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Sandia National Laboratories

Exceptional service in the national interest

Supporting end-to-end workflows for the design and analyst communities through an intuitive frontend and extensible backend grounded in user experience

ASC S³C Tri-Lab Advanced Simulation & Computing Sustainable Software Conference

Next Generation Simulation Development Team, NGS(D)

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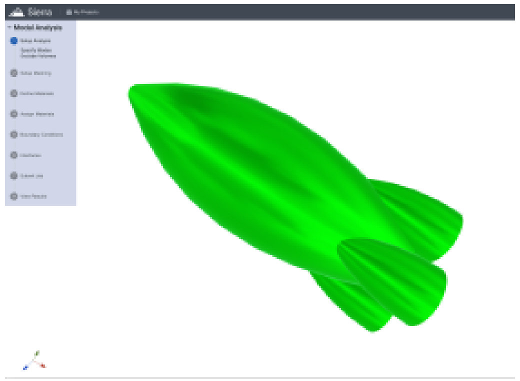
U.S. DEPARTMENT OF ENERGY

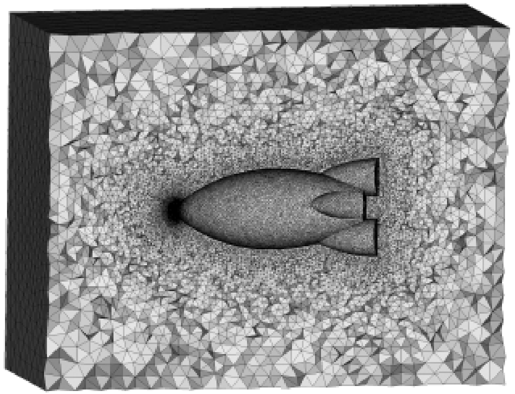
NNSA

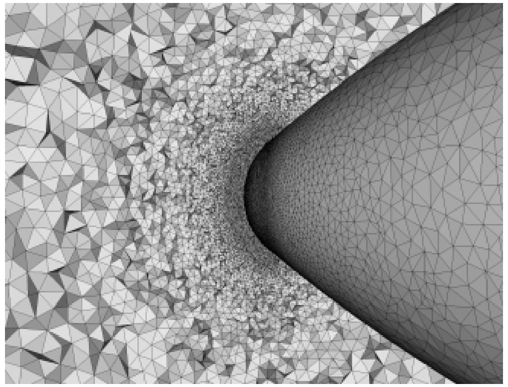
Next Generation Simulation Development – NGS(D)

Originally motivated by the Lab goal of cycle reduction

The NGS project is a strategic initiative to reduce the turn-around time of ModSim-based problem solving in design, qualification and surveillance.







Key strategy:

- Separate user intent from tedious steps of executing it
- Robust automated meshing & scripting enables *workflows*
- Componentized technologies provides scalability

Intuitive user experience:
Support the users intent!
Consistent, simplified user experience across the toolchain,
context-specific workflows

Fast model creation:
Minimize CAD clean-up!
Capture important features, gracefully ignore others
Automated, parallel in-situ tet meshing

Solutions with credibility evidence:
Solution verification (geometry capture metrics, solution error estimation), sensitivities, reproducibility

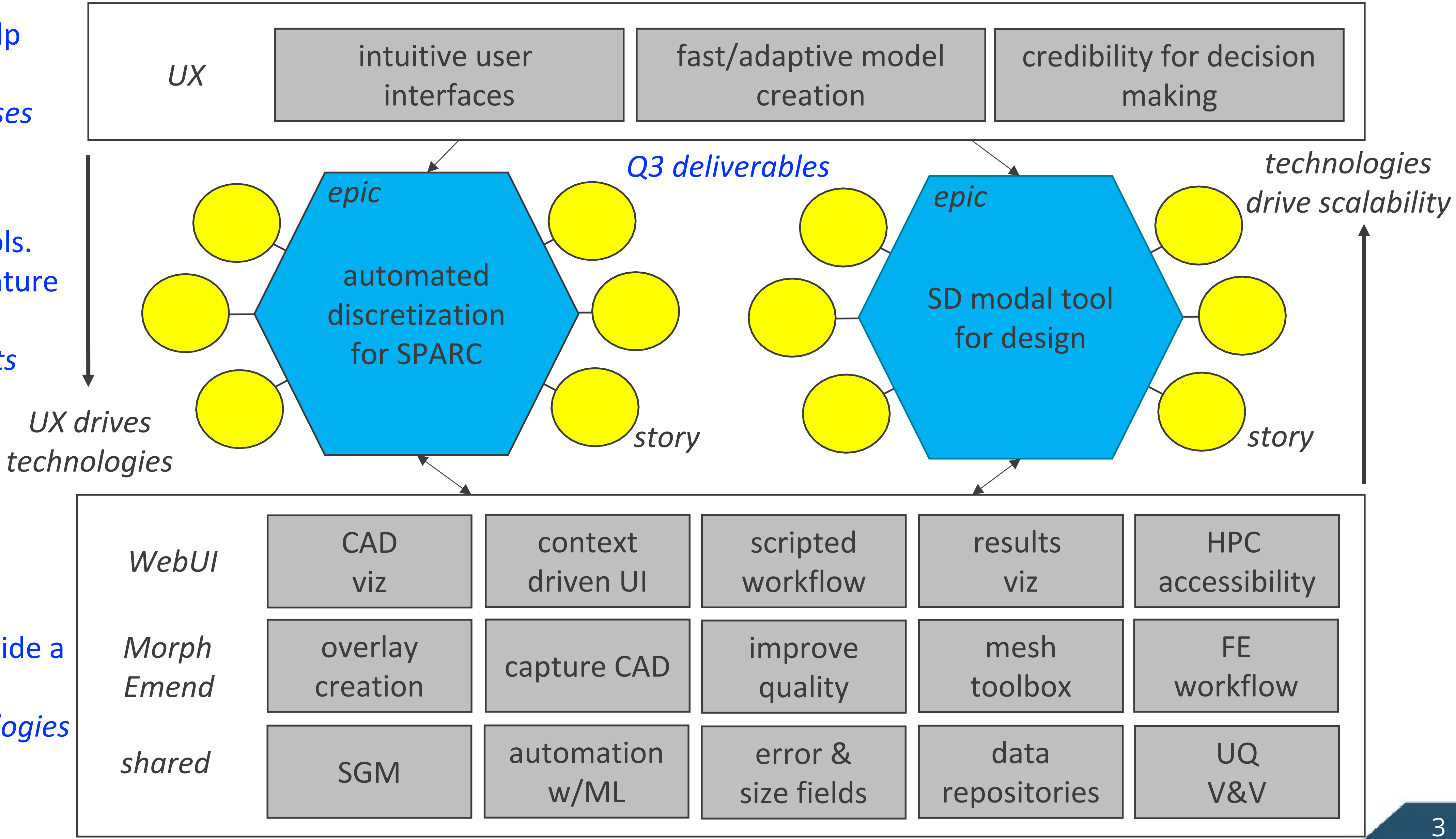
How does NGS(D) deliver?

