

# An overview of ExaConstit and its use in the ExaAM project

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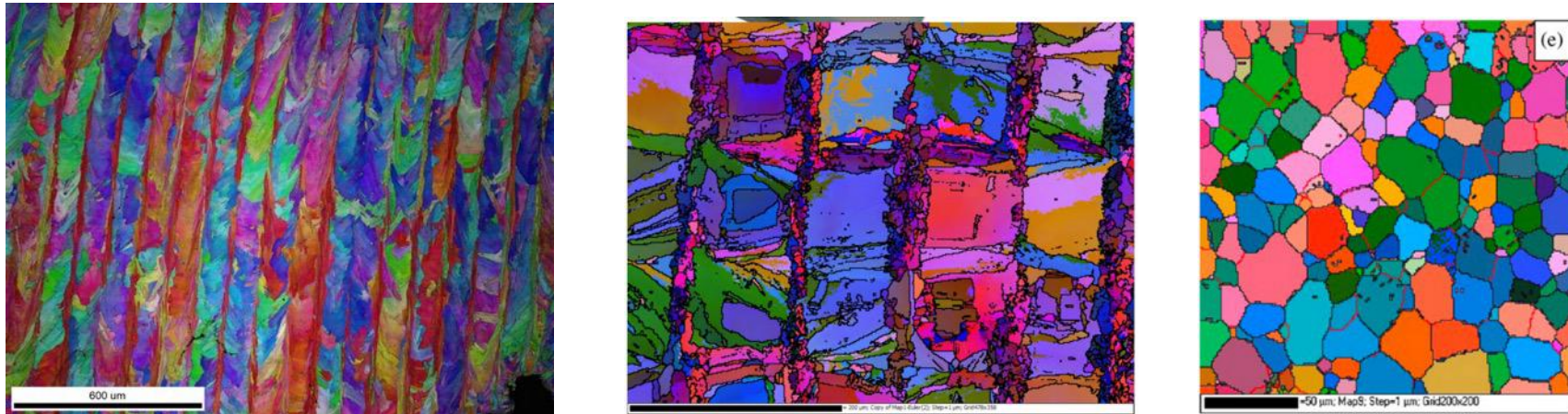


# Outline

- Motivation and overview of project
- Overview of ExaConstit
  - FEM formulation
- Overview of GPU Porting Efforts
  - Element assembly formulation
  - Exascale readiness of ExaConstit
- Overview of local property calculation workflow
- ExaConstit's use in other areas
- Conclusion/On-going work

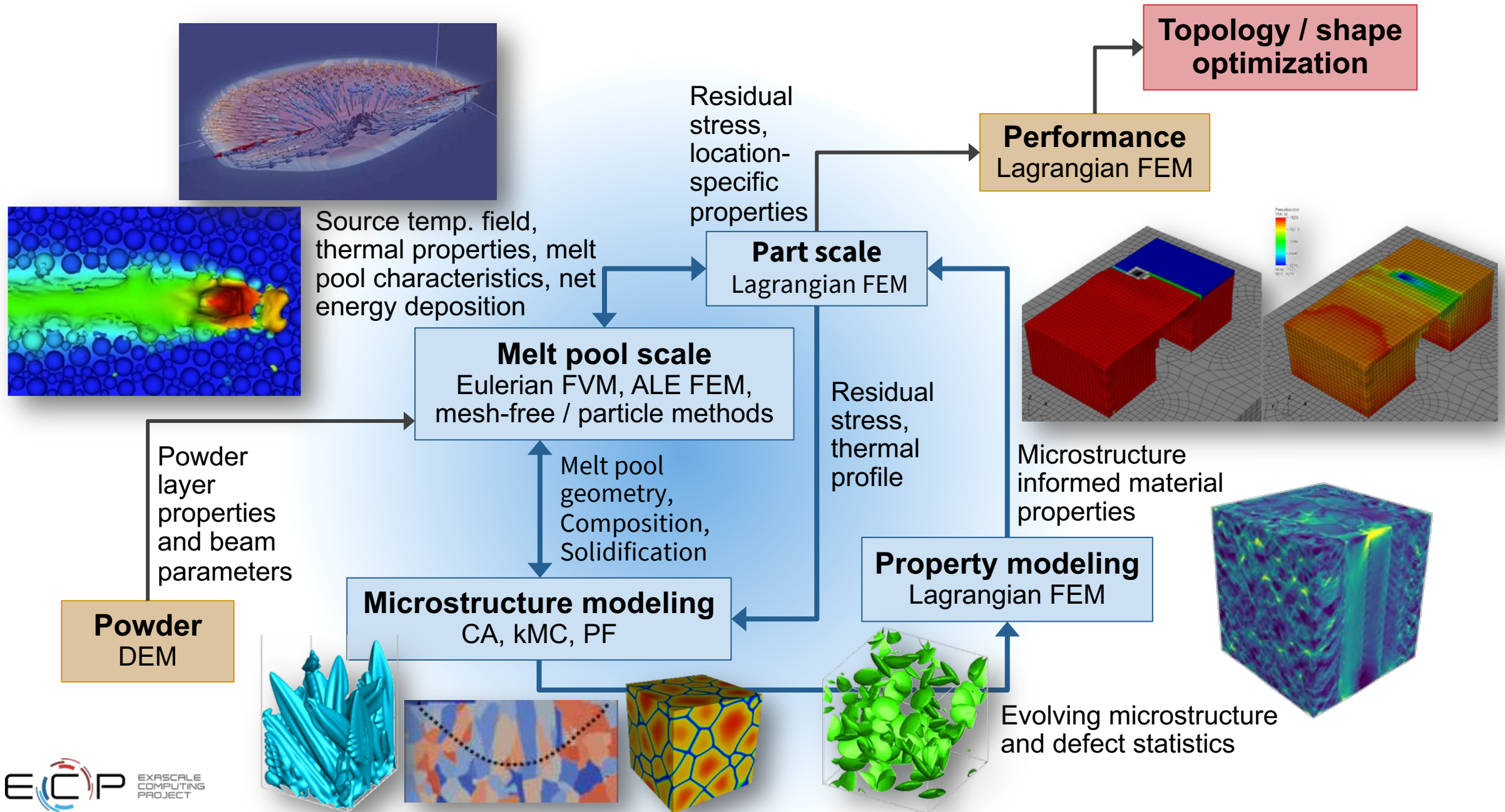
# Motivation

- AM produces as-built metals that are characteristically quite different from typical manufacturing processes in both the microstructure and mechanical response [2]
- Want to couple the microstructure development and the local macroscopic properties
  - Can be accomplished through crystal plasticity models that utilize finite elements



Microstructure of an AM part at 2 different locations (Left and Middle) [3] and a traditional manufacturing microstructure [4]

# ExaAM focus (blue) fits within a larger modeling and design optimization context



# A full ExaAM simulation consists of five stages

**0: Full-part build simulation**



**1: As-built microstructure**



**2: Late-time Microstructure**

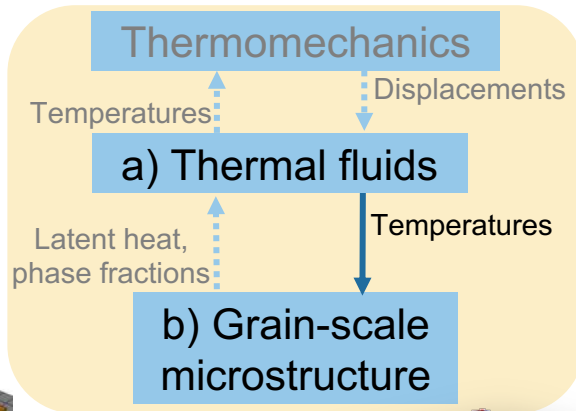


**3: Micromechanical properties**



**4: Full-part build simulation**

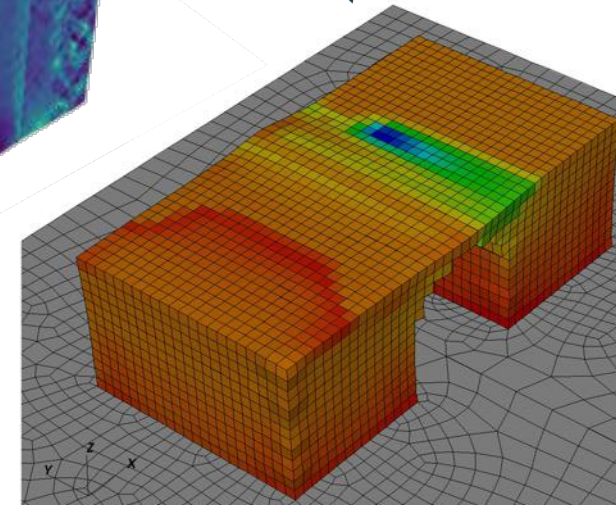
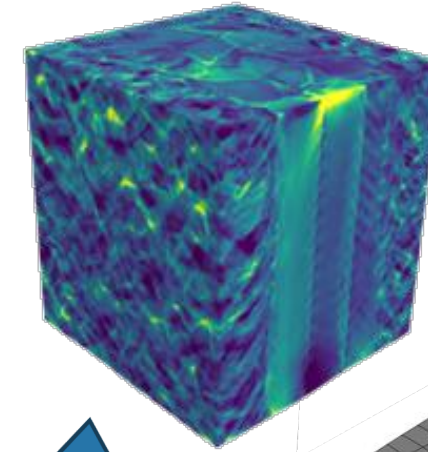
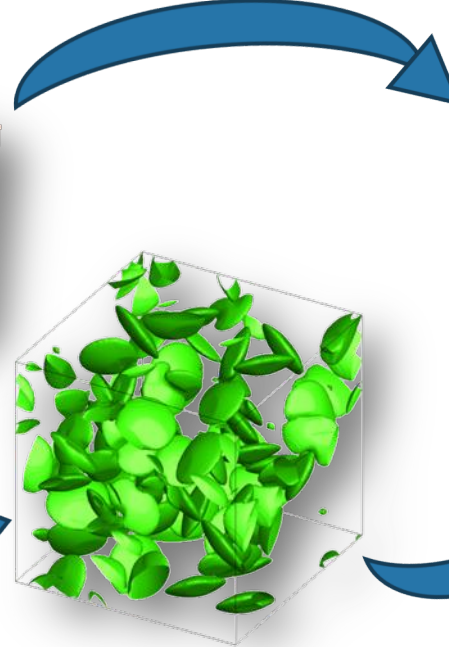
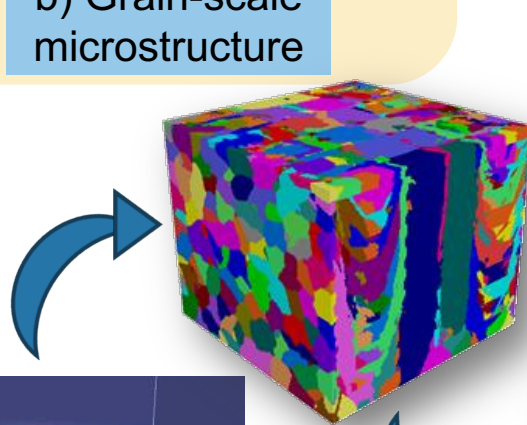
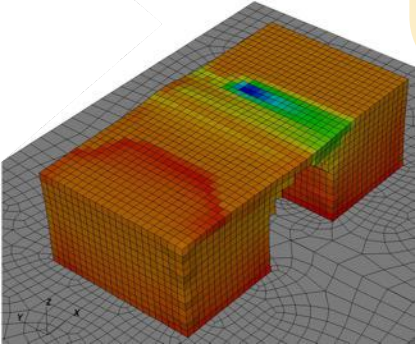
Coarse macroscale thermo-mechanics using assumed properties



