Introduction to NEESShub

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Overview of NEES

NEES Tools and Resources

Data Management Tools

High Performance Computing Tools

Project Warehouse

Project Curation
Safer buildings and civil infrastructure are needed to reduce damage and loss from earthquakes and tsunamis.

To facilitate research to improve seismic design of buildings and civil infrastructure, the National Science Foundation established NEES.

**NEES Objectives**

- Develop a national, multi-user, research infrastructure to support research and innovation in earthquake and tsunami loss reduction.
- Create an educated workforce in hazard mitigation.
- Conduct broader outreach and lifelong learning activities.
Facilitate access to the world's best integrated network of state-of-the-art physical simulation facilities.

Build a cyber-enabled community that shares ideas, data, and computational tools and models.

Promote education and training for the next generation of researchers and practitioners.

Cultivate partnerships with other organizations to disseminate research results, leverage cyberinfrastructure, and reduce risk by transferring results into practice.
NEES has a broad set of experimental facilities
- Each type of equipment produces unique data
- Located at 14 sites across the United States

- Shake Table, Tsunami Wave Basin
- Large-Scale Testing Facilities
- Centrifuge, Field and Mobile Facilities
- Large-Displacement Facility
- Cyberinfrastructure
https://www.nees.org
Data Management Tools

- Workspace
- SynchroNEES
- PEN
- inDEED (visualization)
Data is the 4th Paradigm

- Producing an avalanche of high resolution digital data
- All (or most) of the data needs to be accessible over a long period of time
  - Much of the data is not reproducible
- Example – NEES project
  - Structure or sample destroyed through testing
  - Very expensive to rebuild for more tests
Need for High Performance Computing (HPC) Simulation

- Earthquake engineering problems:
  - Involves intense computation on large volumes of data
  - Will take days to complete simulation on normal computers

- Earthquake engineering problems on an HPC resource takes hours to complete

- Using HPC resources for solving computationally intensive problems results in huge time savings

- Different HPC resources include:
  - XSEDE: Kraken, Stampede
  - Purdue: Hansen, Carter
  - Open Science Grid (OSG)
Why Batchsubmit?

Different steps of job submission on an HPC resource includes:

- Login to the remote venue and copy all input files
- Ensure that the simulation program is available on the remote venue and copy program to the venue if necessary
- Prepare venue specific script file specifying parameters for job submission
- Submit the job to the correct job class and wait for the result
- Copy the results to a local system for analysis and visualization
Why Batchsubmit?

- Repeating this process for multiple simulations is tedious and time consuming.
- Batchsubmit automatically performs all the steps for submitting a job in an HPC resource.
- User can submit jobs using batchsubmit to multiple venues.
- Batchsubmit will intimate the user when job finishes execution and all results will be available in user job directory.
- Batchsubmit makes job submission easier and results in huge time savings.
Batchsubmit Features

- Simple command line interface and GUI interface
- Easy to do parallel processing
- Asynchronous job submission
- Select HPC resource (venue) to run the job
- Send executables to the venue, if required
Batchsubmit Features

- Automatic retrieval of results
- Email notification once results are available
- Monitor job status
- Monitor queue traffic at different venues
- Cancel a job
batchsubmit date

batchsubmit --venue carter --ncpus 16 OpenSeesMP/apps/opensees/NEEShubExamples/SmallMP/Example.tcl

batchsubmit --venue stampede --ncpus 64
--appdir /apps/share64/opensees/stampede
--rcopyindir OpenSeesMP /LargeMP/Example.tcl
OpenSees Laboratory

OpenSees Application: Parallel Job Submission

Main Script: /apps/openseesbuild/current/NEEShubExe
Resource: Carter

Carter Options
- Application: OpenSeesMP
- # Processors: 16
- Walltime: 00:30:00

Parallel Job Submission Tool

This tool can be used to submit parallel OpenSees jobs. The user is asked which parallel OpenSees application to use, which parallel machine to run on, how many processes to run and which parallel machine to run these on.

The results from the analysis when completed will be placed in the user's scratch directory. The actual directory location will be shown in the result screen.

IMPORTANT NOTES:
1) the main script CANNOT be located in your home directory. II and all the files it requires must be in a subdirectory.

2) control will return after the job has been submitted, AND NOT after the job has completed. This means you may have to wait awhile before the actual results are located in your output directory.