Delivering processes, products, & technologies for engineering

How do we help engineers?
Deliver processes

Make good tools. Do it again. Mature solutions.
Deliver products

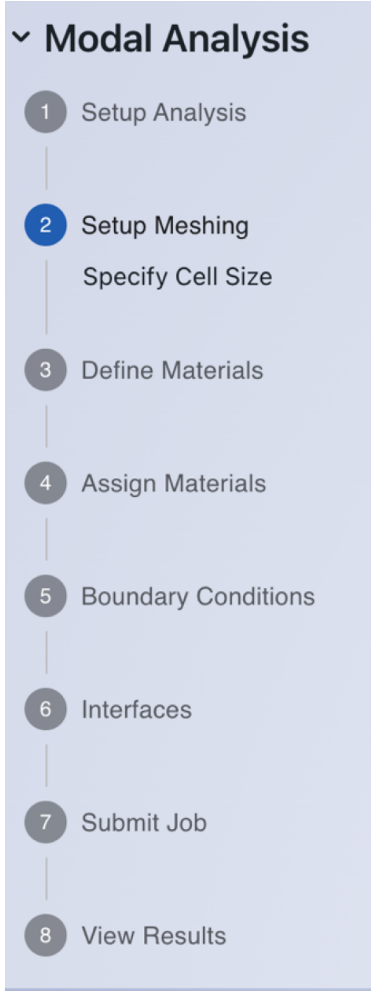
Common components & strategies provide a path forward
Deliver technologies



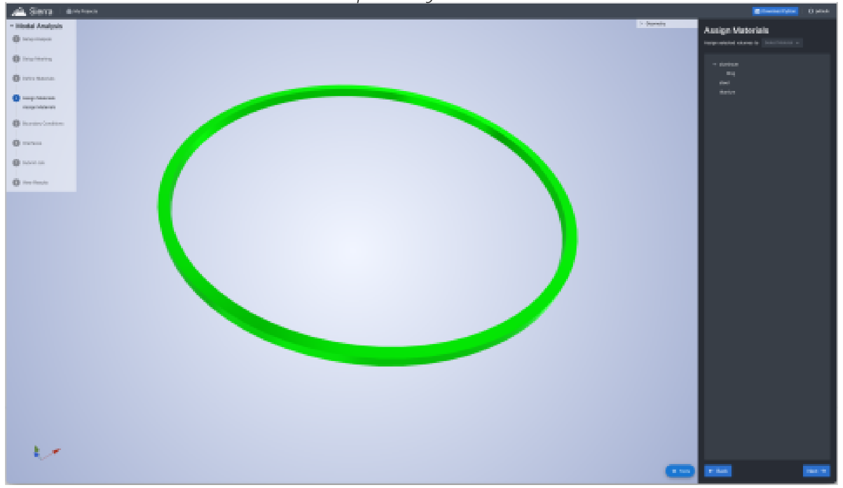
Deliver context driven workflows on the frontend

intuitive user interfaces

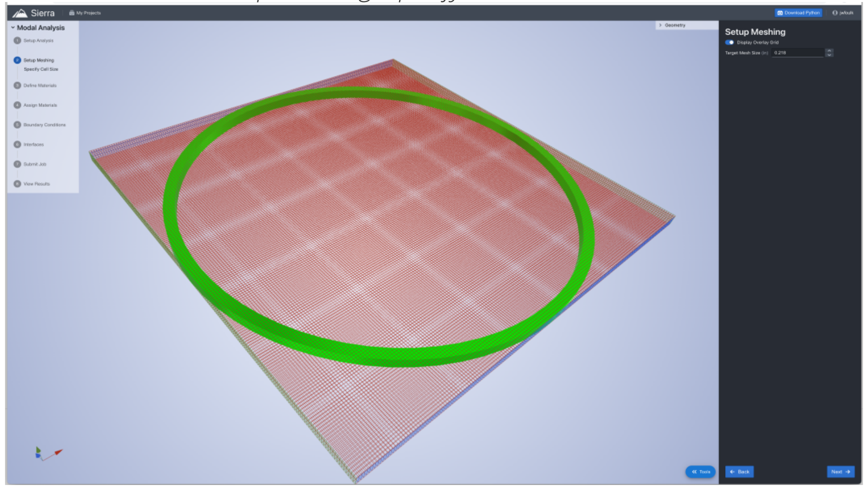
With exposed left-hand navigation, we provide a context-specific workflow to users.

