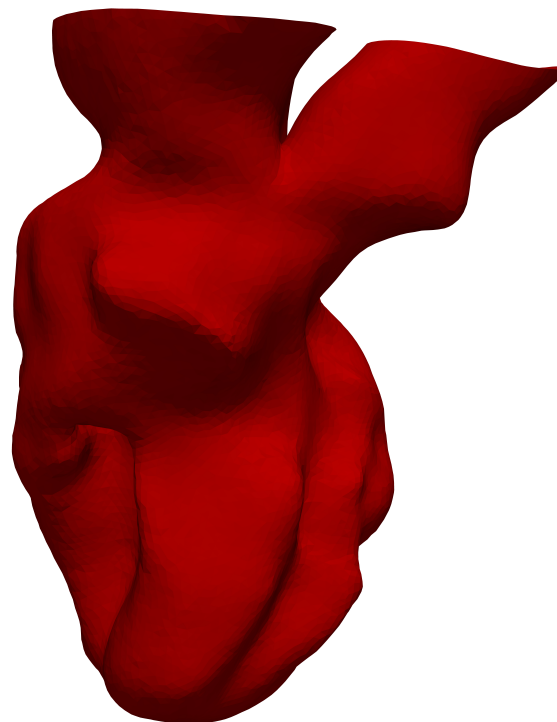
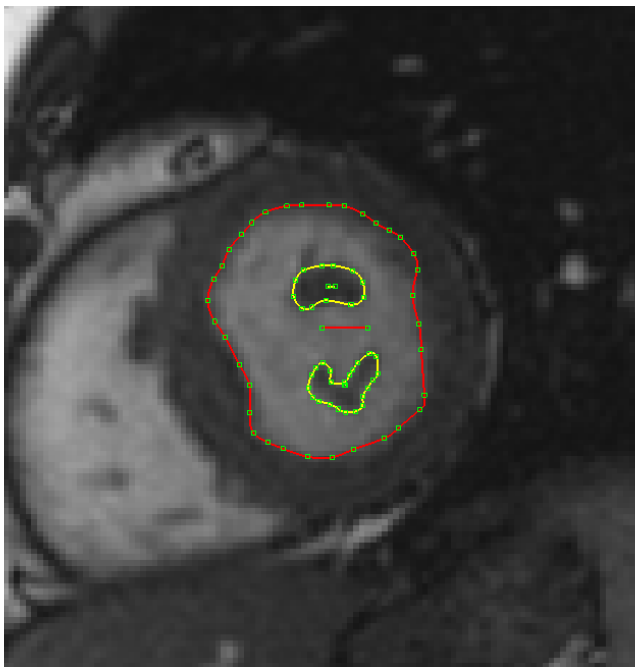
# SimCardio

Open-Source, Multi-Physics, Cardiac Modeling and Simulation

Alexander D. Kaiser, PhD, Cardiothoracic Surgery, Stanford; Vijay Vedula, PhD, Cardiology, Stanford;

Nathan M. Wilson, PhD, MBA, Open-Source Medical Software Corporation; Shawn C. Shadden, PhD, Mechanical Engineering, UC Berkeley;

Ellen Kuhl, PhD, Mechanical Engineering, Stanford; Alison L. Marsden, PhD, Pediatrics and Bioengineering, Stanford



Major support for this work was provided by the NSF SI2-SSI Collaborative Research Program (Awards #1339824 and #1663671).

# HydroShare: Cyberinfrastructure for Advancing Hydrologic Knowledge through Collaborative Integration of Data Science, Modeling and Analysis

David Tarboton, Ray Idaszak, Shaowen Wang, Jeffery Horsburgh, Dan Ames, Martyn Clark, Jon Goodall, Alva Couch, Hong Yi, Tony Castronova, Christina Bandaragoda, Rick Hooper

## Advancing Hydrologic Understanding

- requires integration of information from multiple sources
- is data and computationally intensive
- requires collaboration and working as a team/community

HydroShare is a system to advance hydrologic science by enabling the community to more easily and freely share products resulting from their research, not just the scientific publication summarizing a study, but also the data and models used to create the scientific publication.

- **F**indable
- **A**ccessible
- **I**nteroperable
- **R**eusable

- Open data
- Transparency
- Research Reproducibility
- Enhanced trust in research

The screenshot shows the HydroShare website homepage. At the top, there is a navigation bar with the HydroShare logo on the left and a 'SIGN IN' button on the right. Below the navigation bar is a large hero image of a river flowing over rocks. Overlaid on this image is the text 'Share your data and models with colleagues' and a subtext 'Upload, share, and access a broad set of hydrologic data types and models. Manage who has access to the content that you share.' Below the hero image, there is a section titled 'Join the community to start sharing' with a subtext 'HydroShare is an online collaboration environment for sharing data, models, and code.' and a 'Sign up now' button. To the left of this section is a list titled 'What you can do with HydroShare' with six bullet points, each preceded by a green checkmark. To the right of this list is an image of a laptop displaying the HydroShare interface. Below these sections is a 'How it works' section with a four-step process: 1. Create data, 2. Upload to HydroShare, 3. Describe with metadata, and 4. Share with colleagues.

<http://www.hydroshare.org>

Share your data and models with colleagues

Upload, share, and access a broad set of hydrologic data types and models. Manage who has access to the content that you share.

Join the community to start sharing

HydroShare is an online collaboration environment for sharing data, models, and code.

Sign up now

What you can do with HydroShare

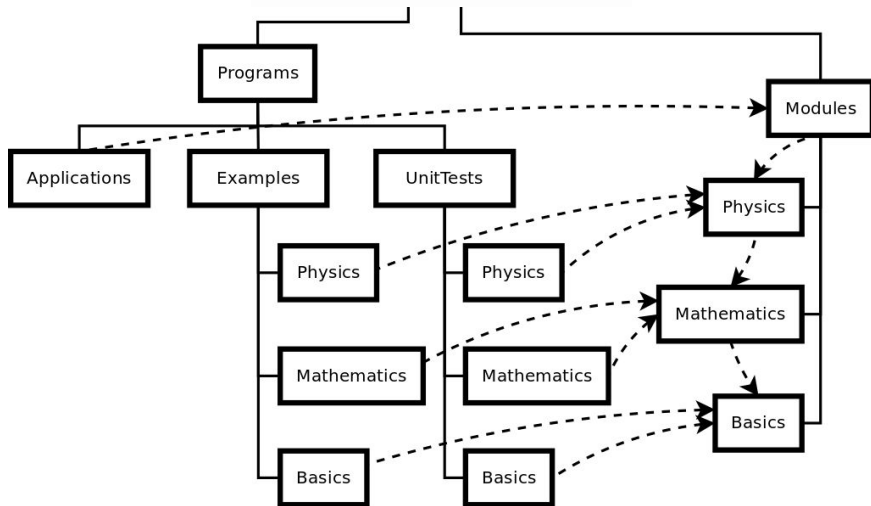
- ✓ Share your data and models with colleagues
- ✓ Manage who has access to the content that you share
- ✓ Share, access, visualize and manipulate a broad set of hydrologic data types and models
- ✓ Use the web services API to program automated and client access
- ✓ Publish data and models to meet the requirements of your data management plan
- ✓ Discover and access data and models published by others
- ✓ Use web apps to visualize, analyze and run models on data in HydroShare

How it works

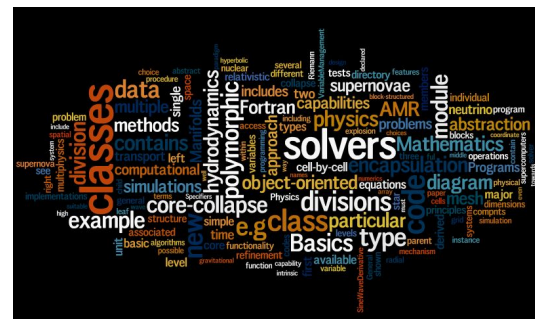
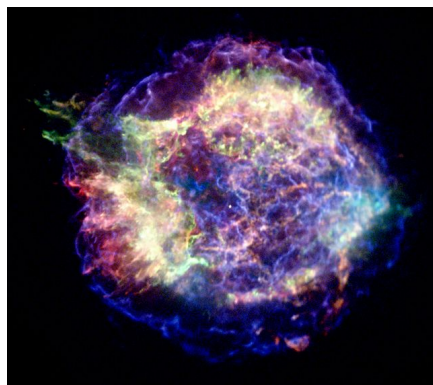
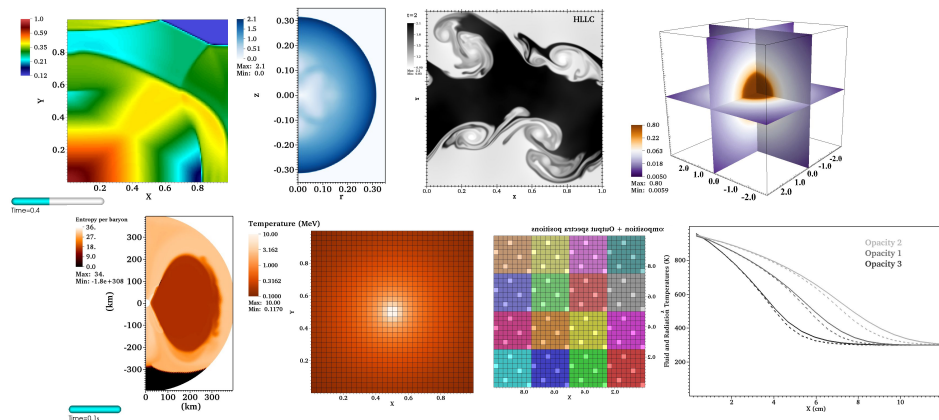
- 1 Create data
- 2 Upload to HydroShare
- 3 Describe with metadata
- 4 Share with colleagues

- Includes a repository for users to share and publish data and models in a variety of formats
- Includes tools (web apps) that can act on content in HydroShare

Reuben D. Budiardja, Eirik Endeve, Christian Y. Cardall, R. Daniel Murphy  
The University of Tennessee -- Oak Ridge National Laboratory



