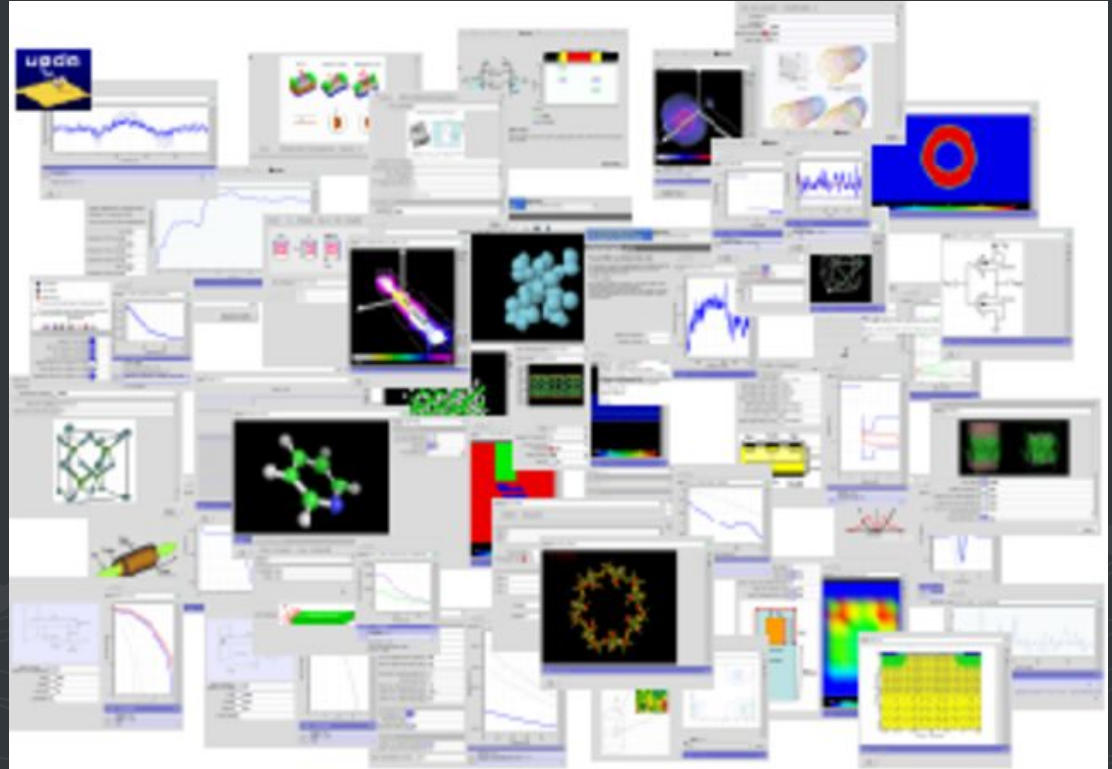


Evolution of the nanoHUB Tool

Steven Clark
nanoHUB.org
HUBzero.org
San Diego Supercomputing Center

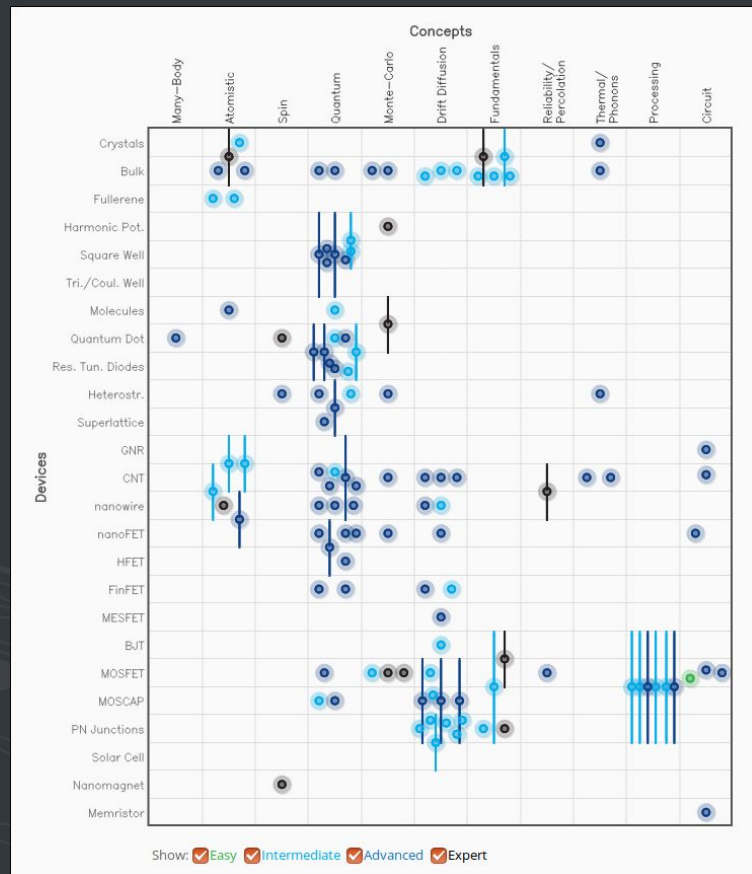


- Collaborate
- Simulate
- Explore
- Learn



PLATFORM FOR COLLABORATIVE SCIENTIFIC COMPUTATION

- 1.9 million users annually
- 220,000+ registered users
- 23,000+ simulation users
- 675+ published tools
- Varying degrees of skill required
- Wide range of topics covered
- Diagram highlights tools related to nanoelectronics, concepts vs devices