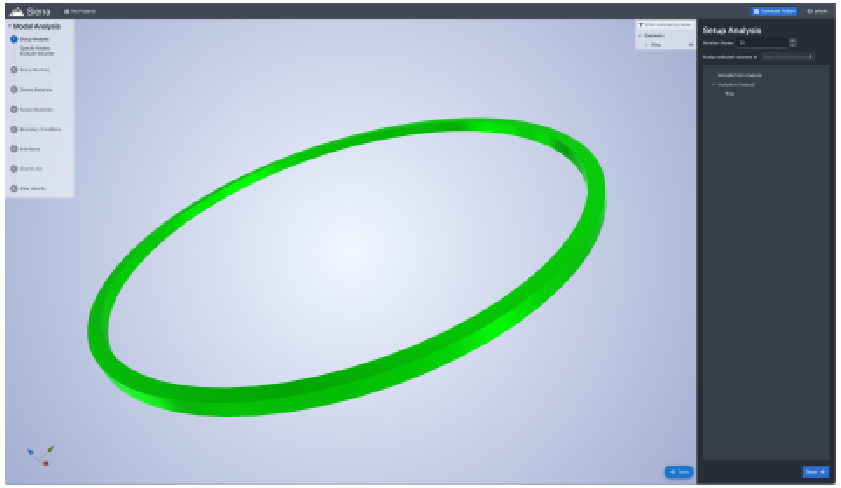


Setup Analysis

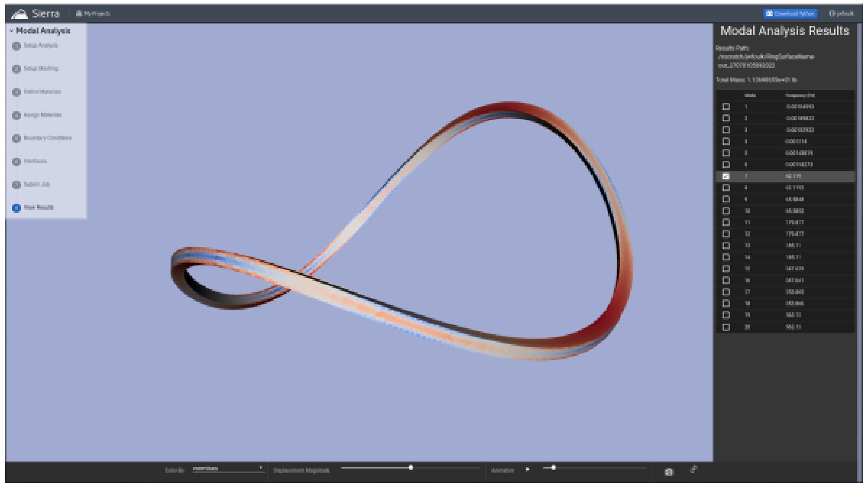


Setup Meshing, Specify Cell Size





Assign Materials

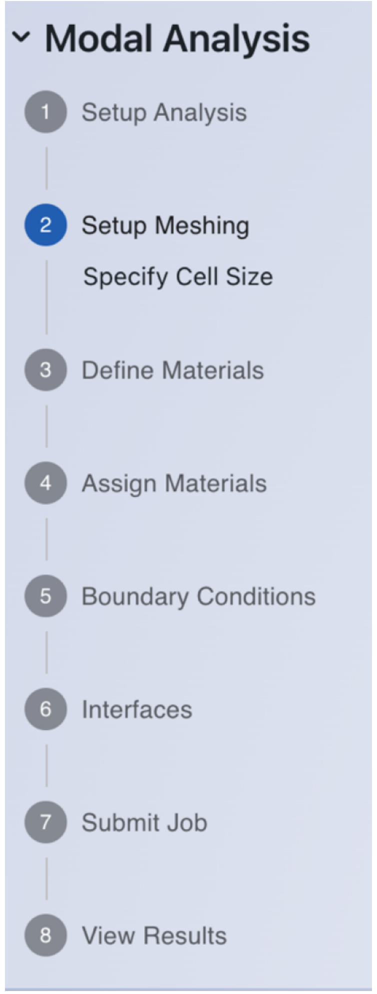


View Results

Deliver Python scripting on the backend

fast/adaptive model creation

Consistent w/left-hand navigation, we provide the corresponding Python script




```
import sierra

# Setup Analysis
geometry = sierra.Geometry()
geometry.import_file('./RingSurfaceName.stp')
hpc = sierra.HPCJobSubmission()

# Setup Meshing, Specify Cell Size
morph = sierra.Morph()
morph.set_size(0.218)
morph.set_geometry(geometry)
morph.set_excluded_volumes({})

# Define Materials for SD
sd = sierra.SDEigenAnalysis()
sd.set_wtmass(0.00259)
sd.add_material(2.75e+7,0.265,0.285,'steel')
sd.add_material(9.86e+6,0.320,0.0928,'aluminum')
sd.add_material(1.88e+7,0.350,0.162,'titanium’)

# Assign Materials for SD
sd.assign_material(3, 'aluminum')
sd.set_number_of_modes(20)
sd.set_mesh(morph)
sd.set_output_filename('RingSurfaceName.e’)
```

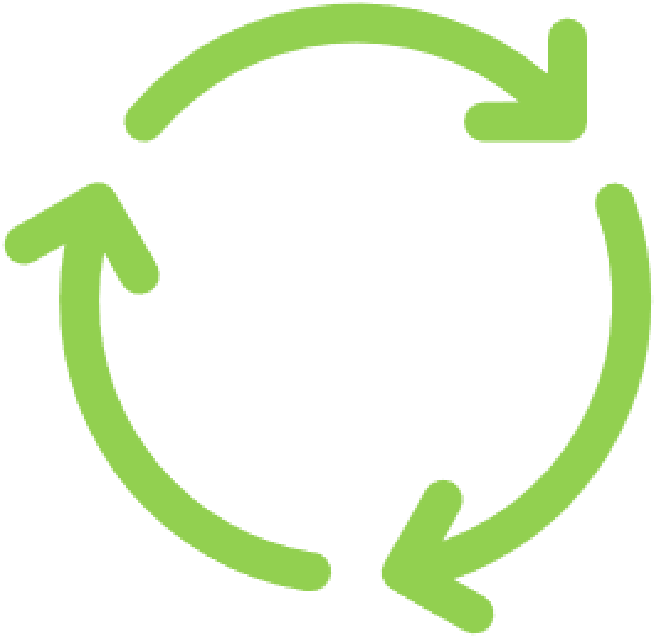
```
# Boundary Conditions and Interfaces
connections = sierra.MorphSDConnections()
connections.set_morph(morph)
connections.set_sdeigenanalysis(sd)

# Submit Job
hpc.set_runnable(connections)
hpc.set_machine_name('ghost')
hpc.set_number_processors(8)
hpc.submit_job('fy150075','/nscratch/jwfoulk')
hpc.download_return_files()

# View Results
sd.write_viz_input_deck(sd.get_output_filename(),hpc.get_remote_path(),"lb")
```

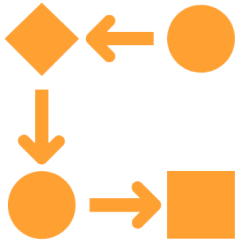
Continuous improvement through user feedback

Step 1: Users provide feedback while attempting to work through the workflow



Step 2: Document feedback; discuss & prioritize as a team

Step 3: Implement changes rapidly & iteratively

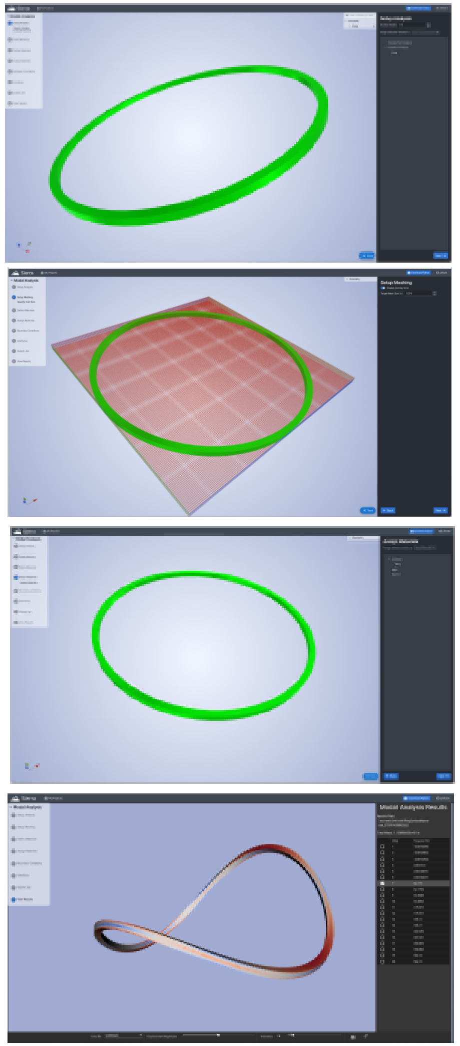


Technologies let the workflow do more

intuitive user interfaces

fast/adaptive model creation

workflow



WebUI

- CAD viz
- context driven UI
- scripted workflow
- results viz
- HPC accessibility