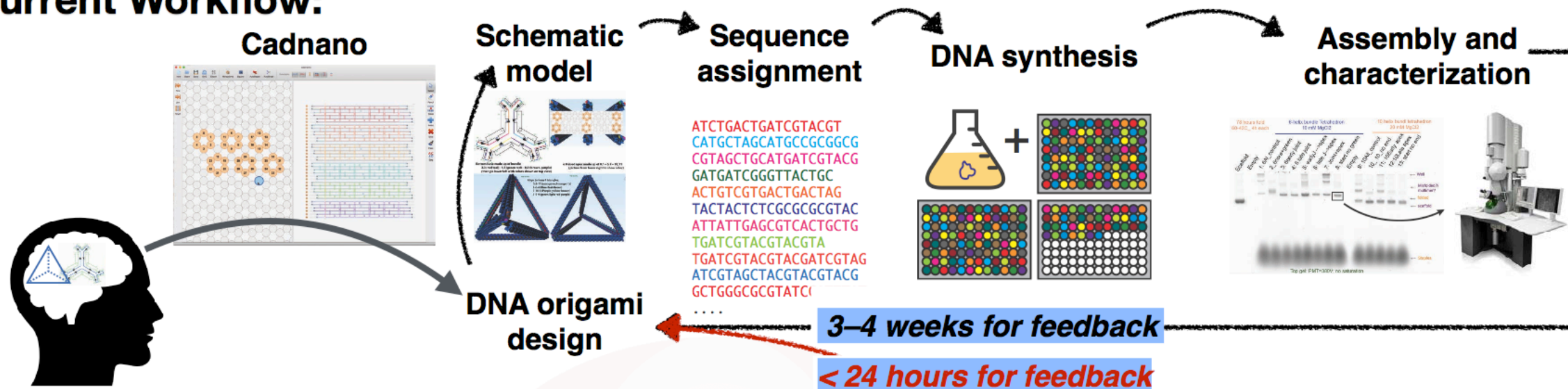
<http://genasis.xyz>



# SI2-SSE: Collaborative Research: Integrated Tools for DNA Nanostructure Design and Simulation

PIs: Shawn Douglas (UCSF) and Aleksei Aksimentiev (UIUC)

## Current Workflow:



## Future Workflow:



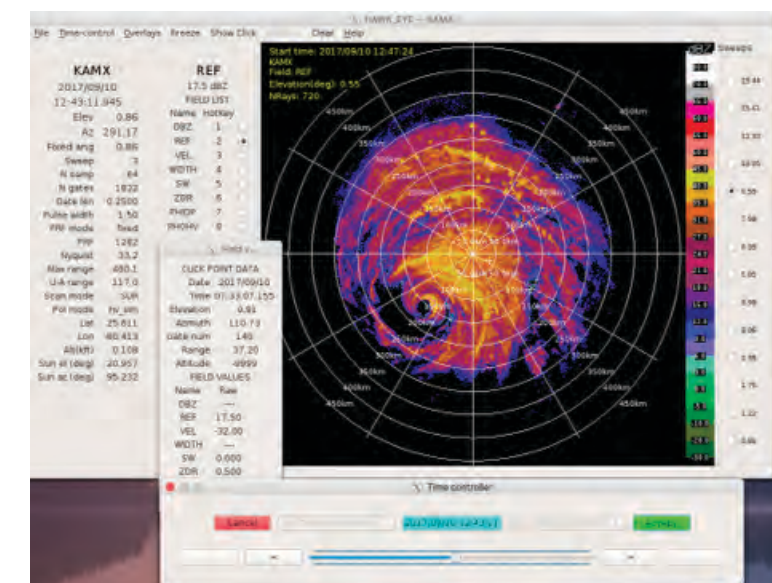
NSF OAC-1740212



# **LROSE:** **Lidar-Radar Open Software Environment**



- LROSE is a joint 4-year project between Colorado State University and the National Center for Atmospheric Research funded by NSF SI2-SSI to develop common software for the LIDAR, RADAR and Profiler community
- The 1st LROSE community workshop was held in April 2017. Focus on key applications as ‘building blocks’, allowing users to assemble trusted, reproducible workflows to accomplish more complex scientific tasks
- LROSE **“Blaze”** released in 2018 in a **“Virtual Toolbox”** Docker container or as C++ compiled native apps focused on data Conversion, Display, and Gridding. Additional tools for QC, Echo, and Wind analysis are in development

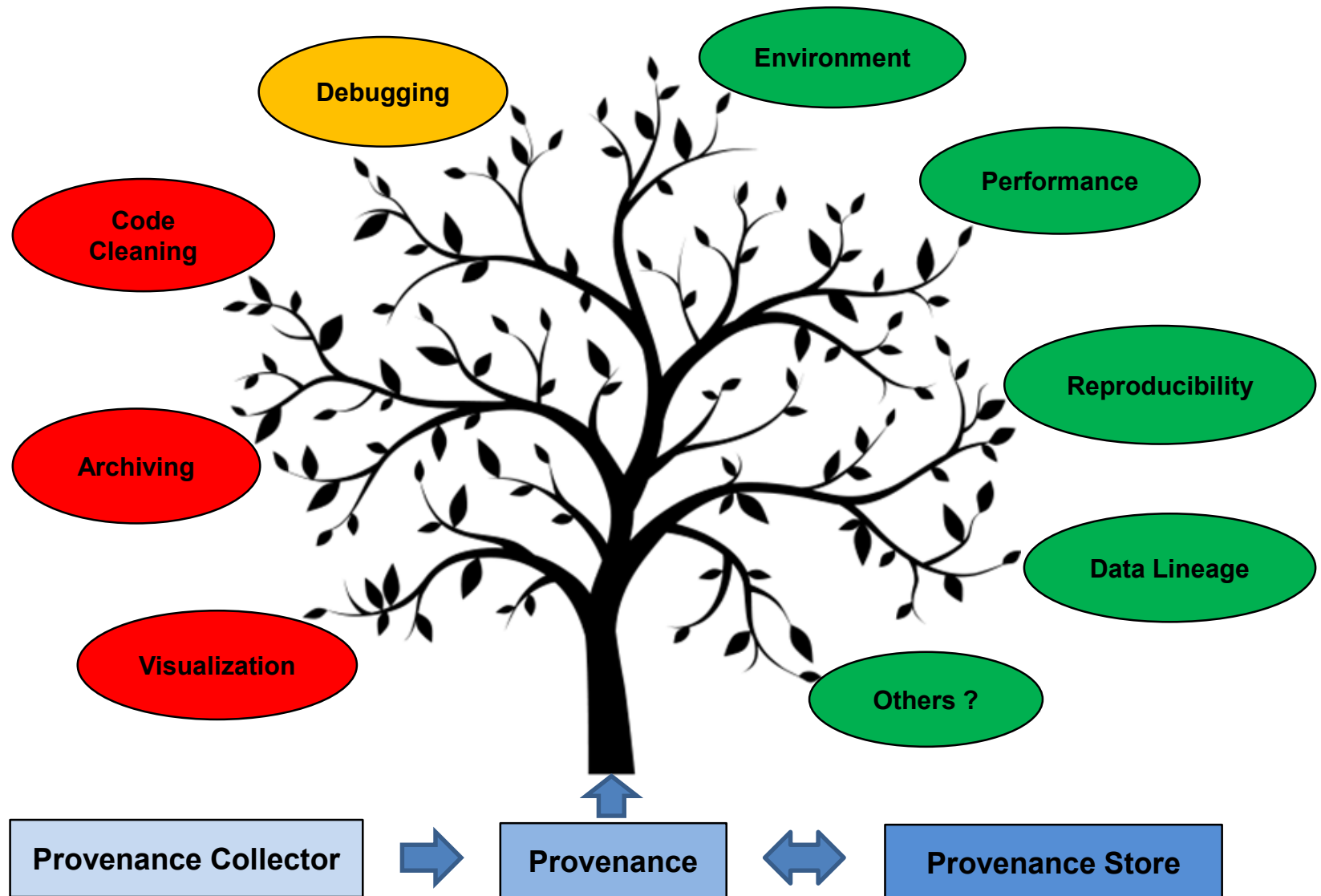


**HawkEye Display of  
Hurricane Irma (2017)**

***[nsf-lrose.github.io](https://nsf-lrose.github.io)***

# The Fruits of Provenance

Emery R. Boose, Aaron M. Ellison, Elizabeth Fong, Matthew Lau,  
Barbara S. Lerner, Jackson Okuhn, Thomas Pasquier, Margo Seltzer





# Harmonically Mapped Averaging for Everyone

## Ensemble Averages

- Core of statistical mechanics
- Relate molecule coordinate averages to material properties
- Example: Pressure tensor

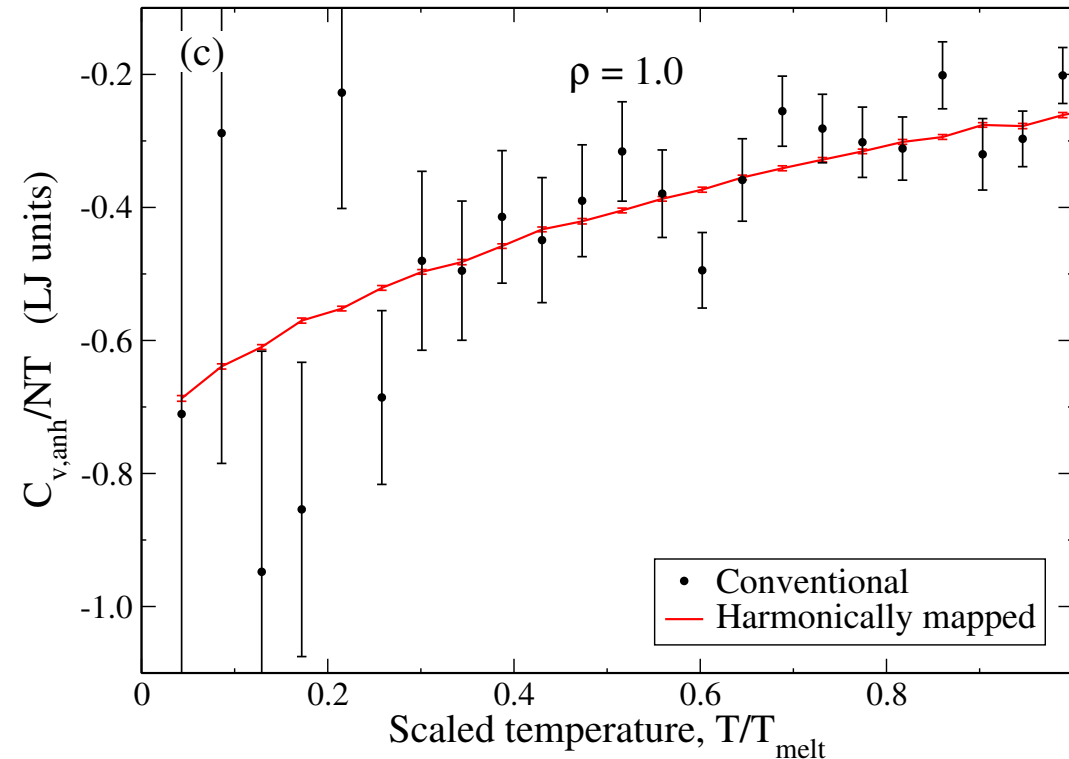
$$\mathbf{P} = \rho kT \mathbf{I} + \frac{1}{3V} \left\langle \sum_{i < j} \mathbf{f}_{ij} \mathbf{r}_{ij} \right\rangle$$

