Center for Shock Wave-processing of Advanced Reactive Materials (C-SWARM)

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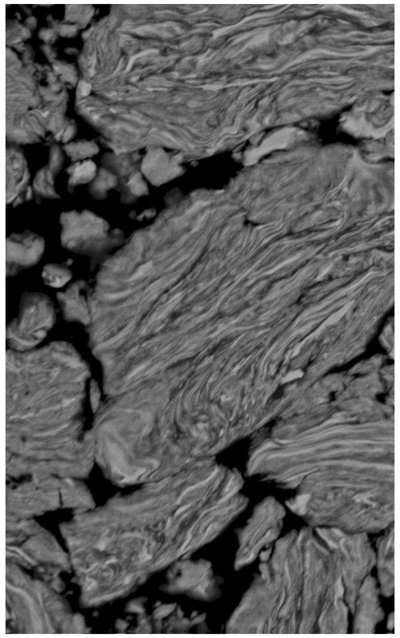
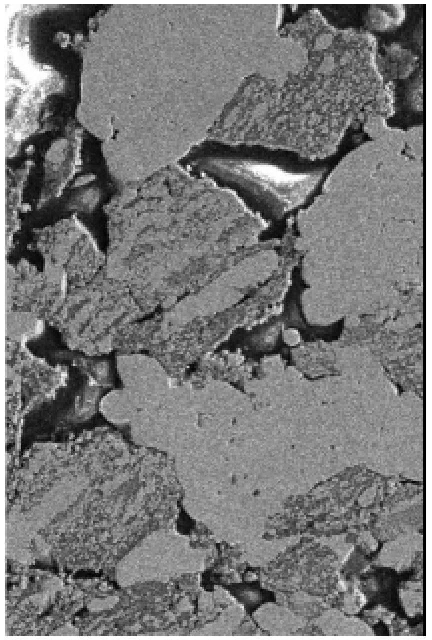
Shock Wave-processing of Advanced Reactive Materials



High Energy Ball Milling (HEBM)

C-SWARM
Verification
Prediction



Validation/UQ
Discovery

- Continuum modeling framework
- Truly multiscale in space, time, and constitutive equations
- Chemo-thermo-mechanical behavior
- Solid-solid state transformations

Physical Problem Description

- Formation of controlled microstructures
  - unique mechanical, thermal and chemical properties
- Heterogeneous reactive materials
  - higher energy density, multi-functionality
  - potential for fabrication of novel materials
- High strain rate processes
  - 10^{-3} s^{-1} quasi-static, 10^{2} -10^{4} s^{-1} high, 10^{4} -10^{7} s^{-1} very high
- Shock synthesis
  - shock induced - time scale of mechanical equilibrium (ns)

Specific Goals of C-SWARM

- Predict behavior of heterogeneous materials undergoing shock-induced chemo-thermo-mechanical transformations.
- The transformations are governed by a plethora of physics/ chemistry.
- Use adaptive Exascale simulations to predict conditions for synthesis of novel materials-by-design.
- The work will enable us to discover materials with unique and tailored characteristics; e.g., porosity, yield stress.

How are the Goals Accomplished?

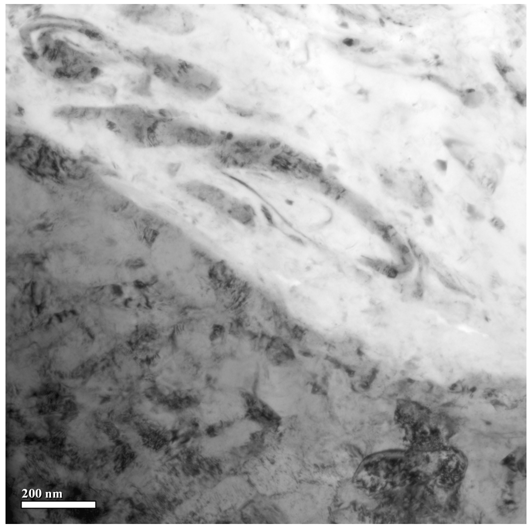
Implementation of five plans:

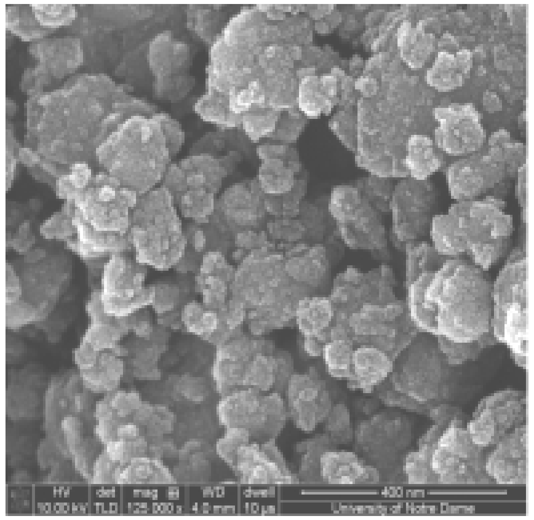
- Predictive Science
- V&V/UQ and Experimental Physics (EP)
- Exascale
- Software
- Integration

Applied to:

Demonstration System: simulation of the shock-induced synthesis of a nickel-aluminum (Ni-Al) composite in a reverse Taylor impact experiment performed every year.

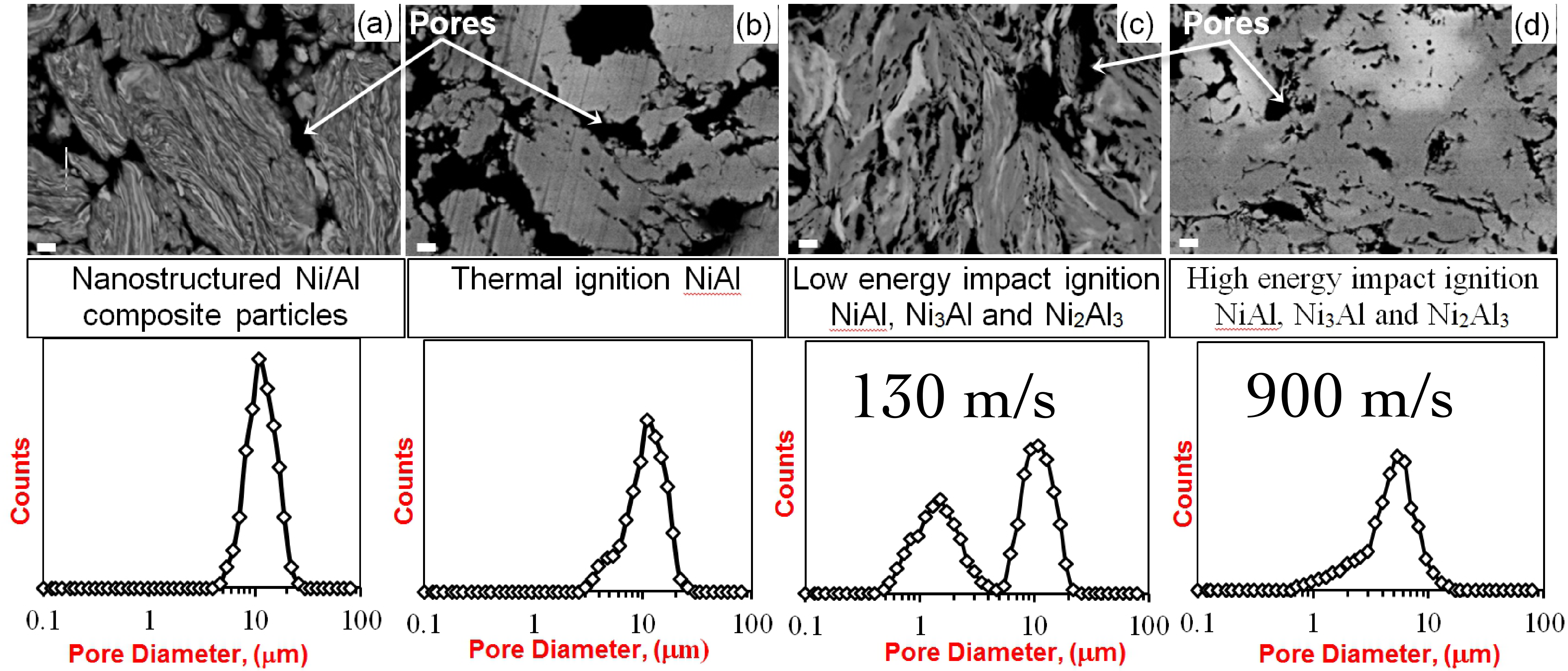
Discovery System: identification of conditions under which we can synthesize cubic boron nitride (*c*-BN) through a reverse Taylor impact experiment.





