Center for micromorphic multiphysics porous and particulate materials simulations within exascale computing workflows

Multi-disciplinary Simulation Center (MSC)

PSAAP III Virtual Kickoff Meeting

18, 19 August 2020
University of Colorado Boulder

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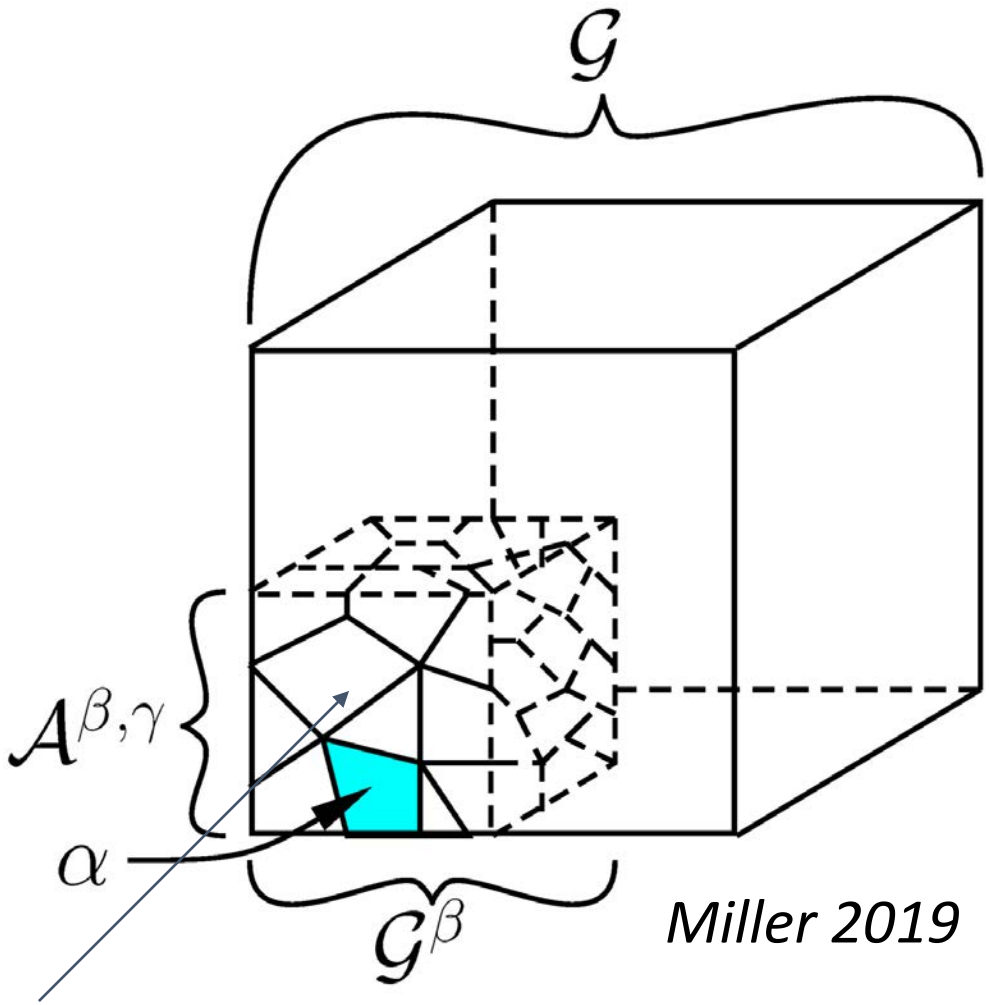
Rich Regueiro (PI), Henry Tufo (Co-PI)

Objectives

- (I) simulate with <u>quantified uncertainty</u>, from **pore-particle-to-continuum-scales**, a *class of problems* involving **granular flows, large deformations,** and **fracture/fragmentation of unbonded** and **bonded particulate materials**

Objectives (cont.)

- (II) **to achieve higher fidelity multiscale multiphysics computation through large deformation micromorphic continuum field theories,** *informed by DNS through the latest ML techniques,* <u>with DNS calibrated and validated against rich experimental data set</u>



Miller 2019

DNS domain, fully-overlapped with micromorphic continuum point

Overarching Problem

- **(I)** Processing and Thermo-Mechanical (TM) behavior of **compressed virgin and recycled mock HE material** subjected to *quasi-static and high-strain-rate confined and unconfined compression, in-situ (static) X-ray computed tomography (CT)*, and *dynamic Kolsky bar and gas gun experiments with ultrafast imaging at the APS and pRad*

- **mock HE** = mix of 10-600 micrometer diameter particles of idoxuridine (IDOX) with polymeric binder (Estane)

Processing Effects on Thermo-Mechanical Behavior of virgin and recycled mock HE

Figure 1. Post-test compression specimen from virgin PBX 9502 lot HOL83H890-019 [3].

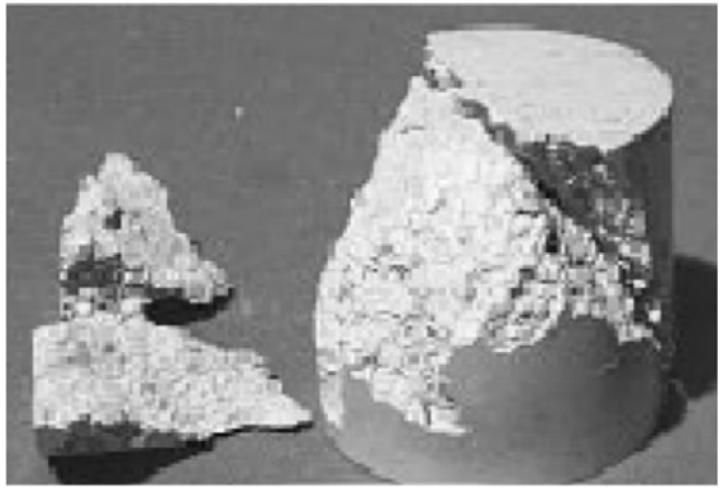


Figure 2. Post-test compression specimen from recycled PBX 9502 lot HOL88A891-005 [3].

