

# ***Cross Cutting Research Initiatives (CCRI)***

***Mark Foster, Jeff Davis***

*(July 21-22, 2020)*



**MSEE**

MATERIALS SCIENCE IN  
EXTREME ENVIRONMENTS  
UNIVERSITY RESEARCH ALLIANCE





# Long-term Goals and Strategies

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- Cross-Cutting Research Initiative (CCRI)
  - Bring cutting-edge tools to bear on MSEE URA research activities
    - Diagnostics
    - Modeling
    - Data Science
  - 5 targeted research efforts
    - Advanced Optical Diagnostics
    - Structural Visualization
    - Uncertainty Quantification (UQ)
    - Machine Learning (ML)
    - Data Management



# IPP Goals and Strategies

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- IPP → 5 areas
  - Advanced Optical Diagnostics
    - High-Speed Hyperspectral Imaging
    - Spectroscopy and Pyrometry
    - Velocimetry (PDV, VISAR)
  - Structural Visualization
    - Time-resolved, *in situ* structural visualization (XPCI, pRAD)
    - *Ex situ* imaging and diffraction microscopy
  - Uncertainty Quantification (UQ)
    - Disseminate UQ methods
    - UQ subgroup
  - Machine Learning
    - Object Detection
    - Automatic Characterization
    - Anomaly Detection
    - Prediction
  - Data Management



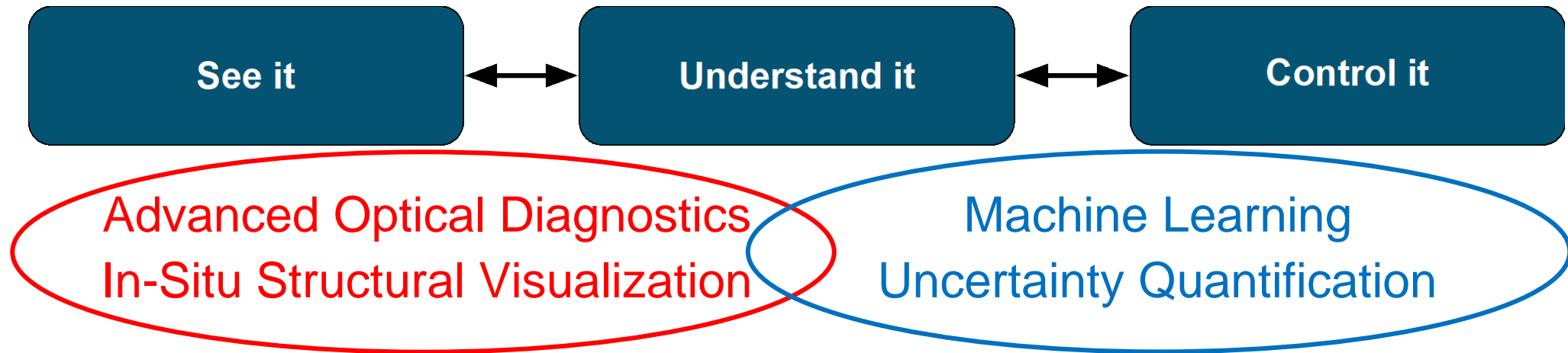
# Personnel

Investigators and Collaborators	Position	Institution	Workforce
<b>Mark Foster</b>	<b>CCRI Coord</b>	<b>JHU</b>	<b>1 PhD</b>
Mike Shields	PI	JHU	0.5 PD
Brian Barnes	PI	CCDC ARL	self
Tim Mueller	PI	JHU	0.67 PD
Todd Hufnagel	PI	JHU	0.5 PD
Farhat Beg	Collaborator	UCSD	
Davide Curreli	Collaborator	UIUC	
Jim Gaffney	Collaborator	LLNL	
Sivanandan Harilal	Collaborator	PNNL	
Ryan Hurley	Collaborator	JHU	
Dave Elbert	Collaborator	JHU	
Suresh Menon	Collaborator	GT	
Gena Miloshevsky	Collaborator	VCU	
Harry Radousky	Collaborator	LLNL	
Sean Regan	Collaborator	UR LLE	
Betsy Rice	Collaborator	ARL	
Neeraj Sinha	Collaborator	CRAFT Tech	
Rick Spielman	Collaborator	UR LLE	
John Volakis	Collaborator	FIU	
Tim Weihs	Collaborator	JHU	
Bryan Wong	Collaborator	UCR	
Jacob Calkins	Collaborator	DTRA	
Dave Peterson	Collaborator	DTRA	
Jeff Davis	Collaborator	DTRA	