Demonstration System (Ni-Al)

- Reversed ballistics Taylor impact experiment



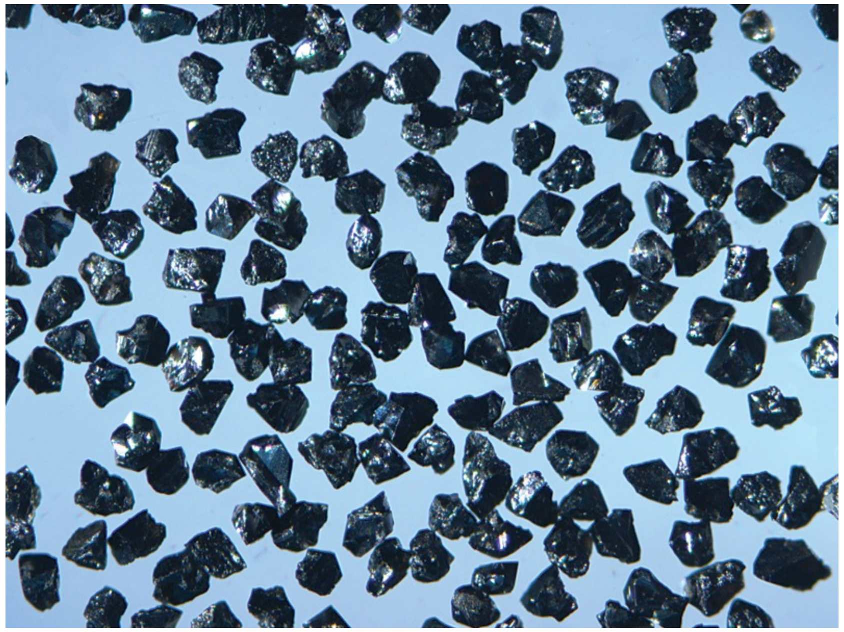
- Chemo-thermo-mechanical behavior
- Solid-solid state transformations
    - Intermetallic crystals (e.g., Ni_3Al), Arrhenius kinetics

Discovery System (*c*-BN)

- Identify initial material morphology and, *P* and *T* conditions for shock synthesis of *c*-BN

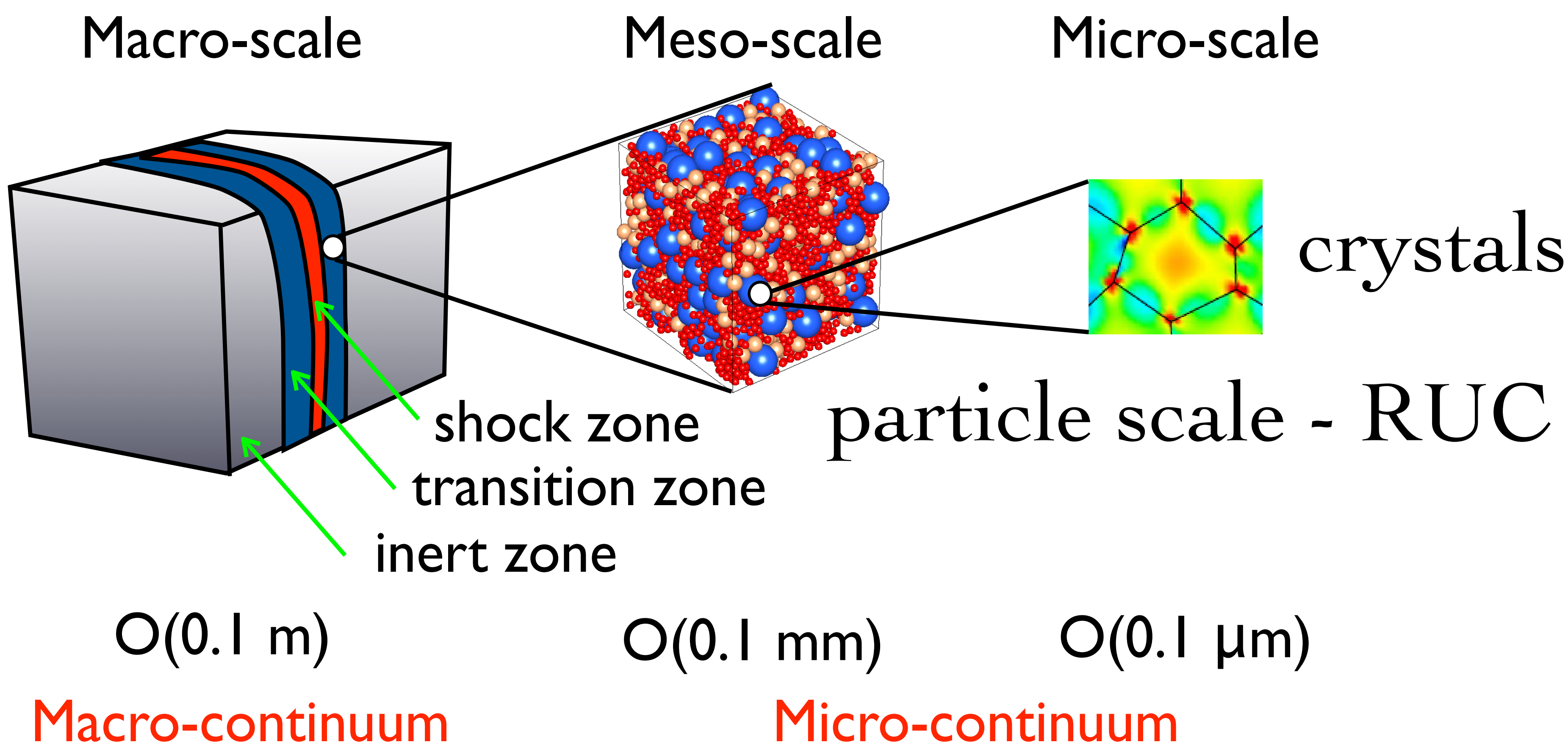
$$3\,\mathrm{B} + \mathrm{TiN} \xrightarrow{P,T} c\text{-BN} + \mathrm{TiB_2}$$

- *c*-BN is not found in nature; it can only be produced synthetically.
- Hardness of *c*-BN is similar to diamond, but its thermal and chemical stability is superior.
- *c*-BN surpasses diamond in high temperature applications (steel machining, i.e. tool bits, cutting tools).
- Contrary to diamond, larger *c*-BN pellets can be produced by fusing (sintering) *c*-BN powders.



Modeling and Computational Aspects

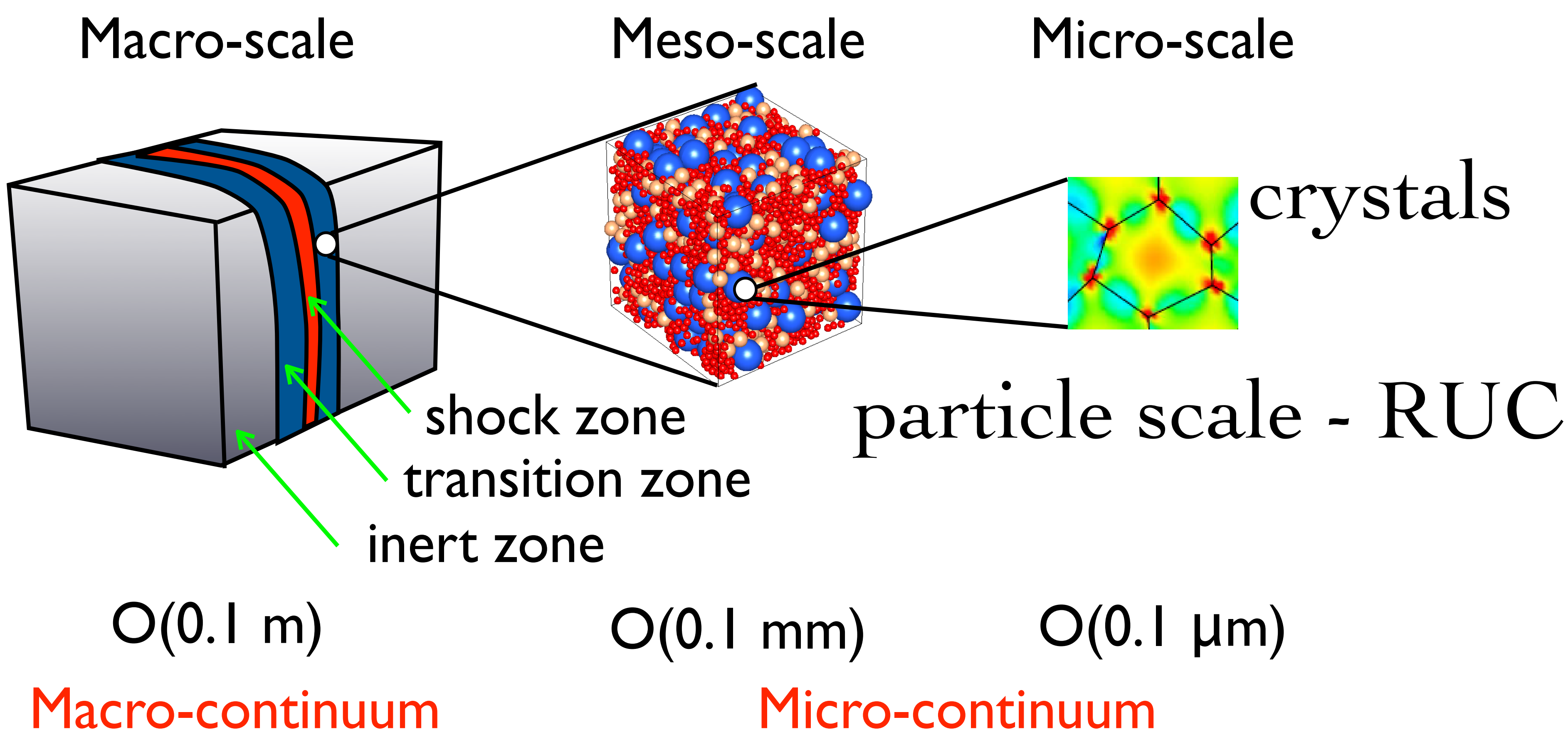
- Hierarchical multiscale modeling concept
- Macro(M) and micro(m) codes - M&m