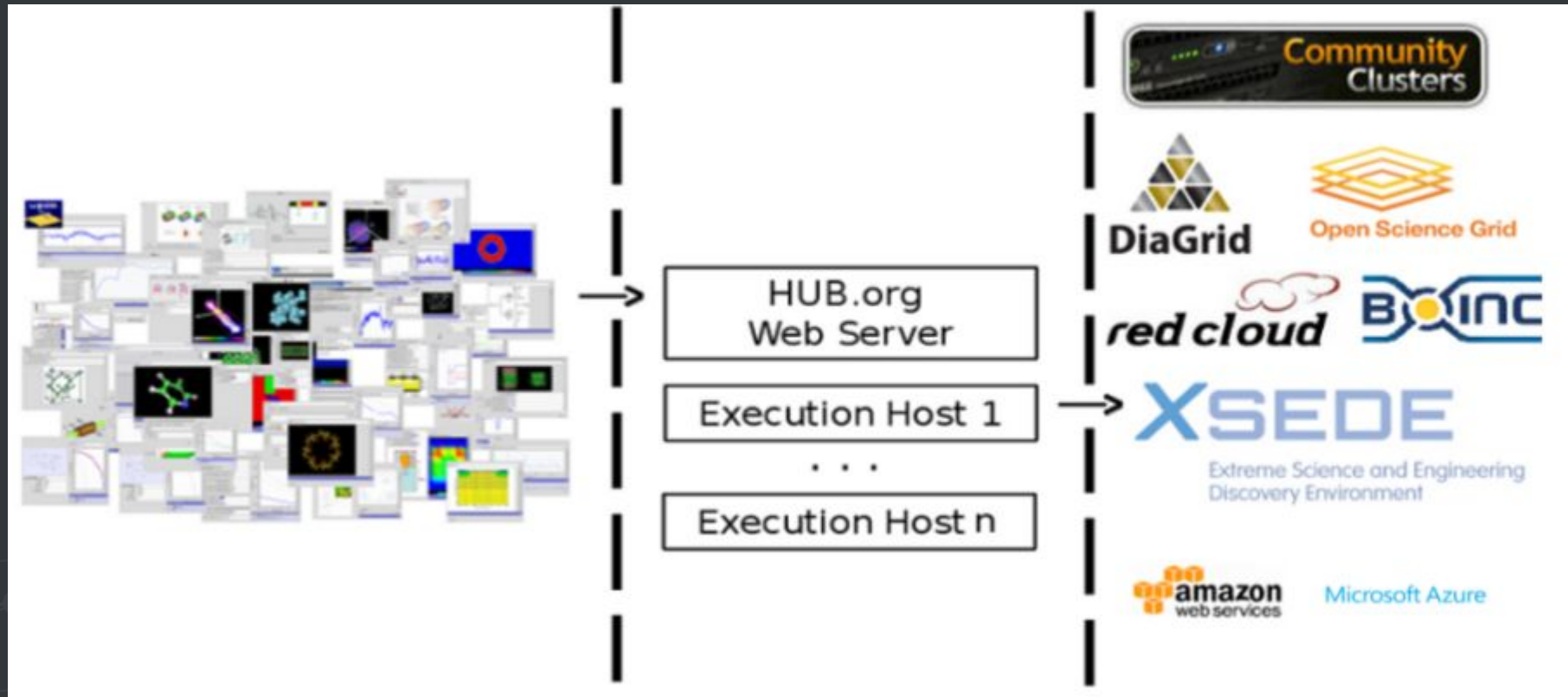


PLATFORM FOR COLLABORATIVE SCIENTIFIC COMPUTATION

- User perspective
 - Production level code
 - Powerful computing resources
 - No downloading, no compiling, ...
 - Automatically runs most updated version
 - Access regardless of location
- Developers perspective
 - GUI development environments
 - RAPPTURE
 - Jupyter Notebooks
 - Source code management - GIT/SVN/GitHUB
 - Rich development platform
 - Powerful computing resources



