# Use Case Teams: Enabling HPC in DesignSafe

Clint Dawson

# Goal:

*"To further promote the use of HPC by the broader NHE research community, members of this Use Case team will develop innovative use cases that take advantage of not only the HPC resources, but also seamlessly integrate data analysis and visualization."*

- How does DesignSafe enable HPC now?
- Plans for future years and example Use Cases

# HPC and Archival Storage Resources at TACC


Stampede2 Supercomputer


Lonestar5 Supercomputer


Corral disk farm

# Current DS HPC Allocation Policy

- A base allocation of 2000 node hours and 50 GB of disk storage is provided to all registered users.
- A startup allocation for 20000 node hours and 1 TB of disk storage can be requested for fast track review.
- A research allocation of around 100000 node hours and 100 TB of disk storage can be submitted and awarded after full review.
- An education allocation of 10000 node hours and 1 TB of storage can be requested for instructional purposes.

# HPC Codes in the Research Workbench

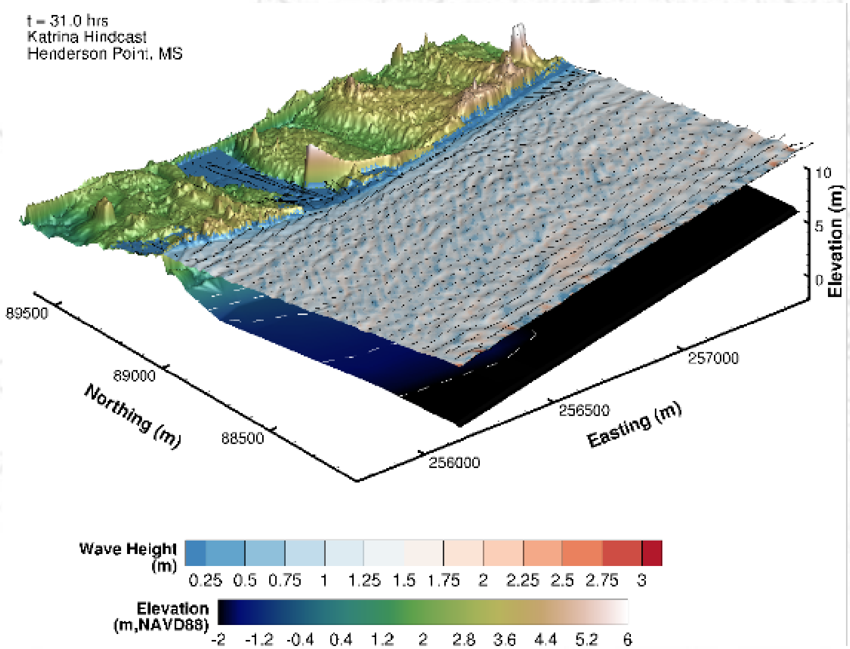
- OpenSees-MP: earthquake model
- ADCIRC: storm surge
- ADCIRC+SWAN: storm surge + spectral wave
- LS-DYNA: FE analysis, fluid dynamics, multi-physics
- OpenFOAM: wind and general CFD
- CLAWPACK: tsunamis

Other codes being considered:

- ANSYS (in negotiation)
- FUNWAVE (phase-resolving wave model)
- ABAQUS

# Research highlight using HPC

Brett Webb (U. of South Alabama): Using ADCIRC+SWAN and XBEACH to study storm surge, waves and sediment erosion/depositon to study resilience of built coastal infrastructure. FigureGen and QGIS are used for visualization. Matlab is used for data analysis. Simulation outputs are shared in MyProjects.