Morph Emend

- overlay creation
- capture CAD
- improve quality
- mesh toolbox
- FE workflow

shared

- SGM
- automation w/ML
- error & size fields
- data repositories
- UQ V&V

workflow

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# Boundary Conditions and Interfaces
connections = sierra.MorphSDConnections()
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```

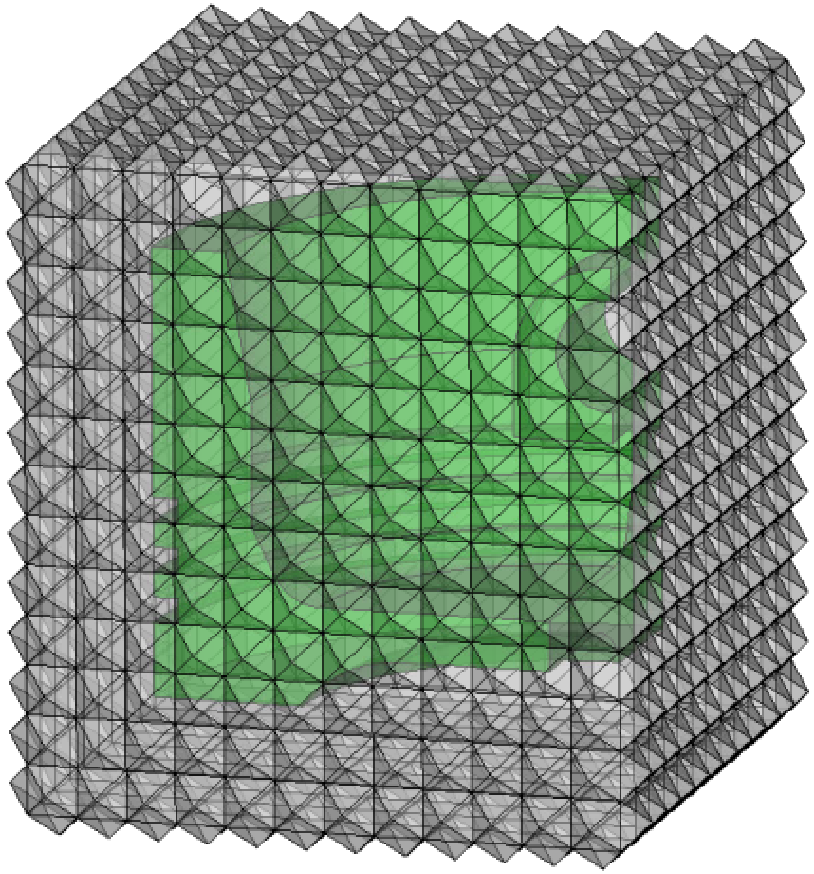
Enabling technology: Morph/Emend

overlay creation

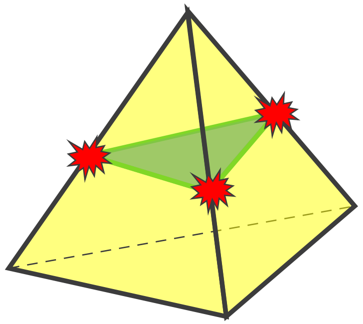
capture CAD

A: If we employ improved tetrahedral elements, we can conduct TF/SD/SM with tets
A: Filling a well-defined volume is easy. Filling it with high-quality tets is harder
A: Filling an ill-defined volume, “bad CAD”, with high-quality tets is even harder

BCC Lattice background grid

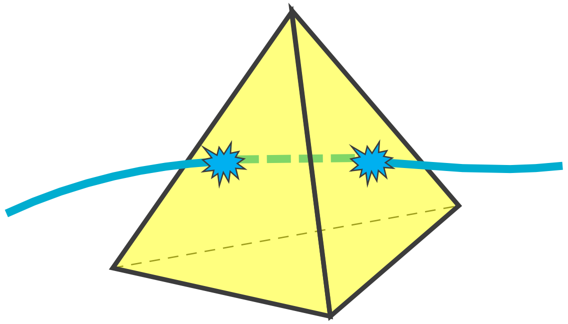


CAD Surface-Edge



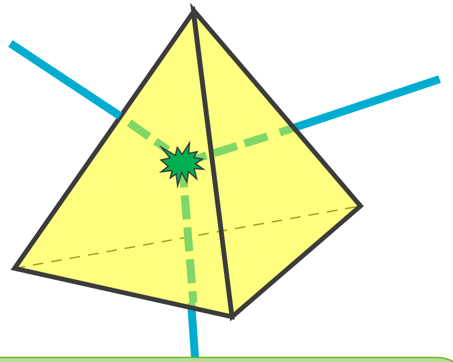
1 Cutting Option
+ 2 Snapping Options
3 Total Options