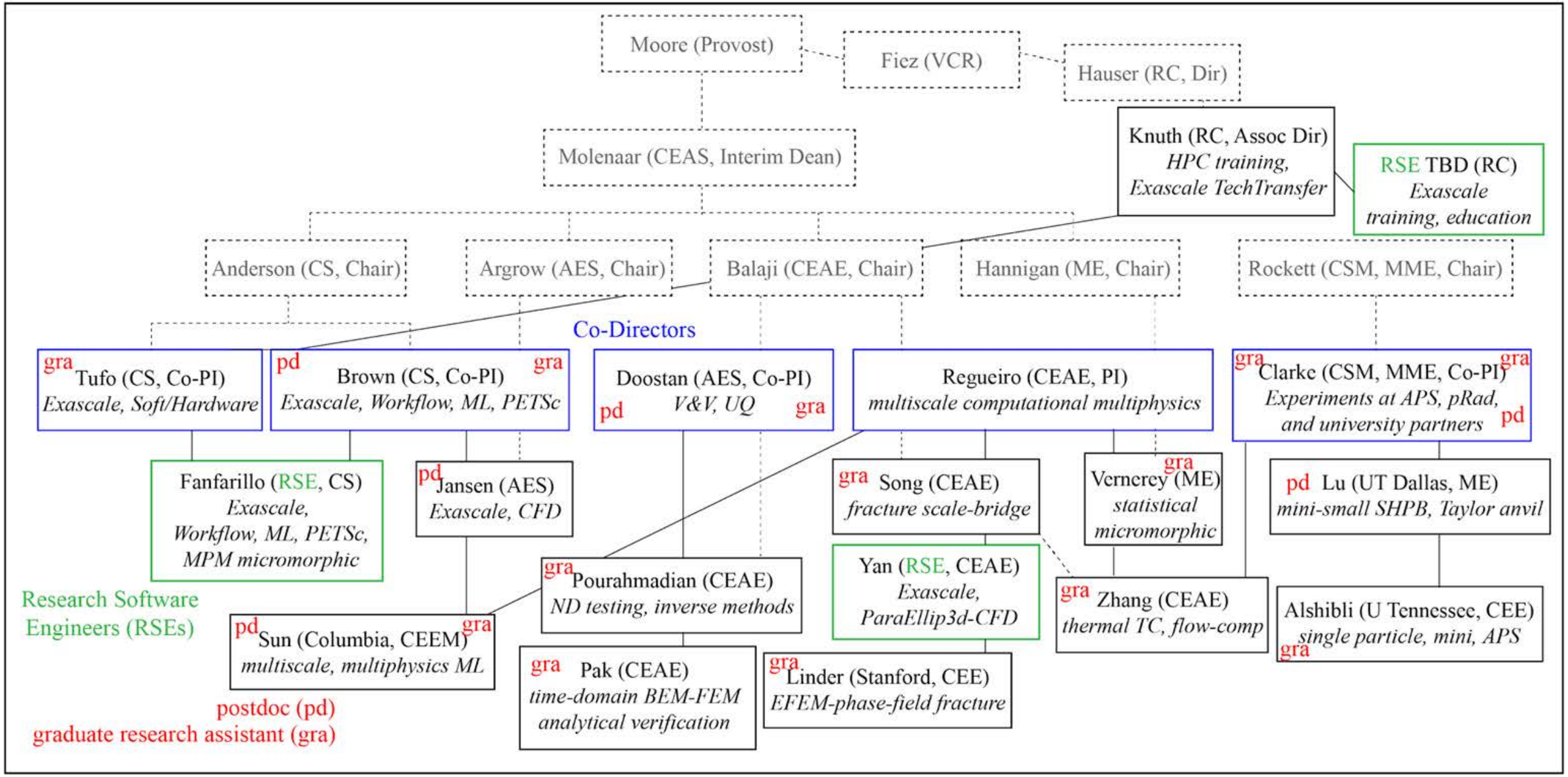
Peterson & Idar 2005

(a) Pressing Assembly (b) PBX 9502 Billet

Buechler et al. 2015

LANL 2015

Organizational Chart



Overarching Problem (cont.)

- **Processing:**
  - **(i)** flow and partial pressing of ~125M particles (~200 micrometer diam) of mock HE (IDOX-Estane) through pluviator into die shape (~10cm diam), or heated and flowed into die shape, with DNS coupled non-spherical oriented particle (crystalline) Discrete Element Method (DEM) – Material Point Method (MPM, for binder) – Computational Fluid Dynamics (CFD, air); ~125M non-spherical DEM particles, ~500 MPM material points for binder per particle, ~1000 CFD grids per particle = ~***125M non-spherical DEM particles coupled to (~500*125M=)~62.5B MPM points, both coupled to (~1000*125M=)~125B CFD grid blocks***
    -quantities of interest: density/porosity, texture distributions

Buechler et al. ASME 2016

(a) Pressing Assembly (b) PBX 9502 Billet

FIGURE 7: PHOTOGRAPHS OF PBX 9502 COMMON CHARGE AFTER PRESSING. PRESSED BILLET (A) INSIDE NEOPRENE BAG AND (B) REMOVED FROM BAG.

  - **(ii)** using (i) as initial state for DNS MPM (~1000 material points per particle and binder, or ***~1000*125M=~125B MPM material points per simulation***) for large deformation pressing (particle deformation and fracture, re-orientation for texture)
    -quantities of interest: density/porosity, texture

- **Q2**: "Why will it require exascale level computing?"
- **A2:** *Simulations (i)-(ii) push the limits of current Petascale machines, not including UQ; thus, when including UQ, Exascale is justified*

Overarching Problem (cont.)

- **Thermo-Mechanical (TM) behavior:**
  - **(iii)** machine ~1-2cm diam cylinders out of large pressed mock HE material for TM - Embedded Finite Element Method (EFEM) and phase field (phase) <u>simulation of frictional cracking under quasi-static and high rate</u> compression (with **scale bridging**; ~3 orders of magnitude less resolution than (ii) for ~2000 FEs per 1cm diam cylinder simulation (with scale-bridging, ~1000 MPM points per FE, or ~1 DE + 500 MPM points per FE)

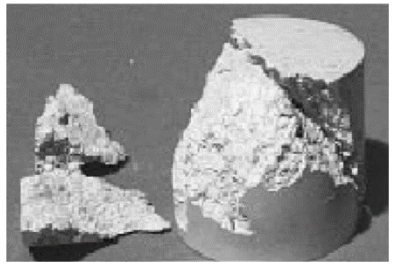
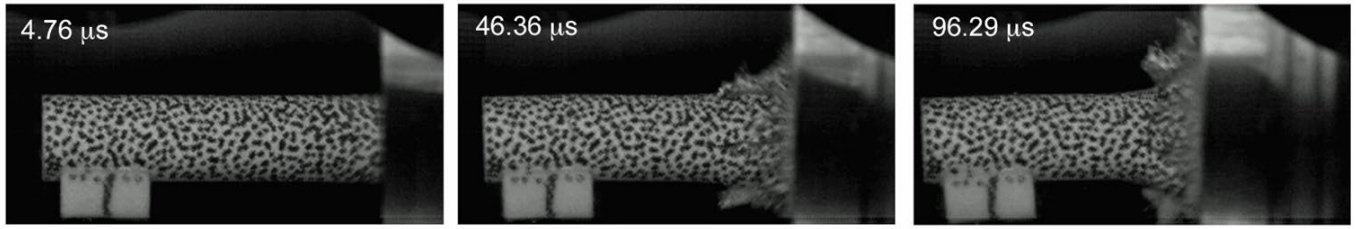


Figure 2. Post-test compression specimen from recycled PBX 9502 lot HOL88A891-005 [3].