Solid-solid phase transformation and other mesoscale phenomena during cooling

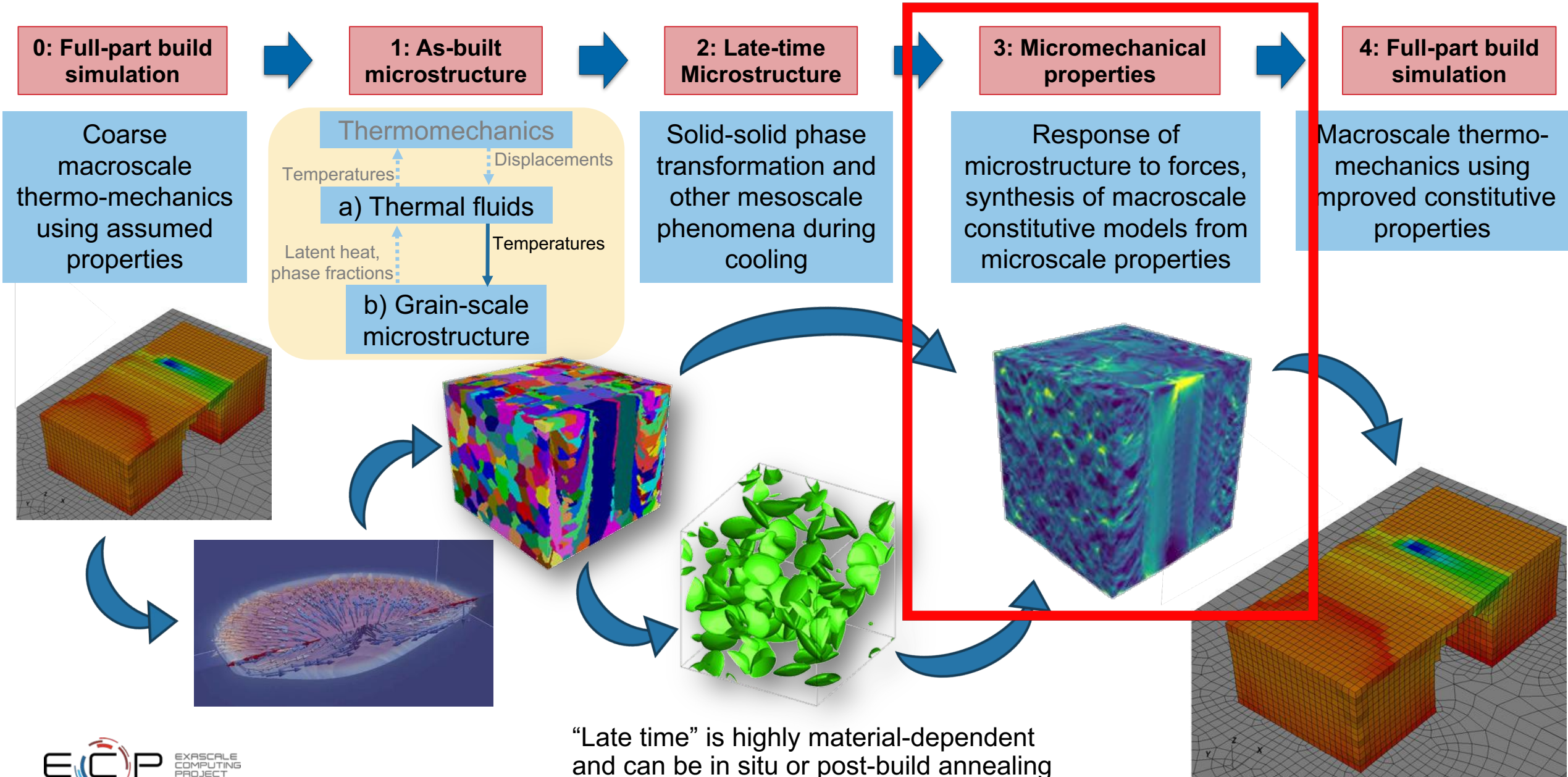
Response of microstructure to forces, synthesis of macroscale constitutive models from microscale properties

Macroscale thermo-mechanics using improved constitutive properties



"Late time" is highly material-dependent and can be in situ or post-build annealing

# A full ExaAM simulation consists of five stages



# Overview of ExaConstit

- A new nonlinear quasi-static, implicit FEM solid mechanics code built on the MFEM library
  - Development began in 2018 for ExaAM project
  - Updated Lagrangian formulation (velocity based)
  - Natively supports a wide range of element types
  - Supports complex parts and non-trivial/changing Dirichlet BCs
  - Available at <https://github.com/LLNL/ExaConstit>

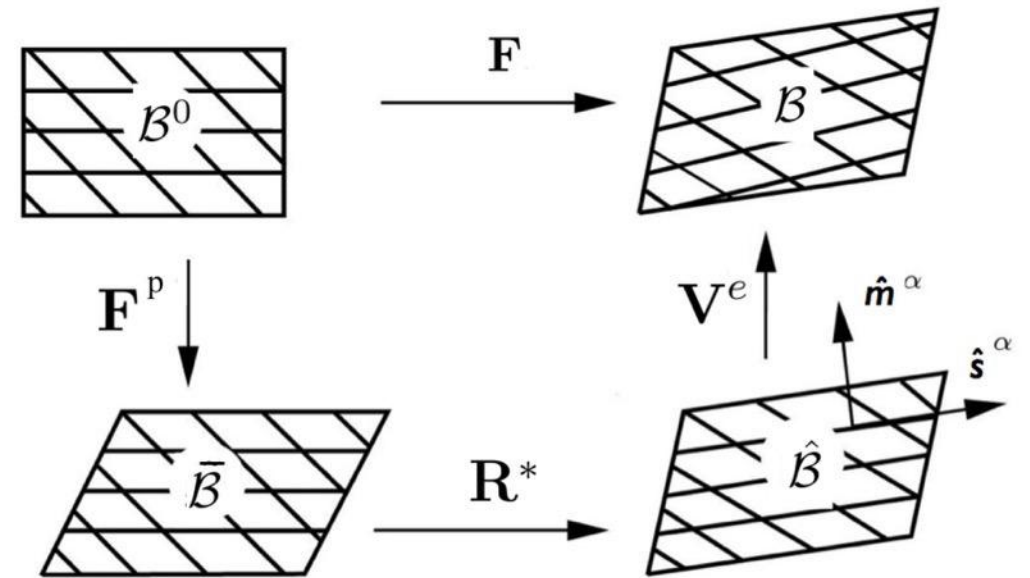
# Overview of ExaConstit

- Designed with exascale computers in mind but performant even on desktop machines
- New features, workflows, and post-processing tools are constantly being added
- Bread and butter is crystal plasticity type problems
  - Crystal plasticity models are provided through ExaCMech library
    - ExaCMech is available at <https://github.com/LLNL/ExaCMech>
    - Models can be upwards of 75-90x faster than Abaqus UMAT runs
  - Users can also run UMAT problems as well
    - UMAT framework enables us to run a wide range of industry and research models

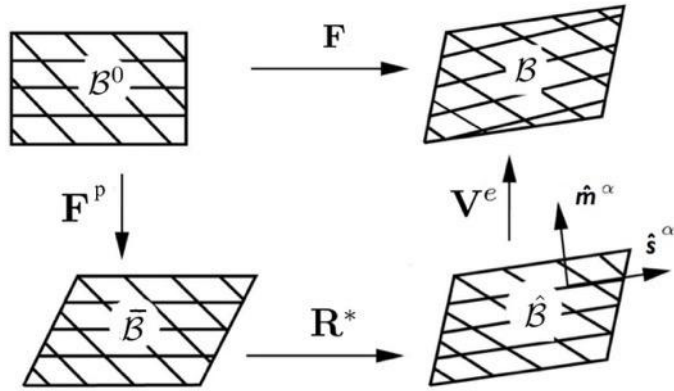
# Model Overview

- A large strain single crystal elasto-viscoplastic model is being used
  - Small deviatoric elastic strain assumption is made

$$\mathbf{F} = \mathbf{F}^e \mathbf{F}^p$$



# Model Overview



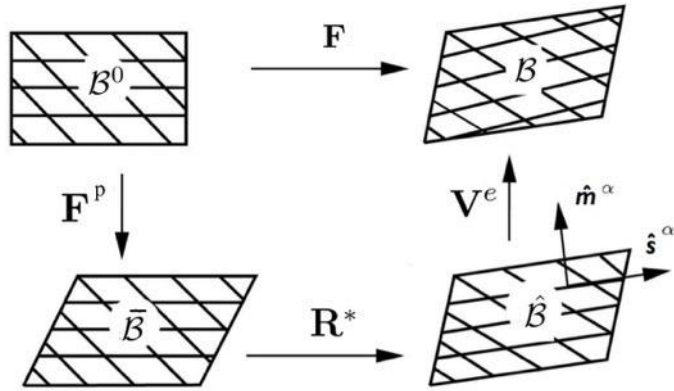
$$\mathbf{L} = \dot{\mathbf{V}}^e \mathbf{V}^{e-1} + \mathbf{V}^e \hat{\mathbf{L}}^p \mathbf{V}^{e-1}$$

$$\hat{\mathbf{L}}^p = \dot{\mathbf{R}}^* \mathbf{R}^{*T} + \mathbf{R}^* \dot{\mathbf{F}}^p_n \mathbf{F}^{p-1} \mathbf{R}^{*T}$$

$$\bar{\mathbf{L}}^p = \dot{\mathbf{F}}^p \mathbf{F}^{p-1} \quad \bar{\mathbf{L}}^p = \sum_{\alpha=1} \dot{\gamma}^\alpha \bar{\mathbf{s}}^\alpha \otimes \bar{\mathbf{m}}^\alpha$$

$$\dot{\gamma} = \dot{\gamma}_0 \left( \frac{\tau^\alpha}{g^\alpha} \right)^{\frac{1}{m}} \text{sgn}(\tau^\alpha)$$

# Model Overview



$$\mathbf{L} = \dot{\mathbf{V}}^e \mathbf{V}^{e-1} + \mathbf{V}^e \hat{\mathbf{L}}^p \mathbf{V}^{e-1}$$

Small elastic strain assumption

$$\mathbf{V}^e = \mathbf{I} + \boxed{\boldsymbol{\varepsilon}^e}$$

$$\hat{\mathbf{L}}^p = \dot{\mathbf{R}}^* \boxed{\mathbf{R}^*}^T + \mathbf{R}^* \dot{\mathbf{F}}^p_n \mathbf{F}^{p-1} \mathbf{R}^{*T}$$

$$\bar{\mathbf{L}}^p = \dot{\mathbf{F}}^p \mathbf{F}^{p-1}$$

$$\bar{\mathbf{L}}^p = \sum_{\alpha=1} \dot{\gamma}^\alpha \bar{\mathbf{s}}^\alpha \otimes \bar{\mathbf{m}}^\alpha$$

$$\boxed{\dot{\gamma}} = \dot{\gamma}_0 \left( \frac{\tau^\alpha}{g^\alpha} \right)^{\frac{1}{m}} \text{sgn}(\tau^\alpha)$$