CAD Curve-Tri



4 Cutting Options
+ 3 Snapping Options
7 Total Options

CAD Vertex-Tet

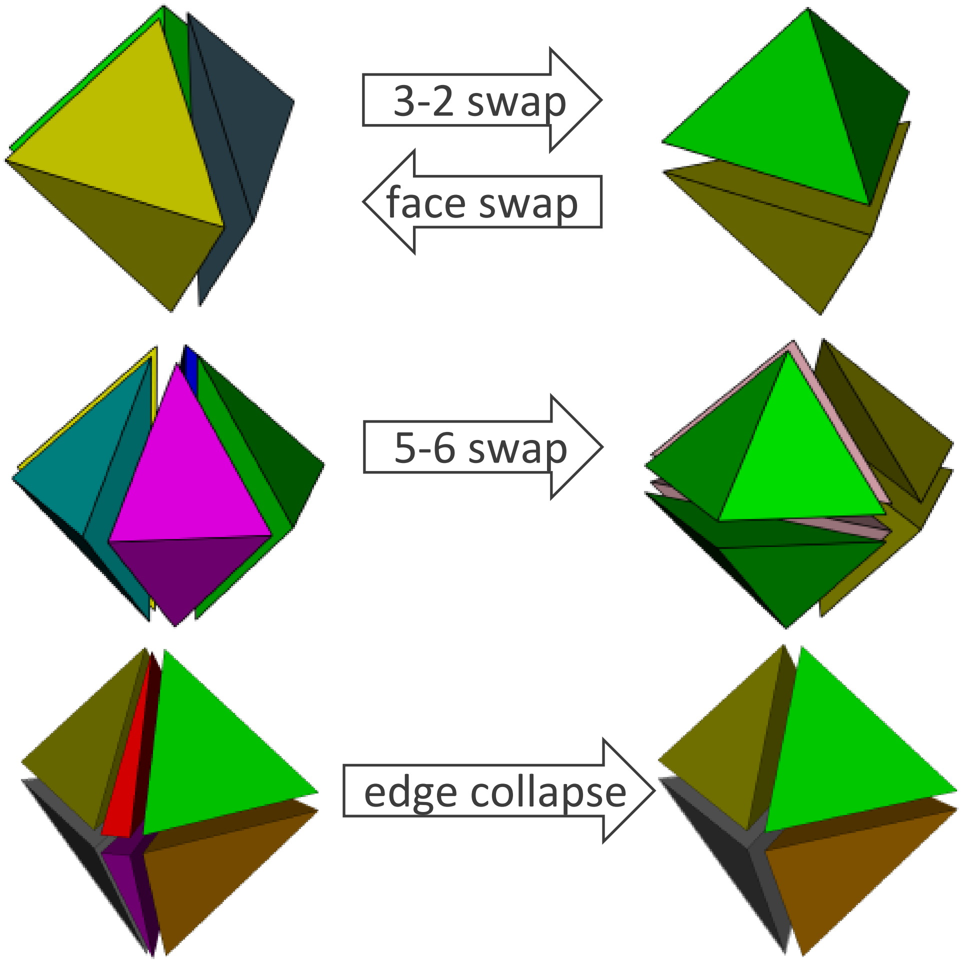


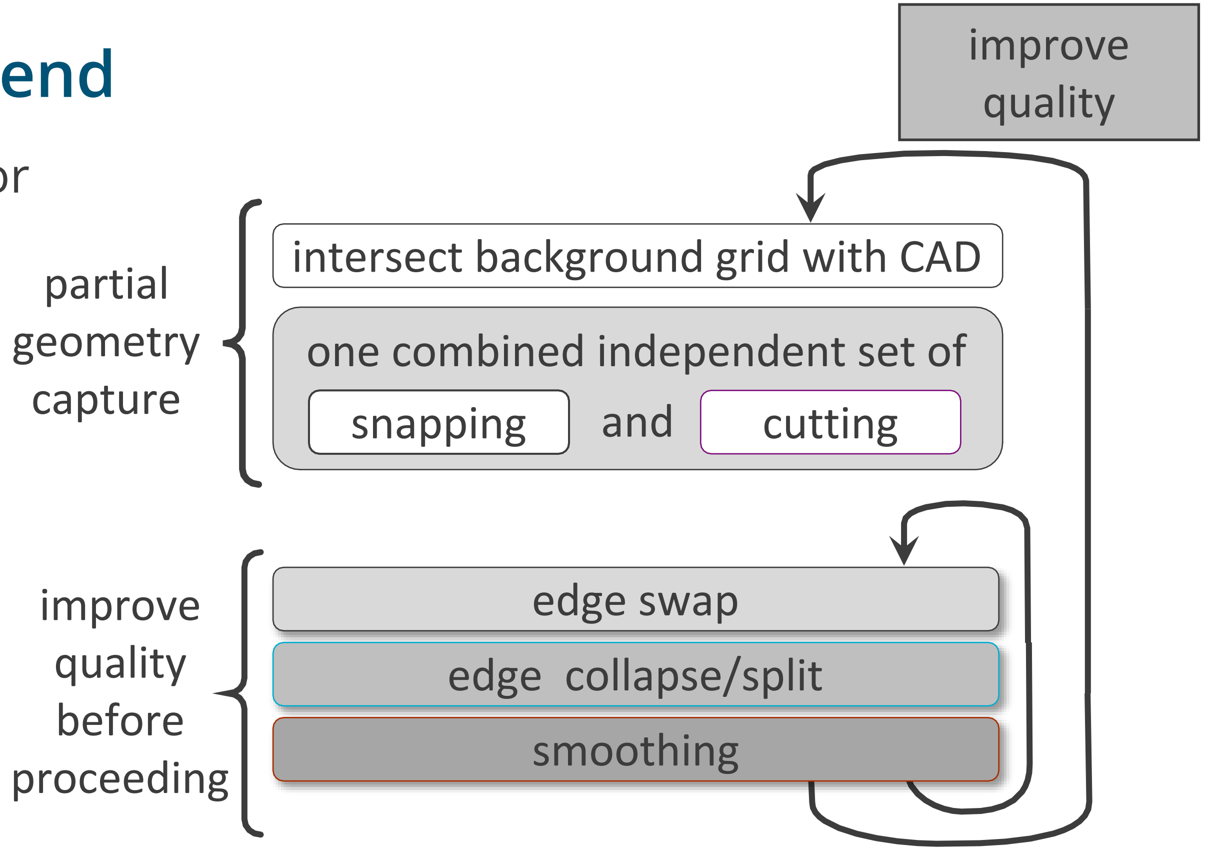
11 Cutting Options
+ 4 Snapping Options
15 Total Options

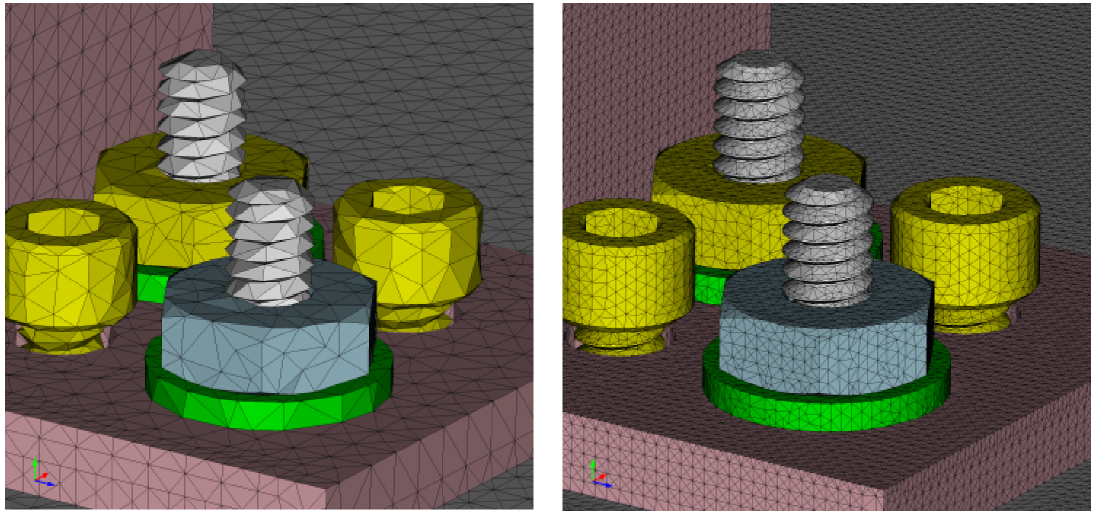
NOTE: Choose the option with highest element quality (> 1 metrics)

Enabling technology: Morph/Emend

Emend builds on Omega_h, an open source library for mesh adaptivity with a focus on topological operations such as swaps and collapses.