- Image-driven modeling - Representative Unit Cell (RUC)
- Shock thickness ~ 1-5 particle diameters
- Need to resolve sub-crystal levels - ~0.02 μm

▸ Continuum modeling concept

Computational Complexity



Shock zone

$\sim 10^4$ cells x 10^{10} dofs/RUC

$\approx 10^{14}$ dofs

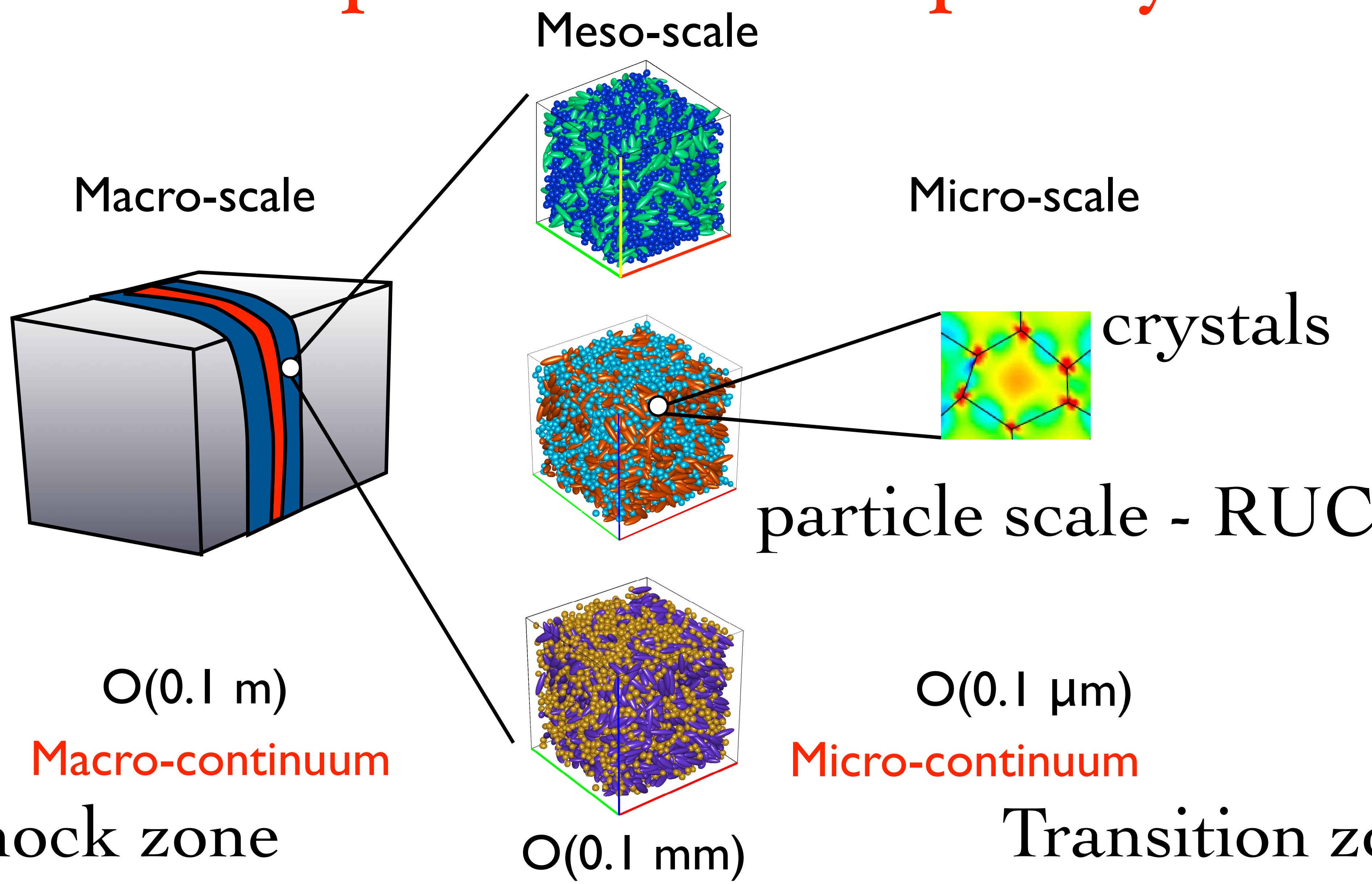
Transition zone

$\sim 10^3$ cells x 10^8 dofs/RUC

$\approx 10^{11}$ dofs

- This is just one deterministic simulation

Computational Complexity



Shock zone

~10^4 cells x 10^{10} dofs/RUC

≈10^{14} dofs

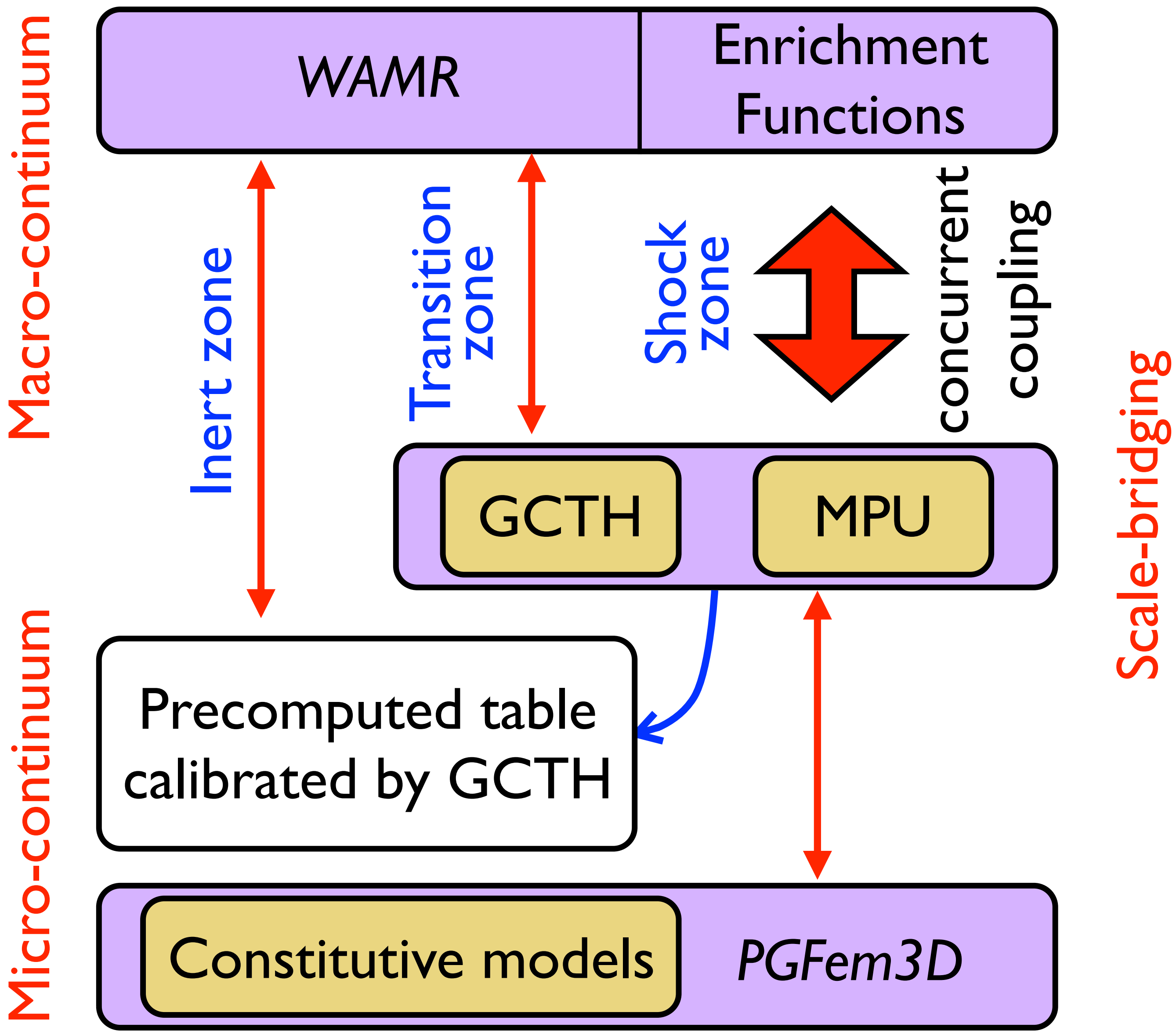
Transition zone

~10^3 cells x 10^8 dofs/RUC

≈10^{11} dofs

Scale Bridging - M&m

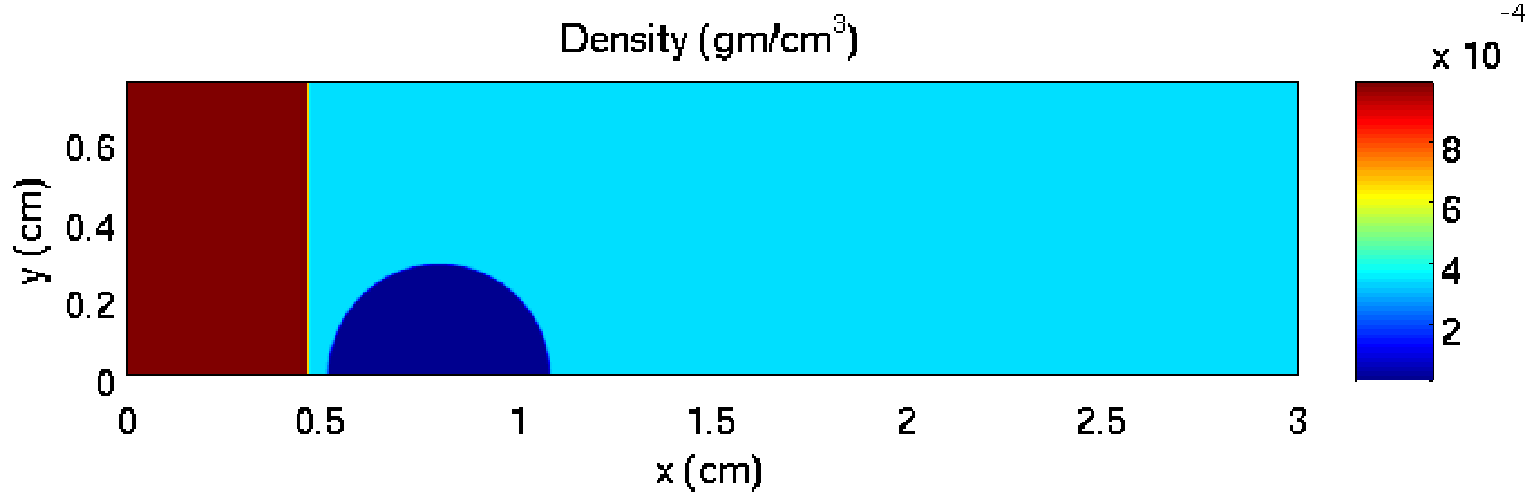
- Generalized Computational Theory of Homogenization (GCTH)
- Multiscale Partition of Unity (MPU)



- Model Selection
  - Localization knowledge from *WAMR*
  - Principal stress/strain
  - V&V/UQ
  - *A posteriori* constitutive model error estimates
- I^2-ASLib, ParalleX model

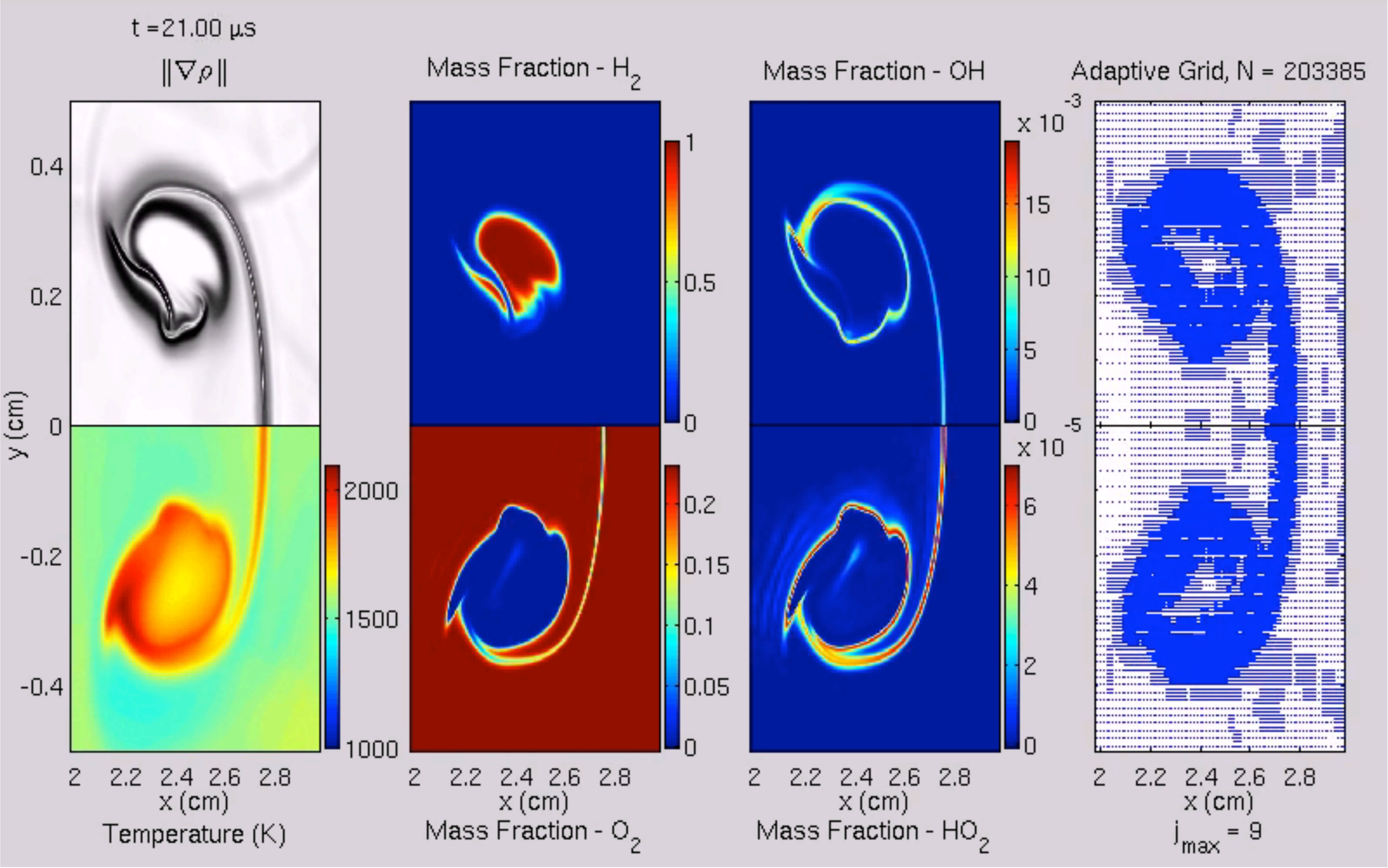
▸ We propose vertical coupling across scales

