RA1-FA2: Material Constitutive Models

Prof. Ryan Hurley
Johns Hopkins University
(July 21-22, 2020)
Scientific Driver

**Scientific Driver:**
- Develop validated constitutive models for the deformation, flow, and thermal fields in geomaterials

**Thrust 1:** REAL-TIME X-RAY AND THERMAL IMAGING
  - IN SITU X-RAY RADIOGRAPHY
    - Multi-angle x-ray radiography at HyFIRE; time-resolved imaging
  - IN SITU X-RAY PHASE CONTRAST IMAGING
    - Advanced Photon Source; time-resolved imaging
  - IN SITU THERMAL IMAGING
    - Near-penetrator heating

**Thrust 2:** CONSTITUTIVE MODEL DEVELOPMENT & VALIDATION
  - MODEL SELECTION
    - Bayesian model selection using UQpy
  - MODEL IMPLEMENTATION AT MICRO- AND MACROSCALES
    - Material Point Method; hydrocodes at LLNL
  - MODEL VALIDATION AT MICRO- AND MACROSCALES
    - Validation against in situ time-resolved 3D fields

**Thrust 3:** MATERIAL AND MICROSTRUCTURE CHARACTERIZATION
  - MATERIAL SELECTION
    - Probabilistic active learning to identify materials with most uncertainty
  - MATERIAL CHARACTERIZATION
    - X-ray computed tomography; image and microstructure analysis

MULTI-SCALE CHARACTERIZATION AND IMAGING
• To develop validated constitutive models for deformation, flow, and thermal fields in geomaterials
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<tr>
<th>Investigators and Collaborators</th>
<th>Position</th>
<th>Institution</th>
<th>Workforce</th>
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<td>KT Ramesh</td>
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<td>Mike Shields</td>
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<td>Jeff Davis</td>
<td>Collaborator</td>
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Long-term Goals and Strategies

- **Thrust 1**: develop real-time X-ray imaging and quantitative image interpretation capabilities (e.g., for pore sizes, porosity, etc.) and disseminate throughout URA through CCRI efforts

- **Strategies**: develop *in-situ* lab (HyFIRE), synchrotron (e.g., DCS, CHESS), and other user-facility capabilities (e.g., pRad)

**Wedge impact on sandstone (APS 32)**

**In-situ XPCI data from DCS**
Long-term Goals and Strategies

- **Thrust 2**: develop, implement, and validate constitutive models
  - **Strategies**: UQ-informed model selection with measurable internal variables describing material microstructure and mechanisms

Material Point Method (MPM) Simulation of Oblique Asteroid Impact by a Projectile

Charles El Mir / KT Ramesh
Long-term Goals and Strategies

- **Thrust 3**: material and microstructure characterization
  - **Strategies**: MicroCT and use of novel AXIS system (to be described)
Initial Program Plan (IPP) Goals and Strategies

- **Goal 1**: UQ-informed selection of canonical model: specific materials, chemistries, behaviors, and mechanisms of interest
  - **Strategies**: initial focus on sand, sandstone, granite, cement

- **Goal 2**: UQ-informed identification and development of computational model and supporting experiment diagnostics
  - **Strategies**: *measurable* internal variables; ML for experiment design

![Diagram of Model Design, Calibration and Validation, Bayesian UQ and Active Learning, Experiment Design, Microstructure Analysis]
Initial Program Plan (IPP) Goals and Strategies

- **Goal 3**: integrated future roadmap within UQ framework

- **Broad strategies during IPP**:
  - Weekly RA1/FA2 meetings with PIs, students
  - CCRI, GCAP/LLNL, RA1/FA1 collaborations
  - Preliminary *in-situ* data analysis
  - Use of user facilities (DCS, CHESS, pRad)
  - Development of HyFIRE, a novel AXIS instrument
  - Extensive review of literature and repositories (e.g., dtic) to ensure roadmap builds upon prior advances
What is Revolutionary and/or Unique About this Research (HyFIRE)