# What is Revolutionary and/or Unique About this Research

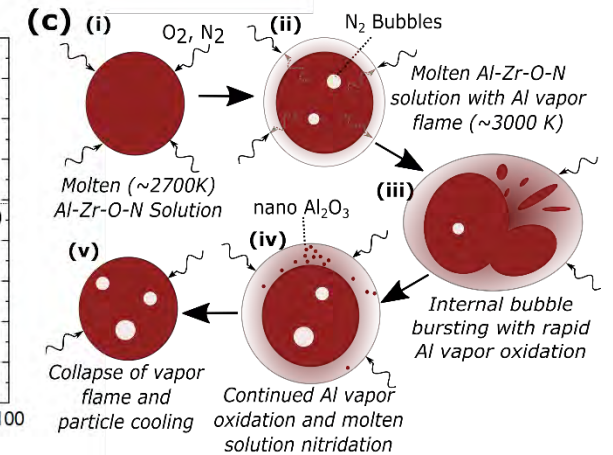
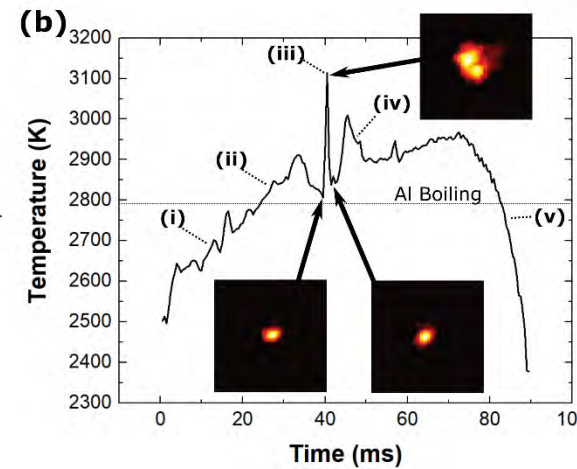
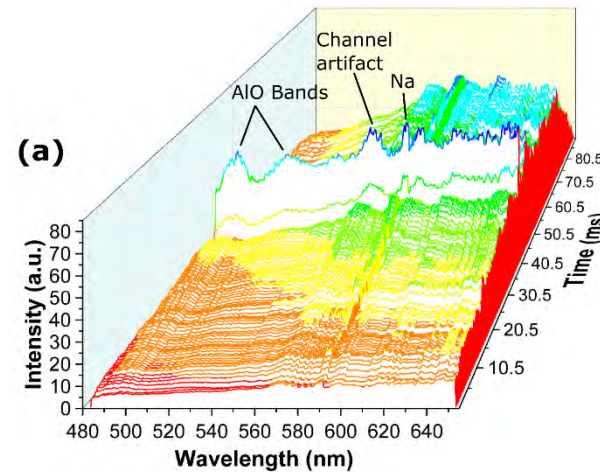
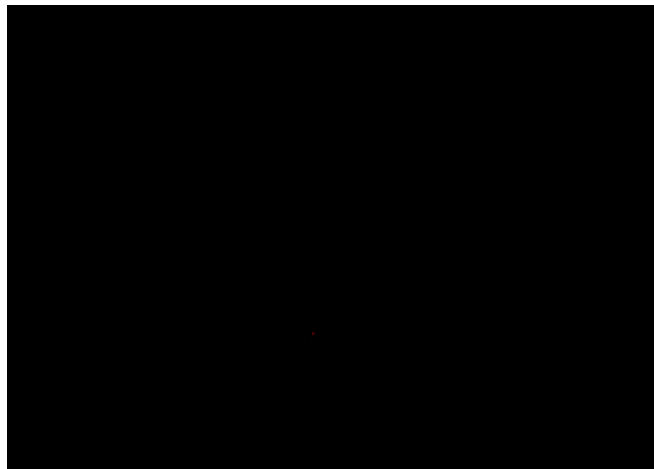
- CCRI → Emerging Computational and Experimental Tools
  - Strong foundational understanding in disparate research communities
  - Poised to impact unique challenges of MSEE research interests
  - URA offers unique collaborative opportunities





# Description of PI Activities

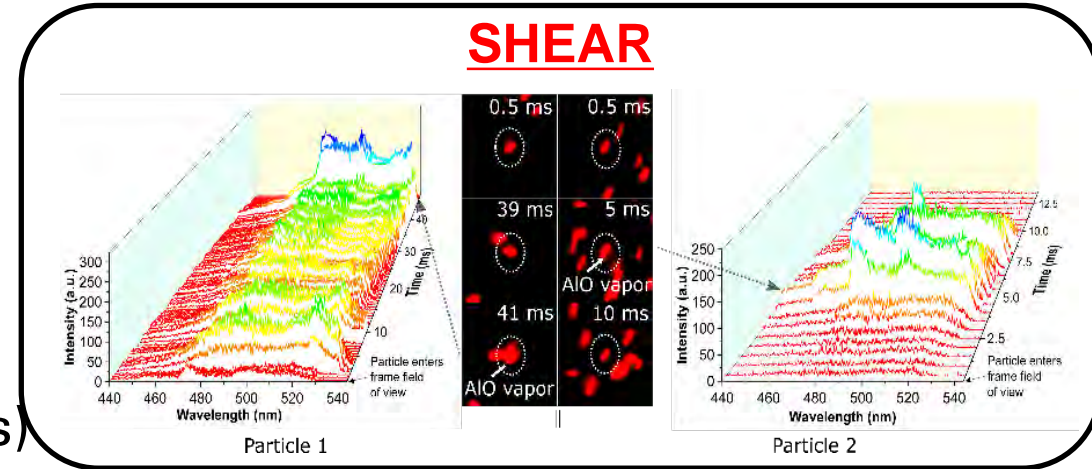
- PI: Mark Foster
- Advanced Optical Diagnostics
  - Links to RA1-FA2, RA2-FA2/FA3, RA3-FA1/FA2, RA4-FA2
  - e.g. Hyperspectral Imaging, Spectroscopy, Pyrometry, Velocimetry