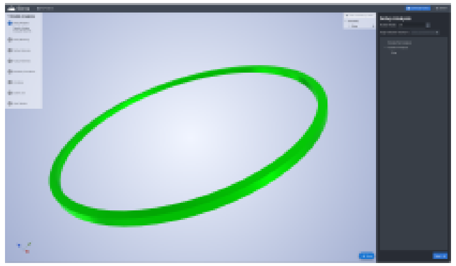


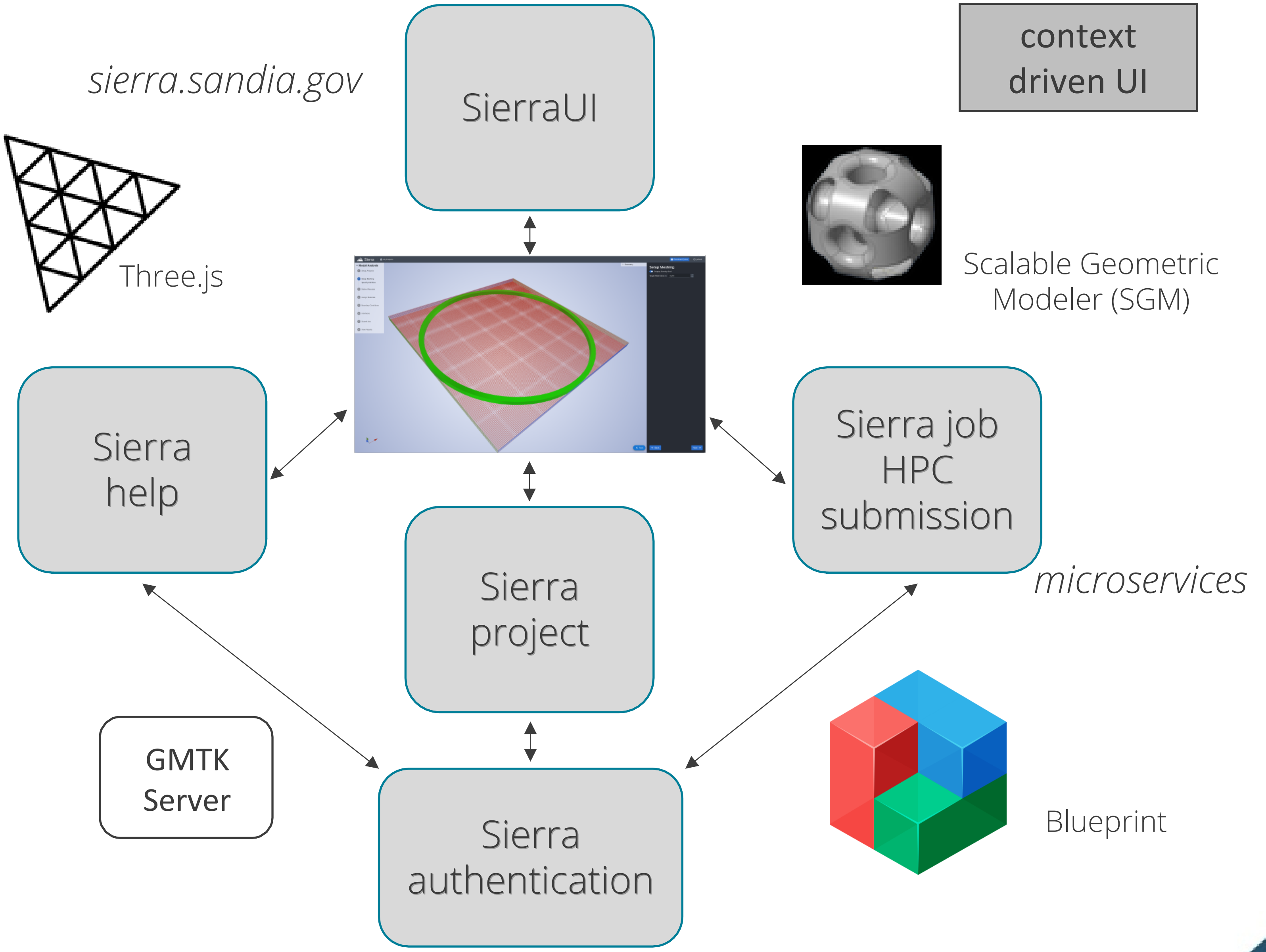


Enabling technology: Context driven WebUI

CAD viz	HPC accessibility
context driven UI	

web browser





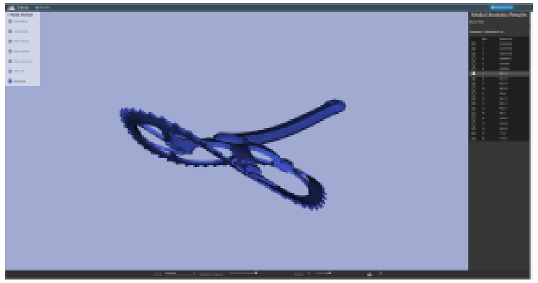
Premise

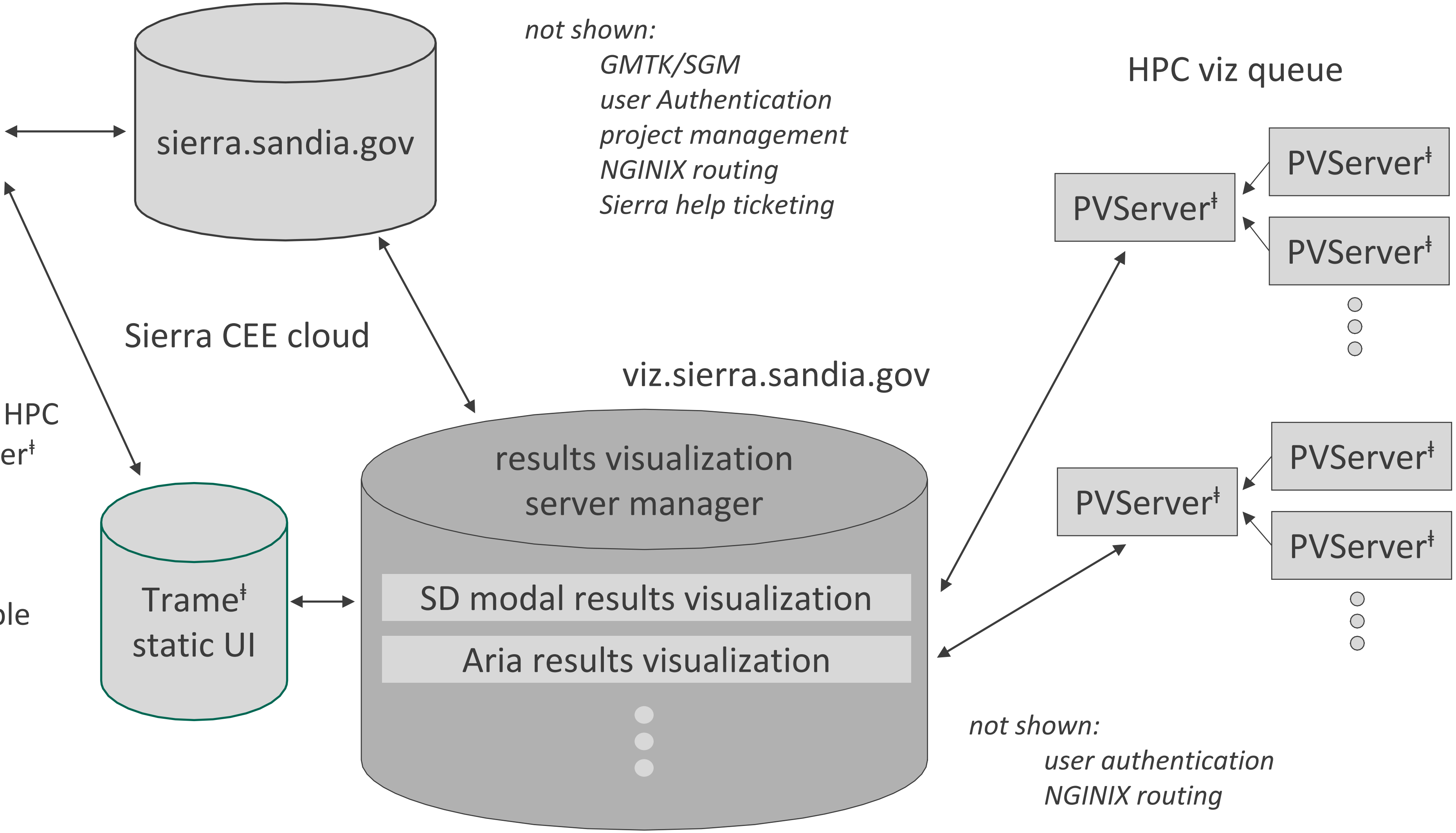
- Have an idea
- Jump into a browser
- Get work done
- Go to a meeting
- Go to another meeting
- Plan to do work. Meet to discuss.
- Report progress on work not completed
- Remember that you are an engineer
- Hide. Go back to browser.
- Confirm hypothesis. Make decision.
- Move forward

Enabling technology: Future web-based visualization

HPC accessibility | results viz

web browser





- Results rendered directly from HPC
- Limitations with ParaView serverǂ prevents use of OpenShift
- Revised architecture
  - Cleaner