# FEM Formulation

- We're solving for the conservation of linear momentum using a Newton Raphson scheme
  - Our finite element formulation takes on a form very similar to linear elasticity
  - We make use of an updated Lagrangian formulation here

$$[K_{tan}]\{-\Delta\mathbf{V}\} = \{f_{int}\}$$

$$[K_{tan}] = \int_{\Omega} [\mathbf{B}]^T [\mathbf{C}^{\sigma\tau}] [\mathbf{B}] d\Omega \quad [\mathbf{C}^{\sigma\tau}] = \frac{d\boldsymbol{\sigma}}{d\mathbf{d}}$$

$$\{f_{int}\} = \int_{\Omega} [\mathbf{B}]^T \{\boldsymbol{\sigma}\} d\Omega$$

$$\{\mathbf{V}\}^{i+1} = \{\mathbf{V}\}^i + \{\Delta\mathbf{V}\}$$

$$\{\mathbf{x}\}^{t+\Delta t} = \{\mathbf{x}\}^t + \Delta t \{\mathbf{V}\}^{i+1}$$

**Note: This formulation uses the velocity rather than the typical displacement**

# Transitioning over to the GPU: Separate Material Model and FEM code

- ExaConstit originally had the material model calculation tied in with the linearized RHS calculation and compute stiffness matrix
  - This strategy does not scale well as different assembly operations are added
- Refactored code into a set-up phase, pre-processing step before assembly, RHS calculations, and gradient calculation / operation

# Set-up phase

- Calculate necessary parameters to use within our material model
  - Pre-processing stage for material kernel
- Material kernel stage
- Post-processing material kernel stage
  - Perform what-ever steps are necessary for material kernel's data to be used by the rest of the code
- MFEM\_FORALL loops are used for pre & post processing steps
- Material model uses its own parallelization strategy

# An Element Assembly Formulation

- We're making use of efficient formulations developed back in the 80s [5]
- $\{f_{int}\}$  is just calculated using partial assembly formulation
- This formulation allows us an efficient way to compute sub-blocks of  $[K_{tan}]$ 
  - Could further specialize this for tensor-type elements for further performance gains

$$[K_{tan}] = \int_{\Omega} [\mathbf{B}]^T [\mathbf{C}^{\sigma\tau}] [\mathbf{B}] d\Omega$$

$$[K_{tan}] = \int_{\Omega} [\mathbf{b}_1 \mathbf{b}_2 \dots \mathbf{b}_N]^T [\mathbf{C}^{\sigma\tau}] [\mathbf{b}_1 \mathbf{b}_2 \dots \mathbf{b}_N] d\Omega$$

$$[\mathbf{b}_1 \mathbf{b}_2 \dots \mathbf{b}_N] = [\mathbf{B}]$$

$$\{f_{int}\} = \int_{\Omega} [\mathbf{B}]^T \{\boldsymbol{\sigma}\} d\Omega$$

$$\det(J) w_{qpt} \nabla_{ij} \phi_{\xi}^T J_{jk}^{-T} \sigma_{kl}$$

# Incompressible Material Support within ExaConstit

- An initial integration formulation for incompressible has been implemented
  - Based on the work presented in [6]
  - New integrators are not as simple to port over to the element assembly formulation
- This formulation brings linear hexahedron response much more in line with response from higher order elements
  - Runtime is comparable to full integration approach

$$\mathbf{B}_a = \begin{bmatrix} B_1 & 0 & 0 \\ 0 & B_2 & 0 \\ 0 & 0 & B_3 \\ \hline B_2 & B_1 & 0 \\ 0 & B_3 & B_2 \\ B_3 & 0 & B_1 \end{bmatrix}$$

Full integration  
gradient matrix



$$\bar{\mathbf{B}}_a = \begin{bmatrix} B_5 & B_6 & B_8 \\ B_4 & B_7 & B_8 \\ B_4 & B_6 & B_9 \\ \hline B_2 & B_1 & 0 \\ 0 & B_3 & B_2 \\ B_3 & 0 & B_1 \end{bmatrix}$$

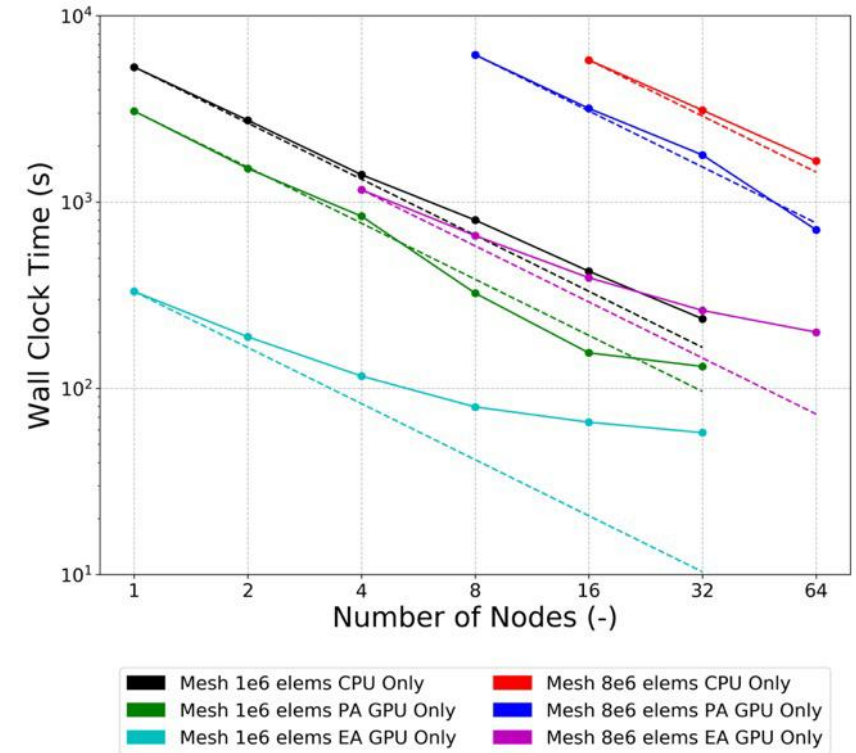
Incompressible integration  
gradient matrix

Contains a mean  
dilation and full  
deviatoric response

# Exascale Readiness Status: ExaConstit

## Summit performance

- 15x speed-up with GPU implementation over CPU
- GPU strong and weak scaling for most performant assembly method (element assembly)
- Poor strong and weak scaling is due to start-up cost of reading in the mesh and partitioning it
  - Recent work-in-progress within MFEM is expected to drastically improve this area (Thanks Veselin!)
- Ported ExaCMech over to HIP this past year
  - ExaConstit port will follow this year

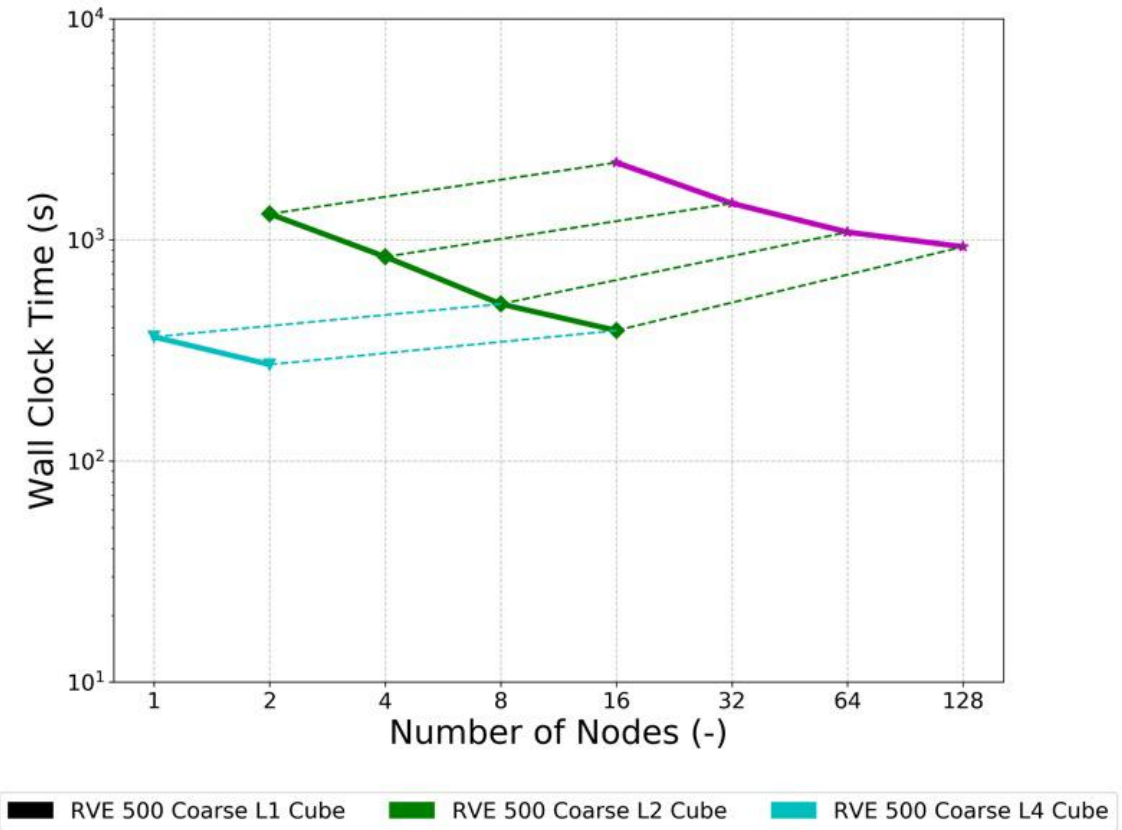


Strong scaling across different assembly methods

# Exascale Readiness Status: ExaConstit

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Strong and weak scaling of  
a typical AM microstructure

# Computational shifts between GPU and Host Runs

## Summit performance

- How do computational costs shift when moving from CPU to GPU?
  - Looking at a 450k element mesh run with Caliper
- Krylov solver still dominates run time
- What's going on with the MPI calls?
  - MPI is taking up a larger % of our runtime now
    - Partially due to issues with MPI D2D calls not being as performant as possible
  - MPI times are 40% less on the GPU though
- Improvements could be made by looking at communication hiding Krylov solvers