# Description of PI Activities

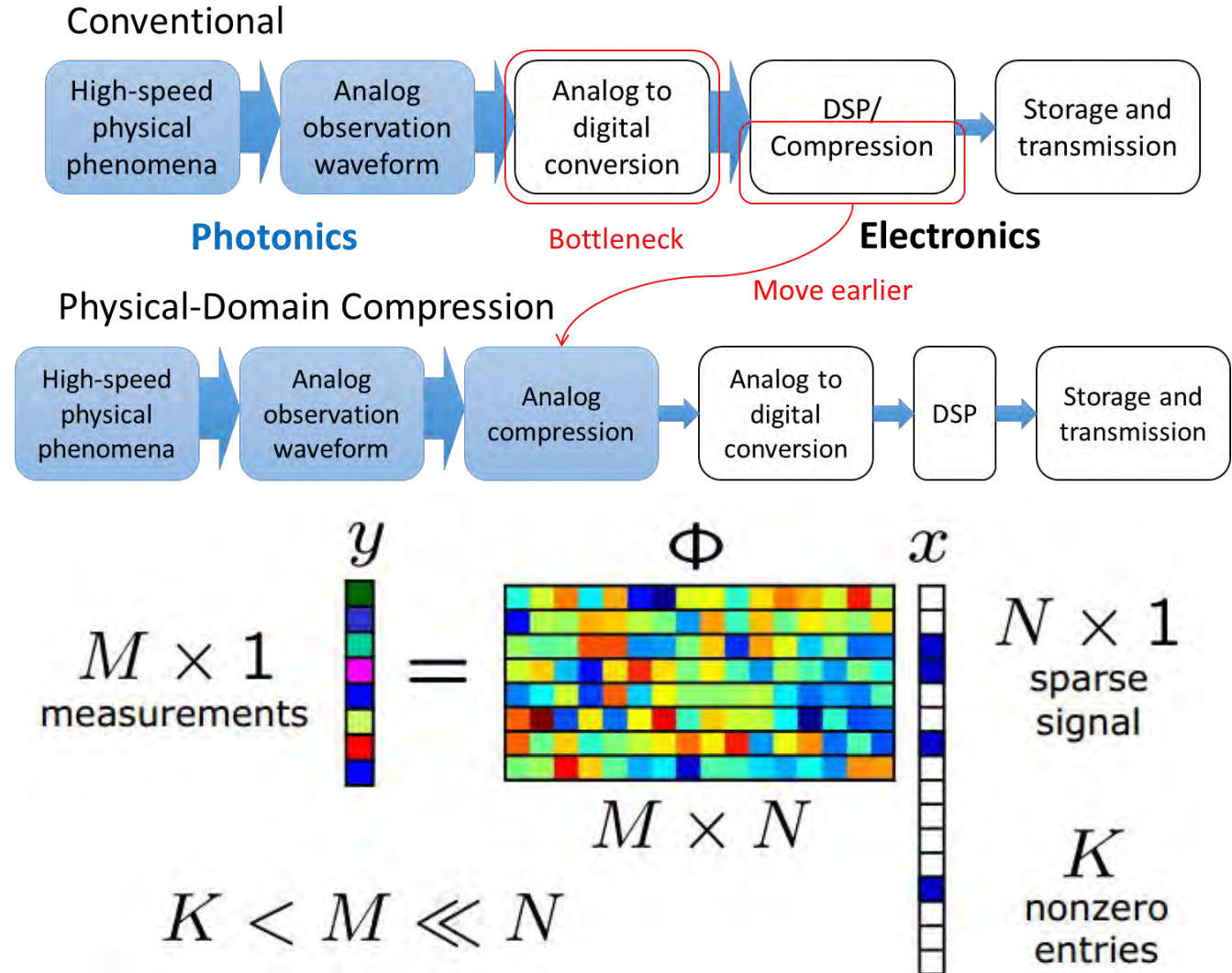
- PI: Mark Foster
- Advanced Optical Diagnostics
  - High-speed hyperspectral imaging
    - Disseminate SHEAR (particulate scenes)
    - Develop for diffuse scenes (e.g. flames, fireballs)
  - Photon Doppler Velocimetry
    - Dramatically increase spatial points using compressive acquisition
    - Increase temporal resolution and velocity range using optical signal processing
  - Fiber-optic VISAR
    - Investigate telecom hardware to decrease cost and increase performance





# Description of PI Activities

- PI: Mark Foster
- Compressed Sensing
  - More efficient sampling
  - Increase the *information* acquired in *measurement constrained* experiments
  - e.g. rapid, destructive, costly experiments
  - Applicable beyond optical diagnostics