## Mapped Averages

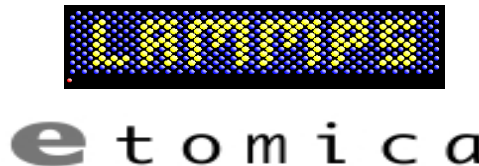
- Writes averages rigorously as deviation from an approximate starting point
- For crystals, a good starting point is a harmonic lattice
- Example: internal energy

$$U = \frac{3}{2} NkT + \left\langle U_{\text{config}} + \frac{1}{2} \mathbf{F} \cdot \Delta \mathbf{r} \right\rangle$$

## Performance: Heat capacity



## SSE project: Implement in these codes

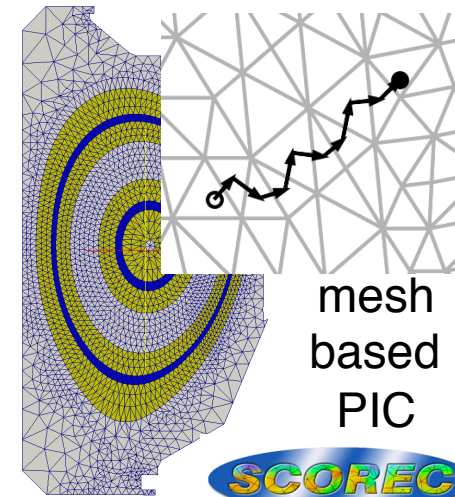
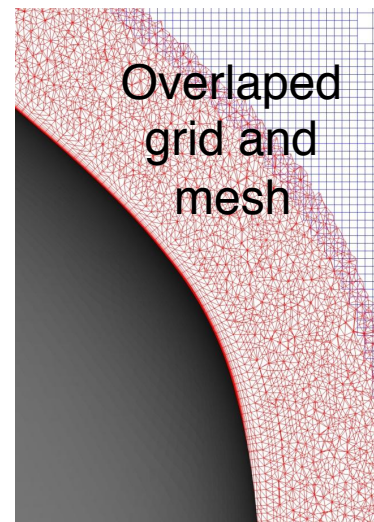
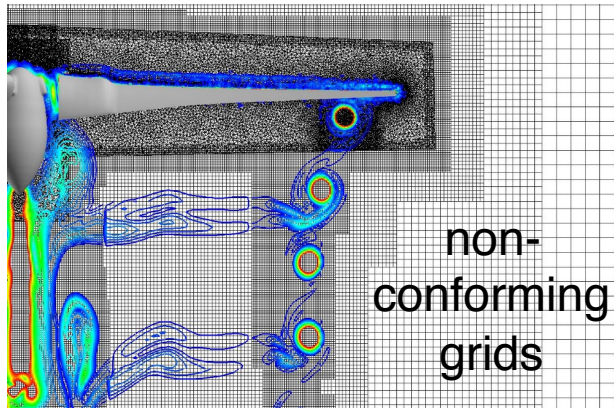
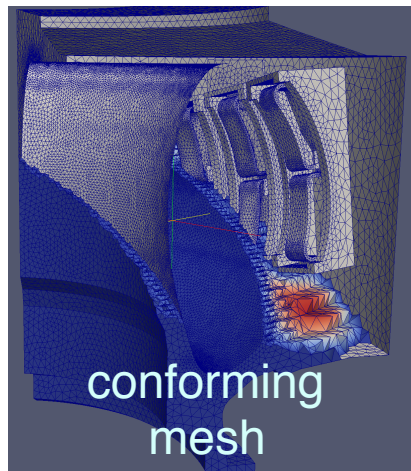
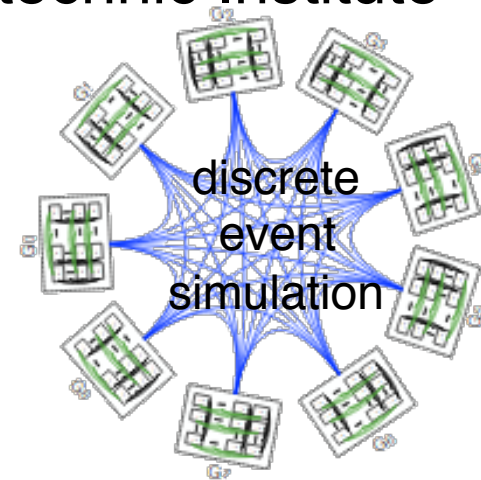


# Fast Dynamic Load Balancing for Extreme Scale Systems

Cameron W. Smith, Gerrett Diamond, M.S. Shephard

Computation Research Center, Rensselaer Polytechnic Institute

- Dynamic load balancing is a core tool needed to support automated simulations
- Goal: Generalize a multicriteria procedure to:
  - Applications past conforming unstructured meshes
  - Execute on accelerator supported systems
- Developing the EnGPar multicriteria partition improvement procedures based on a distributed N-graph





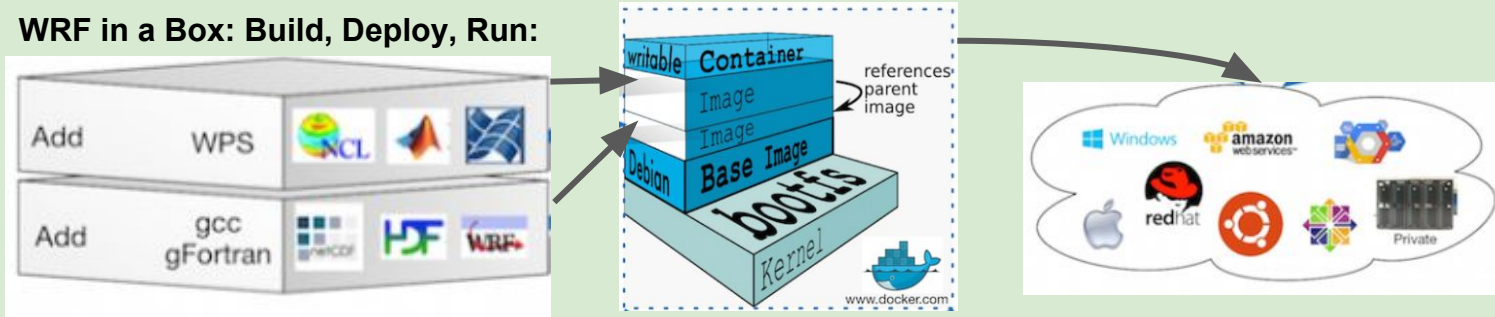
# BIG WEATHER WEB

Carlos Maltzahn, Ivo Jimenez (UC Santa Cruz), Mohan Ramamurty (Unidata), Gretchen Mullendor (UND), Brian Ancell (Texas Tech), William Capehart (SD Mines), Clark Evans (UW Milwaukee), Robert Fovell, Kevin Tyle (UAlbany), Steven Greybush (PennState), Russ Schumacher (Colorado State), Kate Fossell (NCAR), Joshua Hacker, John Exby (Jupiter Intelligence)

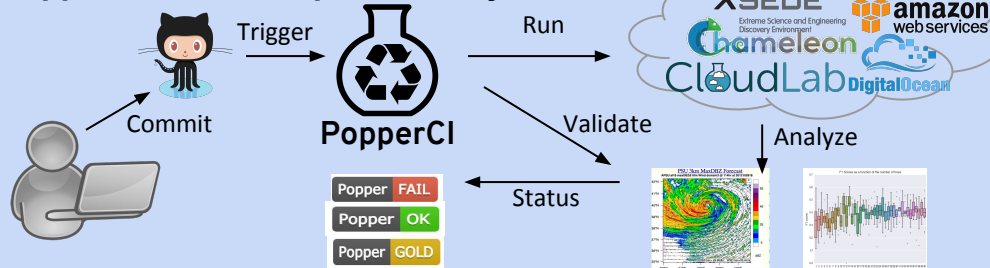
## Large ensemble shared among 7 universities:

Gretchen Mullendore (UND), Brian Ancell (Texas Tech), William Capehart (SDSM), Clark Evans (UW Milwaukee), Robert Fowell (U Albany), Steven Greybush (Penn State), Russ Schumacher (CSU).

## WRF in a Box: Build, Deploy, Run:



## Popper: Practical Reproducibility



BWW-funded grad student wins Better Scientific Software (BSSw) Fellowship



Ivo Jimenez

Crystallization Points: easily shared artifacts, community-improved over time



# SI2-SSE: Analyze Visual Data from Worldwide Network Cameras (Continuous Analysis of Many CAMeras, CAM<sup>2</sup>), NSFACI-1535108

PI: Yung-Hsiang Lu, [yunglu@purdue.edu](mailto:yunglu@purdue.edu) <https://cam2.ecn.purdue.edu>

## SUMMARY OF 2017-2018

- New Collaborators:



- Open-Source in github
- REST interface

facebook

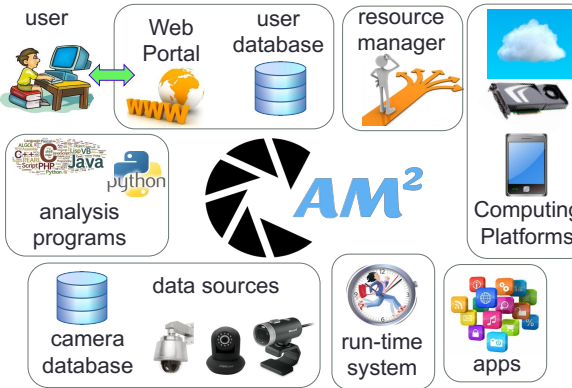
## NEW PUBLICATIONS

- IEEE Transactions on Cloud Computing
- IEEE International Conference on Multimedia Information Processing and Retrieval 2018.
- ACM Multimedia 2017
- IEEE International Conference on Information Reuse 2017
- "Parallel Video Processing using Embedded Computers", IEEE Global Conference on Signal and Information Processing 2017
- "Creating the World's Largest Real-Time Camera Network", Imaging and Multimedia Analytics in a Web and Mobile World 2017
- "Internet of Video Things in 2030: a World with Many Cameras", IEEE International Symposium of Circuits and Systems 2017.