Peterson & Idar PEP 2005

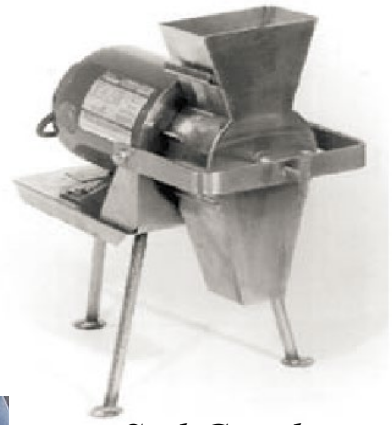
Ferranti et al LLNL 2010



-quantities of interest: force (magnitude, duration) of impact, fracture/fragmentation pattern, particle size distribution, local heating/strain-rate

Overarching Problem (cont.)

- **Grind, Recycle, Repeat (i)-(iii):**
  - **(iv)** simulate with DNS DEM-MPM-CFD the ***grinding and/or washing of mock HE for recycling***, into <0.5mm particle size (similar simulation resolution as (i) and (ii), but more effort because of grinding and mixing)
    -***quantities of interest: particle size distribution***
  - **(v) repeat steps (i)-(iii)**

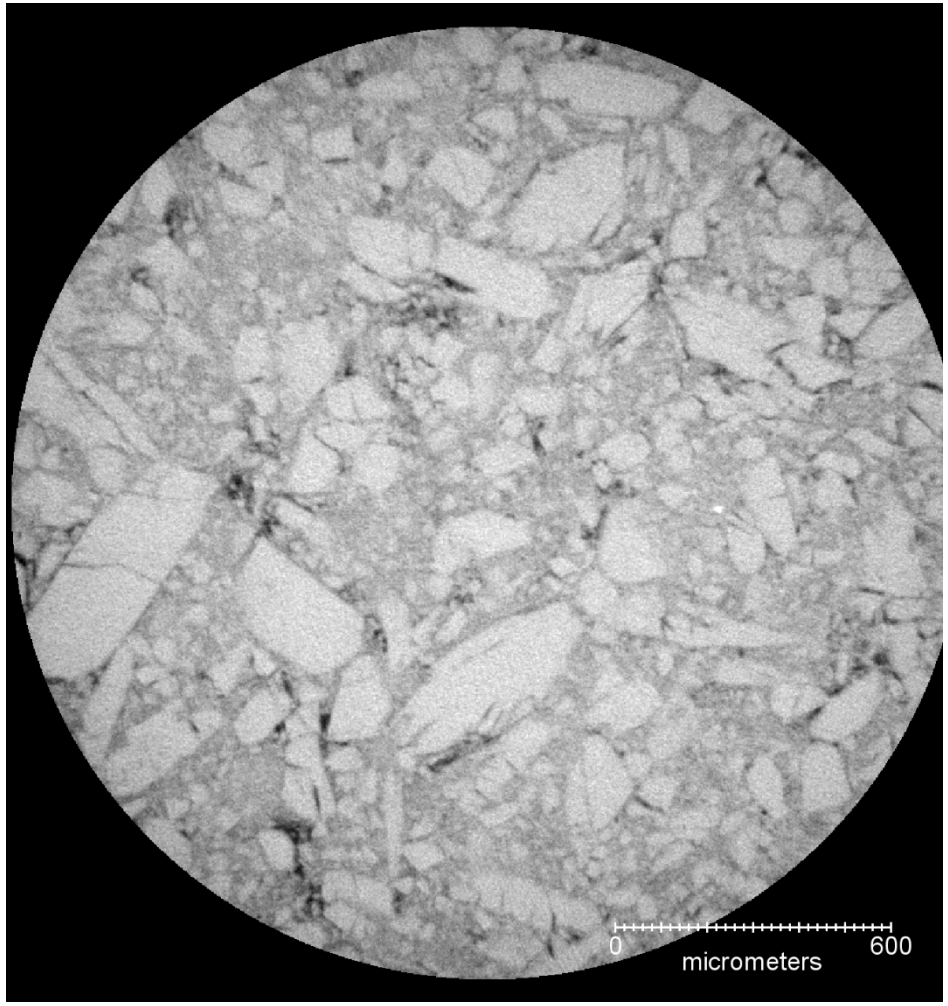


Soil Grinder

heated and flowed (LANL 2015)

- **Poro-Mechanical (PM) scale-bridging for (i)-(ii)** (pouring and pressing)
- **Thermo-Mechanical (TM) scale-bridging for (iii)** (thermal TC, SHPB, gas gun)
- **add Statistical Micromorphic Continuum features with offline DNS ML for all scale-bridging simulations**

Example IDOX + binder CT



CT POC: Brian Patterson (bpatterson@lanl.gov)

IDOX POC: John Yeager (jyeager@lanl.gov)

Overarching Problem: *Simpler Materials*

- **Simpler Materials studied before mock HE:**

  - **(a)** ***glass beads of various size and shape, and various gradations, and/or aluminum particles with similar specs, with bonded 10-20 particles***, 1cm diameter cylinders, with same binder (Estane) as used for mock IDOX HE (same experiments and simulations (no HPC required) as for (iii))

  - **(b)** ***silica (Ottawa) sand with various grain size distributions, unbonded and bonded***, with different binders (HTPB, HYTEMP, HYCAR, Estane); processing into ~10cm dies, and machining or direct formulation of 1mm, 1cm, 5cm cylinders; and individual particle experiments (same experiments and simulations as for (i)-(v), HPC required)

Predictive Science Plan

- **annual full system simulations:**
  - **Year 1:**
    i. develop full V&V/UQ workflow (no HPC required) for **simpler 10-20 ~5mm diam glass beads or aluminum particles with binder** in 1-2cm diam cylindrical specimens, with *all experiments and modeling tools brought to bear* (TDBEMC, DEM, DEM-MPM, DEM-CFD, MPM, EFEM, phase field, micromorphic upscaling with fracture, statistical micromorphic, ML micromorphic)
    ii. DEM simulation of ~1M ~1mm diameter **silica sand** pouring into ~10cm diameter die (vacuum; simulations currently on DoD HPCs; need to compile and run *ParaEllip3d-CFD* on DOE NNSA HPCs)

Predictive Science Plan (cont.)