# Goals for Next Phase of DesignSafe

- Training on HPC
- Promoting the use of HPC through Use Cases
  - Developing Jupyter notebooks to execute ensemble suites of simulations in parallel for parameter estimation
  - In-situ visualization
  - Improving workflows for codes in the research workbench

# Training

- Provide novice users with guidance on appropriate use of HPC resources through the portal and command line interfaces.
- Writing an effective research allocation proposal. This could also include writing XSEDE proposals.
- Integrating HPC into workflows and Jupyter notebooks.
- Visualization of results of HPC applications.
- Lessons learned from Use Cases

## Use Case Project 1: Development of ensemble simulation capabilities using ADCIRC and Jupyter notebooks
## PI: Clint Dawson

- Accurate prediction of storm surge impacts requires ensemble calculations through suites of parameters and across multiple scenarios.
- A Jupyter notebook will be developed that can serve as a template for performing parallel ensemble calculations using ADCIRC on an HPC platform. We will study estimating wind drag parameters in ADCIRC based on observations.
- Explore and demonstrate the capabilities of Jupyter notebooks, ADCIRC, python, and statistical inversion software within the DesignSafe-CI to support data and modeling needs of the storm surge research community.

Jupyter Notebook:

- Obtain field data
- Generate and sample from prior parameter PDFs
- Run ensemble ADCIRC simulations
- LUQ (learning uncertain quantities statistical inversion package)
- Output and visualize PDF’s of most likely parameters

Pylauncher

ADCIRC Parameter 1

ADCIRC Parameter N

# Preliminary result: estimation of two wind drag parameters using statistical inversion.

```
# Plot predicted marginal densities for parameters

fig, axs = plt.subplots(1, 2, figsize=(20,10))

for i in range(params.shape[1]):
    x_min = min(min(params[:, i]), min(params_obs[:, i]))
    x_max = max(max(params[:, i]), max(params_obs[:, i]))
    delt = 0.25*(x_max - x_min)
    x = np.linspace(x_min-delt, x_max+delt, 100)
    axs[i].plot(x, unif_dist(x, param_range[i, :]),
           label = 'Initial', linewidth=4)
    mar = np.zeros(x.shape)
    for j in range(learn.num_clusters):
        mar += param_marginals[i][j](x) * cluster_weights[j]
    axs[i].plot(x, mar, label = 'Updated', linewidth=4, linestyle='dashed')
    axs[i].plot(x, true_param_marginals[i](x), label = 'Data-generating',
             linewidth=4, linestyle='dotted')
    axs[i].set_title('Densities for parameter ' + param_labels[i])
    axs[i].legend()
```

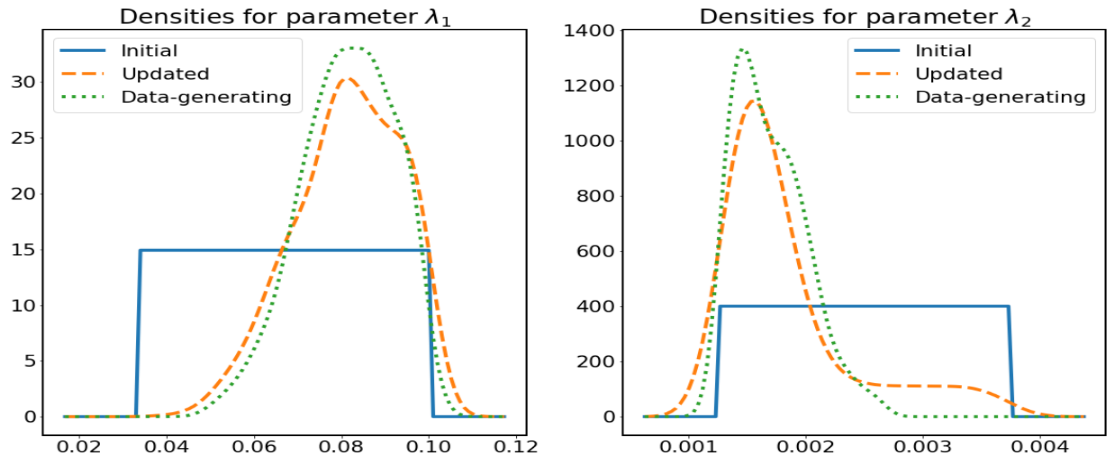



Figure. Jupyter notebook that utilizes the LUQ framework to solve for the probability distribution of the ADCIRC wind drag coefficient parameters based on observed storm surge water surface elevations.