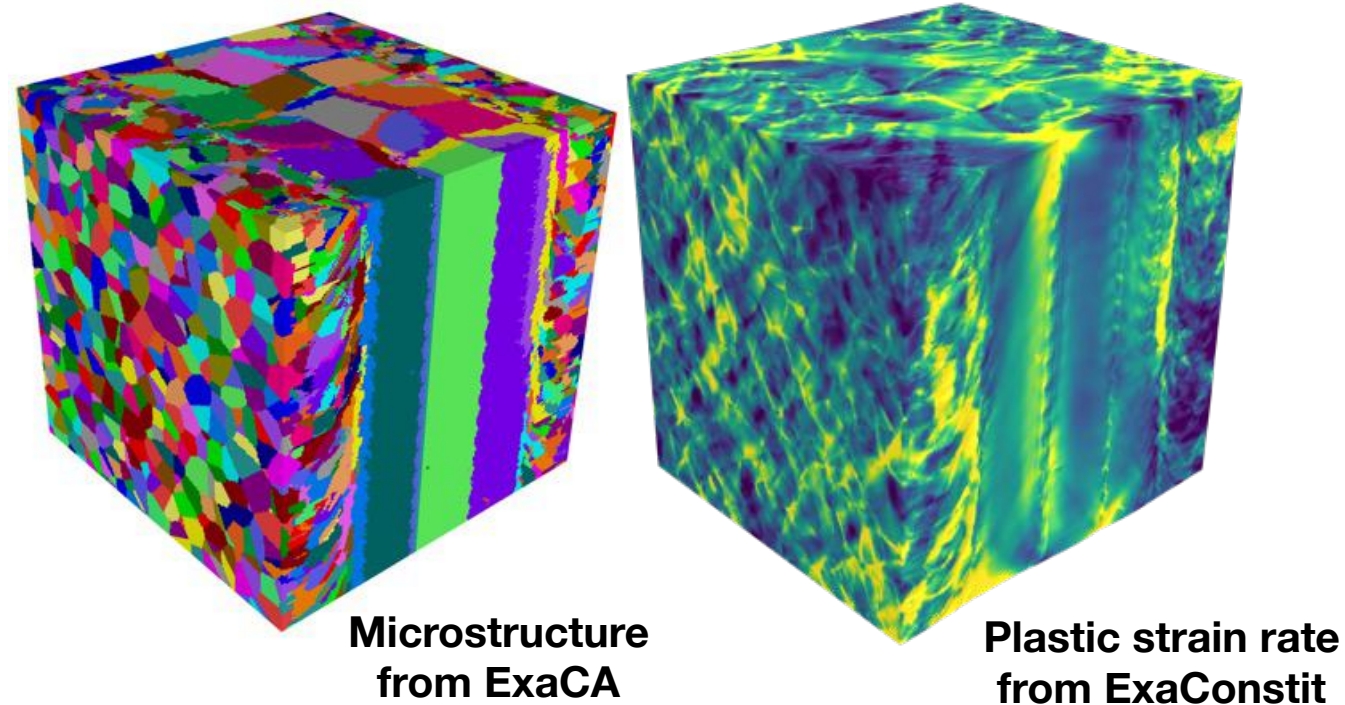
CPU Kernel Name	Time % (total)
Krylov Solver	84.534
Material Model	7.091
MPI Calls	6.778
Element Assembly	0.577
Simulation Initialization	0.295
Material Model Setup	0.283
Integrator Setup	0.137
Total	99.69

GPU Kernel Name	Time % (total)
Krylov Solver	55.16
MPI Calls	18.83
Element Assembly	15.80
Material Model	6.28
Simulation Initialization	1.39
Integrator Setup	0.93
Main Driver	0.88
Assemble Diagonal	0.47
Post-processing step	0.14
Total	99.87

# Stage 3: Micromechanical properties (ExaConstit)

- We now have a performant code but what do we need that for?
- ExaAM requires local property to be calculated from microstructures obtained through out an AM part
- Local properties are calculated by running tons of crystal plasticity simulations under varying loading conditions and temperatures
  - Simply running 1 simulation per microstructure is not adequate for AM parts
  - Complex macroscopic models are needed for part scale simulations (not computed by ExaConstit)

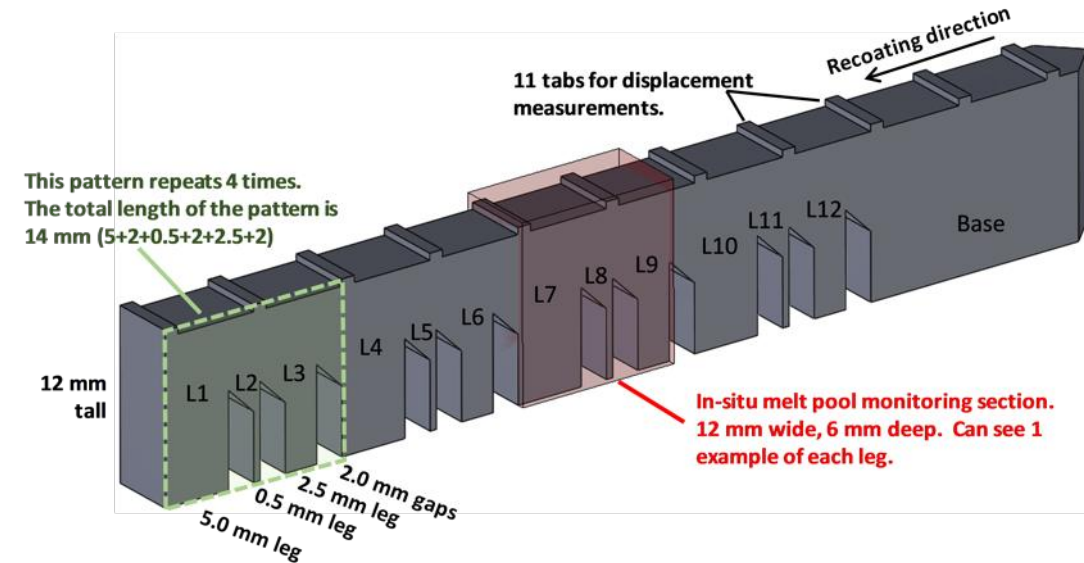
AMB2018-01 L8 microstructure generated by ExaCA  
0.5<sup>3</sup> mm domain, 3475 grains



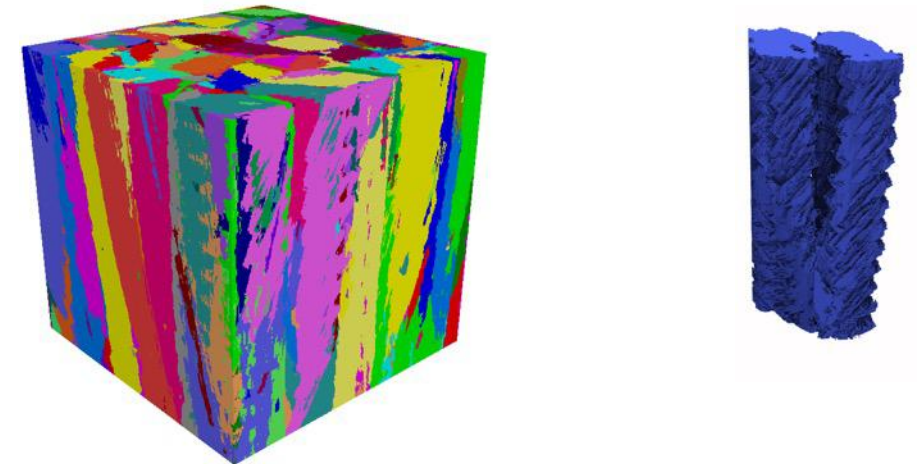
- Localization of plastic strain is non-trivial for these complex AM microstructures - What is an appropriate RVE?
- Hydrostatic stress is commonly used to drive porosity models - How can we appropriately homogenize?

# Representative Volume Element for Macroscopic Calculations

- Microstructure was obtained from a cellular automata simulation based on scan paths of the NIST AM benchmark problem AMB2018-01. Thermal histories provided by either TruchasPBF or OpenFOAM simulations of the scan path
  - Inconel 625 material
    - Voce hardening model parameterized against AFRL MIDAS challenge 3 data [7]
  - Scan pattern mimics one of the larger legs of the AMB2018-01
  - Microstructure used is away from edge boundaries
  - $500^3$  microns sample with  $300^3$  voxel size



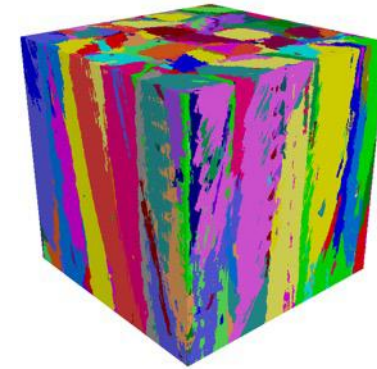
AMB2018-01 part



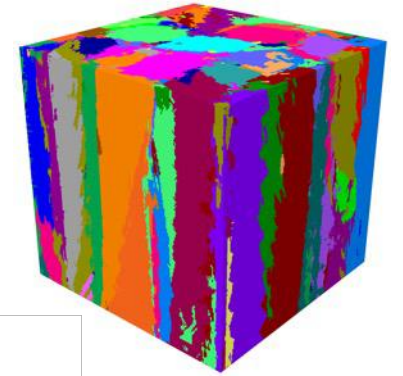
Initial CA microstructure

# Domain Size Microstructures

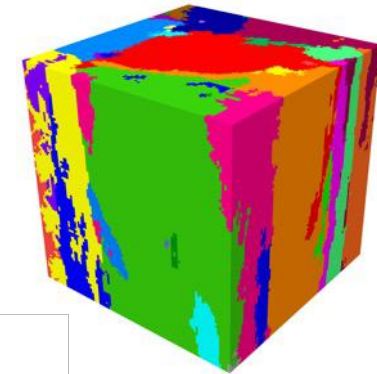
- Microstructures are all taken from the middle of the initial  $500^3$  microns sample
- Microstructures have dimensions:  $500^3$  microns,  $333.3^3$  microns, and  $166.7^3$  microns
  - 27, 8, and 1 million linear hexahedron elements respectively
- Uniaxial tension tests out to 5% were taken on these samples
  - Symmetry boundary conditions were applied to all samples
  - Large strains are not of great interest to our AM applications



Large Microstructure



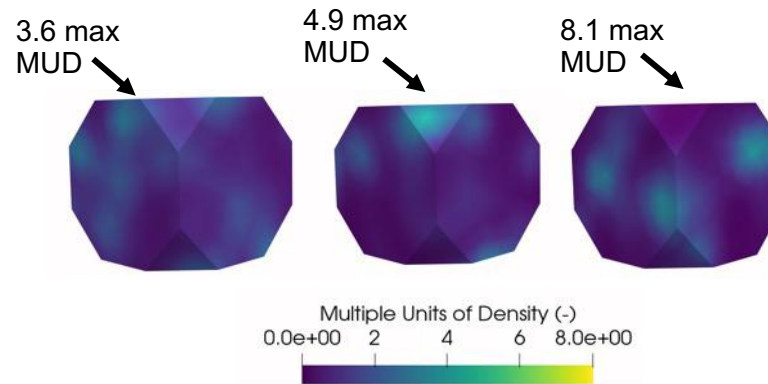
Medium Microstructure



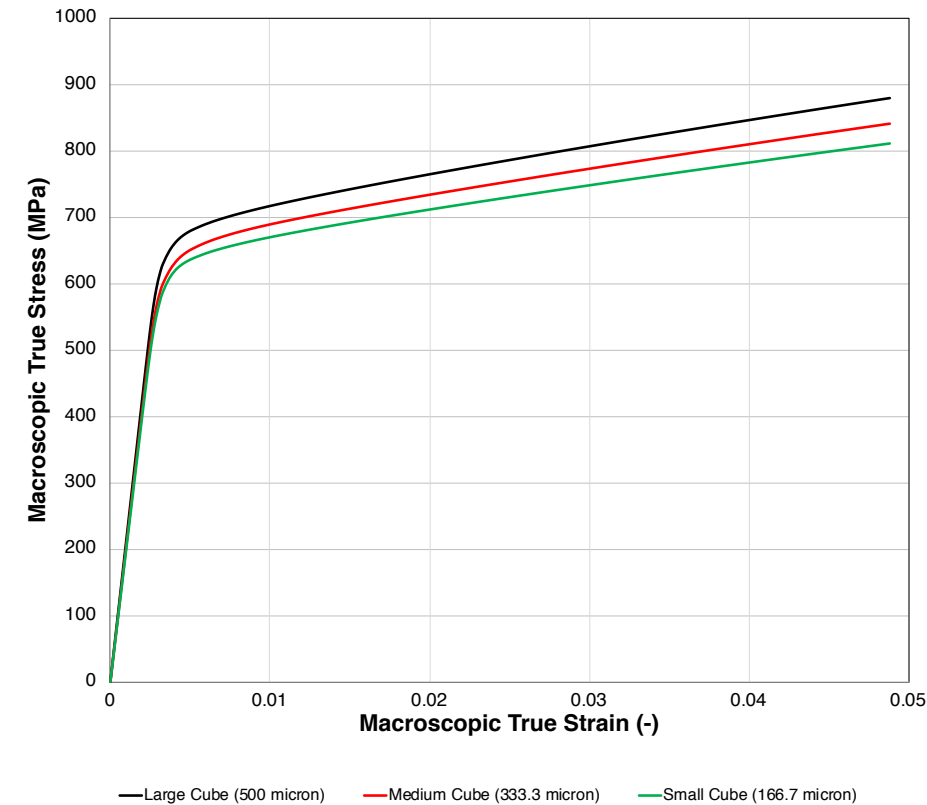
Small Microstructure

# Macroscopic Stress Strain Response

- The medium cube was below 5% error for the entire loading history
  - Error continues to grow as sample enters fully developed plastic flow
- The small cube started around 6% error and continued to grow as simulation progressed
- Differences in responses was largely driven by differences in crystallographic texture
  - Follows historical trends already observed