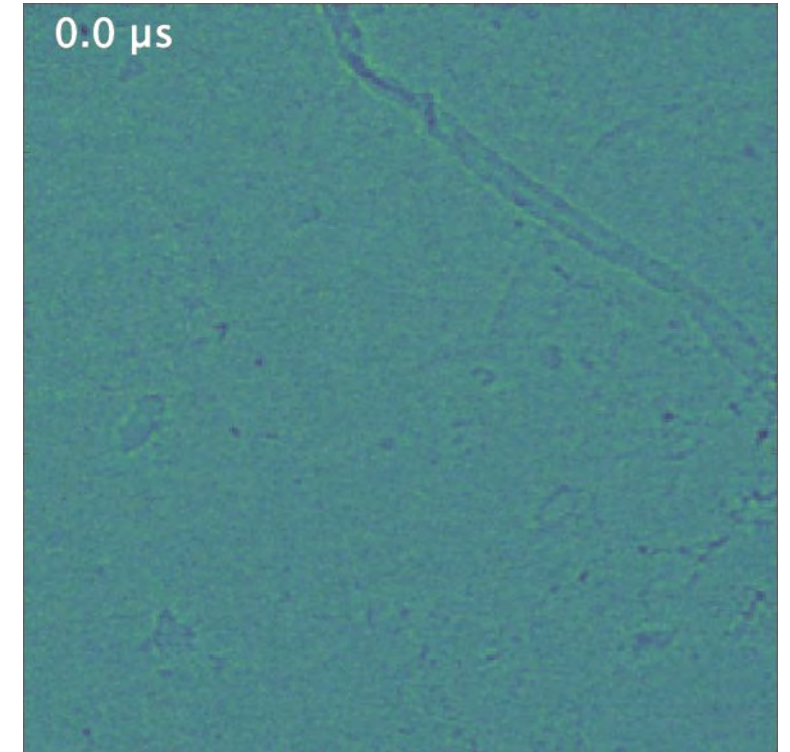






# Description of PI Activities

- PI: Todd Hufnagel
- Links to RA1-FA1/2, RA2-FA2/3, RA3-FA1
- Time-resolved, *in situ* structural visualization with multiple diagnostics
  - XPCI (APS/CHESS)
  - pRad (LANL)
- *Ex situ* imaging and diffraction microscopy
  - Advanced X-Ray Imaging System (AXIS) (to be installed September 2020)

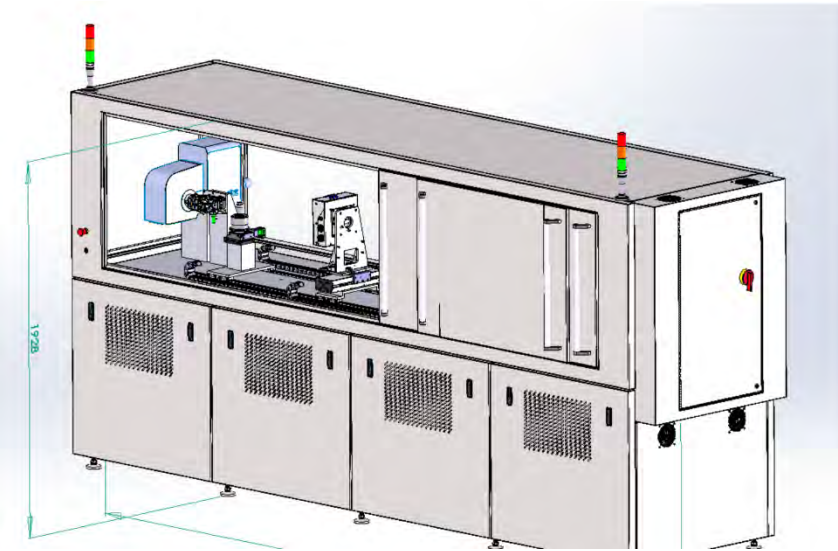


Dynamic compression of boron carbide  
Strain rate  $\sim 5000 \text{ s}^{-1}$   
3  $\mu\text{m}$  resolution, 0.75 mm FOV  
APS Sector 32