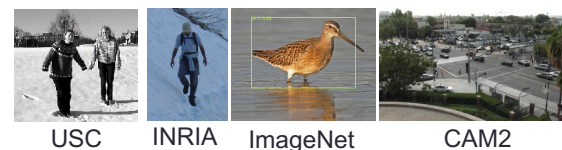
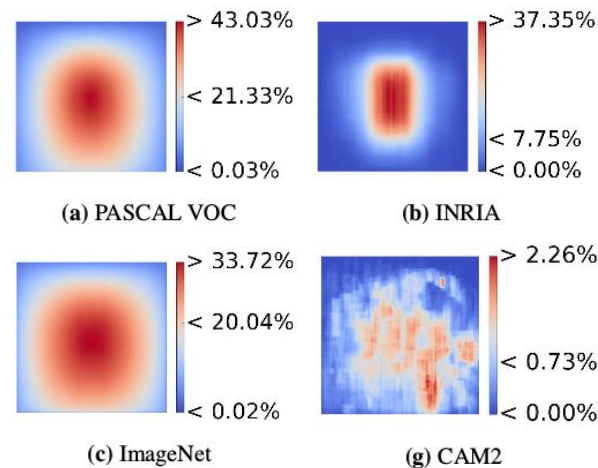
## MEDIA COVERAGE



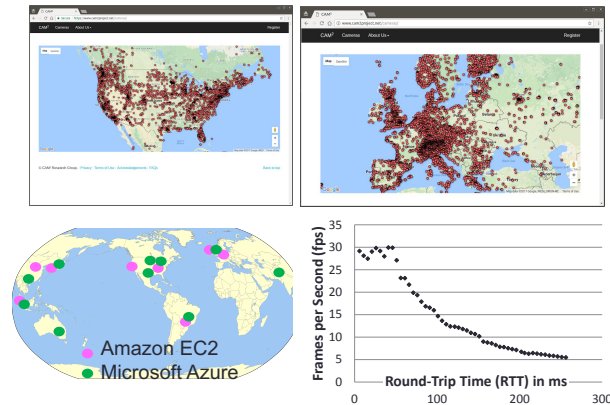
## CAM2 COMPONENTS



## UNDERSTAND DATA BIAS



## GLOBAL SCALE

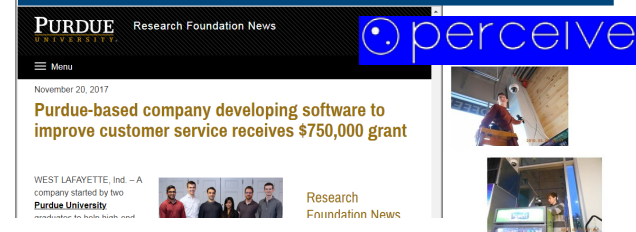


## USER RECRUITMENT AND OUTREACH

Vertically Integrated Projects  
Midwest Undergraduate Research Workshop



## COMMERCIAL SPIN-OFF



Collaborative Research: Building Sustainable Tools  
and Collaboration for Volcanic and Related Hazards  
Program: Software Infrastructure for Sustained  
Innovation

**Abani Patra**

An open source multi-physics platform to advance  
fundamental understanding of plasma physics and  
enable impactful application of plasma systems

**Davide Curreli and Steve Shannon**





# Parsl: A Python-based Parallel Scripting Library

<http://parsl-project.org>

Yadu Babuji\*, Kyle Chard\*, Ian Foster\*, Daniel S. Katz°, Mike Wilde\*, Anna Woodard\*, Justin M. Wozniak\*

\*Computation Institute, University of Chicago and Argonne National Laboratory

°National Center for Supercomputing Applications, University of Illinois at Urbana-Champaign



**Goals:** Easily write Python workflows that glue together external programs and Python functions; run them quickly and easily in parallel on diverse resources

## Simple installation:

```
pip install parsl
```

Annotate functions to make Parsl **apps**

- Bash apps call external applications
- Python apps call Python functions

Apps run concurrently respecting data dependencies via futures. Natural parallel programming!

Parsl scripts are independent of where they run. Write once run anywhere!

Features: Multi-site work distribution, automatic elasticity, Globus data staging, resilience, containers.

```
from parsl import *
from parsl.configs.local import localIPP, localThreads

dfk = DataFlowKernel(config=localIPP)

@app('bash', dfk)
def generate(outputs=[]):
    return "echo $(( ( RANDOM )) >> {outputs[0]})"

@app('python', dfk)
def total(inputs=[]):
    total = 0
    for i in inputs:
        with open(i, 'r') as f:
            total += sum([int(line) for line in f])
    return total

# Create 5 files with random numbers
output_files = []
for i in range(5):
    output_files.append(generate(outputs=['random-%s.txt' % i]))

# Calculate the sum of the random numbers
t = total(inputs=[i.outputs[0] for i in output_files])
print (t.result())
```

# MetPy - A Python GEMPAK Replacement for Meteorological Data Analysis

**Ryan May**

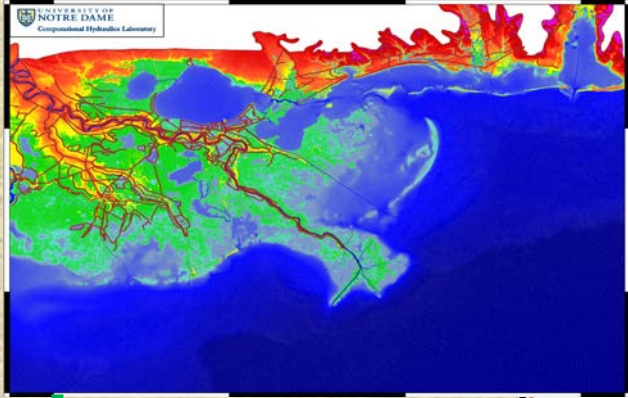


# STORM: a Scalable Toolkit for an Open Community Supporting Near Real-time High Resolution Coastal Storm Modeling

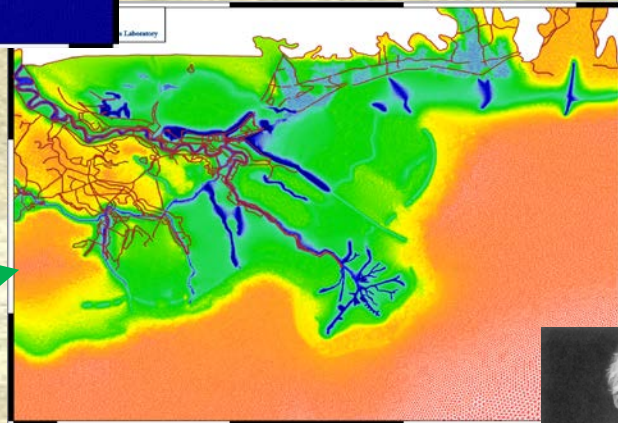
Hartmut Kaiser<sup>1</sup>, Joannes Westerink<sup>2</sup>, Rick Luettich<sup>3</sup>, Clint Dawson<sup>4</sup>

<sup>1</sup>Louisiana State University, <sup>2</sup>University of Notre Dame, <sup>3</sup>University of North Carolina, <sup>4</sup>University of Texas at Austin

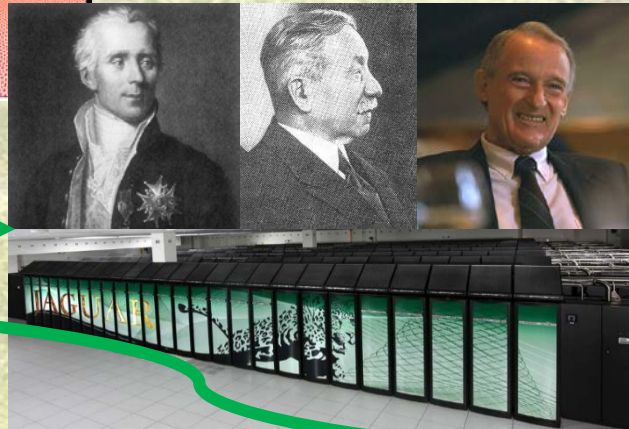
Geophysical systems



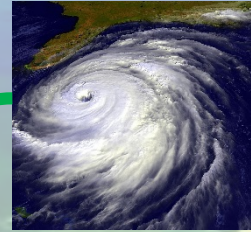
Unstructured grids



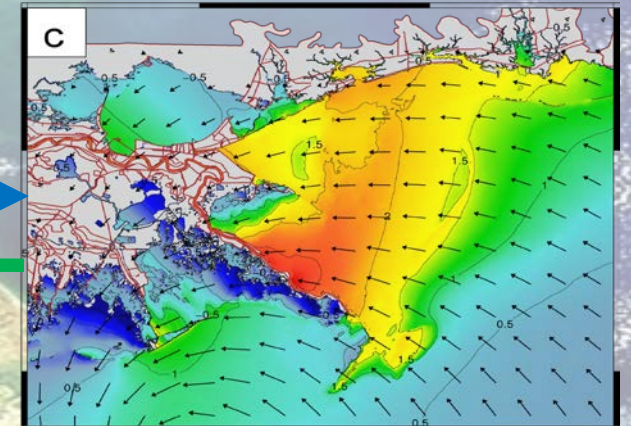
Pde's + FEM + HPC



Physics & forcing functions  
Model interfacing and interleaving



Ocean Responses



Dynamic  
grids/domains  
HPX & MPI-Zoltan

# SI2-SSE: 3DSIM: A Unified Framework for 3D CPU Co-Simulation

**ANKUR SRIVASTAVA**

# SI2-SSI: Sustainable Open-Source Quantum Dynamics and Spectroscopy Software

**Xiaosong Li**



# SI2-SSI: EVOLVE

## Open MPI for Next Generation Architecture and Applications

George Bosilca, Aurélien Bouteiller, Thomas Herault, and Edgard Gabriel

*Augment Open MPI to evolve and adjust to the challenges of new hardware environments, and to maintain the same level of efficiency for parallel scientific applications in a quickly transitioning hardware ecosystem.*

- Efficient **threading**, including for **MPI + X** programming models, **high injection rate**
- Support hybrid architectures with direct data movement to/from **accelerators**
- **Event-driven, architecture-aware collective** communications
- Highly **efficient MPI I/O** support via OMPIO
- Fast and scalable **runtime (PMIx)** providing **reduced memory** consumption, **fast startup** and **resilient** capabilities





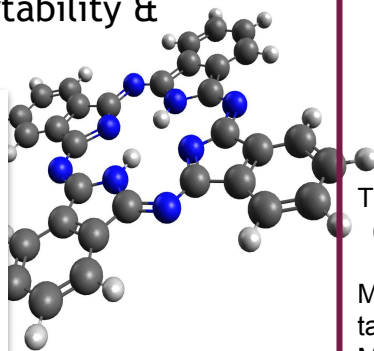
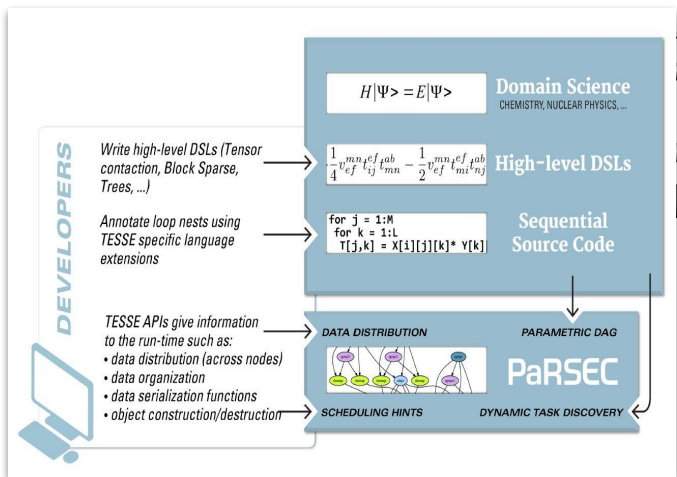
# SI2-SSI: TESSE