Macro-continuum Example - *WAMR*



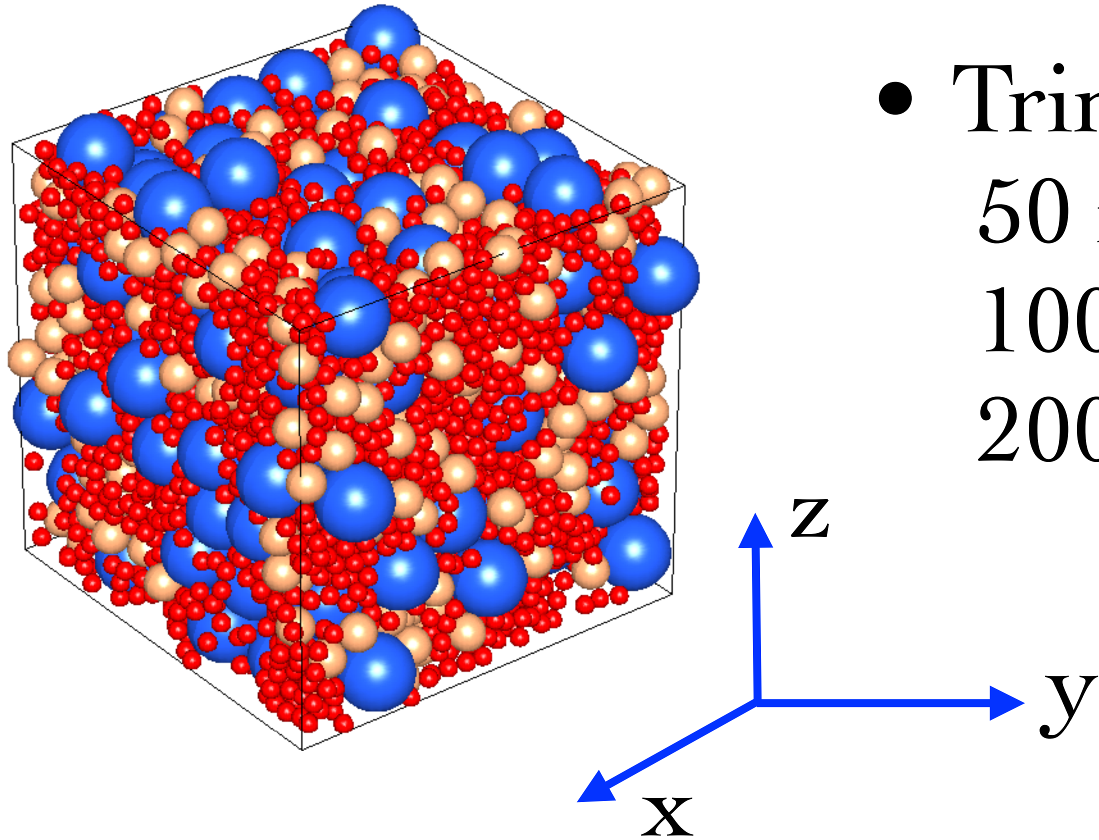
- Domain
  $[0, 5] \times [0, 0.75]$ cm
- Ambient mixture
  $Y_{N2} = 0.868$, $Y_{O2} = 0.232$
  P = 101.3 kPa
  T = 1000 K
- Hydrogen bubble
  $Y_{H2} = 0.99$, $Y_{air} = 0.01$
  $x = 0.80$ cm
- Chemical model
  9 species, 38 reactions
- Loaded by shock Ms = 2.0 at $x = 0.46$ cm
- Wavelet parameters
  $\varepsilon = 10^{-3}$
  p=6
  $[N_x \times N_y]_{coarse} = [50 \times 8]$
  J = 14
- 256 cores