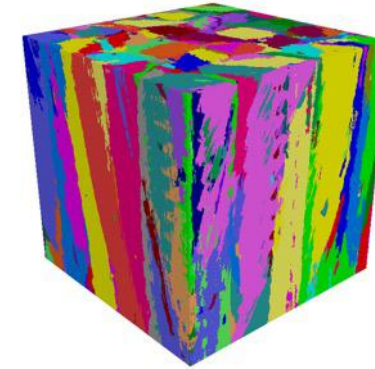
Orientation distribution plots of large, medium, and small cube



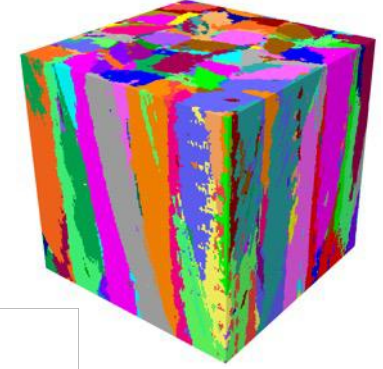
Macroscopic stress strain curves for different size microstructures

# A Need for Mesh Coarsening

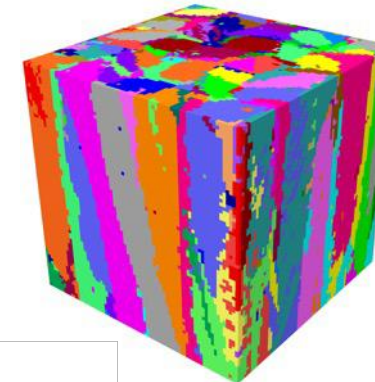
- Cellular Automata simulations produce microstructures with fine voxel sizes (1.667 microns)
  - Results in large number of elements for our simulations
    - $500^3$  micron sample had 27 million elements
  - Similar issues could come from either near-field high energy x-ray diffraction (nf-HEXD) or 3D-serial sectioned EBSD mapped microstructures
- Coarsening voxel data set reduces this issue
  - But what effects does this have on property calculations and intragrain heterogeneity responses?
- We're examining four levels of coarsening
  - Coarsen large microstructure 2, 3, 4, and 6 levels
  - Levels refer here to number of neighbor voxels averaged into 1 voxel in coarser mesh



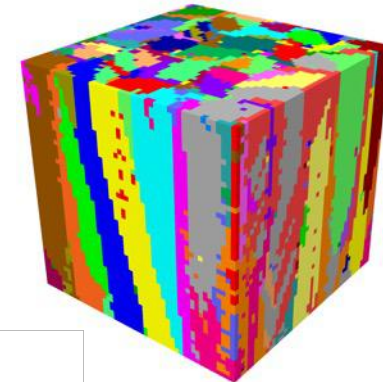
Original  
Microstructure



Coarsen L2  
Microstructure



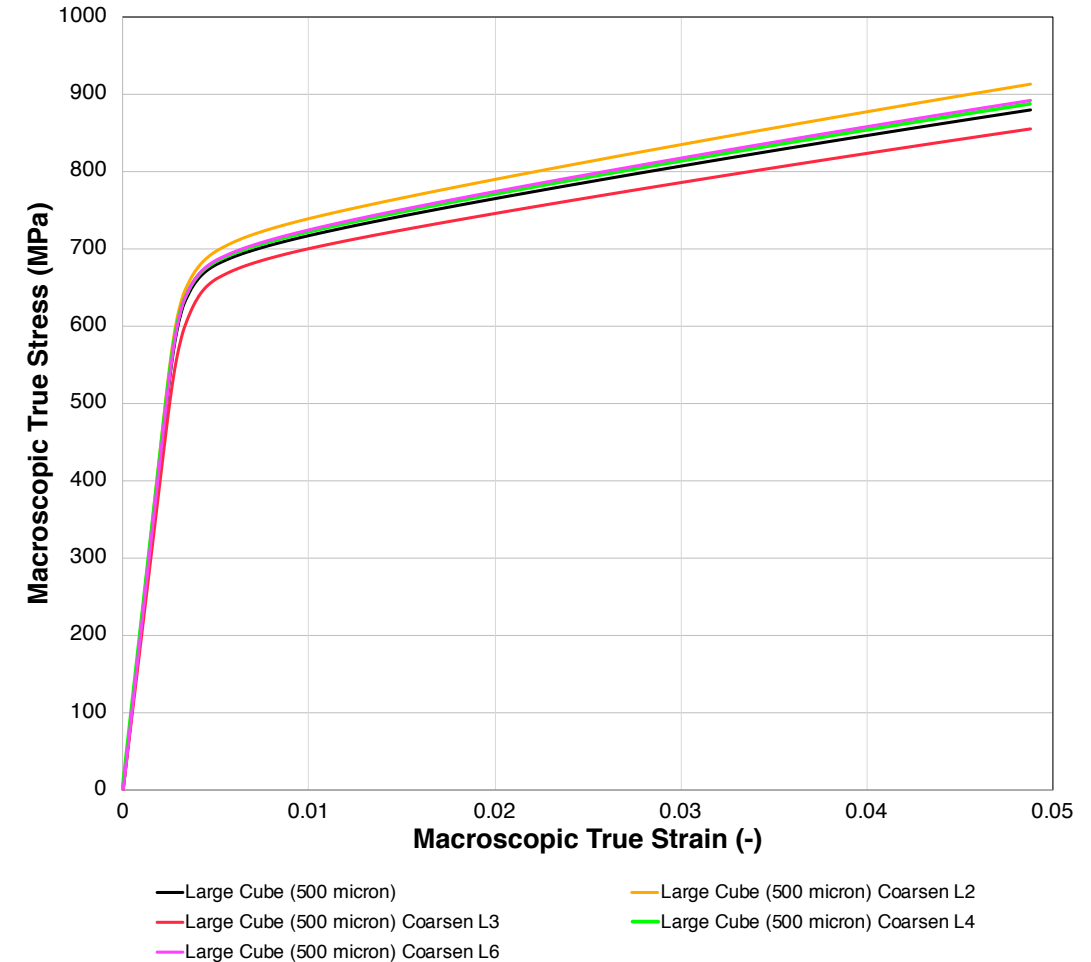
Coarsen L4  
Microstructure



Coarsen L6  
Microstructure

# Macroscopic Stress-Strain Response

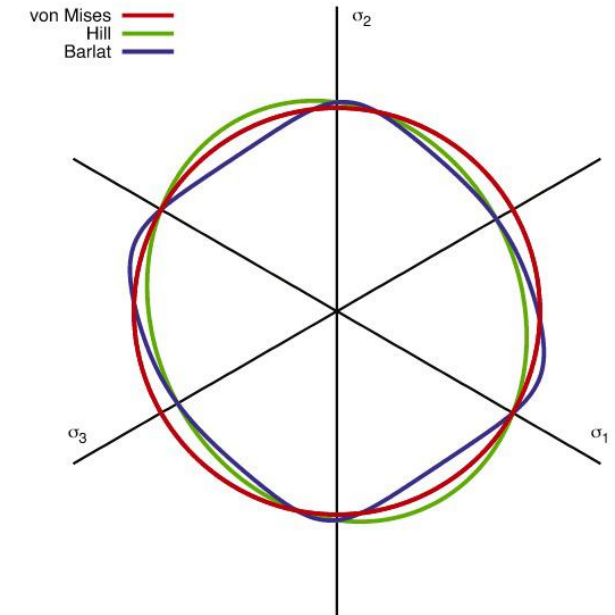
- Uniaxial tension tests out to 5% were taken on these samples
  - Symmetry boundary conditions were applied to all samples
- Stress-strain responses differed by at most 3% from the original mesh for all cases
- Crystallographic texture driving similarities in response
  - Voce hardening model lacks size dependence which could affect the trends seen here



Macroscopic stress strain curves for different size microstructures

# Why an anisotropic yield surface?

- If you're dealing with a strongly textured material a J2-type model probably isn't going to cut it
  - Rolling process to create sheet metal is well known for creating a textured materials that have orthotropic like behavior
- As-built AM materials can develop strong textures in the build direction
  - Post-build heat treatments and manufacturing processes such as HIP (high isostatic pressure) can reduce this issue
- Examine how varying the anisotropic properties of the material affects desired performance of a part



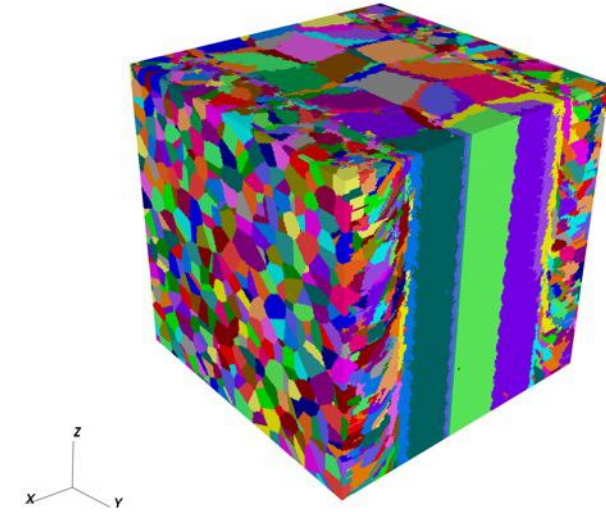
Yield surface comparison in the  $\pi$ -plane for 2090-T4 Al parameterization given in [9,10]

# Barlat Yield Surface Model (Yld2004-18p)

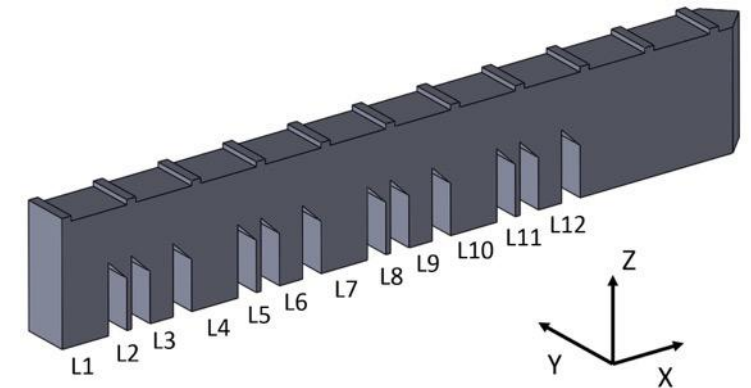
- Barlat and his associates have created several yield surfaces over the year to improve modelling of manufacturing processes
  - Sheet metal processes was one of the largest drivers in this process
- The Yld2004-18p model is one of his more famous ones
  - 18 parameter model that's largely orthotropic with some out of plane behavior
  - Nice properties in that it can reduce to several famous models such as J2, Hill, and Tresca yield surface model
  - As of end of 2021, we have this implemented in one of LLNL's in-house material library
    - An open-source version will be coming to ExaCMech within a year or so