## Task Based Environment for Scientific Simulation at Extreme Scale

Robert J. Harrison, Mohammad M. Javanmard, George Bosilca, Thomas Herault, Damien Genet, Edward F. Valeev

### Challenge:

- Execute dynamic algorithms over irregular data on extreme scale hybrid machines using a task-based runtime
- Guarantee performance portability & productivity



### Recent Development

#### New Programming Model:

##### Templated Task Graph (TTG)

- General purpose programming model implemented in C++
- Applications composed as graphs of templated Ops encoding DAG of tasks instantiated at runtime
- Abstracts out the details of the execution runtime (PaRSEC and MADNESS already supported)

Tasks are parameterized (loop index, label of node, couple of indices)

Minimize the known task graph

Match tasks with keys

Explicit send / implicit receive

```
void Plus::op(const keyT &key,
              baseT::input_values_tuple_type &&t,
              baseT::output_terminals_type &out) {
    auto x = baseT::get<0>(t);
    auto y = baseT::get<1>(t);
    ::send<0>((int) (key), x+y, out);
}

Plus plus;
Times times;

connect<0, 0>(&plus, &times);
```

```

graph TD
    x --> plus
    y --> plus
    plus --> t
    t --> times
    times --> z
    z --> r
    
```

*TensorFlow for general-purpose workloads*

### Project Objectives

- WorldWide Telescope visual front-end for Astrolabe repository of legacy data.
- Tools for processing raw data into Astrolabe and visualization formats needed by WWT.
- Integration of the Unified Astronomy Thesaurus (UAT) into both Astrolabe and WWT.
- Data manipulation tools necessary to use WWT as a first look in archive browsing and retrieval.
- Workshops to identify community need for years 2 and 3.

### Year 1 Development

- Port of key WWT functions to web interface.  
~20k users/month since Oct

### Year 2 Development Status

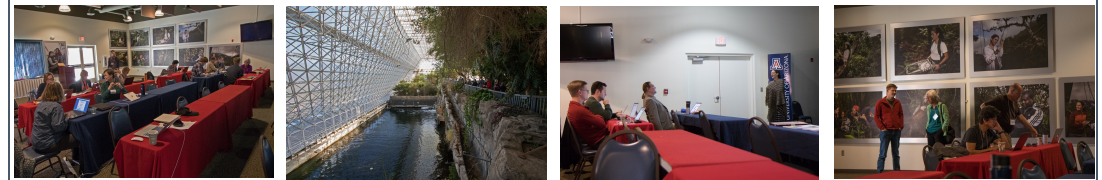
- Integrating software with CyVerse
- Community outreach
- Ingesting data and metadata

### Year 2 Astrolabe Tools

- JS9 - WWT
- Glue
- Jupyter Notebook
- Topcat
- Customized metadata template
- UAT keywords
- DataCite DOIs

### Year 2 Outreach

- Splinter session workshop held at American Astronomical Society annual meeting in January 2018
- Workshop and hackathon held at Biosphere 2 in March 2018
- Paper to be published in ApJS: *"Astrolabe: Curating, Linking and Computing Astronomy's Dark Data"*



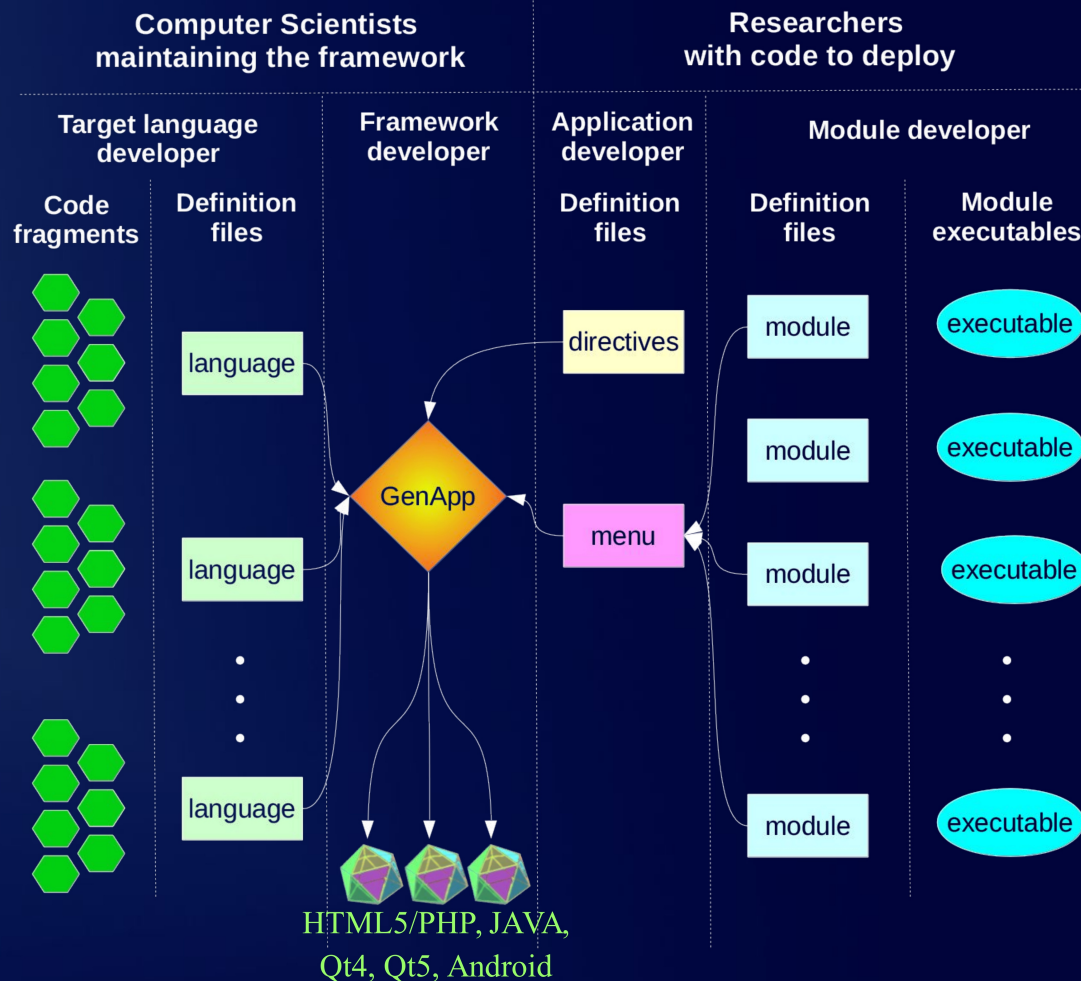
# SI2-SSE: GenApp - A Transformative Generalized Application Cyberinfrastructure

E. H. Brookes<sup>a</sup>, J. E. Curtis<sup>b</sup>, D. Fushman<sup>c</sup>,  
S. Krueger<sup>b</sup> and A. Savelyev<sup>a</sup>

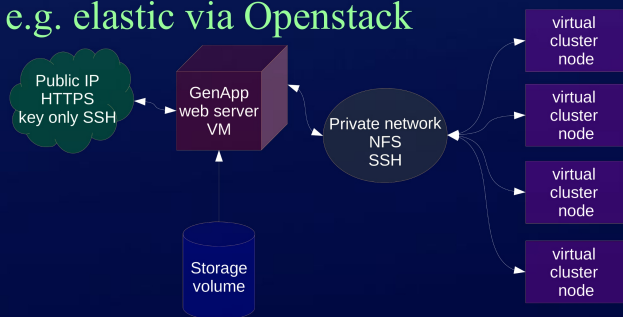
<sup>a</sup>Department of Biochemistry & Structural Biology, University of  
Texas Health Science Center at San Antonio, San Antonio, Texas

<sup>b</sup>NIST Center for Neutron Research, Gaithersburg, Maryland

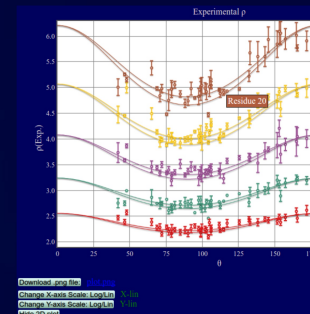
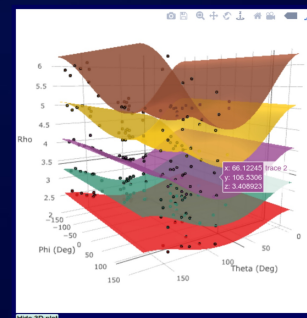
<sup>c</sup>Department of Chem. & Biochem., University of Maryland, College  
Park, Maryland



Multiple Execution models  
e.g. elastic via Openstack

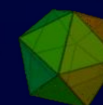


Full featured: job  
management, “cloud” files,  
messaging, integrated  
feedback, context help, 2 &  
3d plots, atomic structures  
audio, video



OAC-1740097  
OAC-1739549

<https://genapp.rocks>



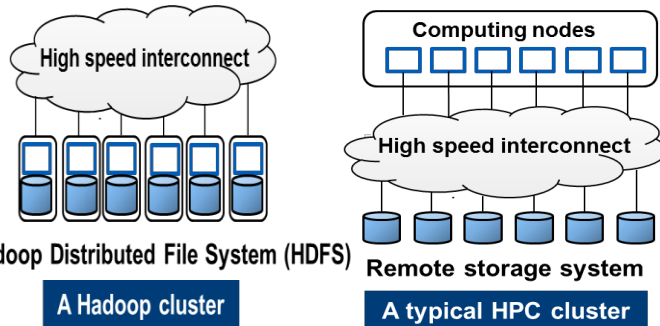
GenApp

# Application Characterization for Adaptive Computing Platform Determination for Computational and Data-Enabled Science and Engineering

Haiying Shen, Associate Professor  
University of Virginia, USA  
hs6ms@virginia.edu

Walter B. Ligon, Associate Professor  
Clemson University, USA  
walt@clemson.edu

## MOTIVATION



- Hadoop platforms with local storage and dedicated storage
- Different applications may benefit differently from the two platforms

## SOLUTIONS

- Determine thresholds to decide whether use:
  - local storage or remote storage
  - scale-up or scale-out nodes

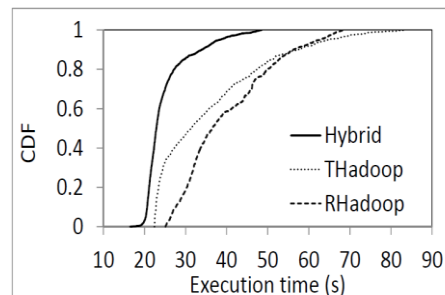
## PROJECT

- Application performance comparison (I/O, data, and CPU intensive)
- Best platform determination
- Adaptive hybrid Hadoop platform construction

## OBSERVATIONS

- Remote file system Orange File System (OFS) outperforms local file system HDFS when the data size is large due to the fast I/O.
- HDFS outperforms OFS when the data size is small due to the network latency.
- Scale-up machines are better for small jobs but not large jobs.
- Scale-out machines bring more benefits to process a larger amount of data than scale-up machines.