Macro-continuum Example - *WAMR*



- Resolution required < 1 micron

Micro-continuum Example - *PGFem3D*



- Trimodal Pack 70% volume fraction

  50 microns - 0.15

  100 microns - 0.15

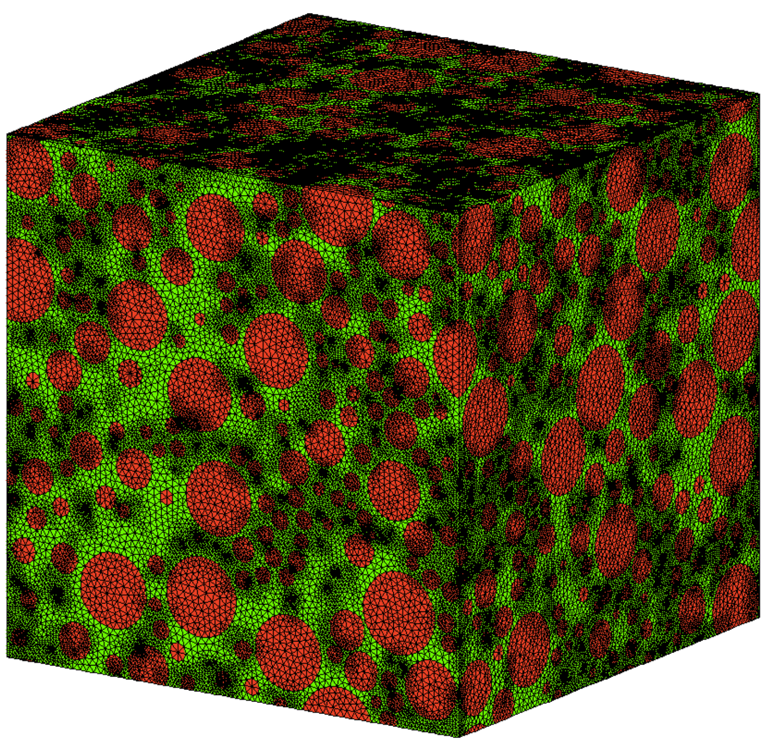
  200 microns - 0.4

4501 particles

Cell size 1.2x1.2x1.2 mm^3

E_m = 1 MPa - rubber

E_p/E_m = 100



3,232,787 nodes

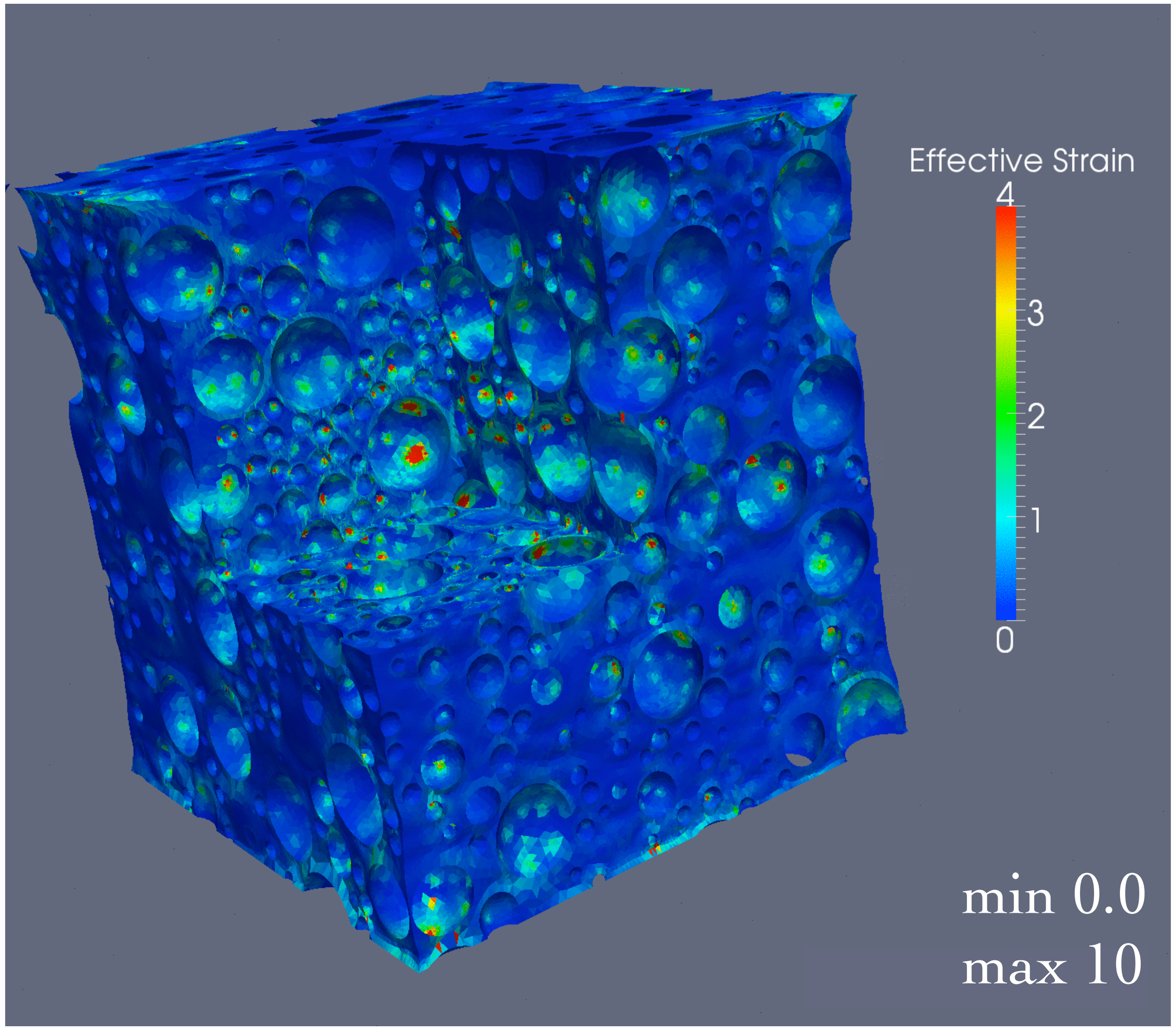
18,561,290 elements

12,897,386 degrees of freedom

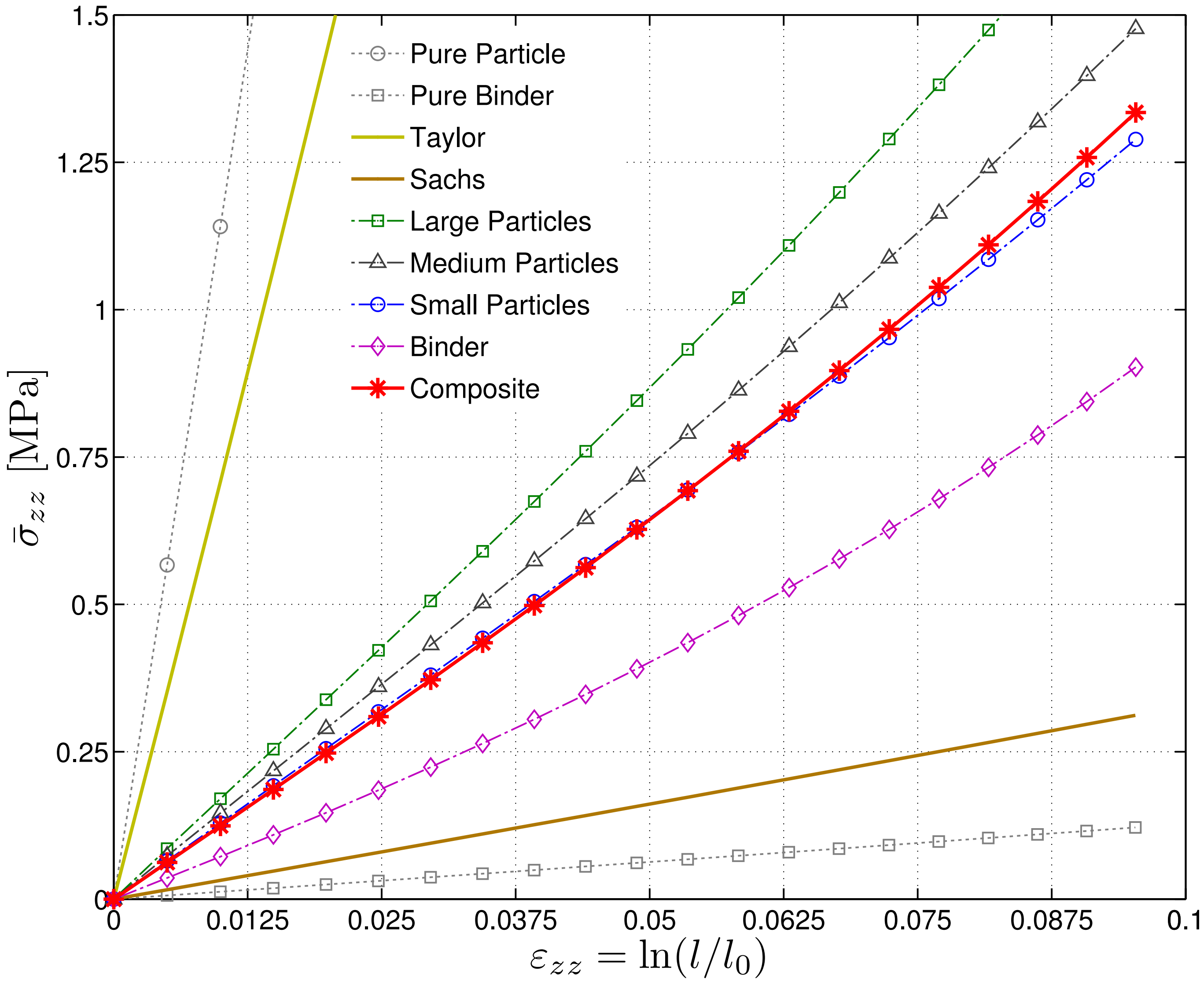
- Fixed in x-y, 10% stretch in z-direction

Micro-continuum Example - *PGFem3D*

Strain in Binder



Overall Stress-Strain Response



- 20 nonlinear steps
- Mixed FEM - $P_1/P_1 + \nabla P$
- 12,897,386 nonlinear equations
- 512 cores

V&V/UQ Experimental Physics Plan

- C-SWARM will be a predictive tool which yields solutions with verified spatio-temporal fidelity to the underlying mathematical model, calibrated and validated against micro- and macro-scale and scale-bridging experiments; uncertainty will be quantified at and across all scales.
- We will couple deterministic verification with stochastic validation/UQ strategies.
- The co-designed simulations and experiments will be refined continuously to support our advancing physical models.
- Our plan is informed by and consonant with the 2011 PSAAP II V&V/UQ Whitepaper.

Verification

- **Code Verification:**
  - Convergence studies
  - Sandia-developed Enhanced Verification Test Suite
- **Solution Verification on Well-designed Problems:**
  - Macro-continuum (*WAMR*): a priori adaptive refinement
  - micro-continuum (*PGFem3D*): a posteriori refinement
- **Scale-bridging Verification Between M&m:**
  - Direct simulation of a challenging multi-scale test problem with WAMR
- **Non-traditional Issues:**
  - numerical precision
  - failure of processors and/or memory banks
  - fault-detection and self-healing remediation built into the HPX runtime system

Quantities of Interest (QOIs)