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TEXAS The University of Texas at Austin
UCLA
TACC
RICE
Florida Tech

## Project 2: Enabling interactive in-situ viz systems for natural hazards modeling.
## PI: Krishna Kumar

- **Objective:** ***Enable interactive in-situ exploration of the data sets through a flexible framework for specifying and emphasizing different aspects of the natural hazard data.***

- In-situ visualization is a rendering technique for visualizing the simulation data in real-time.

- This work will explore and demonstrate the in-situ viz capabilities with integration to Jupyter notebooks on DesignSafe-CI through a VTK data model. Integrations will be developed for existing DesignSafe apps through ParaView Catalyst and TACC Galaxy.

## This is a multiyear project. Year 1 tasks:

- Enabling In-situ viz through ParaView Catalyst and TACC Galaxy using a Jupyter interface with VTK data model
- Demonstrate a proof-of-concept for asynchronous distributed petascale simulation visualization of landslides using TACC Galaxy and CB-Geo MPM code.

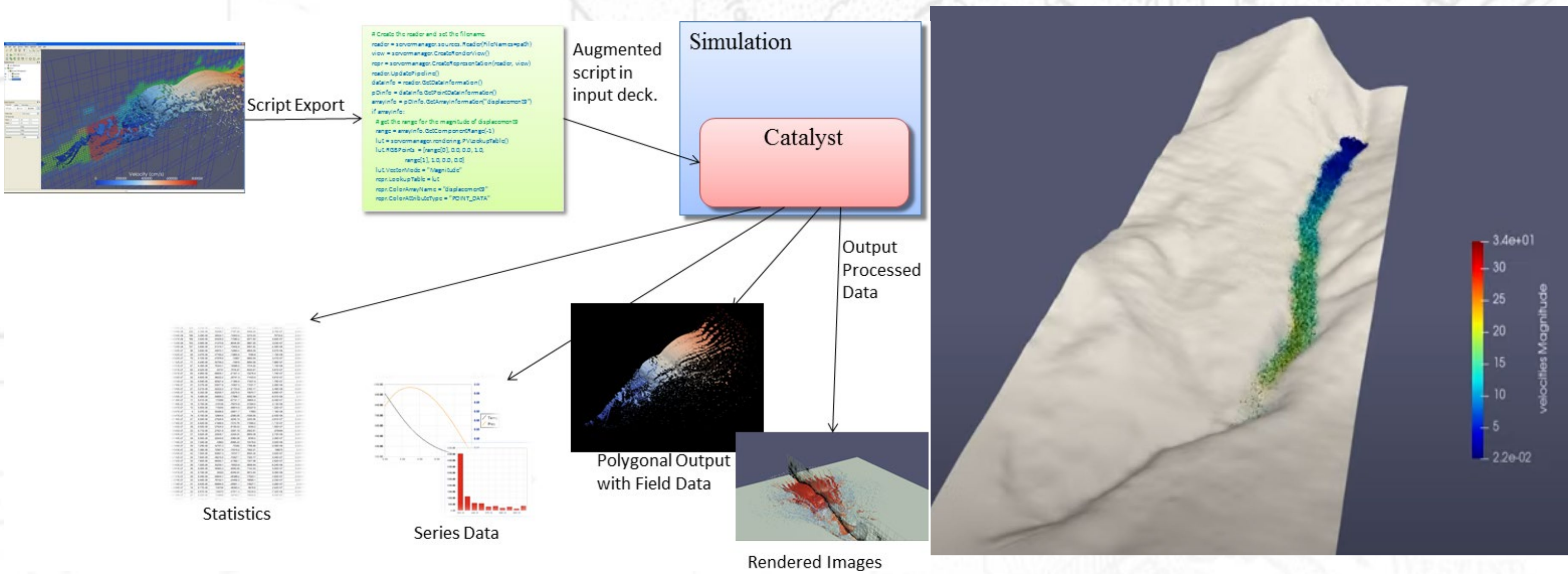


Figure: (a) ParaView Catalyst integration with Python scripts (Paraview., 2020)
(b) Rendering of the Hong-Kong Yu Tung road debris flow in June 2008 using CB-Geo MPM with 200,000 material points