COMPUTATIONAL RESOURCES



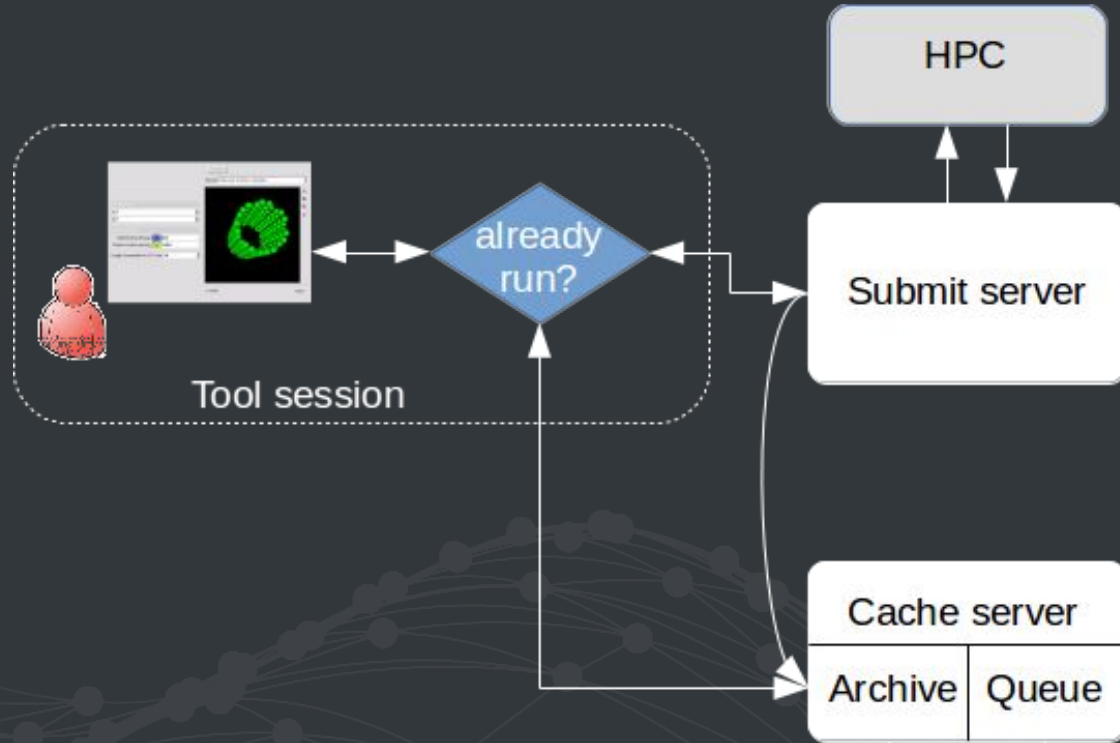
SIMULATION USE CASES

- **On demand**

- UI used to declare inputs for simulation
- Command line
- Single simulation or parametric sweep
- If archive result exists no simulation is required simply pull the existing result
- Faster response time provides better user experience
- Generated results are immediately archived
 - Number of hits running slightly behind number of publications