We will study several QOIs which we hypothesize will be relevant, both pre- and post-processing, including

- space-time fields of grain size, porosity, pressure, temperature, chemical composition,
- shock speed and thickness,
- necessary milling conditions and impact velocity to achieve desired end.

All measurements will be sufficiently repeated so as to determine their aleatoric uncertainty for use in UQ studies.

Material Characterization/Calibration

Mean material properties, e.g. specific heat, and their uncertainty at the micro-scale is a **statistical inverse UQ problem** and will influence **forward UQ propagation**. Some of these are available in the literature; many will need original calibration experiments.

- Representative Unit Cell (RUC) construction of the pre-shock microstructure will be performed.
- Effect of High Energy Ball-Milling (HEBM) on material properties (M&m) will need to be measured.
- Reaction rates will be measured at the micro-scale.

Validation

Carefully co-designed, in-house simulations and experiments for validation will be a hallmark of C-SWARM.

- micro: quasi-steady properties at the RUC level, conductivity, dynamic elasto-visco-plastic properties; post-mortem characterization of final morphology.
- micro-Macro: Asay shear impact allows viewing of thermal response, ignition, and local surface strain field in response to impact — quasi-2D.
- Macro: full 3D reversed Taylor impact, allows i) strain under dynamical loading, ii) initiation threshold and resulting reaction propagation via impact experiments, and iii) properties of the resulting synthesized material. **Embodies all scales**.

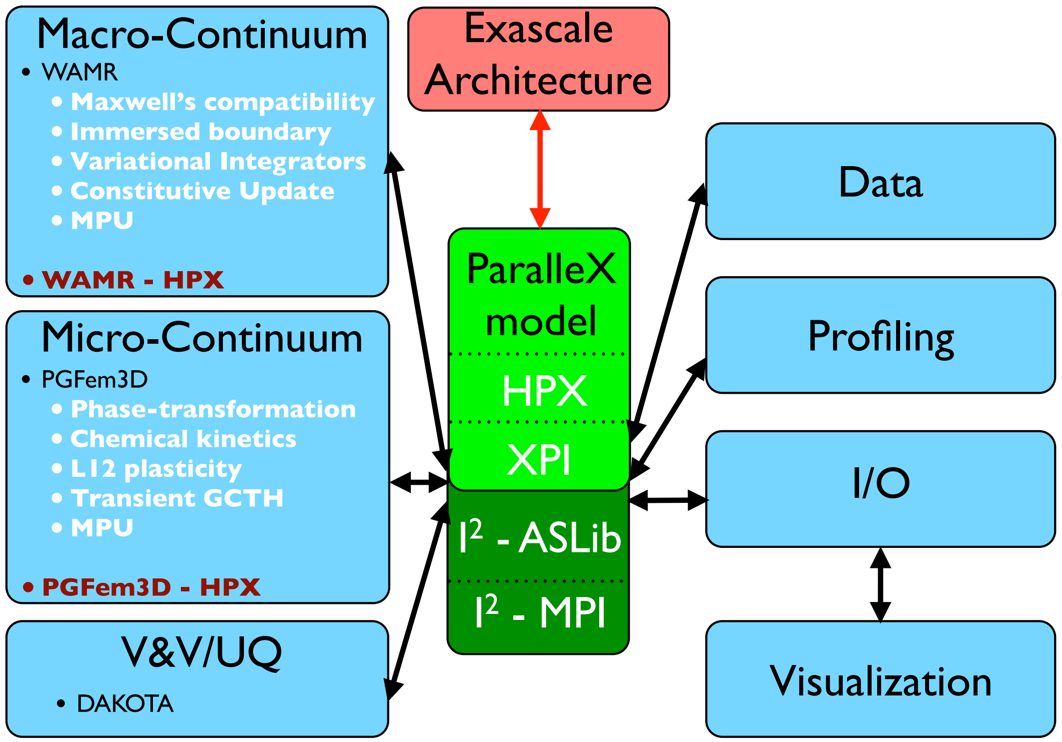
Uncertainty Quantification (UQ)

UQ is a synergistic process, two-way coupled to validation. We will stay abreast of ongoing developments in this area in cooperation with colleagues at SNL, and focus our UQ efforts on tools available and being developed within DAKOTA.