- **annual full system simulations (cont.):**
  - **Year 2:**
    i. (cont.) complete full V&V/UQ workflow (no HPC required) for **simpler 10-20 ~5mm diam glass beads or aluminum particles with binder** in 1-2cm diam cylindrical specimens, with *all experiments and modeling tools brought to bear* (TDBEMC, DEM, DEM-MPM, DEM-CFD, MPM, EFEM, phase field, micromorphic upscaling, statistical micromorphic, ML micromorphic)
    ii. DEM-CFD **exascale** simulation of ~1M ~1mm diameter **silica sand** with ~1B CFD grids (air) pouring into ~10cm diameter die (air)
    iii. ~250k ~125M DEM-MPM and ~250M MPM-MPM simulations of ~250k ~1mm diameter **silica sand with binder** in 1-5cm diameter cylindrical specimens (thermal TC, SHPB, Taylor anvil)
    iv. upscaling of Y2.iii to micromorphic continuum with fracture

Predictive Science Plan (cont.)

- **annual full system simulations (cont.):**
  - **Year 3:**
    i. DEM-MPM-CFD **exascale** simulation of ~1M ~1mm diameter **silica sand with binder** with ~500M MPM points and ~1B CFD grids (air) pouring and pressing into ~10cm diameter die (air); machine out 1cm diam specimens for testing as in Y2.iii and upscale as in Y2.iv
    ii. DEM-CFD simulation of ~250k ~200 micrometer diameter **IDOX** with ~250M CFD grids (air) pouring into 1cm diameter die (air)
    iii. ~31.25M ~15.625B DEM-MPM and ~31.25B MPM-MPM **exascale** simulations of ~31.25M ~200 micrometer diameter **mock HE (IDOX-Estane)** in 1-5cm diameter cylindrical specimens (thermal TC, SHPB, Taylor anvil)
    iv. upscaling of Y3.iii to micromorphic continuum with fracture

Predictive Science Plan (cont.)

- **annual full system simulations (cont.):**
  - **Year 4:**
    i. DEM-MPM-CFD **exascale** simulation of ~1M ~1mm diameter **recycled silica sand with binder** with ~500M MPM points and ~1B CFD grids (air) pouring and pressing into 10cm diameter die (air); machine out 1cm diam specimens for testing as in Y2.iii and upscale as in Y2.iv
    ii. DEM-MPM-CFD **exascale** simulation of ~125M ~200 micrometer diameter **mock HE (IDOX-Estane)** with ~62.5B MPM points and ~125B CFD grids (air) pouring and pressing into ~10cm diameter die (air); machine out 1cm diam specimens for testing as in Y2.iii and upscale as in Y2.iv

Predictive Science Plan (cont.)

- **annual full system simulations (cont.):**
  - **Year 5:**
    i. DEM-MPM-CFD **exascale** simulation of ~125M ~200 micrometer diameter **recycled mock HE (IDOX-Estane)** with ~62.5B MPM points and ~125B CFD grids (air) pouring and pressing into ~10cm diameter die (air); machine out 1cm diam specimens for testing as in Y2.iii and upscale as in Y2.iv
    ii. Year 5 prediction: *attempt to quantify processing effects on the dynamic, thermo-mechanical behavior of* ***recycled*** *mock HE*

V&V/UQ Plan

- **<u>Verification</u> will follow a Multi-level plan**
- **<u>Validation</u> will use Bayesian inference and DNN-based inversion techniques**
- **<u>Uncertainty Quantification</u> (UQ) will rely on structure-exploiting techniques (sparsity, intrinsic low-dimensionality, etc)**

Multi-Level Verification

- **Numerical:** comparison of numerical methods (DEM, MPM, FEM, CFD, …) to each other and analytical solutions, where available:
  - **Elasticity solutions**: FEM, MPM
  - **Elastic inclusion solutions**: coupled DEM-MPM
  - **Flow around a sphere**: coupled DEM-CFD, and MPM-CFD
  - **Mode I and II loading of elasto-plastic or elasto-damage interfaces**: DEM-MPM, MPM-MPM
  - **MMS**
  - **Micromorphic:** null DNS filtering cases, 1D uniaxial stress/strain, micro-stretch, micro-shear, micro-rotation cases

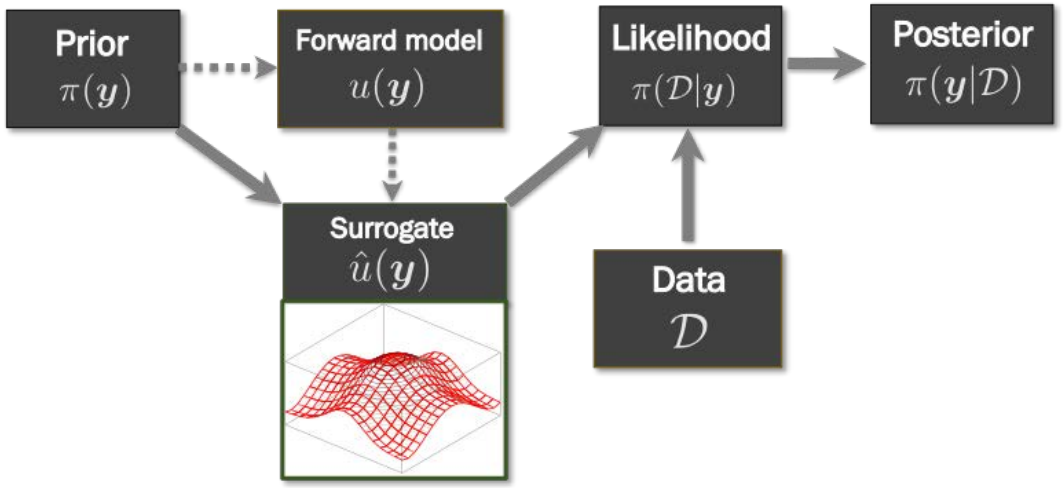
Multi-Level Verification (cont.)

- **Analytical:** develop fundamental rigorous analytical/manufactured solutions for generalized/ micromorphic continuum mechanics theory for comparison:
  - **Suitable combination** of mathematical and numerical techniques
  - **Step-by-step approach**: governing equations, boundary/ interfacial conditions
  - **Linearization:** for poro-thermo-anisotropic-elastodynamic settings
  - **Solution's characteristic features**: number of wave types, nature of wave fronts, attenuation, jumps, shocks, singularities, sharp corners, …
  - **Green's functions** for basic testing and integral formulations