Computation System - Architecture

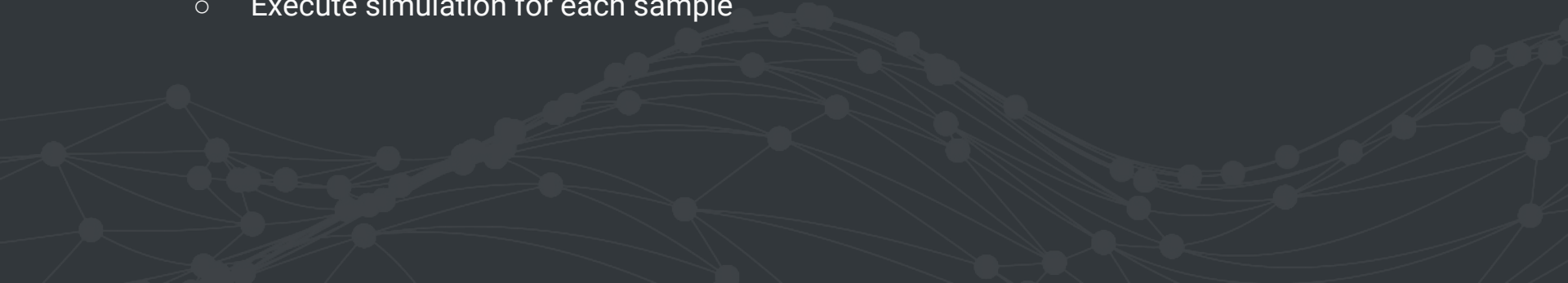


SIMULATION USE CASES

- **Uncertainty quantification**

- Inputs declared as distributions
- Statistical methods used to determine input samples
- A simulation is run for each sample
- Results include a response surface model which can be used to approximate simulation, sensitivity analysis, and probability distribution function (PDF) for outputs.

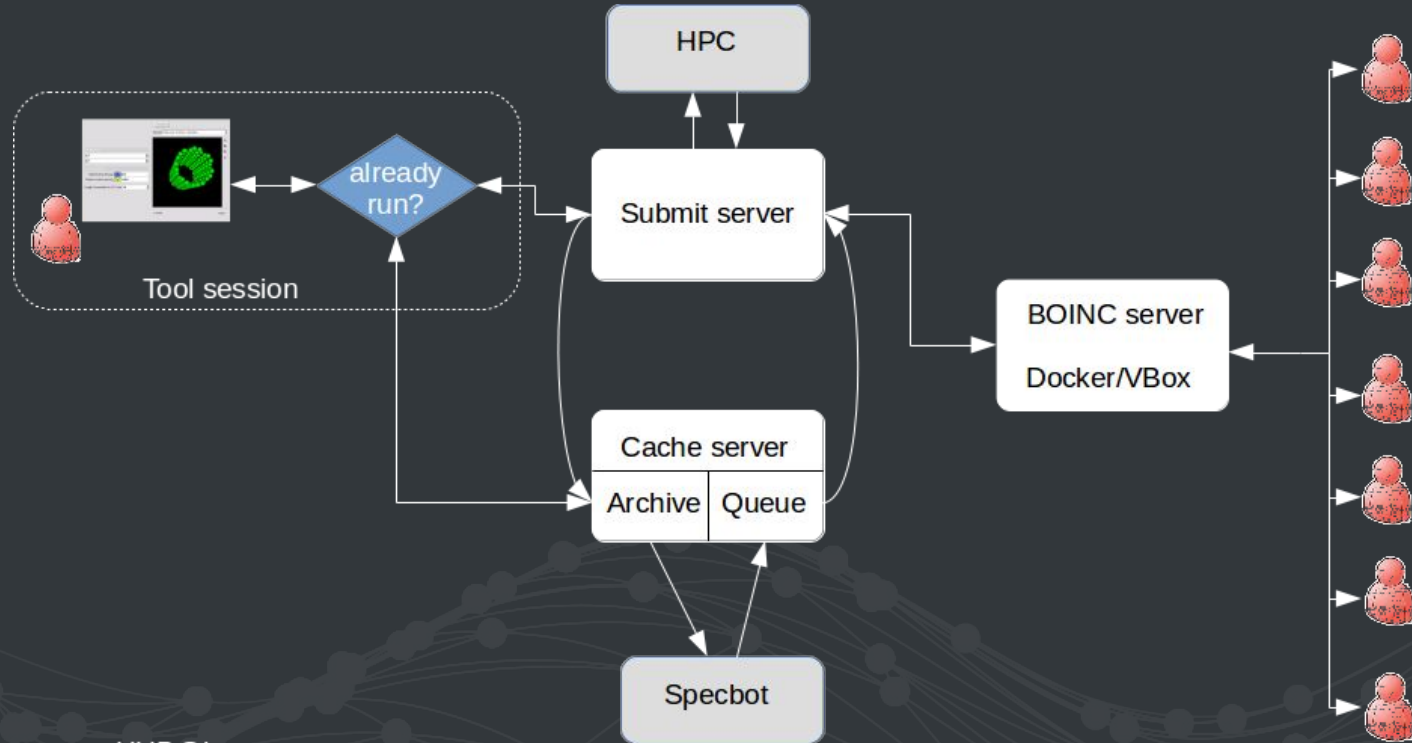
- **Exploratory simulation**

- Automatically generate simulation input samples covering the space
 - Allow for interactive selection of multidimensional input space
 - Execute simulation for each sample
- 