  - Can accommodate multiple applications
  - Hosted on CEE Cloud
  - OpenShift ready pending Paraview Serverǂ
  - Working prototype

ǂ Trame/Paraview from Kitware Inc.

Adopt. Move towards in-core workflows.

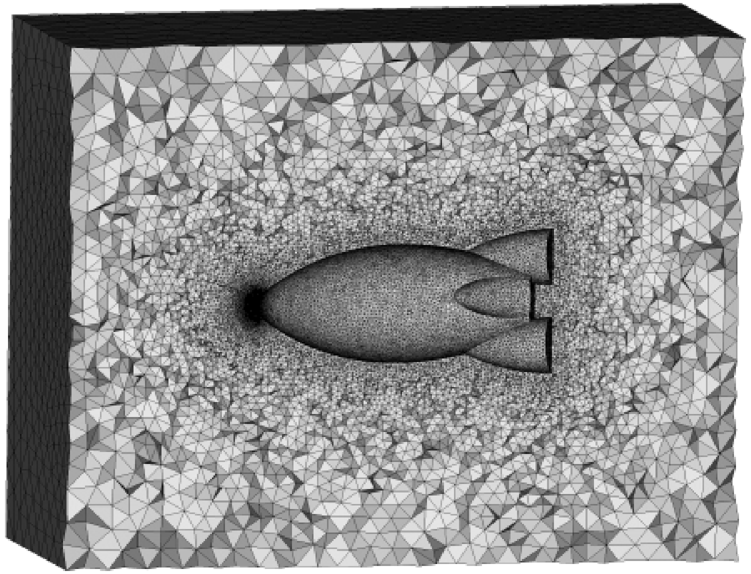
scripted workflow

error & size fields

fast/adaptive model creation

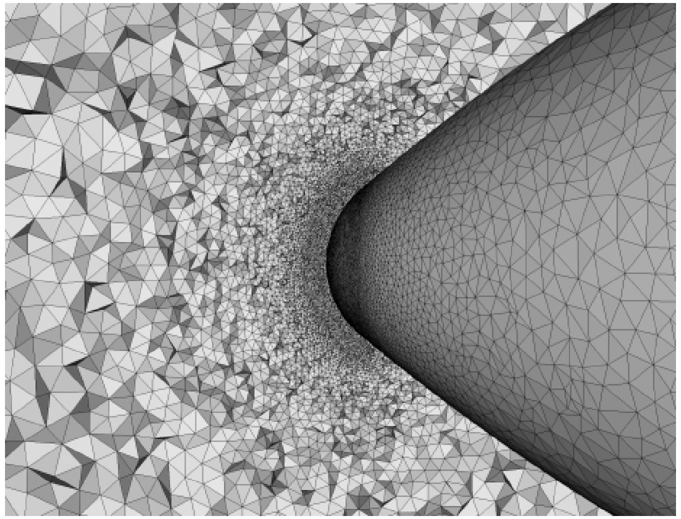
credibility for decision making

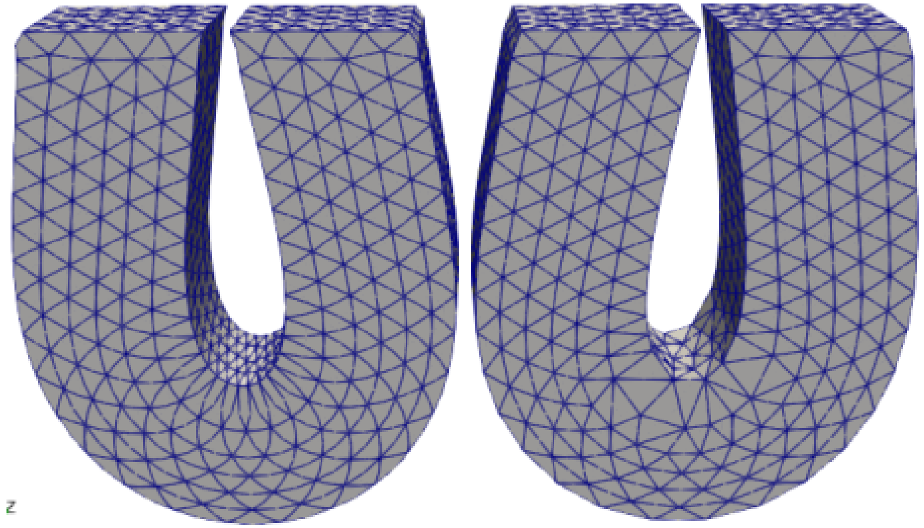
A: Tetmeshing provides the opportunity for mesh adaptivity in 3D
A: Geometric error can provide a metric for coarsening and refinement
A: Physics-specific error indicators provide a metric for coarsening/refinement
A: If we link error to size, we can provide automation via a size field
A: File & in-core capabilities provide the opportunity for remeshing & mapping