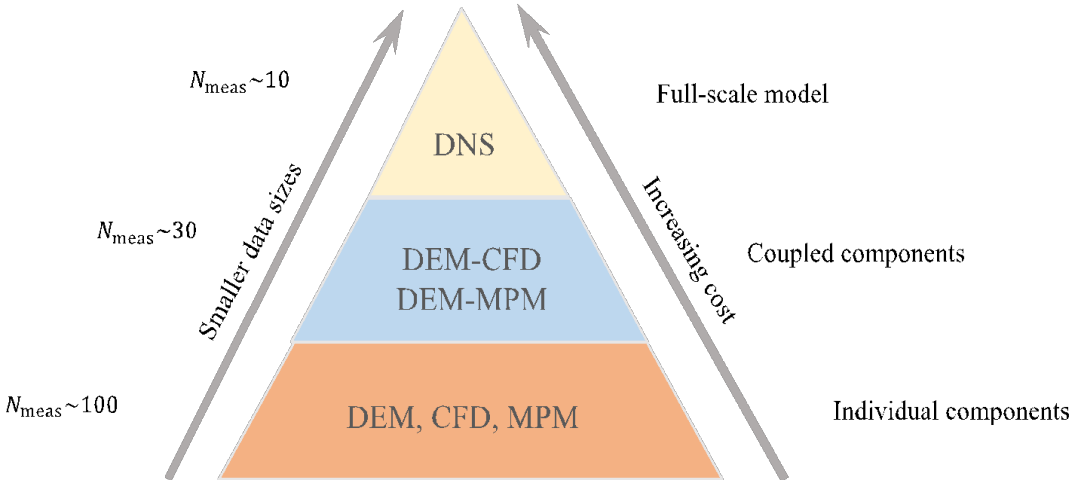
Model Calibration and Validation Strategies

- Model calibration: Surrogate-assisted Bayesian inference and DNN-based inversion techniques – key is the ability to efficiently build accurate surrogates
- Model validation: Hypothesis-testing-based approaches (mean or pdf comparison) at component level
- Focus on model ranking/selection (via the Bayesian framework)
- Hierarchical approach for system model validation

Surrogate-assisted Bayesian Inference



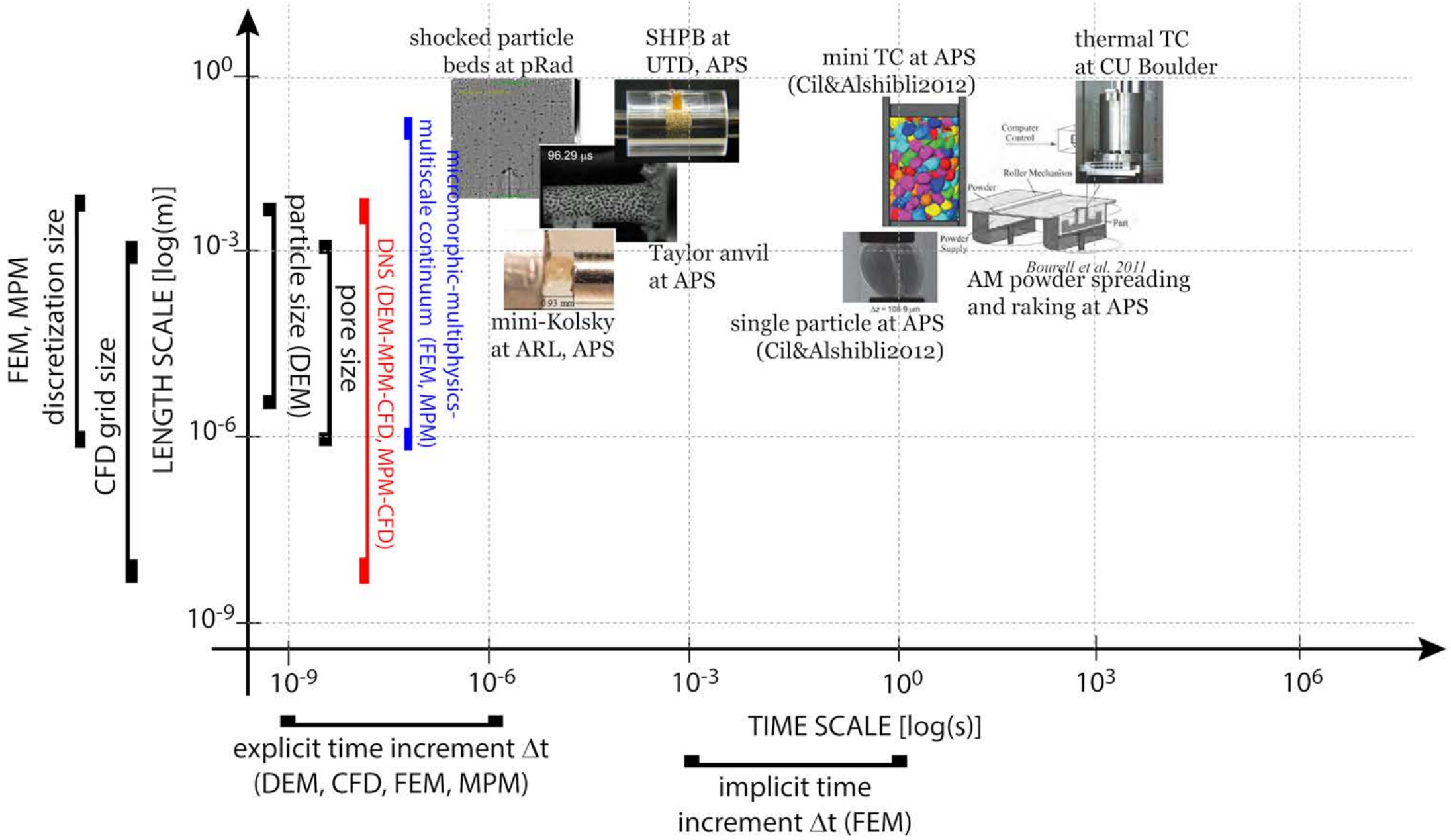
Hierarchical Approach to Model Validation