# Description of PI Activities

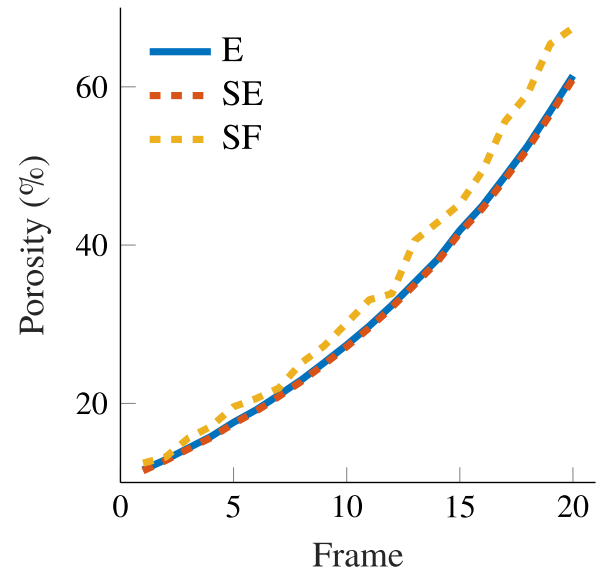
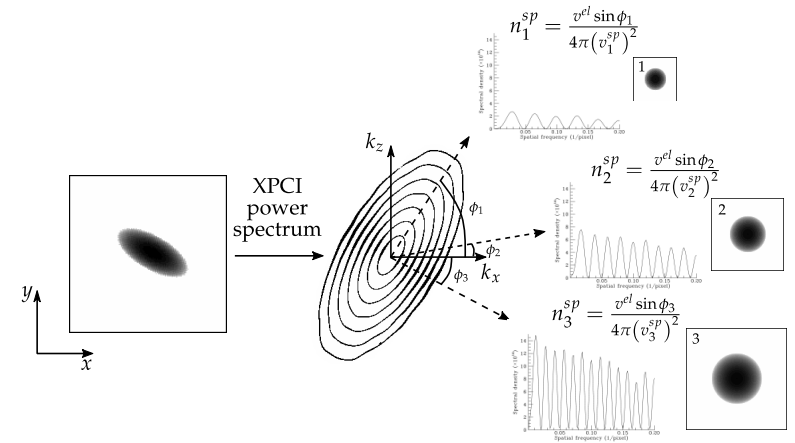
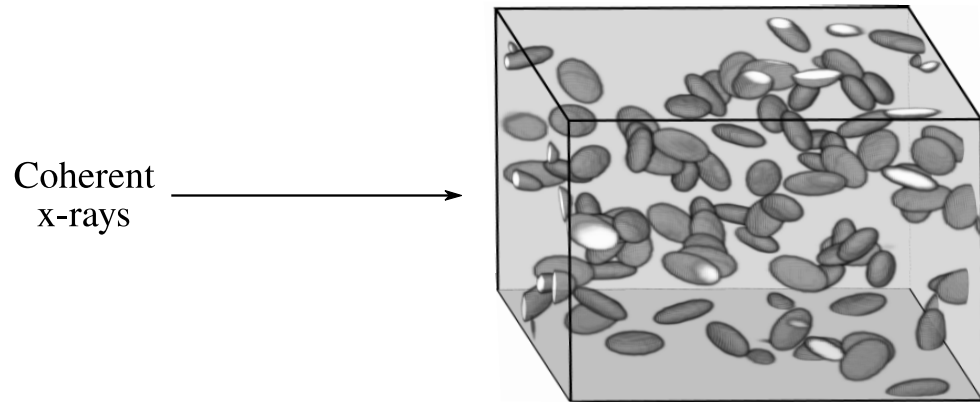
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# Description of PI Activities

- PI: Todd Hufnagel
  - Image analysis and interpretation





# Description of PI Activities

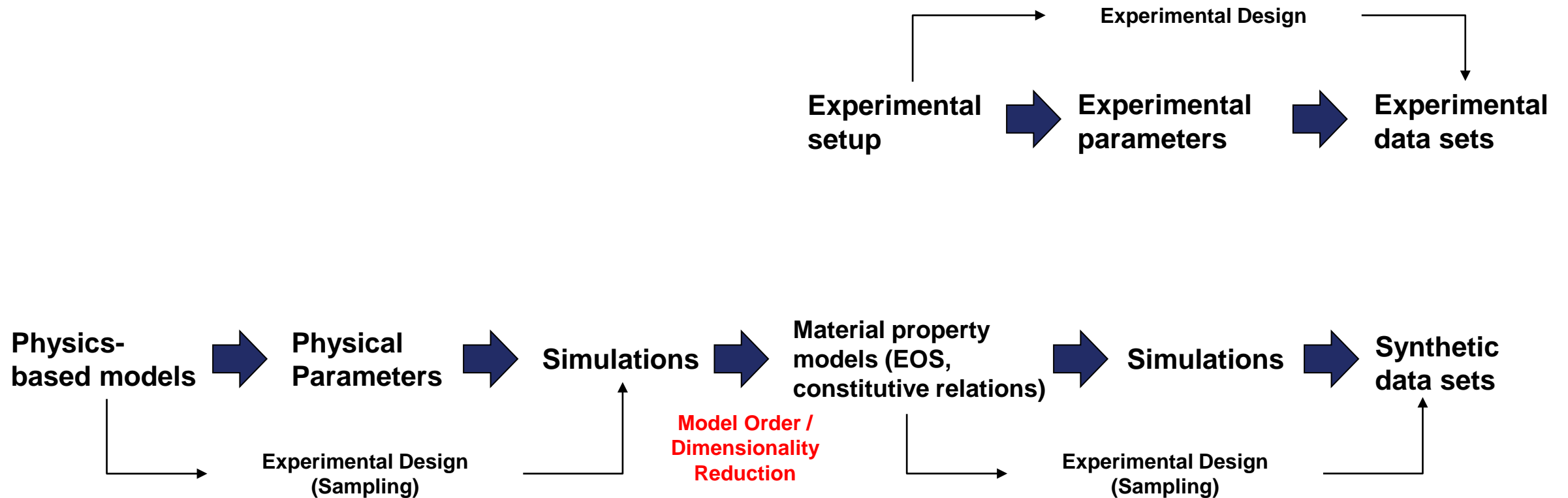
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- PI: Michael Shields
- Uncertainty Quantification (UQ)
  - Objective: Coordinate, formalize and disseminate a consistent UQ strategy and standard practices across the consortium
  - Technical Approach: Bayesian active learning framework tailored to each FA.
    - Bayesian – Allows us to update uncertainty estimates as data are collected.
    - Active learning – Leverages ML formalisms to inform future data collection and simulation efforts.