# Implementation into an AM workflow

- Barlat model has traditionally been parameterized using experimental data
  - Data is not always easy to obtain nor cheap but simulations are “cheap”
  - Crystal plasticity simulations to the rescue
- ExaConstit is going to drive our simulations along with some workflow tools and python
  - Workflow tools will eventually be released as part of ExaConstit repo (contact if interested in them)
- Microstructure provided by an outside code, ExaCA
- Simple SciPy optimization function used to reduce error between the yield function predicted by Barlat model and outputted simulation response
  - Certain load conditions also make use of r-factor

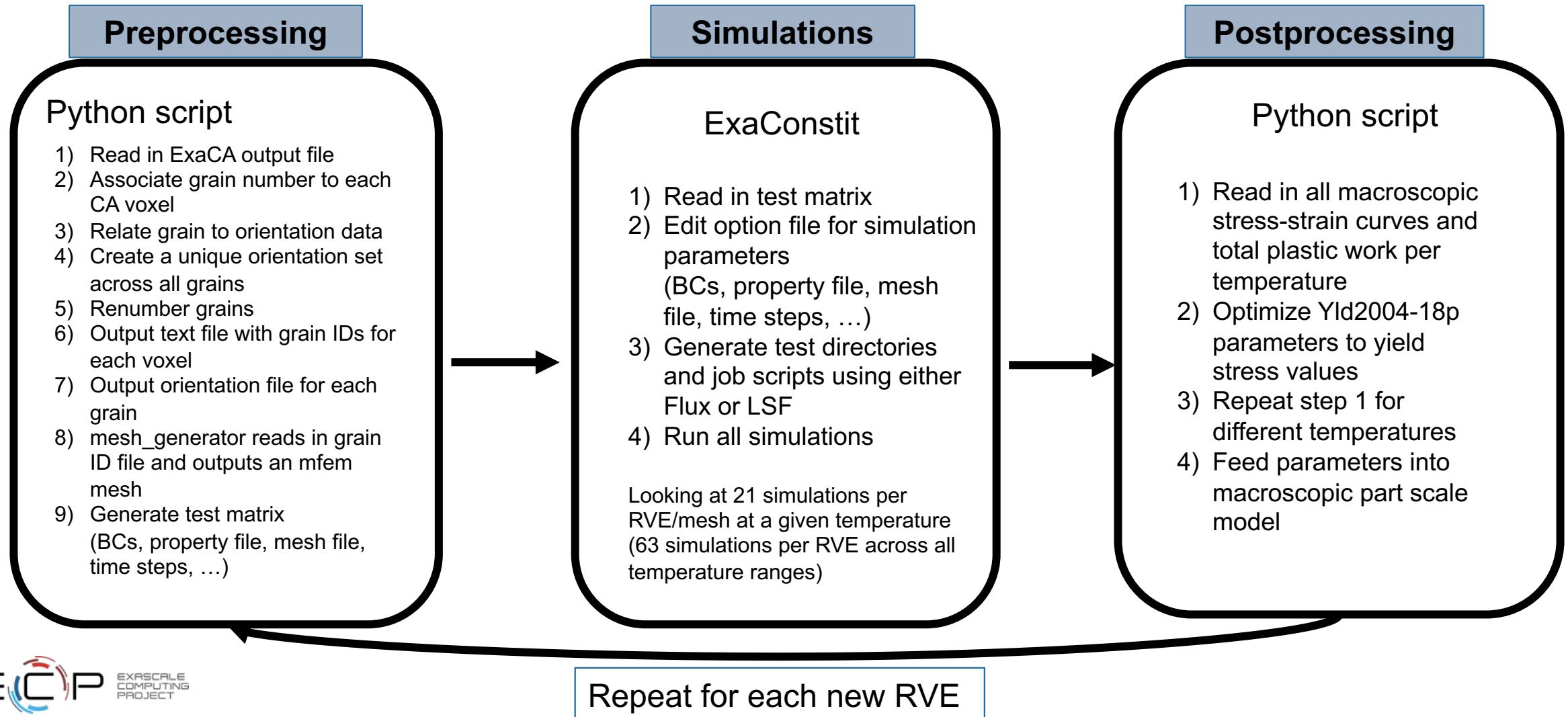


Microstructure of interest  
(L8 leg down below\*)



# We are collaborating with the ExaWorks team to enable execution of ExaAM workflow on Exascale platforms.

- Flux-based implementation of ExaCA-ExaConstit workflow resulted in a 2x improvement



# Preprocessing Step

- Python CLI script takes in a microstructure, generates a mesh, and creates a test matrix
  - Provided multiple temperatures and their corresponding property files
  - Can coarsen microstructure if needed
  - Test matrix generated will be later slurped up by job generation script

```
python3 ./exaconstit_cli_preprocessing.py -ifdir ./ -ifile exaca.csv -ofdir ./output_dir/ -runame
super_cool_microstructure -c 1 -mg -mgdir ./ -t 298.0 -fprops ./props_cp_voce_in625.txt -nprops 17 -fstate
./state_cp_voce.txt -nstates 24
```

```
if (args.mesh_generator):

    with cd(fdiro):
        result = subprocess.run('pwd', stdout=subprocess.PIPE)
        pwd = result.stdout.decode('utf-8')

    with cd(args.mesh_generator_dir):
        cmd = './mesh_generator'
        args = '-nx ' + str(dnx) + ' -ny ' + str(dny) + ' -nz ' + str(dnz)
        args = args + ' -lx ' + str(lx) + ' -ly ' + str(ly) + ' -lz ' + str(lz)
        args = args + ' -grain ' + pwd.strip() + '/' + gr_out
        args = args + ' -o ' + pwd.strip() + '/' + fout + '.mesh'
        args = args + ' -ord 1 -auto_mesh'
        cmd = cmd + ' ' + args
        print(cmd)
        result = subprocess.run(cmd, stdout=subprocess.PIPE, shell=True)
        mesh_file_loc = pwd.strip() + '/' + fout + '.mesh'
```

## Mesh generation code

```
data = {"rve_unique_name" : rve_name, "ori_file_name" : ori_file_name, "ngrains" : grain_num, "tempk" : temperature,
        "prop_file_loc" : lprop_file, "nprops" : nprop, "state_file_loc" : lstate_file, "nstates" : nstate,
        "ess_id_array" : lessential_ids, "ess_comp_array" : lessential_comps, "ess_vals_array" : lessential_vals,
        "loading_name" : lloading_name, "mesh_file_loc" : mesh_file}

df = pd.DataFrame(data)

df.to_csv(fdiro+'/'+fout+'_test_matrix.csv')
```

## Test matrix creation

# Job Generation Step

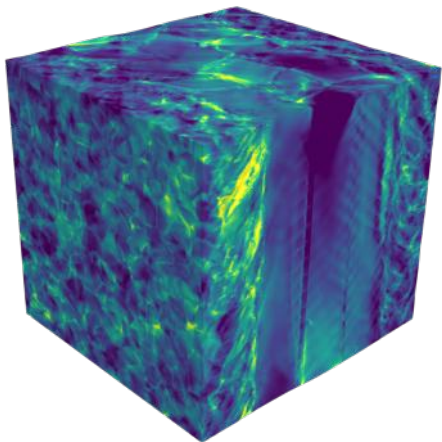
- Python CLI script takes in a test matrix, master option file, and a job submission file
  - Each simulation gets a unique job directory that has symlinks to original shared data
  - Master option file has regex searchable expressions in it that are replaced with test matrix values
  - Supports LSF or Flux job submission systems
    - Flux only required an additional 5 lines of code...
  - Generates a master job script that will submit all jobs for you
- Job generation could easily be extended to parametric studies

```
python3 ./job_cli.py -sdir ./ -odir ../workflow_runs/ -  
imtf file options_master.toml -iotfile options.toml -ijfile  
hip_mechanics.flux -ijfd ./ -iofile options.csv
```

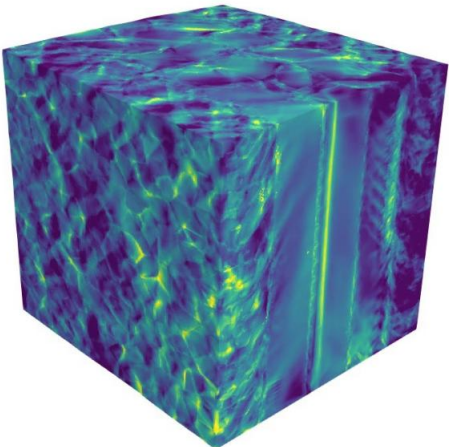
```
for iDir in range(nruns):  
    rve_name = df["rve_unique_name"][iDir]  
    load_dir_name = df["loading_name"][iDir]  
    temp_k = str(int(df["tempk"][iDir]))  
    fdiron = os.path.join(fdiro, rve_name, "")  
    fdironl = os.path.join(fdiron, load_dir_name+"_"+temp_k, "")  
    if not os.path.exists(fdironl):  
        os.makedirs(fdironl)  
    # Create symlink  
    for src in glob.glob(os.path.join(fdirs,"*")):  
        fh = os.path.join(fdironl, os.path.basename(src))  
        if not os.path.exists(fh):  
            os.symlink(src, fh)  
    toml = mtoml  
    for iheader in headers:  
        search = "%%" + iheader + "%%"  
        repl_val = str(df[iheader][iDir])  
        # This line is needed as toml parsers might get mad with just the  
        # 0. and not 0.0  
        repl_val = fixEssVals(repl_val)  
        toml = re.sub(search, repl_val, toml)  
    # Now do the avg_stress, avg_pl_work, avg_dp_tensor replacements  
    # We always want these to be unique names so if they're moved somewhere  
    # else we can always associate them with the correct run  
    # therefore, the name contains the rve name, temperature, and loading dir name  
    # frve_name+"_"+str(temp)+"_"+loading_dir_names[0]  
    ext_name = rve_name + "_" + temp_k + "_" + load_dir_name  
    for iheader in avg_headers:  
        search = "%%" + iheader + "%%"  
        replace = ext_name  
        toml = re.sub(search, replace, toml)  
  
    # Output toml file  
    fh = os.path.join(fdironl, os.path.basename(fotoml))  
    # Check to see if it is a symlink and if so remove the link  
    if os.path.islink(fh):  
        os.unlink(fh)  
    # We can now safely write out the file  
    with open(fh, "w") as f:  
        f.write(toml)  
    # Output job script file  
    fh = os.path.join(fdironl, os.path.basename(fin))  
    # Check to see if it is a symlink and if so remove the link  
    if os.path.islink(fh):  
        os.unlink(fh)  
    # We can now safely write out the file  
    with open(fh, "w") as f:  
        f.writelines(job_script)  
    os.chmod(fh, 0o775)
```

Main code logic

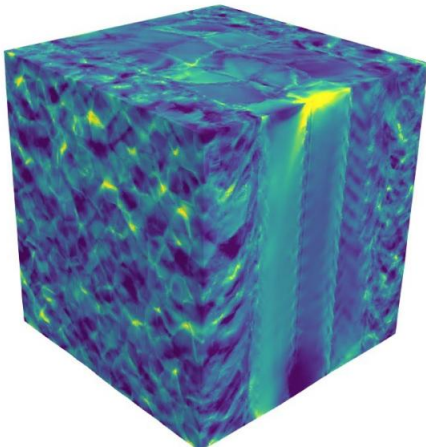
(Aside) AM microstructures have some crazy heterogeneous deformation