3) NEES is a local machine limited to around 16 processors BUT the jobs will start right away. Hansen is an intermediate machine with 96 processors. The others are larger machines. All jobs sent to machines other than the local machine can take awhile to start!

4) as an example set the main script as:
   /apps/openseesbuild/current/NEEShubExamples/SmallMP/Example.lct

DO NOT SELECT OpenSeesSP for this example.
BatchSubmit GUI
BatchSubmit GUI

Submission Command Preview:
```
0:00 --ncpus 16 --nn 1 --ppn 16 OpenSeesMP /home/neeshub/mohan11/examples/SmallMP/Example.tcl
```

Command Options:
- **Job Name**: testjob02
- **Job Prefix**: 
- **Executable**: OpenSeesMP
- **Arguments**: 
- **Env Vars**: 

Input File Options:
- **Infile**: example/SmallMP/Example.tcl
- **Input file is first argument**
- **Input file directory**
- **Input dir + subdirectories**
- **Input file only**

Venue Options:
- **Venue**: carter
- **Queue**: standby
- **Walltime**: 72:00:00
- **NCPUs**: 16
- **NPerProc**: 1
- **MPICh**: 
- **MPICH**: 
- **PPN**: 16
- **MPIargs**: 

Notify upon completion: 

Submit Job
NEES online data repository

- Allows researchers to upload, archive, and disseminate data from their physical, cyber, and hybrid experiments and simulations.
- Provides user with tools to organize data into projects, experiments, trials, and results.
- The data in the Project Warehouse can be cited and shared with researchers across the world, or only within a research group.
- Facility to curate the data in the repository to ensure the long-term preservation of valuable NEES data.
Executive Summary: Download Document

PI(s): Santiago Pujol

Dates: July 20, 2011 - August 09, 2014

Facility: Purdue University at West Lafayette, IN, United States

Organization(s): Purdue University at West Lafayette, IN, United States

Description: Discontinuities in the geometry and the reinforcement of structural walls create stress concentrations that have detrimental effects on wall seismic response. This study focused on discontinuities associated with changes in the geometry of the cross... (more)

Sponsor: ERCO International Corporation - n/a - Experiments 1 through 6

Website(s): Seismic response of RC walls with discontinuities (view)
Seismic response of structural walls with discontinuities (view)
Seismic Response of Structural Walls with Discontinuities (view)

Group Space: Project Seismic Response of Structural Walls with Geometric and Reinforcement Discontinuities
To compare experiments, please select at most four experiments from the experiment list below.

**Experiment-1:** Specimen W-MC-C: Structural wall with mechanical couplers at the base and with boundary-element confinement subjected to lateral displacement reversals of increasing amplitude up to failure

**Dates:** August 01, 2011 - September 01, 2011

**Description:** The longitudinal reinforcement was spliced with mechanical couplers at the base of the wall. It had boundary-element confinement (1.2% volumetric confining reinforcement ratio).

**Facility:** Purdue University at West Lafayette, IN, United States

**Experiment-2:** Specimen W-MC-N: Structural wall with mechanical couplers at the base and without boundary-element confinement subjected to lateral displacement reversals of increasing amplitude up to failure

**Dates:** August 23, 2011 - December 05, 2011

**Description:** The longitudinal reinforcement was spliced with mechanical couplers at the base of the wall. It did not have boundary-element confinement.

**Facility:** Purdue University at West Lafayette, IN, United States

**Experiment-3:** Specimen W-60-N: Structural wall with 60d lap splices at the base and without boundary-element confinement subjected to lateral displacement reversals of increasing amplitude up to failure

**Dates:** May 10, 2012 - June 11, 2012

**Description:** The longitudinal reinforcement was lap spliced at the base of the wall. The length of the lap splices was 80 bar diameters. It did not

**Facility:** Purdue University at West Lafayette, IN, United States
Try It!!!

- **Getting Started**
  - Register for a NEEShub account (Free)
  - Request access to workspace (Support Ticket)
  - Request access to HPC access group (Support Ticket)

- **Download SynchroNEES**
  - [https://nees.org/topics/synchronees](https://nees.org/topics/synchronees)

- **Run batchsubmit**
  - [https://nees.org/resources/batchsubmit/about](https://nees.org/resources/batchsubmit/about)

- **Share results with peers**
  - [https://nees.org/warehouse/welcome](https://nees.org/warehouse/welcome)