smoothly varying background tet mesh via MeshGems for SPARC (T. Fisher, 1541, D. Dinzl, 1515)

local refinement mitigates geometric error





local remeshing/mapping via improve_mesh in SierraRemesh (Andy Sterschic, 8752)

Potential intersection with NGW

scripted workflow

NGS(D) workflow components

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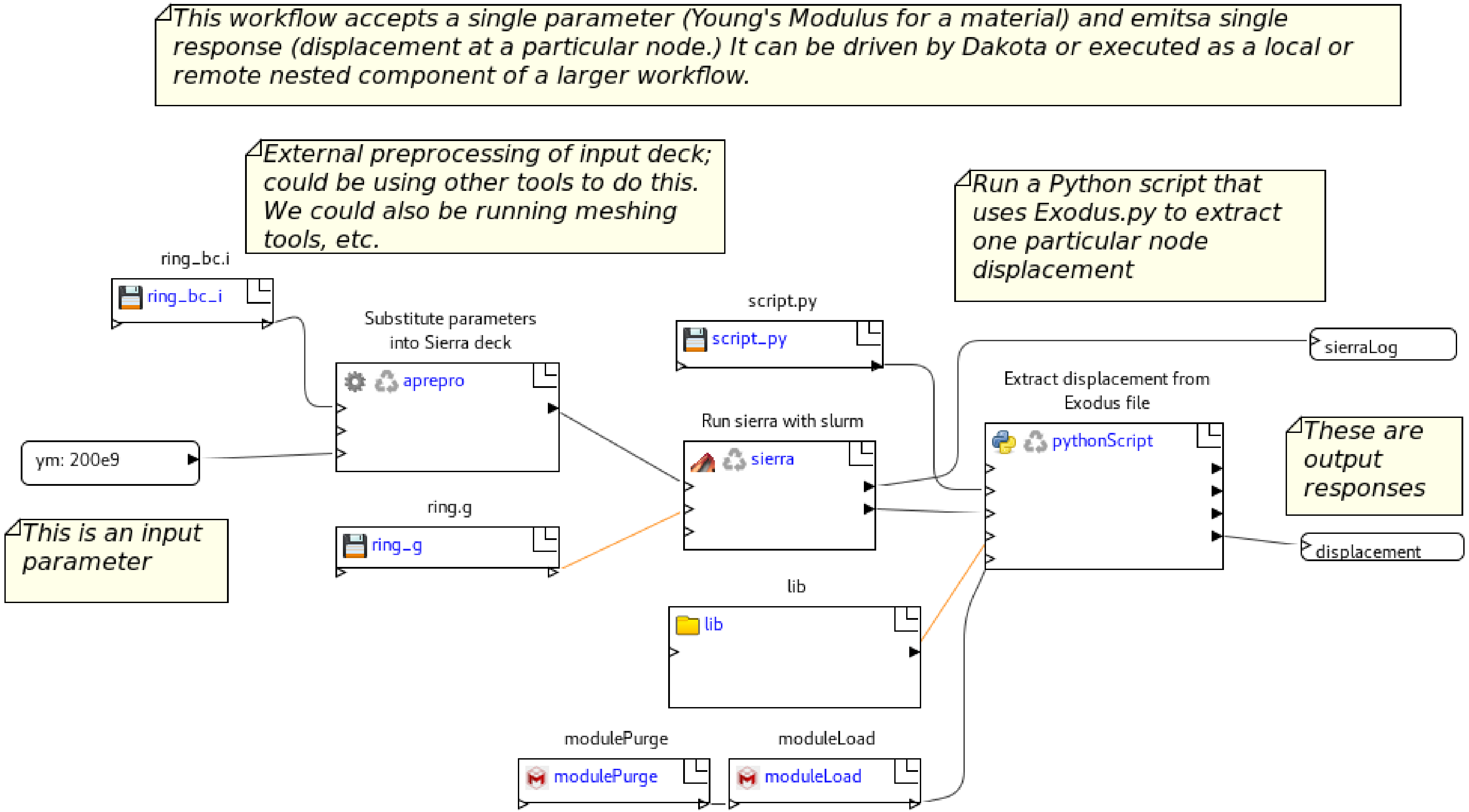
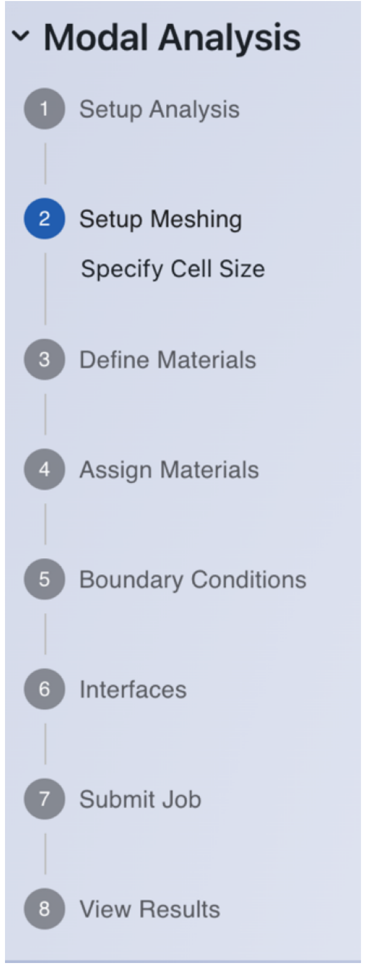


NGS(D) workflow components can be employed in the context of larger, traceable workflows in NGW.

Conclusion: Focus on UX. Generalize. Scale with technologies. Team.

workflow



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UX

- intuitive user interfaces
- fast/adaptive model creation
- credibility for decision making

UX drives products

↓

products drive technologies

↓

technologies drive scalability

↓

impact design, qualification, surveillance

Backup slides