- We will use DAKOTA to propagate uncertainties in boundary conditions, material properties, etc., to put error bounds on our predictions.
- We will employ DAKOTA's Design and Analysis of Computer Experiments (DACE) to develop surrogate models for use in Monte Carlo/Latin hypercube UQ runs.
- Use multiple realizations of the RUC to obtain ensemble averages.
- Estimate uncertainties by sampling the distributions using reduced domain sizes, coarse resolution, and/or response surface models.

Development of C-SWARM Framework

- The demonstration problem will be used to develop and refine the C-SWARM framework
- We propose to use *WAMR* solver in the macro-continuum domain, and *PGFem3D* in the micro-continuum domains
- Coupling of scales is achieved by using two scale-bridging methods (GCTH, MPU)



- The equations and models will be refined continuously to advance the fidelity of our physical models
- I^2-ASLib, ParalleX model
- The plans will be continuously maintained, and updated yearly

▸ Shock synthesis of the novel material *c*-BN will result in a significant scientific achievement

C-SWARM Milestones

Science | Software | Exascale | V&V/UQ | Integration

Predictive Science Plan

- Develop models with comprehensive physics/chemistry
- Develop image-based modeling
- Predict conditions for synthesis of *c*-BN — a major scientific achievement

Software Plan

- Adaptive multiscale macro- and micro-continuum (M&m) solvers
- Coupling of scales using two scale-bridging methods

Integration Plan

- V&V/UQ of Ni-Al problem. Predict synthesis of *c*-BN.
- Prediction based on M&m-HPX codes using scale-bridging, ASLib interface, and linked with DAKOTA.

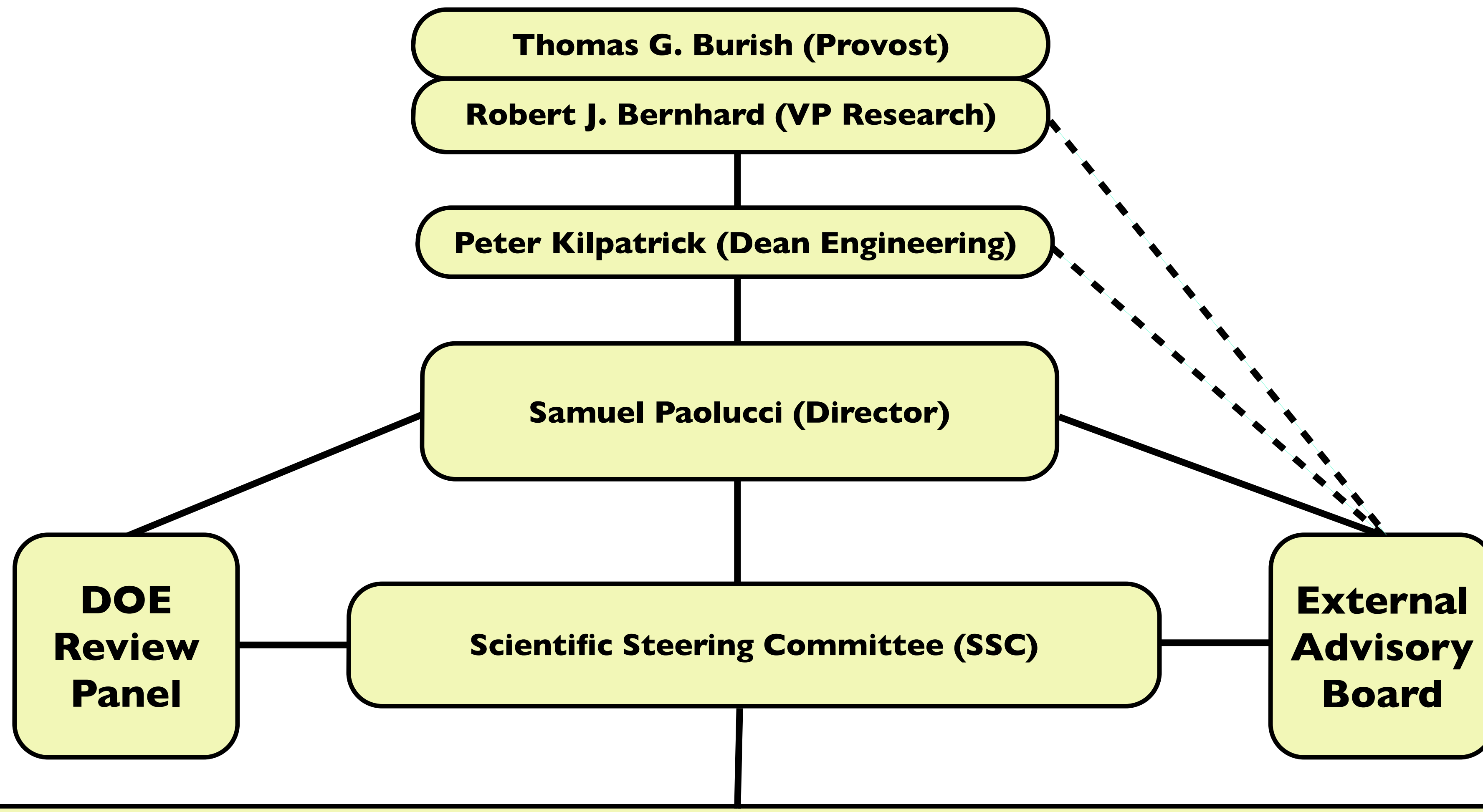
Exascale Plan

- ParalleX model and HPX runtime system
- I^2-XPI and I^2-ASLib libraries
- Performance and reliability metrics

V&V/UQ Plan

- Codes and solutions verified
- Ni-Al validated and *c*-BN predicted using co-designed experiments
- Sensitivity studies and uncertainty quantification analyses

Leadership and Management of Center



Research Groups

Computational Physics	***Computer Science***	***V&V/UQ and Experimental Physics***
K. Matous	P. M. Kogge	A. S. Mukasyan
S. Paolucci	*A. Lumsdaine*	*J. M. Powers*
G. Tryggvason	T. L. Sterling	S. F. Son

C-SWARM Team

Samuel Paolucci – (PI & Director) Former Research Staff Member of Sandia National Laboratories and currently Professor of Aerospace & Mechanical Engineering and Concurrent Professor of Applied and Computational Mathematics and Statistics at the University of Notre Dame; Fellow of ASME and APS; associate editor of Journal of Fluids Engineering; pioneer of wavelet schemes for solution of PDEs.

Gretar Tryggvason – (Associate Director) Viola D. Hank Professor of Aerospace & Mechanical Engineering and Department Chair at the University of Notre Dame; he is a Fellow of ASME and APS; currently the editor-in-chief of the Journal of Computational Physics; world-recognized for his development of numerical methods for direct numerical simulations of multiphase flows.

Peter Kogge – Former IBM Fellow (retired) and currently the Ted McCourtney Professor of Computer Science & Engineering and Concurrent Professor of Electrical Engineering at the University of Notre Dame; world-renowned expert on Exascale computing has served on and chaired influential committees examining potential Exascale technologies and software; 2012 IEEE Computer Society Seymour Cray Computer Engineering Awardee.

C-SWARM Team

Andrew Lumsdaine — Professor in the Department of Computer Science at Indiana University; founding member of the Open MPI effort. Expert in Areas of high-performance scientific computing, parallel, distributed, and concurrent computing and programming, software engineering.

Karel Matous — Associate Professor in the Department of Aerospace & Mechanical Engineering at the University of Notre Dame; Fellow of ASME has 10+ years of academic and industrial experience; international authority on large complex systems of heterogenous mixtures.

Alexander Mukasyan — Research Professor in the Department of Chemical & Biomolecular Engineering at the University of Notre Dame; Director Manager of Laboratory of Advanced Electron Microscopy; author of 3 books of combustion synthesis of advanced materials; holds 20 patents; has 25+ years of research and industrial experience.