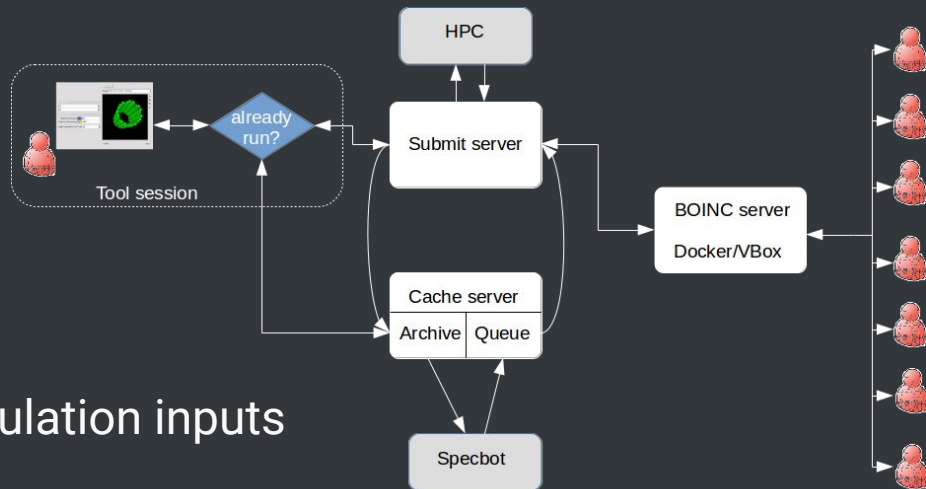
Exploratory Simulation - Motivation

- Probability of exact match with user input is small
- Enhanced visualization techniques
- Machine learning studies
- Surrogate model generation
 - Interpolate between archived results
 - Sensitivity analysis
 - Covariance analysis of results
- Online education services
- All of these require **large** numbers of simulations
 - The challenge is 10,000,000 simulations/yr

Computation System - Architecture



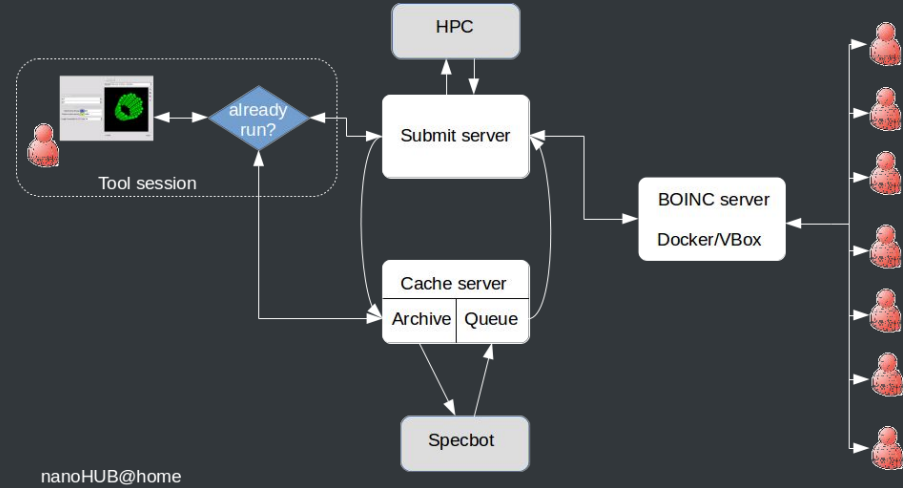
Exploratory Simulation - Generation



nanoHUB@home

- Rappture XML schema defines simulation inputs
 - Scalar numeric inputs
 - Fixed lower and upper bounds
 - Automatically generate simulation input samples randomly distributed in the range
- Input samples are uploaded to cache queue