- **HyFIRE**: Hypervelocity Facility for Impact Research Experiments
  - Two-stage gas gun, 7 km/s launch capabilities
  - Rich *in-situ* diagnostics at intersection of mechanics, physics, chemistry: high-speed camera & hyperspectral imaging; velocimetry & particle tracking system; flash X-ray
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3 mm D 2017 Al Sphere Impacting 2” Borosilicate Glass Cube @ 2.2 km/s. 5 Mfps (Shimadzu HPV-X2). Credit: Gary Simpson, Matt Shaeffer
What is Revolutionary and/or Unique About this Research (AXIS)

• **AXIS**: Advanced X-Ray Imaging System
  • Laboratory XPCI / XRD microscopy system based on Excillum D2+ 700 W liquid metal (In-Ga) anode system
  • 10x brighter than solid anode source in 5-30 µm spot size range
What is Revolutionary and/or Unique About this Research (AXIS)

• Capabilities
  • High-brightness source / long propagation distance for lab-based XPCI
  • Phase-contrast imaging and tomography
  • Deben loading stage for *in situ* studies (quasi-static)
  • 2D parallel beam optics for far-field high-energy diffraction microscopy (crystal size, orientation, strain measurements)

• Status
  • Ordered and under construction (Proto Manufacturing) with delivery and installation of XPCI system in September 2020 (HEDM about 6 months later)
What is Revolutionary and/or Unique About this Research

- Internal variable evolution in 3D from characterization and 2D *in-situ* XPCI and radiography images from user facilities, HyFIRE

- UQ-informed (via Bayesian UQ, active ML) framework for model and experiment design to minimize uncertainty and maximize experimental yield

Wedge impact on sandstone (APS 32)
Initial Program Plan, Thrust 1: Real-Time X-ray and Thermal Imaging

- Planning and preliminary work on radiography and XPCI (HyFIRE, pRad, DCS, CHESS) (Hurley, Hufnagel)
- Characterization and algorithm development supporting CCRI imaging efforts (Hufnagel, Hurley)
- Integration with CCRI PDV & SHEAR (Foster, Ramesh)
- Thermal imaging a long-term goal of RA1/FA2 if future funding allows
Initial Program Plan, Thrust 2: Constitutive Model Development and Validation

- Integrate model/experiment design via Bayesian UQ & active learning (Shields)
- Emphasize history-dependent mechanisms (Ramesh)
- GCAP collaboration with LLNL on constitutive model selection and implementation (Ramesh, Hurley, Hufnagel)
- Careful consideration of measurable internal variables in model selection and development (Ramesh, Hurley, Hufnagel, Shields)
Initial Program Plan, Thrust 3: Material and Microstructure Characterization

• Active machine learning for parameter uncertainty and experiment design to maximize yield (Shields, Hurley, Hufnagel, Ramesh)

• Novel microstructure characterization techniques developed on AXIS and MicroCT (Hufnagel, Hurley)

• Integration with CCRI Data Management plans for characterization and future in-situ data (Elbert, Hurley, Hufnagel)
Plans for Collaborative Exchanges

• Regular discussions with RA1/FA1 investigators to coordinate selection of canonical model materials and regimes of material behavior

• Regular discussions with GCAP collaborators Herbold and Homel (LLNL) to discuss model selection and numerical implementation

• Future development of *in-situ* diagnostics in collaboration with user facilities at APS DCS, CHESS, pRad
**Collaborative Exchanges w/ CCRI**

- **Collaboration with CCRI UQ subgroup**
  - Shields: develop and deploy UQ activities within and beyond RA1/FA2 (and RA1/FA1)

- **Collaboration with CCRI advanced optical diagnostics effort**
  - Foster: adapt high-speed particulate hyperspectral imaging technology to RA1/FA2 (and RA1/FA3, RA2/FA2, RA3/FA1, RA3/FA2)
  - Hufnagel: develop novel data analysis and reduction methods for XPCI in RA1/FA2 (and RA2/FA2)

- **Collaboration with CCRI data management effort**
  - Elbert: integrate image processing in centralized computing environment (maybe data archiving)
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