## RESULTS



**Hybrid:** hybrid scale-up/out cluster with OFS

**THadoop:** traditional scale-out Hadoop with HDFS

**RHadoop:** traditional scale-out Hadoop with OFS





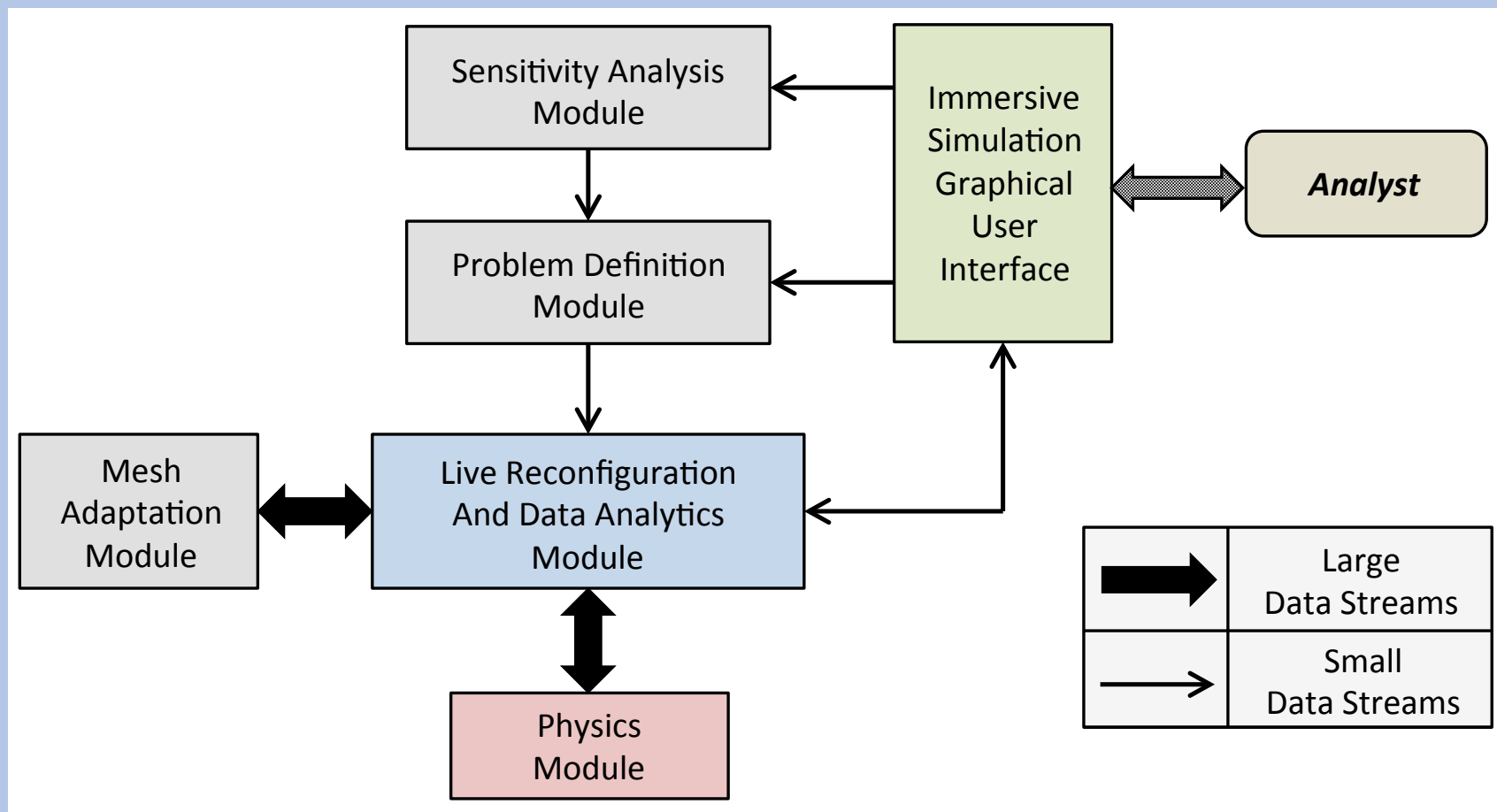
# Software Elements to Enable Immersive Simulation



Corey Nelson, Felix Newberry, John A. Evans, Kurt Maute, Alireza Doostan, Kenneth E. Jansen

*Ann and H.J. Smead Department of Aerospace Engineering Sciences, University of Colorado, Boulder, CO 80309*

**2018 NSF SI<sup>2</sup> PI Meeting**





# A Data-Centric Approach to Turbulence Simulation

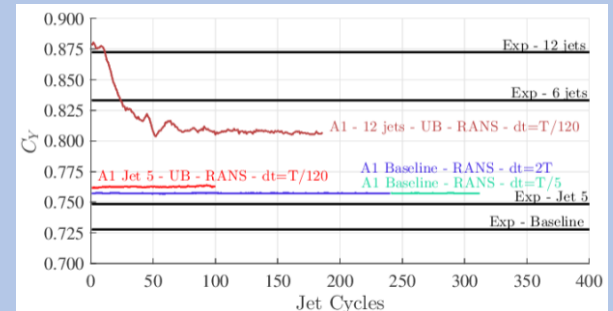
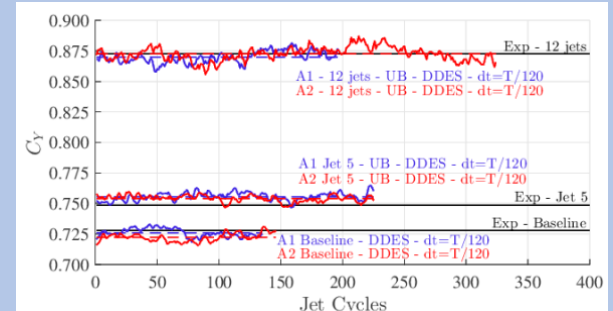
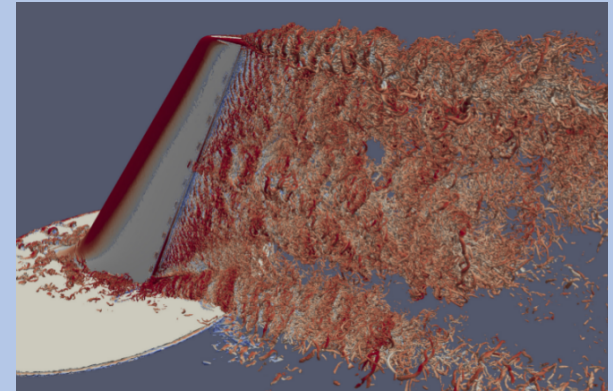


Eric Peters, Riccardo Balin, Ryan Skinner, John A. Evans, Philippe R. Spalart, Alireza Doostan, Kenneth E. Jansen

*Ann and H.J. Smead Department of Aerospace Engineering Sciences, University of Colorado, Boulder, CO 80309*

**2018 NSF SI<sup>2</sup> PI Meeting**

- Separating turbulent boundary layers are poorly predicted by Low Fidelity Models (LFM)
- High fidelity models can predict them but at a cost far too high for design or uncertainty quantification (UQ)
- Goals of this project are:
  - Leverage Multi-Fidelity Modeling (MFM) to accelerate confident design space exploration
  - Contribute to Direct Numerical Simulation (DNS) data base of separating turbulent boundary layers
  - Use Machine Learning (ML) to improve LFM turbulence modeling closures from DNS data
- <https://github.com/PHASTA>





# NSCI SI2-S2I2 Conceptualization of **CFDSI**: Model, Data, and Analysis Integration for End-to-End Support of Fluid Dynamics Discovery and Innovation



University of Colorado  
Boulder

Kenneth E. Jansen Jed Brown,  
Alireza Doostan, John A. Evans,  
John A. Farnsworth, Peter E.  
Hamlington, and Kurt K. Maute