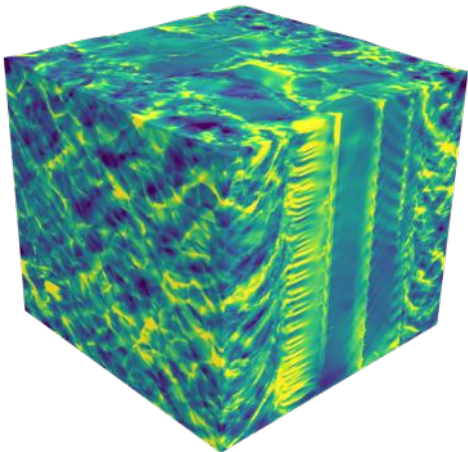
Loading x direction



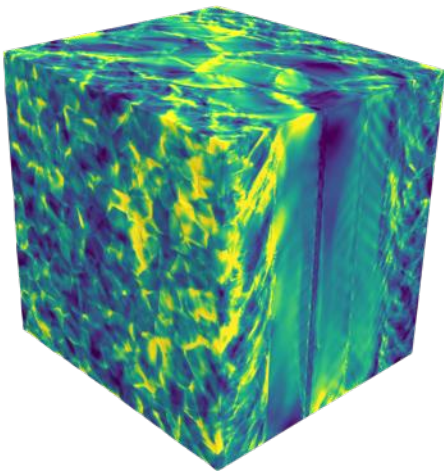
Loading y direction



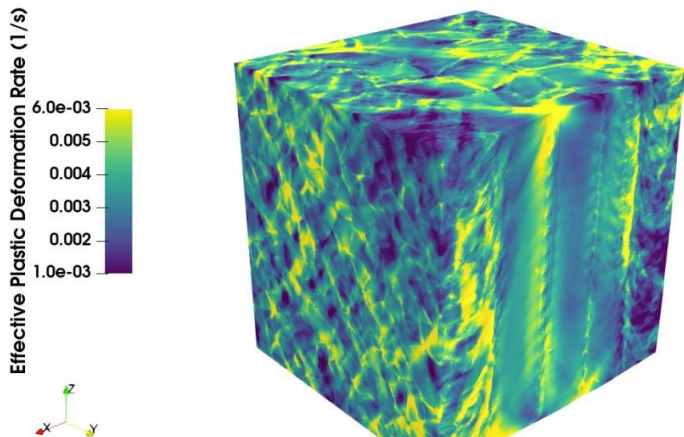
Loading z direction



Equal biaxial loading  
x-y direction

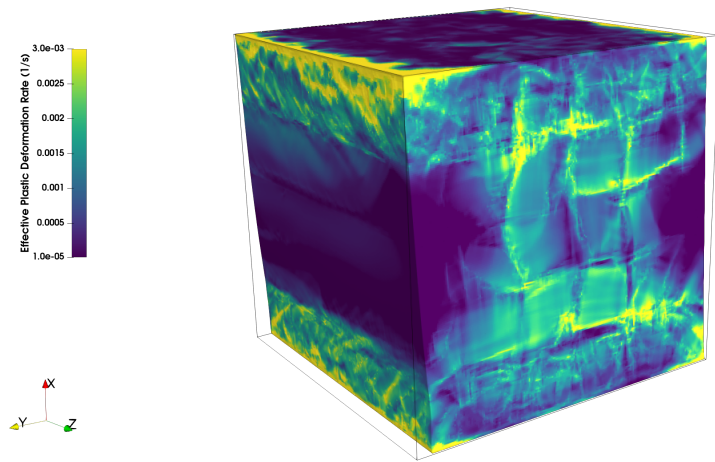


Equal biaxial loading  
y-z direction

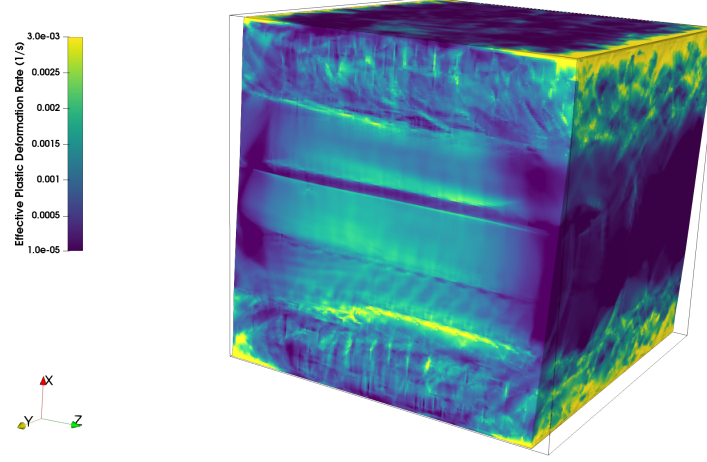


Equal biaxial loading  
x-z direction

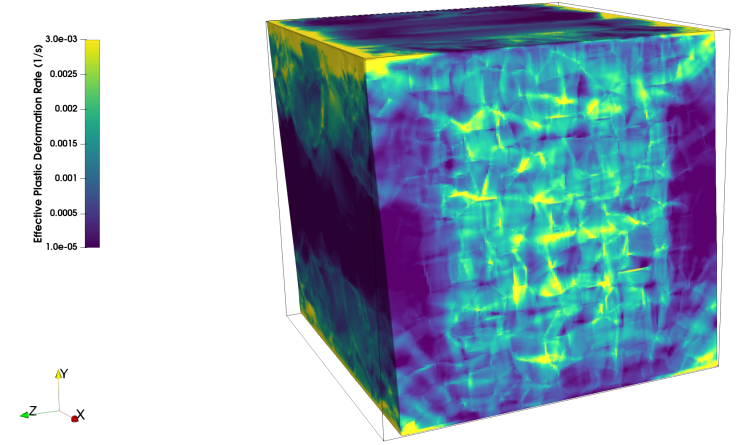
# (Aside) AM microstructures have some crazy heterogeneous deformation



Simple shear xy



Simple shear xz



Simple shear yz

# Optimization Procedure

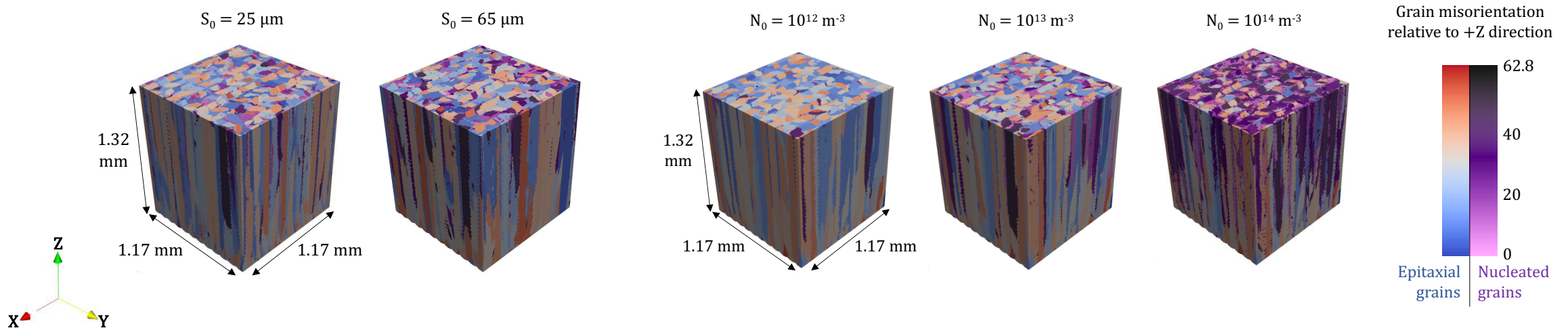
- For each temperature load up all volume average stress-strain responses and total volume plastic work values
  - Loading in the build direction (z-axis) is considered ground-truth for optimization purposes
  - Calculate 0.2% off-set yield and the plastic work associated with that
  - For all simulations find strain step closest to plastic work produce above and use associated stress value to calculate von Mises stress to be used in optimization procedure
  - Let optimization function do its thing (go grab some coffee/do other work)
    - Later temperatures use previous temperature parameters as initial guess to get within ball park

# ExaConstit in other areas

- ExaConstit can be used in areas outside of just the AM field
  - Quantifying variability in microstructure effects on material response
  - Fatigue applications and understanding deformation mechanisms at micro-scale is a large research area
  - Creating better material models to capture single crystal behavior
  - Modelling geological materials to understand how Earth's lower mantle deforms
  - Coupling experiments and simulations by using forward diffraction techniques
  - Modelling texture evolution of materials over large deformations

# Variability in processing conditions and effects on mechanical response

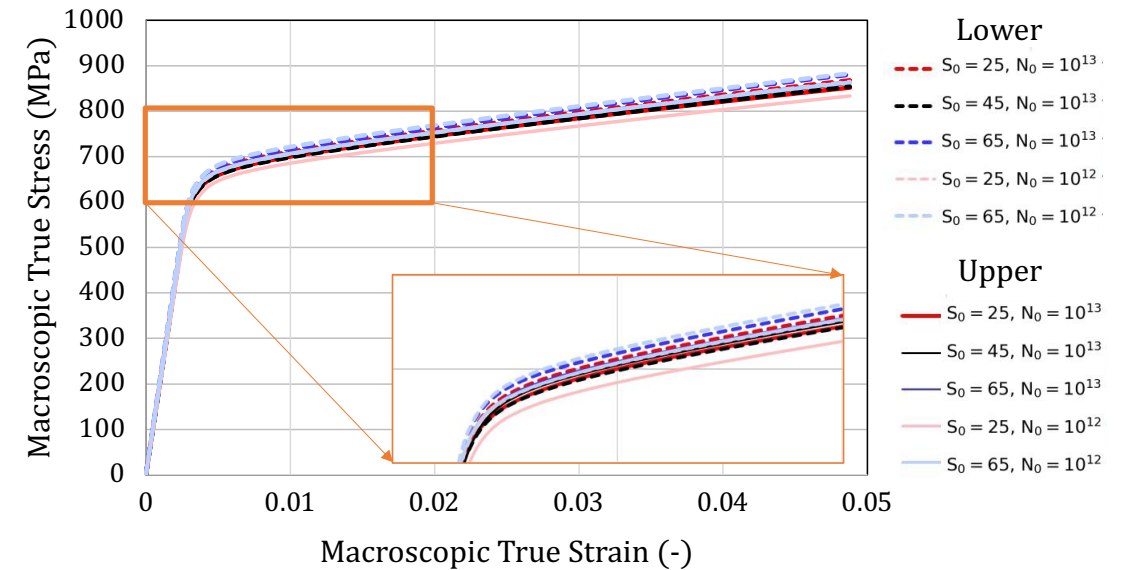
- Varying processing conditions can lead to different microstructures which can effect the micro-mechanical response of a material
  - Wide parameter space so usually best to focus on only a few aspects
- ExaAM team conducted a study on varying parameters that are inputted into ExaCA, microstructure generation code, and effects on micro-mechanical response for AM processes