Exploratory Simulation - Execution



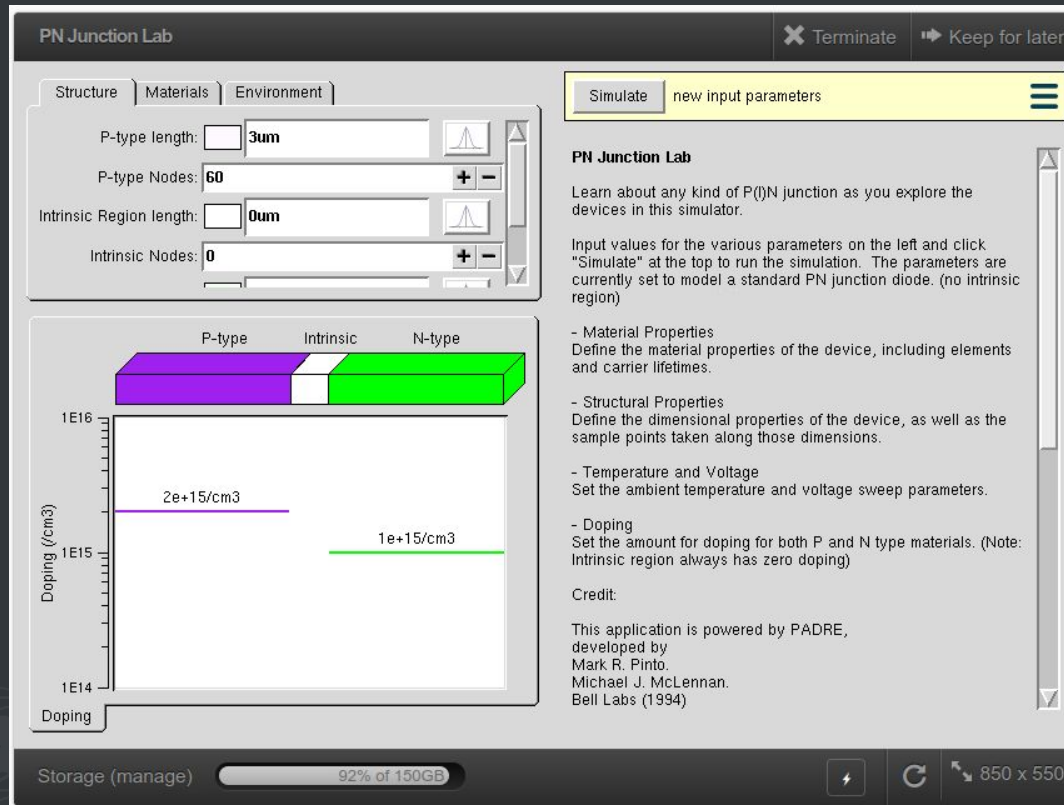
- Automated process pulls driver file inputs from cache queue
- Assemble driver input files into BOINC batches
- Employ submit to execute BOINC batches
- When BOINC batch is complete publish successful results to archive

Exploratory Simulation - 10,000,000 jobs/yr ?