Beverley J. McKeon



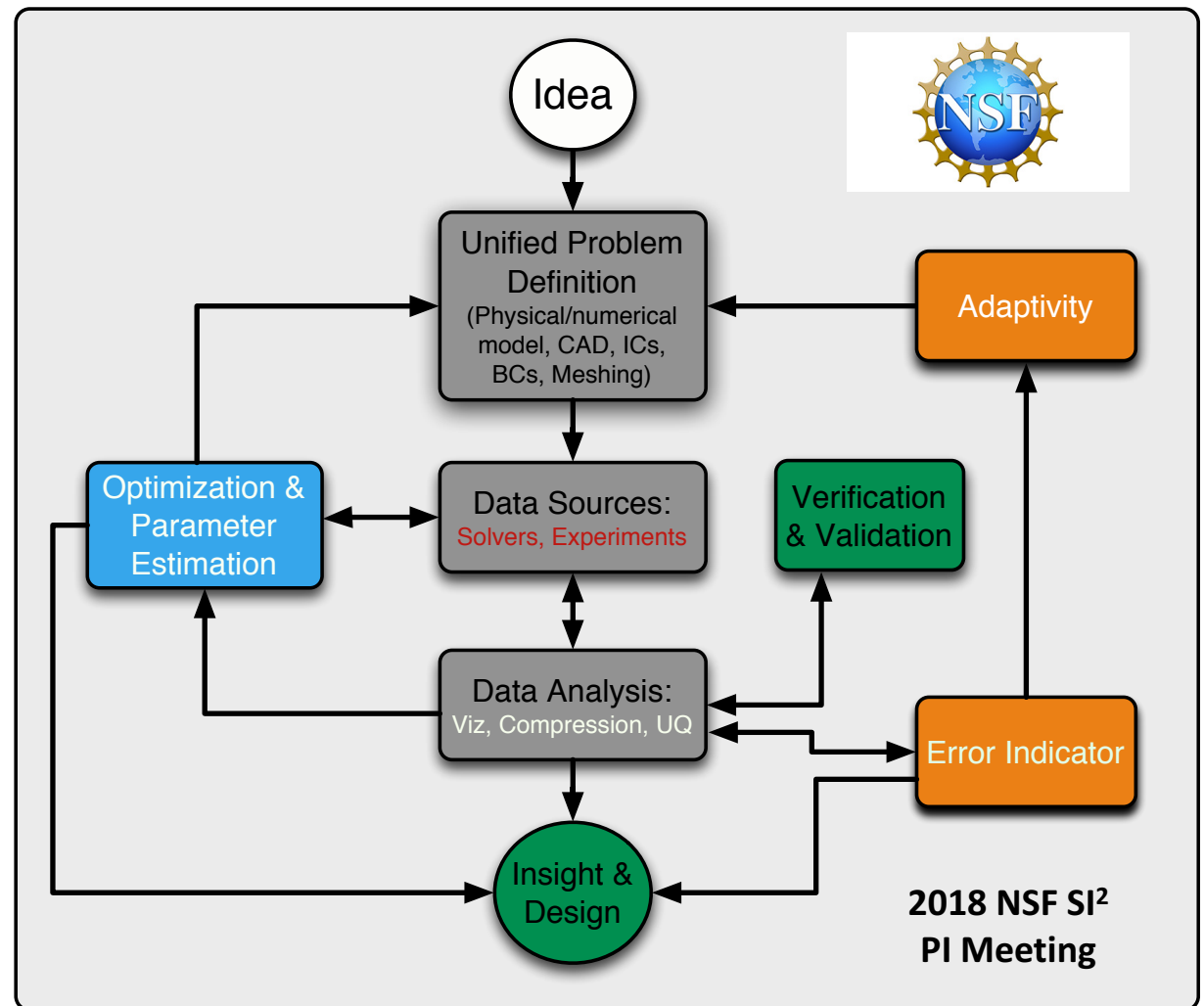
Charles V. Meneveau



Robert D. Moser



Mark S. Shephard, Onkar  
Sahni, and Cameron Smith



# Extending the physics reach of LHCb in Run 3 using machine learning in the real-time data ingestion and reduction system

The LHCb detector is being upgraded for Run 3 (2021-2023), when the trigger system will need to **process 25 exabytes per year**.

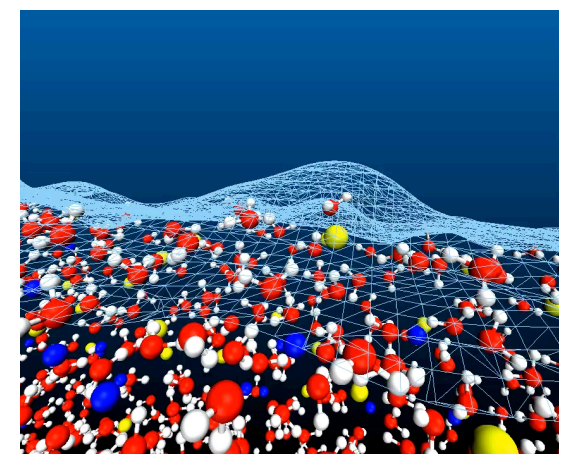
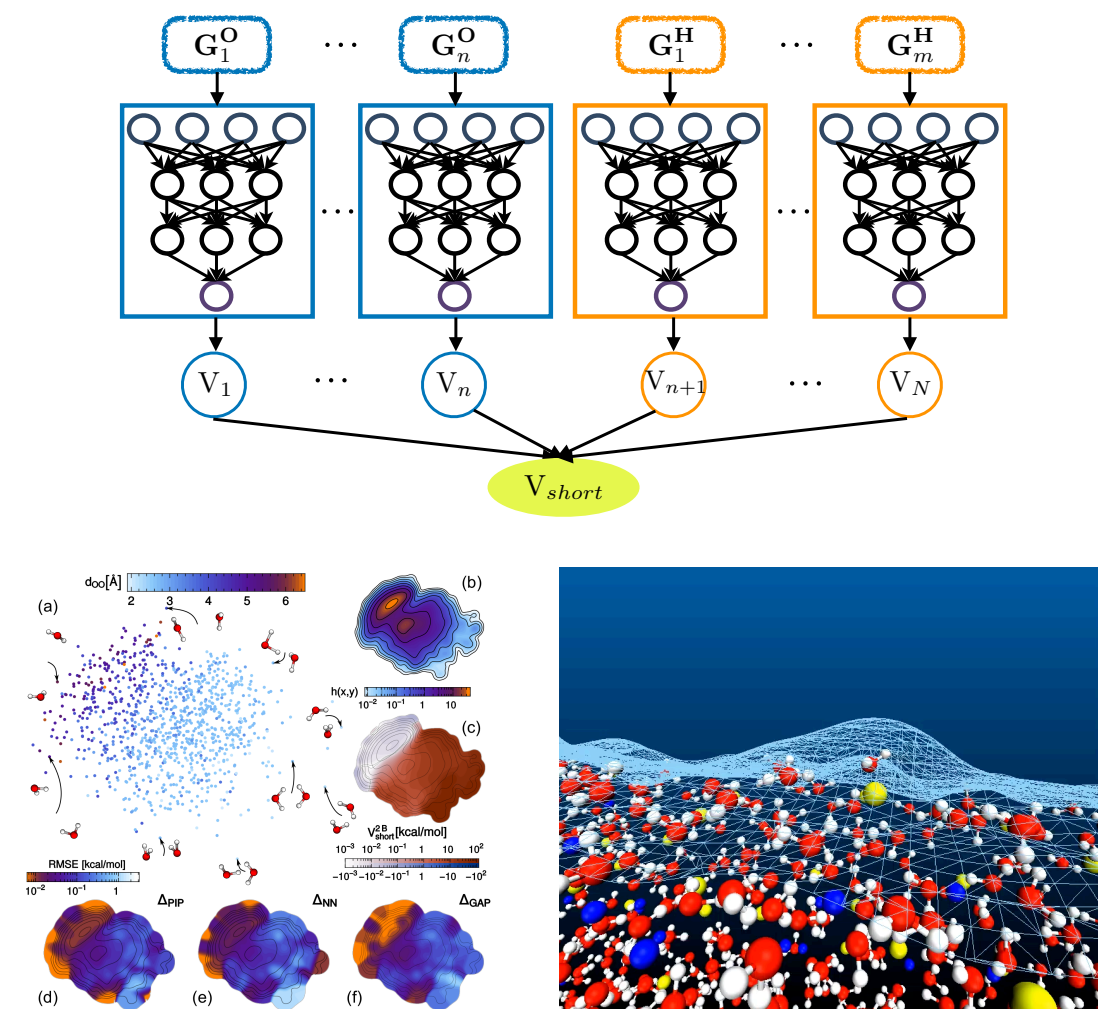
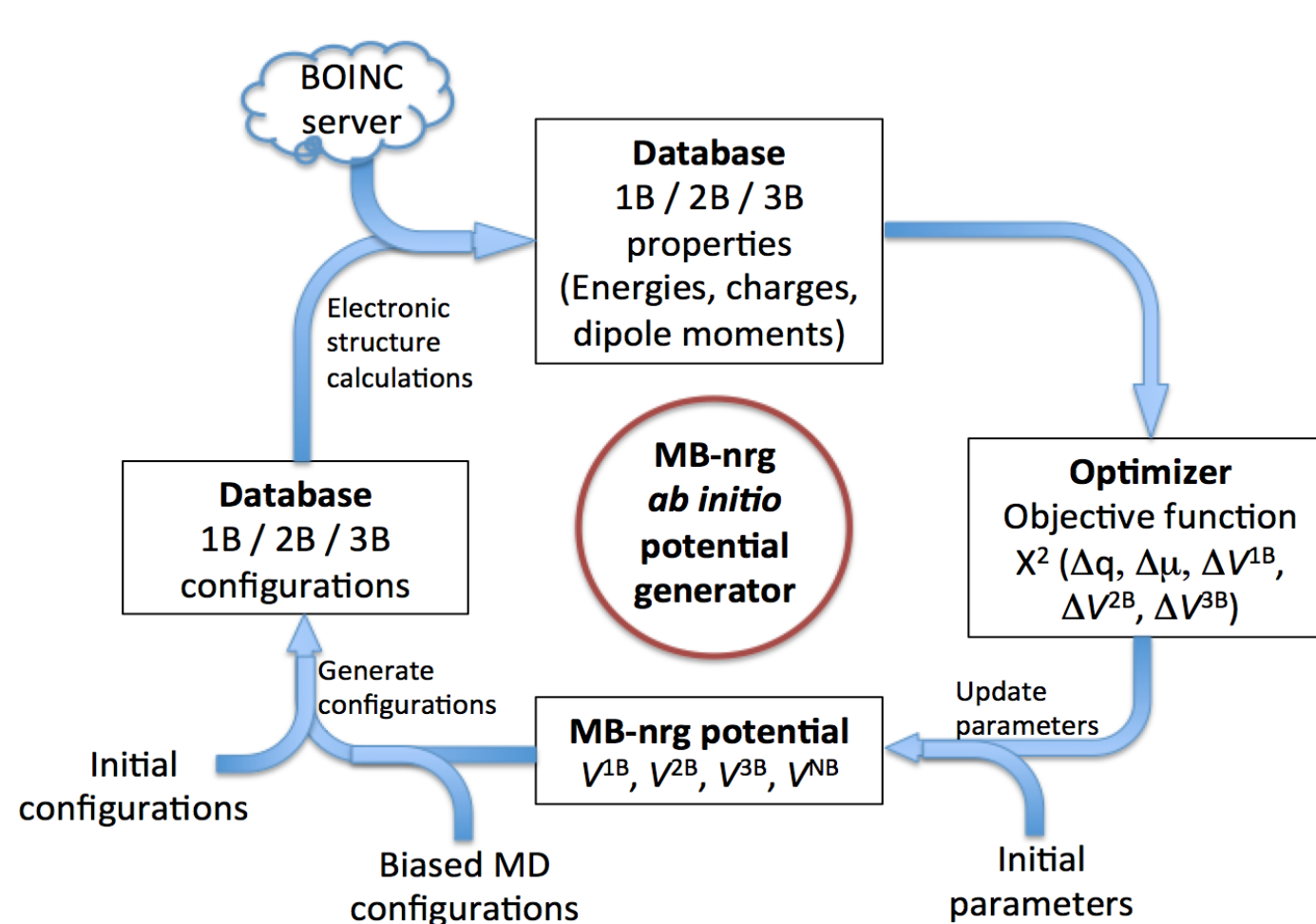
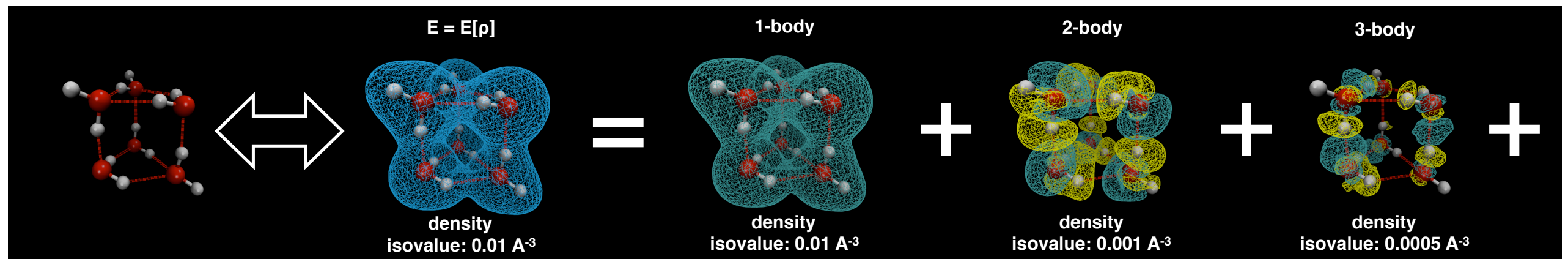
- Currently, only 0.3 of the 10 exabytes per year processed by the trigger is analyzed using high-level computing algorithms; the rest is discarded prior to this stage using simple algorithms executed on FPGAs.
- To significantly extend its physics reach in Run 3, LHCb plans to process the entire 25 exabytes each year using software triggers running on a CPU farm. On average, this will require analyzing events 100 times faster than is possible today.