Variation of AM substrate diameter and nucleation rate effects on microstructure

# Variability in processing conditions and effects on mechanical response

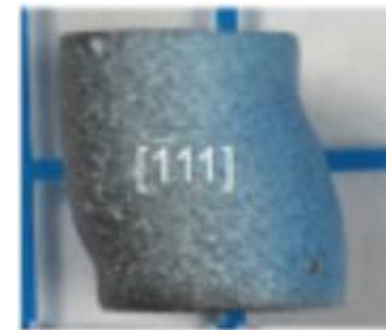
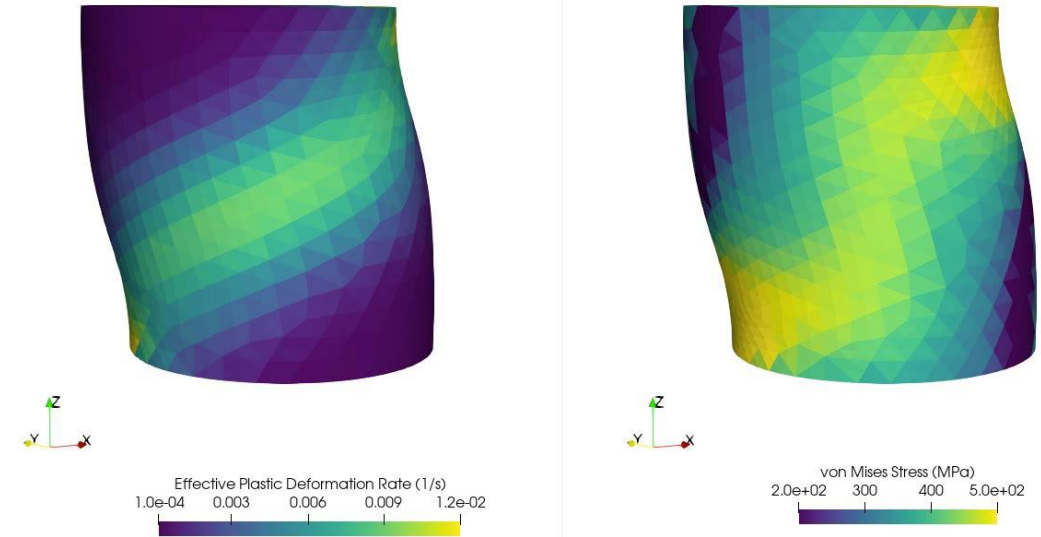
- Varying the substrate diameter and nucleation rate does affect the macroscopic response of the material
  - In cases examined, a difference of ~6% was noted between the min and max stress-strain responses
- Variation within the intragrain response was also noted and a larger variability was noted here as well



Variation of AM substrate diameter and nucleation rate effects on macroscopic response

# Simulating single crystal responses

- Capturing single crystal response of metals is often challenging as traditional crystal plasticity models were designed to capture response of polycrystalline materials
- We have an LDRD set-up to better examine this area and our working on some promising new model formulations
  - Capture buckling behavior as seen in experimental results as well as stress-strain response

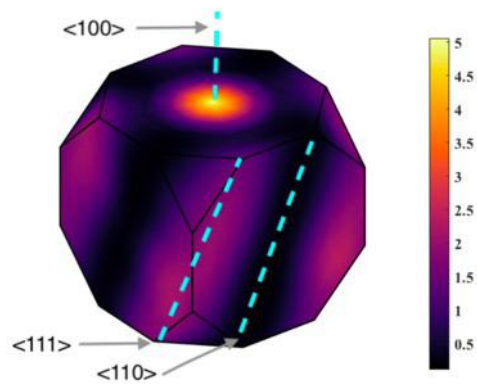


# Crystallographic Texture Evolution

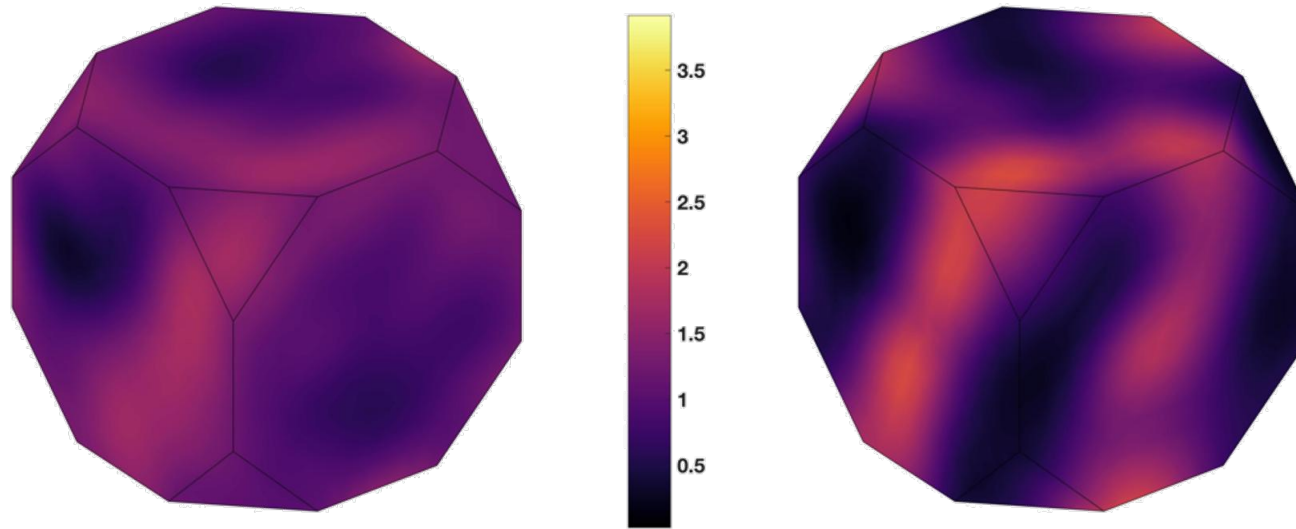
- Crystallographic texture informs of us the orientation dependence of a part in a given direction
- Texture plays a large role in determining how a part will deforms
- Manufacturers use texture to their advantage
  - Gas turbine blades are oriented in the  $\langle 100 \rangle$  direction to improve fatigue life [11]
  - Accounting for texture allows deep forming operations to reduce waste [12]
- Large texture development occurs over large applied strains
  - ExaAM is not concerned with strains typically needed for texture development

# Crystallographic Texture Evolution of AM parts

- A CA microstructure sample was monotonically compressed to 30% strain in order to develop a strong texture in the  $\langle 110 \rangle$  direction

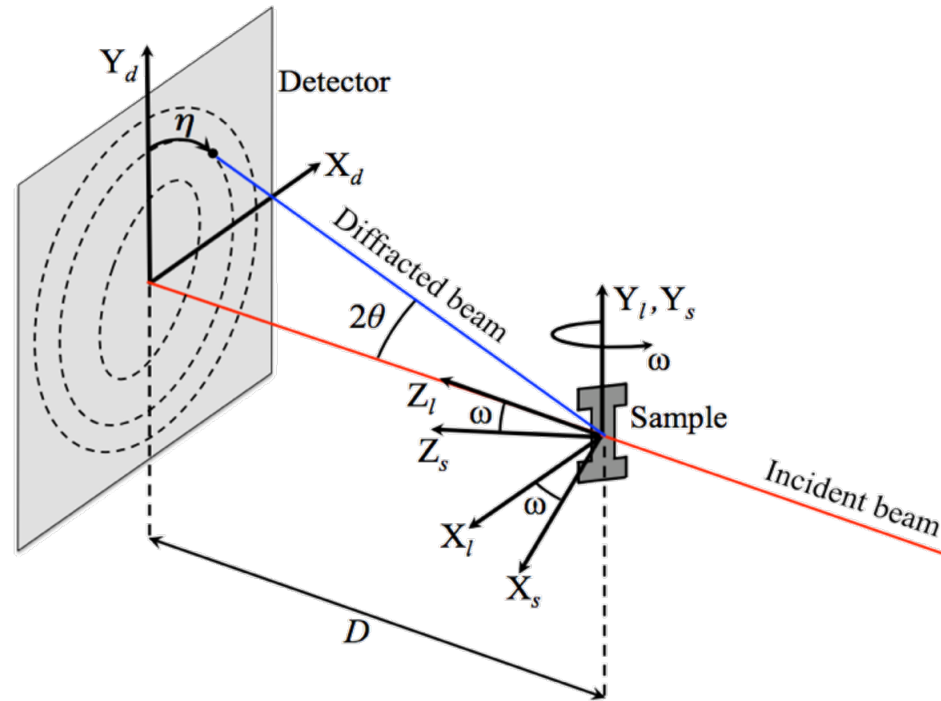


**Example of strongly textured material with various fibers labelled [13]**



**Initial (Left) and final (Right) crystallographic texture of the CA sample**

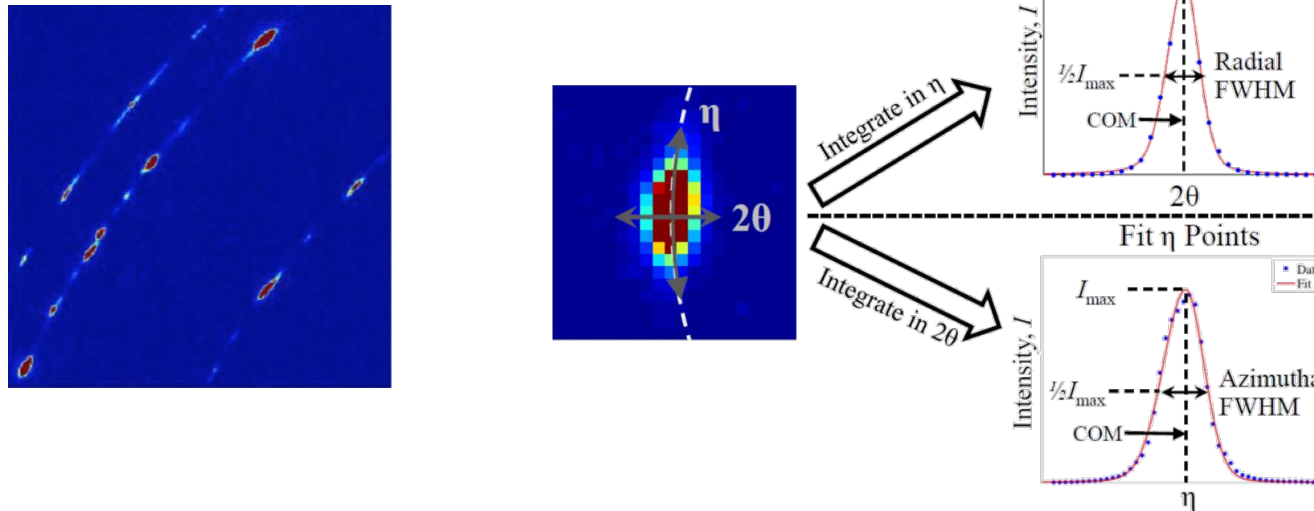
# Simulating High Energy X-ray Diffraction Experiments



**The peak data includes information about strain and lattice orientation of a grain**

# Simulating High Energy X-ray Diffraction Experiments

- Peak data is integrated in  $\omega$  direction and either  $\theta$  or  $\eta$  direction
  - Provides us with info about relative amounts of intragrain heterogeneity in either orientation,  $\eta$  spread, or strain,  $\theta$  spread.
  - Provides direct comparison to experiments



**Spread in peak data tells us relative amounts of intragrain heterogeneity in the elastic deformation**

# Summary

- ExaConstit is an open-source crystal-plasticity FEM code built on MFEM
  - Highly performant on systems ranging from desktops all the way to systems such as Summit
  - Implemented several different integrators for GPU support and different materials models
- Created a workflow in-collaboration with ExaWorks team to efficiently run large number of simulations needed to calculate local properties used in ExaAM's part scale simulations
  - Led to anisotropic yield surface model being added to one of LLNL's material modelling libraries
- ExaConstit is well poised to tackle a wide range of research topics within the crystal plasticity community

# Questions?

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