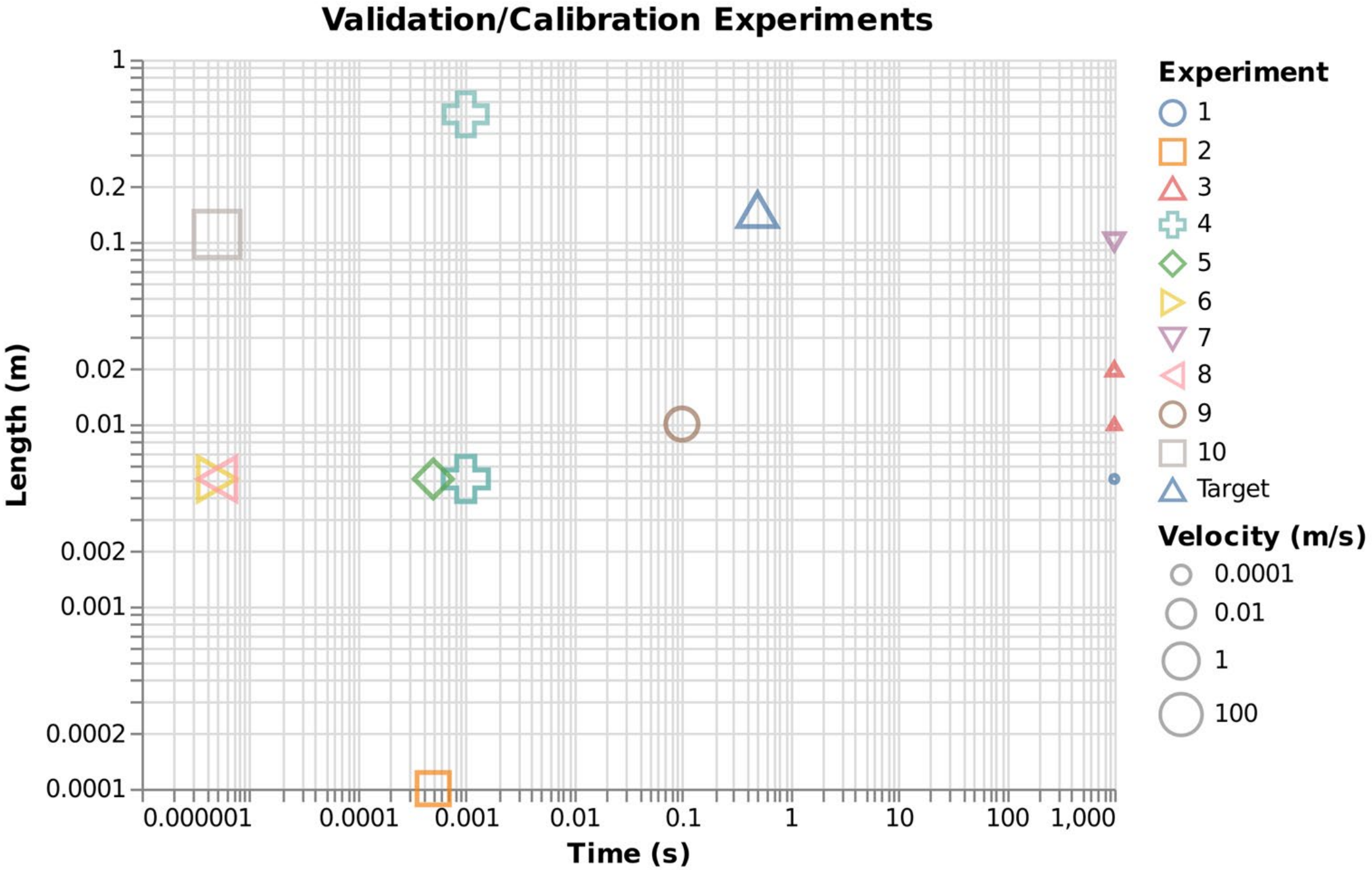


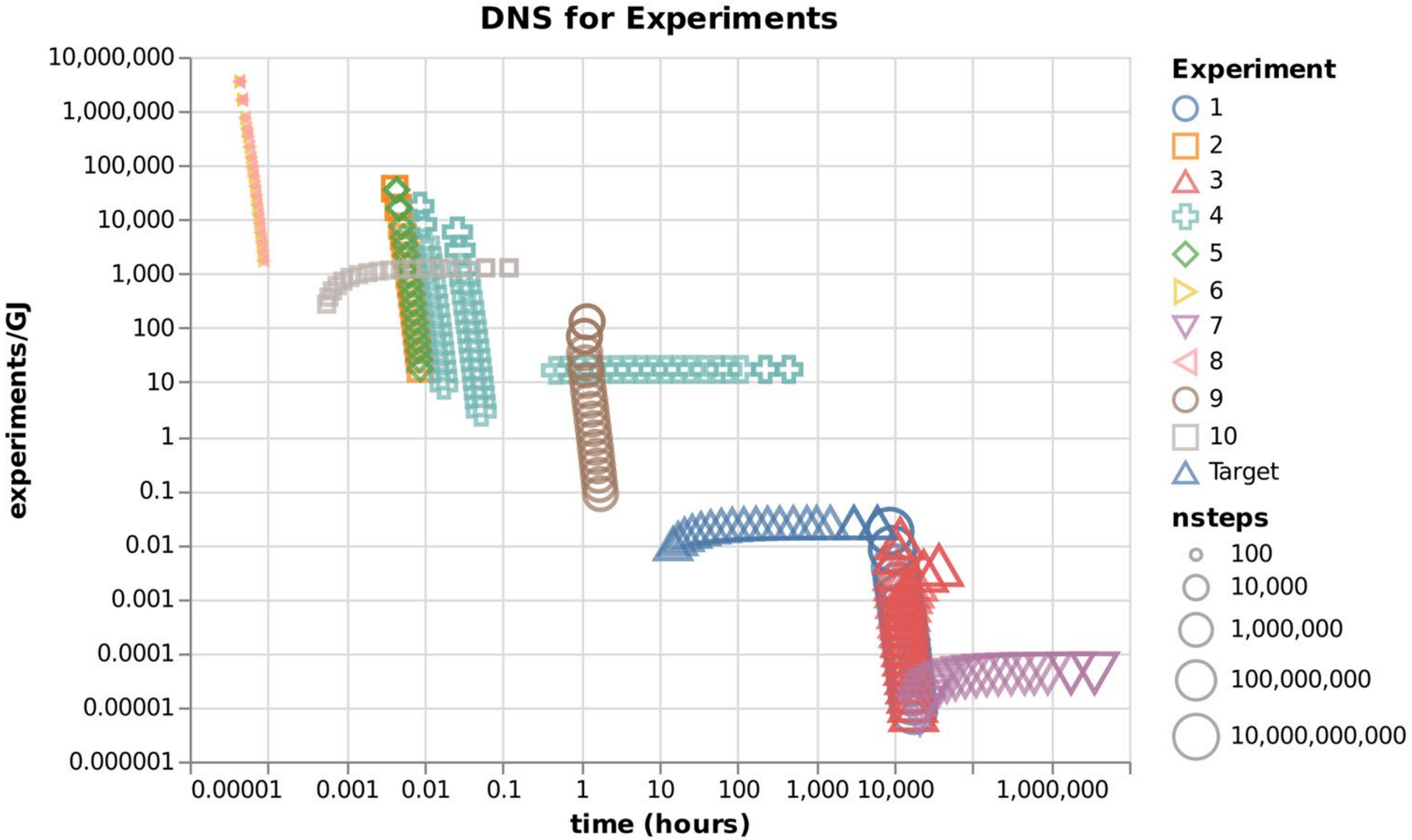
Forward UQ Strategies

- **Structure-exploiting** techniques to tackle curse-of-dimensionality – sparsity, low intrinsic dimensionality:
  - Basis and sample adaptive compressed sensing techniques (sparsity)
  - Data-driven basis learning techniques for compressed sensing (sparsity)
  - Generative modeling assisted compressed sensing
  - …
- **Multi-fidelity DNN** representations
  - Improved variance reduction for training
  - Transfer learning
  - Data-informed regularization
  - …