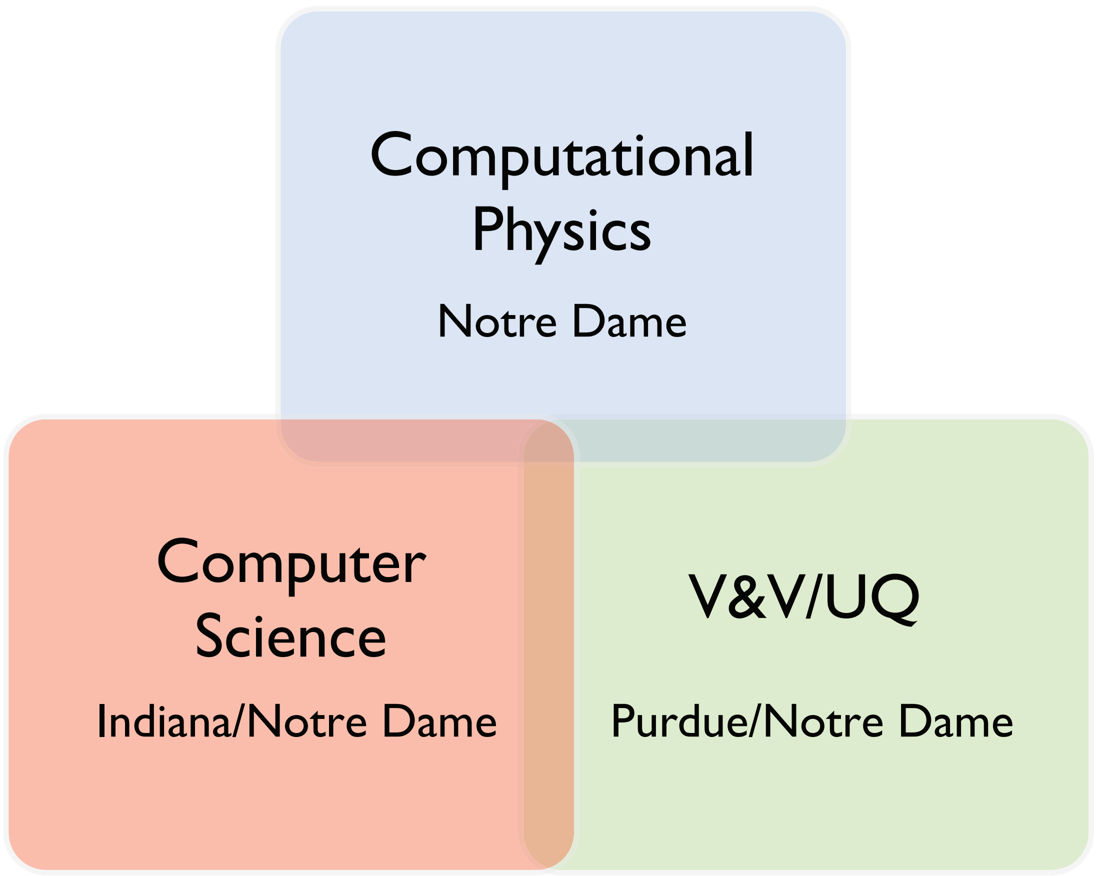
C-SWARM Team

Joseph Powers – Professor in the Department of Aerospace & Mechanical Engineering and Concurrent Professor of Applied and Computational Mathematics and Statistics at the University of Notre Dame; he is an Associate Fellow of AIAA; currently the associate editor of the Journal of Propulsion and Power.

Steven Son – Former J. R. Oppenheimer Fellow and Research Staff Member at Los Alamos National Laboratory and currently Professor and Purdue Faculty Scholar in the Department of Mechanical Engineering at Purdue University; holds four U.S. patents and received a 2007 Distinguished Paper Award from the Combustion Institute.

Thomas Sterling – Professor in the Department of Computer Science and Executive Associate Director and Chief Scientist, Center for Research in Extreme Scale Technologies (CREST) at the Indiana University; co-author of six books and holds six patents; awarded the Gordon Bell Prize with collaborators in 1997; best known as the father of Beowulf clusters.

C-SWARM Integration

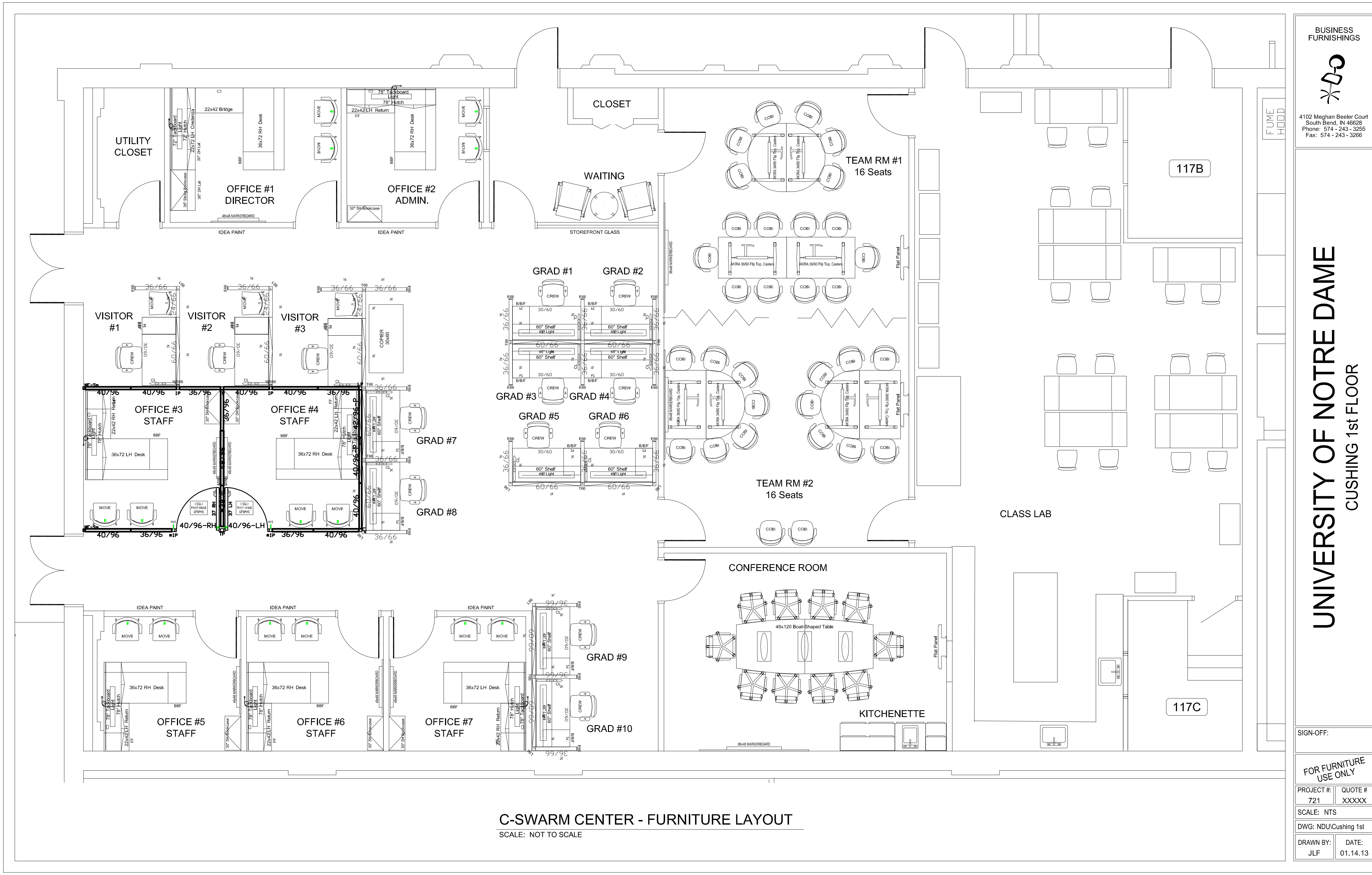


- The Computational Physics Group will oversee primarily the execution of the Predictive Science.
- The Computer Science group will oversee primarily the execution of the Exascale Plan.
- The V&V/UQ and Experimental Physics Group will oversee primarily the execution of the V&V/UQ Plan.
- All groups will contribute to the Software Plan.

Integration Management

- Integration of all plans managed by SSC who will be responsible for the success of the overall project: *Director, Associate Director, and Group Leads*.
- The SSC will meet monthly to monitor progress relative to established milestones, and review and adapt a watch list derived from risk assessments.
- The codes implemented by Karel Matous, the *Software Architect* and *Computational Physics Lead*.
- The *Software Architect* will oversee the overall system integration that the software development is coordinated and integrated effectively.
- Each research thrust group will hold bi-weekly meetings where progress and any problems will be discussed.
- Coupled with educational plan.

C-SWARM Space (2980 ft^2)



Novel Educational Aspects of C-SWARM

- Establish a Computational Science minor between ND and IU with multidisciplinary course requirements encompassing:
  - mechanics
  - applied mathematics
  - scientific computing
  - computer science
  - material science
  - large scale parallel computing
- Host biennial workshop on:
  - "Verification and Validation in Computational Science" or
  - "High-Performance Computational Predictive Science"

Uniqueness of C-SWARM

- We will address a challenging and important problem,
  - shock wave-processing of materials
- that embodies very complex physics/chemistry,
  - heterogeneous reactive materials
- solved by state-of-the-art multiscale algorithms,
  - adaptive macro- and micro-scale (M&m) algorithms
- in conjunction with V&V/UQ,
  - using co-designed simulations and experiments
- executed using unique dynamic programming model and libraries,
  - ParalleX and Active System Libraries (ASLib)
- by an outstanding multidisciplinary research team.

C-SWARM

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