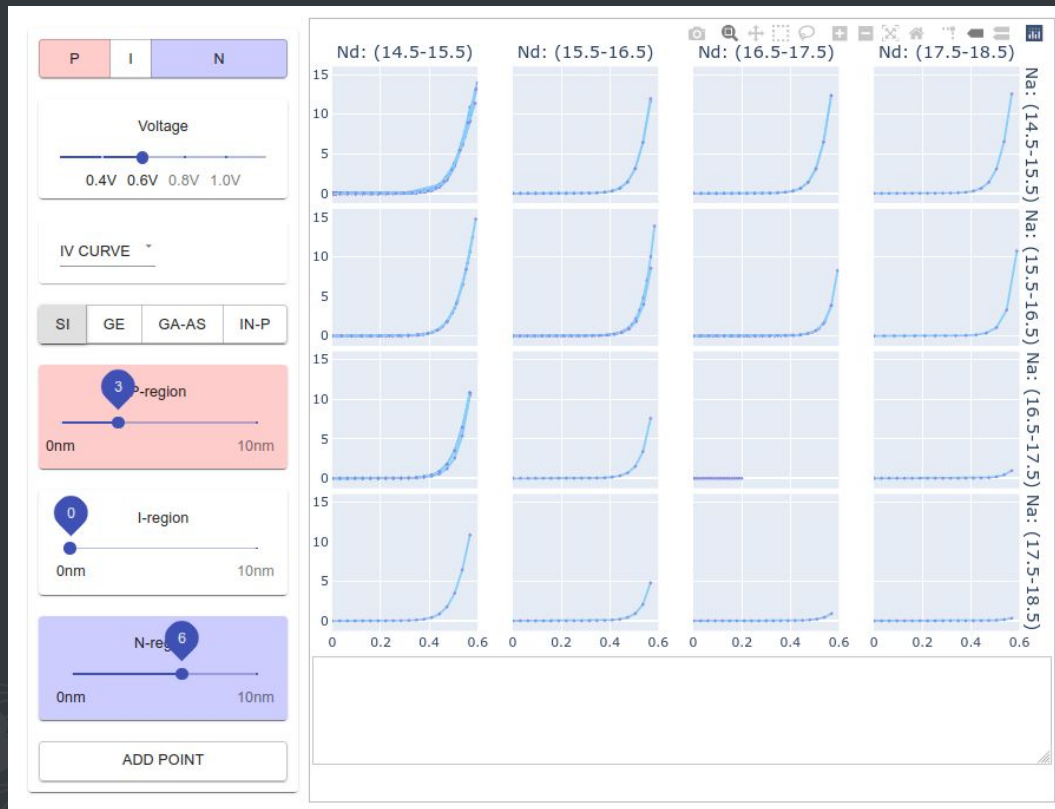
- Achieved late 2019
- Interrupted by HUBzero move to SDSC



Traditional Simulation



Exploratory Simulation



Exploratory Simulation

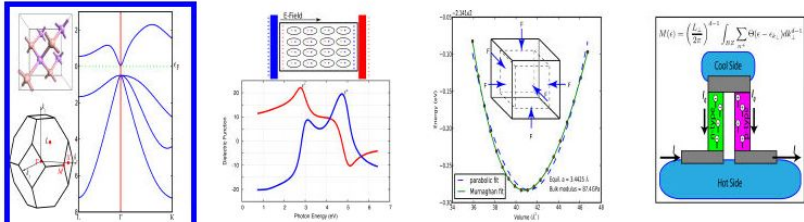
DFT Material Properties Simulator

✕ Terminate ➡ Keep for later

1 Input → 2 Simulate

Basic Input | Geometric Input | Energy Expression | Band Structure/DOS | Dielectric

Task: E-K Diagrams



Material Type: Semiconductor

Semiconductors: Si(Diamond)

Advanced Options: ☐ ☒ yes

Simulate >

Storage (manage) 92% of 150GB

⚡ ↺ 🖨 850 x 650

Exploratory Simulation

File Edit View History Bookmarks Tools Help

nanoHUB.org - Resource x dftviz-0 x +

https://proxy.nanohub.org/weber/1817491/BBM71B75gW5QW2R/26/apps/dftviz.ipynb? 90% Search

nanoHUB jupyter Submit a ticket Terminate Session

Overview

The following tool explores results from density functional theory (DFT) calculations to compute specific properties for a wide range of materials including semiconductors, insulators, and metals.

Getting started and hints

- Results for different properties and different materials can be selected through the dropdown menus.
- Regions of KPoints and KE Cutoff can be explored through the sliders and new calculations can be run as a grid of points in the regions selected.

Explore results database

Material: Si
Functional: LDA
Output: Equilibrium Volume

Run new simulations

Grid KPoint
Min: 2 Max: 6 Points: 2

Grid KECutoff
Min: 2 Max: 6 Points: 2

Run Grid Points

Pearson Correlation

3D Map

2D Map Linear

2D Map Interpolation

Pearson Correlation Coefficient Matrix

input_x_size

input_ke_cutoff

output_eqVol

input_x_size

input_ke_cutoff

output_eqVol

Pearson Correlation

3D Map

2D Map Linear

2D Map Interpolation

$\lambda \sim 3$

42

41.5

41

40.5

40

39.5

39

output_eqVol

input_x_size

input_ke_cutoff

4-k points

The background is a dark gray field filled with a complex, abstract network of thin, light gray lines. These lines connect numerous small, dark gray circular nodes, creating a web-like structure that resembles a molecular model or a data network. The nodes and lines are distributed across the entire frame, with some areas being more densely connected than others.

QUESTIONS & ANSWERS

?