Experiments and Associated Modeling Length and Time Scales

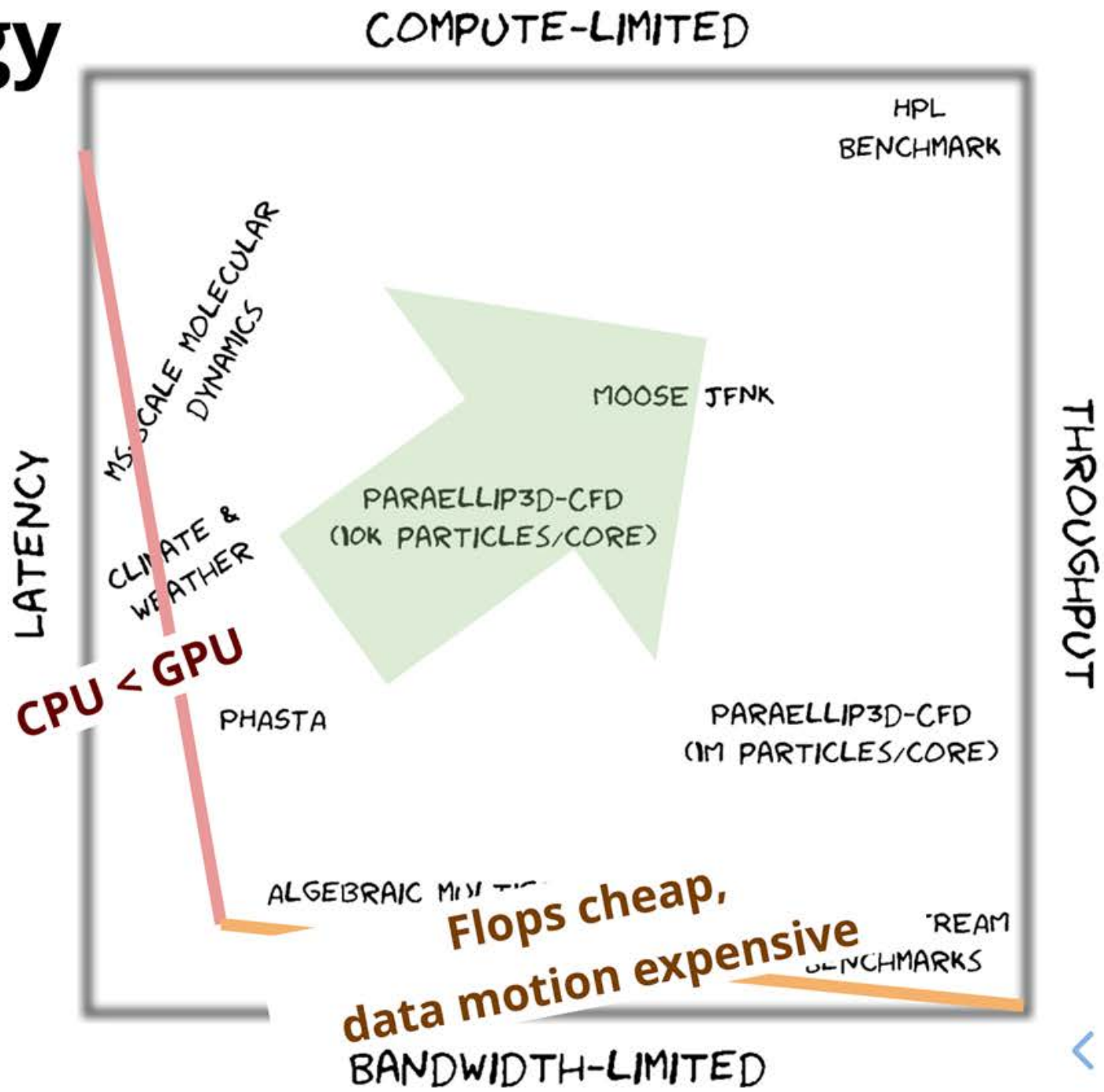



Validation/Calibration Experiments
Length (m)
1
0.2
0.1
0.02
0.01
0.002
0.001
0.0002
0.0001
0.000001
0.0001
0.001
0.01
0.1
1
10
100
1,000
Time (s)
Experiment
1
2
3
4
5
6
7
8
9
10
Target
Velocity (m/s)
0.0001
0.01
1
100

