IOWA STATE UNIVERSITY

Center for Multiphase Flow Research and Education

# Introduction and Overview


1

## CoMFRE: Vision and Mission

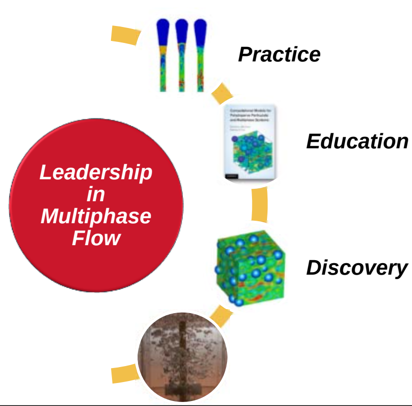
**Center established in Dec 2017**

**Vision**

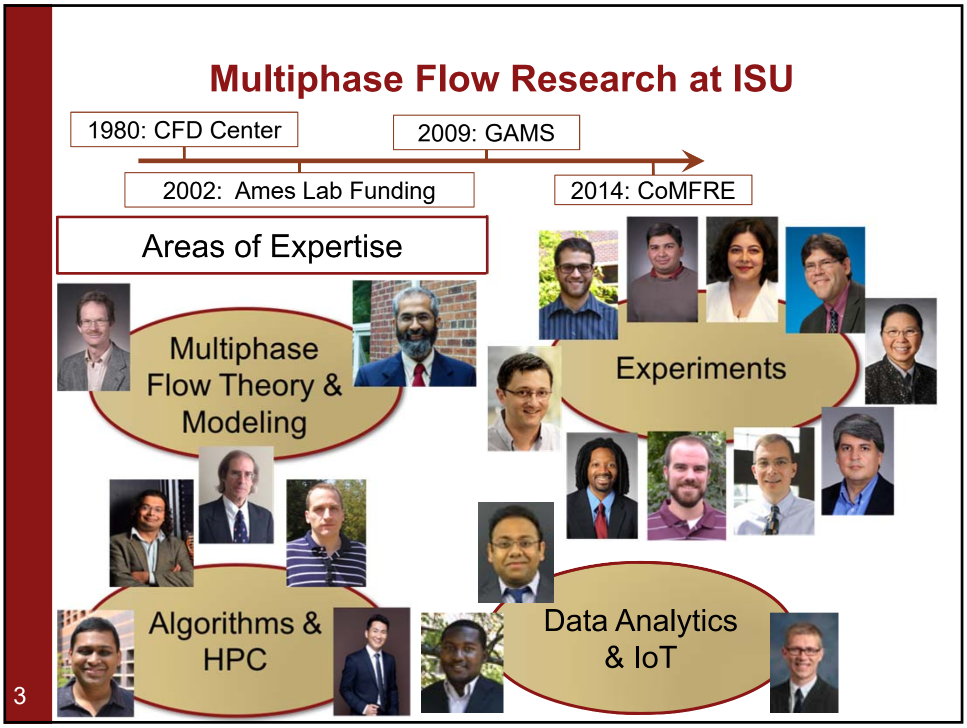
*Iowa State University will be a global leader in multiphase flow science and its engineering application to energy, healthcare, materials design, advanced manufacturing, sustainability and infrastructure*