## Project 3: Enabling modeling of wind effects on structures using a Digital Flow Simulator
## PI: Ahsan Kareem

- Current DesignSafe CI offers the use of OpenFOAM via their portal or direct on Stempede II and tools from SimCenter.
- Need to the "take fear out" of CFD, yet maintain the level of sophistication in the simulation schemes that can address practical problems of wind hazard.
- It is also anticipated that ASCE 7 in its near future revisions may like the Architectural Institute of Japan (AIJ) permit the use of CFD in establishing wind loads on structures, which would expand the user base looking for user friendly yet advanced portals for simulation.

**Objective**: ***Enabling the user base plug and play type end-to-end simulation using jupyter notebook with built in sophistication in the background using OpenFOAM.***

- OpenFOAM and additional pre- and post-processing utilities couched in Jupyter Notebook will launch a new platform currently not available in the open source domain.

- Workflow: Inflow; Computational Module; Data synthesis/detection/analysis; Visualization using *Catalyst* and *ParaView* .

- Modularity of the workflow would offer other options to be added like multi-fidelity simulations, machine learning tools, data assimilation tools and data synthesis/detection/analysis tools.

**This is a Multi-year Project. *First Year Task*: *To develop Jupyter Notebook to undertake simple OpenFOAM based simulation of flow fields around structures and their load effects. The tool will be validated against experiments and benchmarked in data depot for a quick reference for users.***

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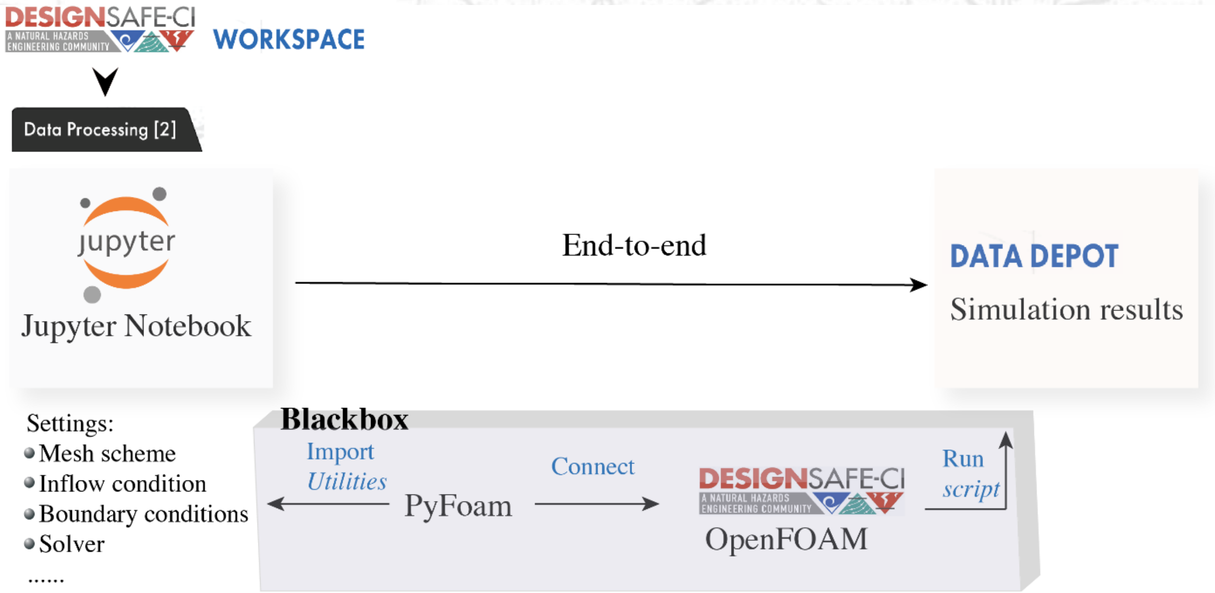

This will be continued beyond the first year to add additional features to offer a platform that can benefit from other computational tools and features needed for advanced and efficient simulations. A possible modular workflow is given below