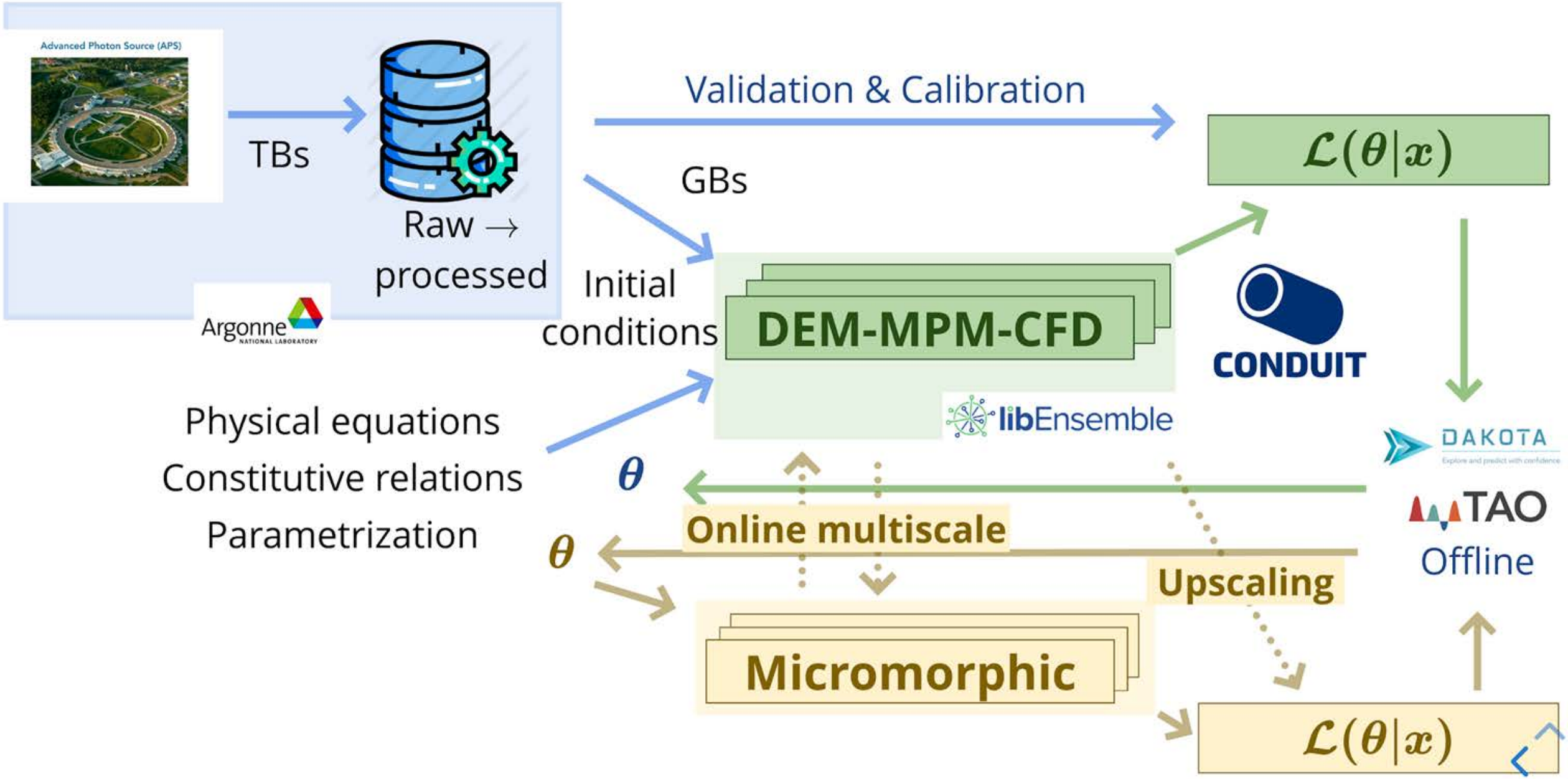

DNS for Experiments
experiments/GJ
10,000,000
1,000,000
100,000
10,000
1,000
100
10
1
0.1
0.01
0.001
0.0001
0.00001
0.000001
0.00001
0.001
0.01
0.1
1
10
100
1,000
10,000
1,000,000
time (hours)
Experiment
1
2
3
4
5
6
7
8
9
10
Target
nsteps
100
10,000
1,000,000
100,000,000
10,000,000,000

Algorithmic strategy

- Latency-hiding algorithms
  - Overlap communication and computation
  - Instruction-level parallelism vs SIMT occupancy
- Data locality
  - Kernel fusion
  - Cache-awareness
- Algorithmic scalability, implicitness
- Data structure transformations
  - Store vs (re)compute
  - Data sparsity, low-rank
  - Kronecker product



Workflow

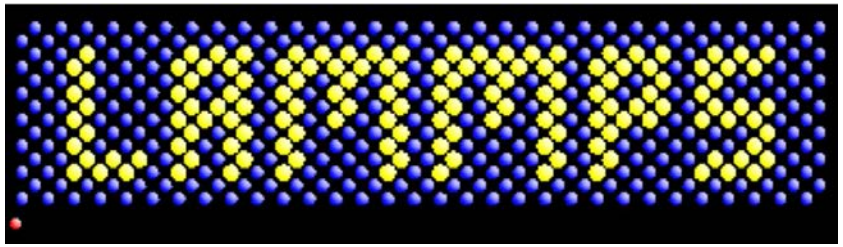

Advanced Photon Source (APS)
TBs
Raw → processed
Argonne NATIONAL LABORATORY
Validation & Calibration
GBs
$\mathcal{L}(\theta|x)$
Initial conditions
DEM-MPM-CFD
CONDUIT
libEnsemble
Physical equations
Constitutive relations
Parametrization
θ
θ
DAKOTA
Explore and predict with confidence
TAO
Offline
Online multiscale
Upscaling
Micromorphic
$\mathcal{L}(\theta|x)$

Software Plan

- **Existing codes in Center:** will develop on ***gitlab.com/micromorph***
  - petascale OpenMP/MPI *ParaEllip3d-CFD* polyellipsoidal, coupled DEM-CFD code (open source, Yan)
  - petascale MPI TDBEM-FEM code (Pak)
  - coupled FEM-DNS upscaling micromorphic continuum code *Tardigrade (MOOSE)* (open source, Miller)
  - 3D fracture models (EFEM, phase-field) in *deal.II* (open source, Linder) to be merged with *Tardigrade* (open source, Song, Linder)
  - multiphase exascale CFD code *PHASTA* (open source, Jansen)

Software Plan (cont.)

- **Existing codes outside Center:**
  - *GEOS-MPM* (limited to LLNL): plan to port over to *GEOS-x* (open source, LLNL); planning collaboration with LLNL
  - *LAMMPS* (open source, Sandia)



  - *PETSc* (open source, ANL)
  - *MOOSE* (open source, INL)
  - *deal.II* (open source)

Software Plan (cont.)

- **Codes/Capabilities to be developed for Center:**
  - MPM extension of *Tardigrade* (postdoc, Miller)
  - MPM coupling (for binder) in *ParaEllip3d-CFD* (Yan)
  - sphero-polyhedral particles shapes, simple fracture model, orientation-dependent particle elasticity in *ParaEllip3d-CFD* (Yan)
  - statistical mechanics extension of *Tardigrade* (Vernerey, GRA, Miller)
  - machine learning (ML) extension of *Tardigrade* (Sun, Brown, Fanfarillo, postdoc, GRA, Miller)
  - Exascale modifications/recoding of all codes (Fanfarillo, Yan, Brown, Jansen, Tufo)

Continuous Integration

GitLab

ECP
EXASCALE COMPUTING PROJECT

- Containerized tests with different operating systems and compilers
- Local testbeds for emerging architectures
- ECP-developed CI at LCFs
  - Correctness tests
  - Performance regression tests
    - Longitudinal monitoring & analysis

Documentation

SPHINX
Python Documentation Generator

- Website
- Manual and API documentation
- Language bindings

binder

- Interactive tutorials

Integration Plan

- During **Year 1,** use **simpler 10-20 ~5mm diam glass beads or aluminum particles with binder** 1-2cm diam cylindrical specimens to **develop full V&V/UQ workflow**, conducting <u>all experiments</u> (except larger 10cm diam die pressing) and <u>all modeling components</u> of project (but no HPC, yet)
- then continue with **silica sand**, toward **mock HE**

Key Challenges

- recruiting US citizen PhD students
- executing Integration Plan in Year 1 (will likely carry over to Year 2)
- demonstrating "exascale readiness" in Year 2 without an exascale machine (will submit proposals to access Frontier at ORNL)
- achieving Y4.ii exascale simulation (DEM-MPM-CFD ~125M ~200 micrometer diameter **mock HE (IDOX-Estane)** with ~62.5B MPM points and ~125B CFD grids)