# Initial Program Plan: UQ Framework

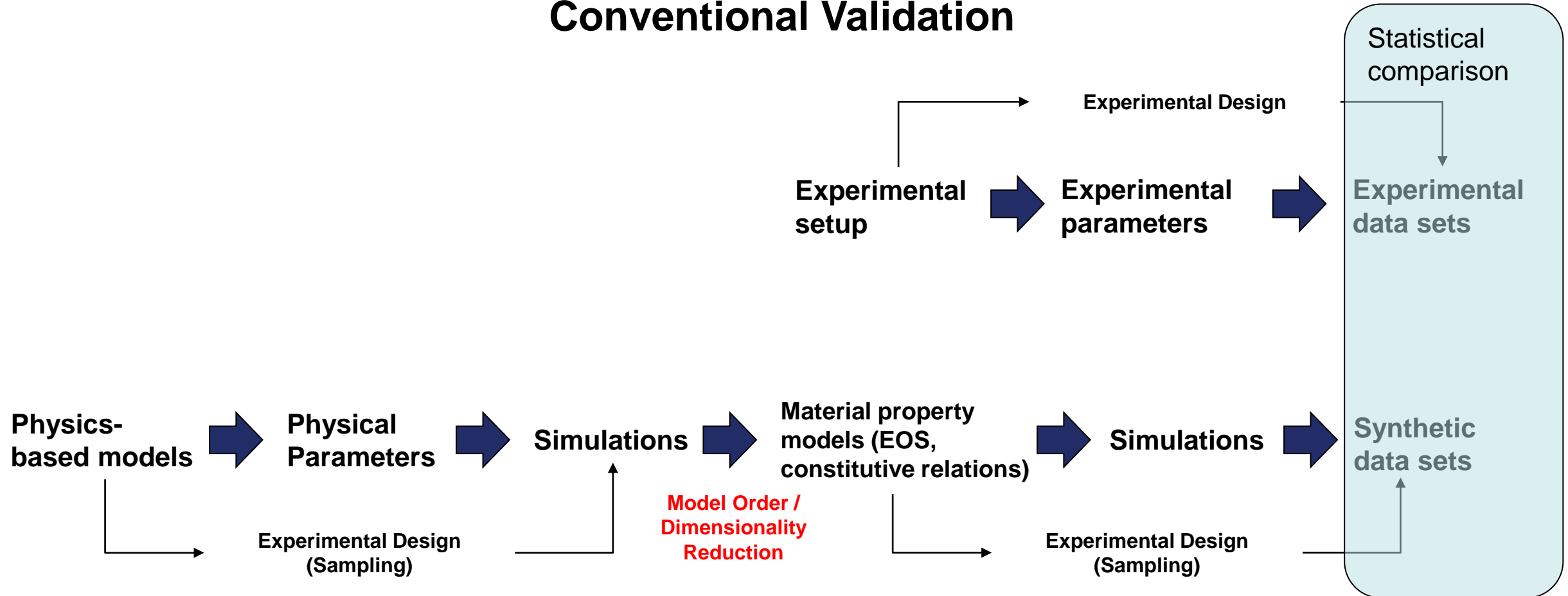
## Experimental/Modeling Paradigm





# Initial Program Plan: UQ Framework

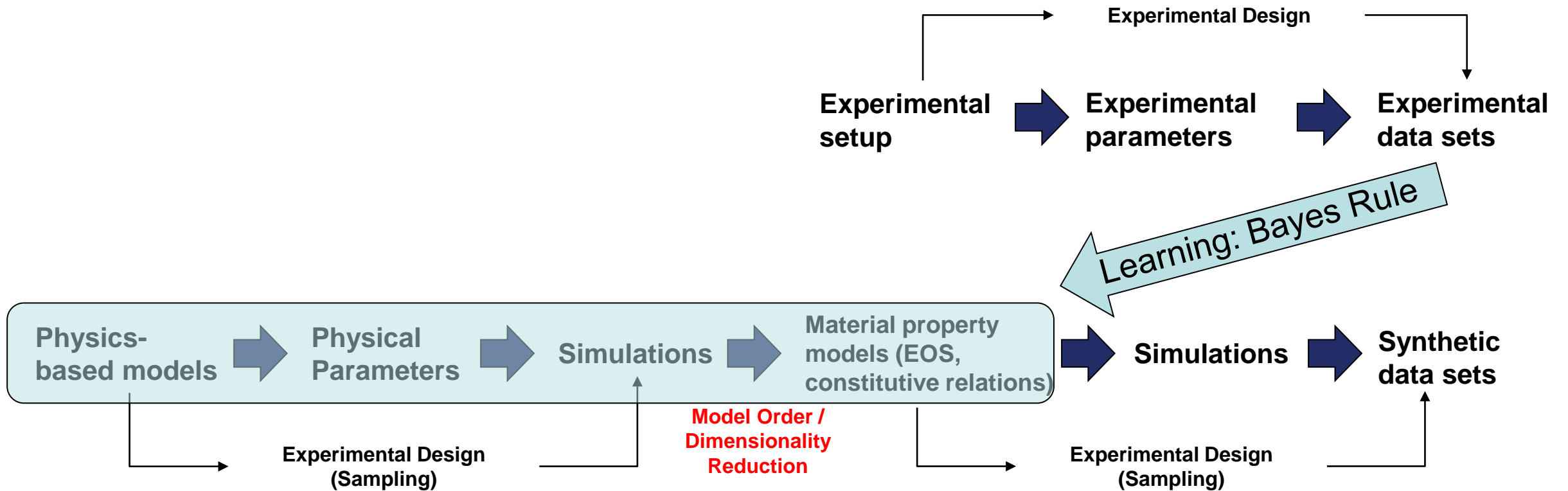
## Conventional Validation





# Initial Program Plan: UQ Framework

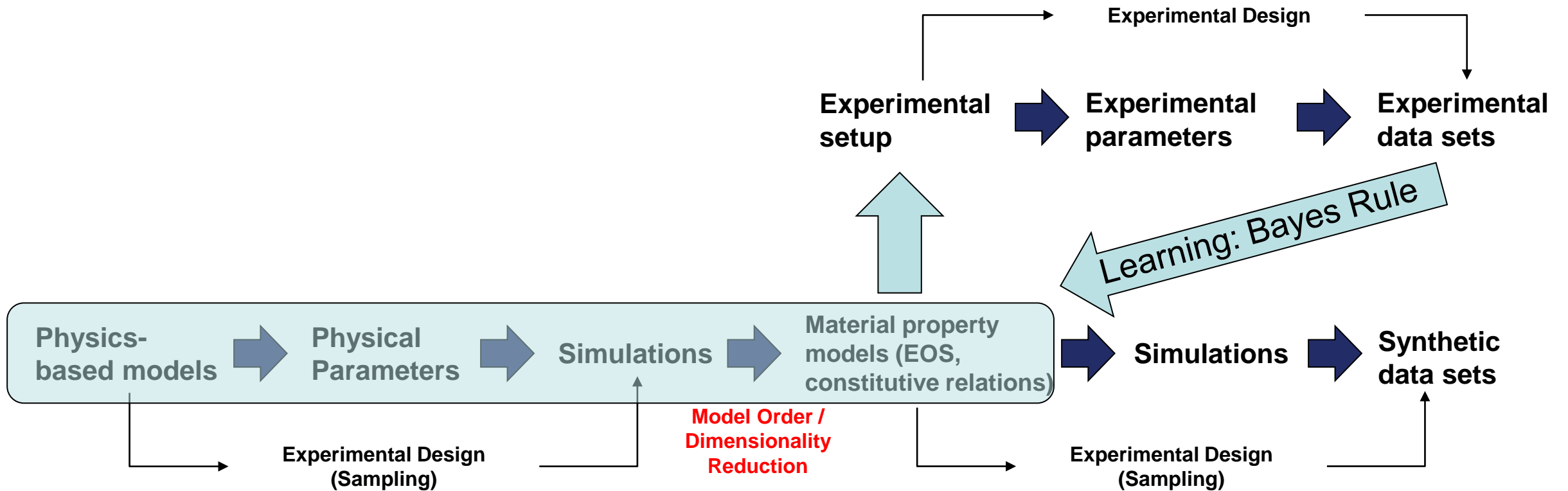
## Static Bayesian UQ





# Initial Program Plan: UQ Framework

## Bayesian Active Learning UQ







# Description of PI Activities

- PI: Michael Shields
- UQ IPP Tasks and Goals
  1. Establish UQ Subgroup
    - Representatives from each focus area (FA)
    - First group meeting in early fall
      - Assess collective needs and goals
      - Get us all on the same page
  2. Establish software foundation
    - UQpy – Python software available across consortium
      - Coordinate with Elbert to set up software backbone on computing systems.
      - Annual software training session
      - Assess software needs across FAs

## UQ subgroup members and their primary RA and FA

Michael Shields - Lead	RA1-FA2, RA1-FA3
Jim Gaffney	RA1-FA1,
Neeraj Sinha	RA3-FA1, RA3-FA2
Suresh Menon	RA2-FA3, RA3-FA2
Gena Miloshevsky	RA1-FA1, RA4-FA1
John Volakis	RA2-FA1
Betsy Rice	RA2-FA2
Bryan Wong	RA2-FA2
Davide Curelli	RA3-FA1
Farhat Beg	RA4-FA2