The primary objective of this project is to **expand the use of machine learning (ML) in the LHCb trigger**, to greatly improve its performance while satisfying its robustness and sustainability requirements. Specifically, ML algorithms will be developed to:

- replace the most computationally expensive parts the event pattern recognition;
- increase the performance of the event-classification algorithms; and
- reduce the # of bytes persisted per event without degrading physics performance.

# Data-Driven Models for Predictive Molecular Simulations

PI: Paesani; Co-PIs: Götz & Zonca



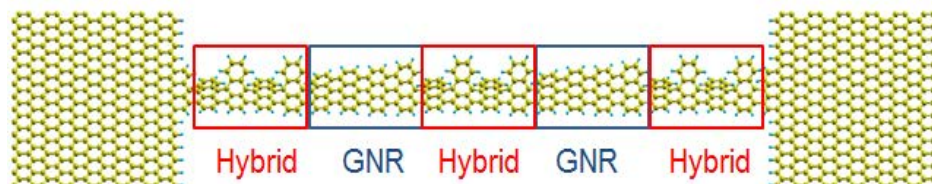
SI2SSI: Collaborative Research: A Robust High-  
Throughput Ab Initio Computation and Analysis  
Software Framework for Interface Materials Science

**Yifei Mo**

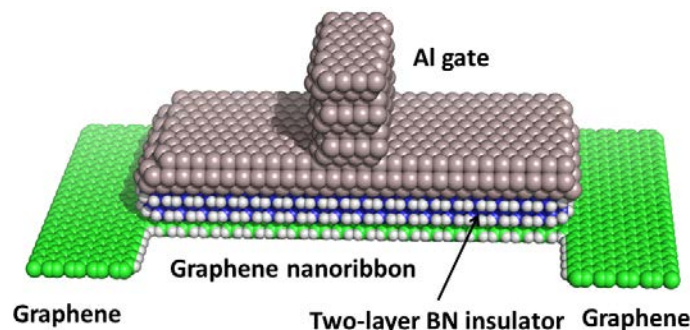
# NSCI SI2-SSE: Multiscale Software for Quantum Simulations of Nanostructured Materials and Devices

J. Bernholc, E. L. Briggs, W. Lu, C. T. Kelley, Z. Xiao, and J. Zhang  
North Carolina State University, Raleigh

- ❖ “Real” materials structures are often complex and cannot be reduced to a few hundreds of atoms
  - Process simulation requires large systems
- ❖ Materials Genome – White House initiative to “deploy advanced materials twice as fast, at a fraction of the cost”
- ❖ National Strategic Computing Initiative (NSCI)
  - Pre-exascale, 150-300 pflops ~2018; Sustained exaflop ~2021
- ❖ Real-space multigrid (RMG) open-source software [www.rmgdft.org](http://www.rmgdft.org)
  - High performance on supercomputers, clusters and desktops
- ❖ RMG-NEGF method for simulating nanoscale devices: I-V, gain, etc.



Novel negative differential resistance device





# The N-Jettiness Software Framework for Precision Perturbative QCD Calculations in Particle and Nuclear Physics

**Frank Petriello**

- Python Analysis Infrastructure
  - Support static/dynamic/symbolic analysis, like LLVM for C/C++ static and KLEE for C
- Use in research
  - Enable researches like software engineering, programming languages, machine learning, AI and data science
  - Improve data processing effectiveness, reliability, stability and efficiency
  - Projects
    - data provenance tracking
    - white box tuning
    - data debugging
    - instability detection in floating point data processing
    - Synthesize workarounds for cross-project bugs in data processing ecosystems
    - Intelligent debugging assistant by probabilistic inference
    - Automated programming assignment grading and synthesis

# Enhancing the **PRIMME** Software for **Eigenvalues** and **SVD** problems

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Andreas Stathopoulos, Computer Science , College of William & Mary

Applicability: Large matrices, a number of smallest / largest / interior e-values

- **Theory**: state-of-the-art, optimized, preconditioned methods
- **Stability and robustness**: solutions close to machine precision
- **Tuned**: full set of defaults and auto-tuning for end-users
- **Flexible**: full customizability for expert users
- **Performance**: HPC, parallel, block (tall skinny) methods, GPUs
- **Interfaces**: F77, MATLAB, Python, R, Julia, Nim

<https://github.com/primme/primme>



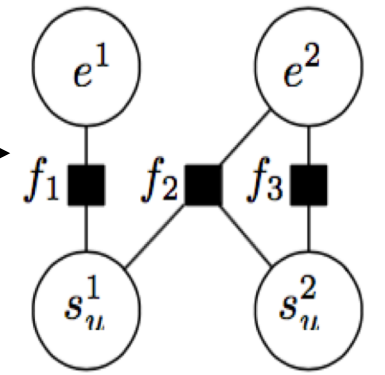
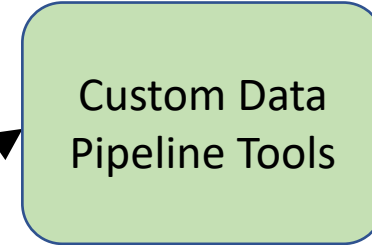
# AttackTagger: Early threat Detection for Scientific Cyberinfrastructure

- Employ factor graphs, a probabilistic graphical model, to capture attacker behavior and detect malicious activities
- Learning graph structure that represents dependencies and their strength among observed events and attack stages

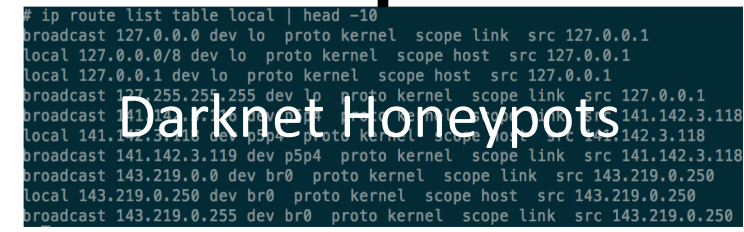
Syslog, netflow, linux auditd, bro IDS logs, etc.



Network Monitoring



AttackTagger



**Goal: transition AttackTagger research into tool easily deployed in security monitoring ecosystems**

Joint project: Cyber Security and Networking Division at the NCSA and the University of Illinois DEPEND Group  
<http://depend.csl.illinois.edu/> <http://security.ncsa.illinois.edu>





# Open Source Matrix Product States: A Simulation Platform for Quantum Computing Technologies



Owner: matjones

 matjones (logout) info about  
 4/8 nodes available

Clone Job

Delete Job

*Daniel Jaschke, Matthew T. Jones, and Lincoln D. Carr*

OpenMPS

Home

Running Jobs (1)



**Quantum simulator** design to support over 300 *analog* quantum computers on 10+ architectures

Beautiful visualizations, In-situ performance metrics, Fully customizable Python output

**A Model Store** maintained by a community of experts: Ising, Hubbard, Exciton, ...

Methods include **strongly correlated entangled dynamics** for open and closed quantum systems

Matrix product states (MPS), exact diagonalization, Lindblad equation, Krylov time propagation, ...

2850 downloads from SourceForge, established code in v3.0

**S12-SSE: Building Science Gateway with SGCI** support on local HPC cluster *Mio*, 200+ dedicated cores

**Large User Community** of Experimentalists, Theorists, Educators, and Citizen Scientists

Two graduate students, PI, undergraduate researchers provide dedicated user support

<https://sourceforge.net/projects/openmps/>

Model Store

Update Model List

Name	Contributor	Affiliate(s)	Notes	Exp. Setups	License
OpenMPS Model Store					
Ising	CSM-CARR			2-Level Systems	GPLv3
Bose-Hubbard	CSM-CARR		Sys. Size: 122	BEC	GPLv3
BBSO	CSM-CARR		Fidelity: 97%	ML-Molecules	GPLv3

Data shape: [ 3 224 224]

Mean: 67.2606

Std deviation: 52.554

population

Statistics

Visualization

Data shape: [ 3 224 224]

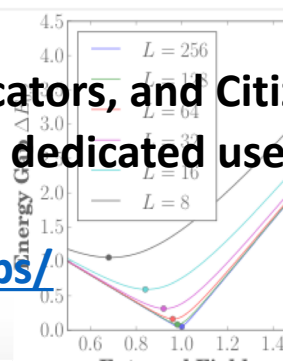
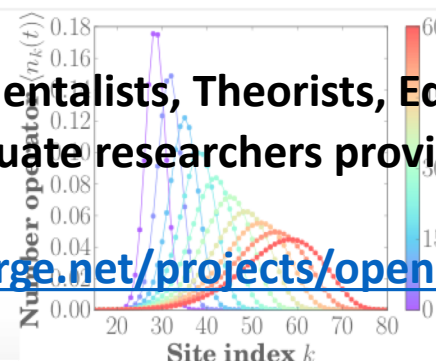
Mean: 67.2606

Std deviation: 52.554

population

Statistics

Visualization





# Coastal Infrastructure Protection



*The entrance the 168th Street subway station in New York City. Taken by Seidenstud - 2006*

# Computing Densities for Stochastic Differential Equations

Harish S. Bhat, Applied Math, UC Merced ([hbhat@ucmerced.edu](mailto:hbhat@ucmerced.edu))

Given an SDE  $dX_t = f(X_t; \theta)dt + g(X_t; \theta)dW_t$   
would you like to compute its PDF? Estimate  $\theta$ ?

Density tracking by quadrature (DTQ) can help!