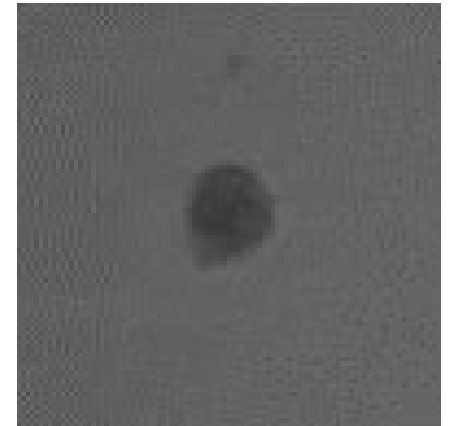


# Description of PI Activities

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- PIs: Tim Mueller and Brian Barnes
- Applied machine learning
  - Automate analysis of large experimental data sets
    - E.g. track and analyze burning particles for biological and chemical agent defeat in support of RA2-FA2.
  - Develop predictive models with uncertainty quantification that can be used to guide decision-making.
    - In collaboration with uncertainty quantification effort.
  - Other applications as needs arise.

High speed video of Al-Zr particle combusting in air

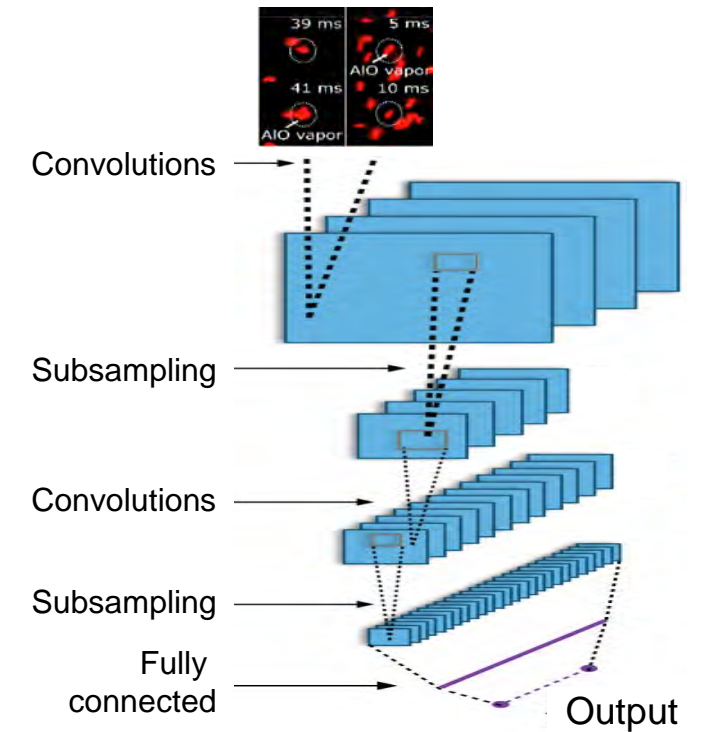




# Description of PI Activities

- Analysis of experiments
  - Terabytes of video data
  - Gaussian mixture models and/or neural networks for object detection and tracking
  - Neural networks for characterization, quantification, and anomaly detection
- Predictive modeling
  - Quantified inputs and outputs from experiments and machine learning analysis
  - Gaussian processes and/or neural networks to predict new outputs with associated uncertainties

## Video analysis using a convolutional neural network



adapted from  
[https://commons.wikimedia.org/wiki/File:Typical\\_cnn.png](https://commons.wikimedia.org/wiki/File:Typical_cnn.png)



# Description of PI Activities

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- PI: Dave Elbert
- Data Management
  - Funded in IPP through F&A return
  - IPP – links to RA1-FA1/2
  - High-throughput data reduction for experiment optimization
    - Foundational work for high-repetition-rate experiments
  - Develop tools within centralized collaborative computing environment
    - Uncertainty Quantification (UQ)
    - Image Processing



# Plans for Collaborative Exchanges

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- Planned Collaborations in IPP Phase
- Advanced Optical Diagnostics: RA1-FA2, RA2-FA2/3, RA3-FA1/2, RA4-FA2
- Structural Visualization: RA1-FA1/2, RA2-FA2/3, RA3-FA1
- Uncertainty Quantification: RA1-FA1/FA2
  - UQ Subgroup – RA1-FA1, RA2-FA2/3, RA3-FA1/2, RA4-FA1/2
- Machine Learning: RA1-FA1/2, RA3-FA1/2
- Data Management: RA1-FA1/2



# Plans for Collaborative Exchanges

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- Disseminate novel diagnostics, methods, modeling as available
- Match-making and shared understanding of challenges is essential
- Monthly CCRI meetings
  - Venue for discussion with URA PIs outside of CCRI
  - Each meeting will focus on identifying applications within one FA
- UQ Workshops and Subgroup
- Tutorials for novel diagnostics, methods, modeling