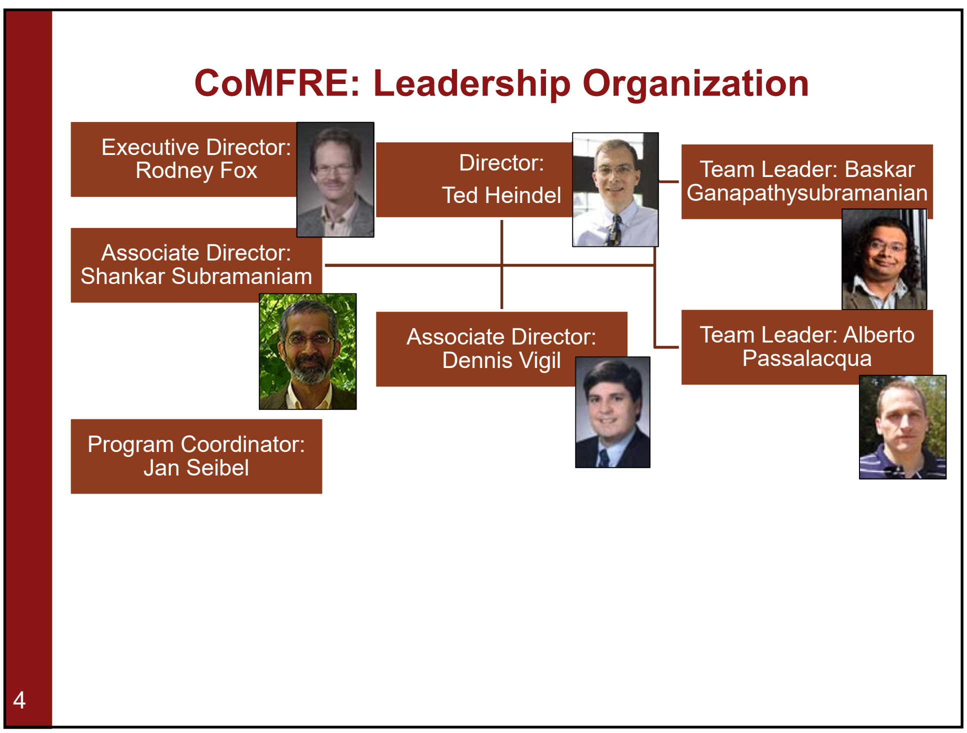
**Mission**

- Conduct critical, unique and high-risk research
- Broaden the impact of multiphase flow research
- Develop a skilled workforce
- Integrate the activities and expertise of individual research leaders to accelerate knowledge transfer

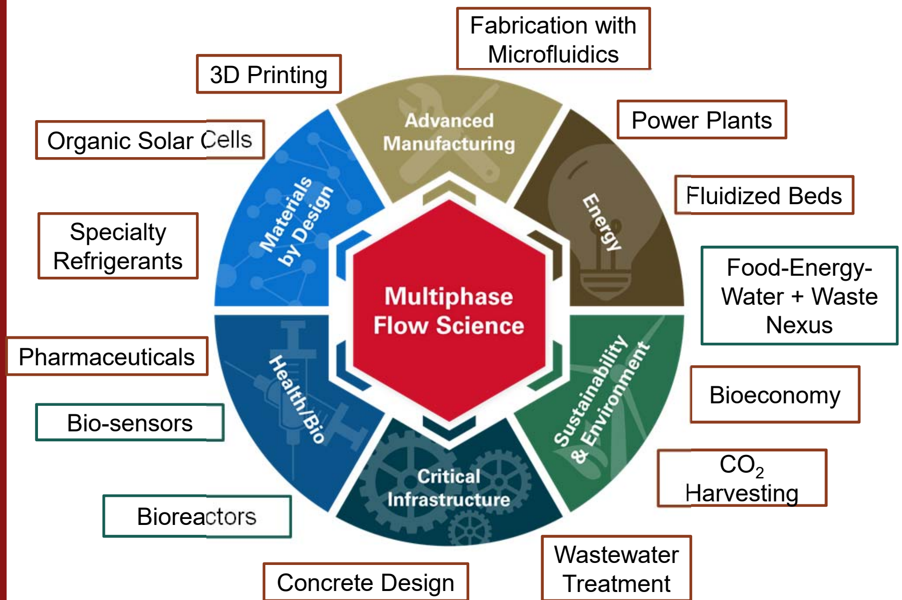



2


Multiphase Flow Research at ISU
1980: CFD Center
2009: GAMS
2002: Ames Lab Funding
2014: CoMFRE
Areas of Expertise
Multiphase Flow Theory & Modeling
Experiments
Algorithms & HPC
Data Analytics & IoT
3


CoMFRE: Leadership Organization
Executive Director: Rodney Fox
Director: Ted Heindel
Team Leader: Baskar Ganapathysubramanian
Associate Director: Shankar Subramaniam
Associate Director: Dennis Vigil
Team Leader: Alberto Passalacqua
Program Coordinator: Jan Seibel
4

## CoMFRE Multiphase Flow Applications




5

IOWA STATE UNIVERSITY

**Center for Multiphase Flow Research and Education**

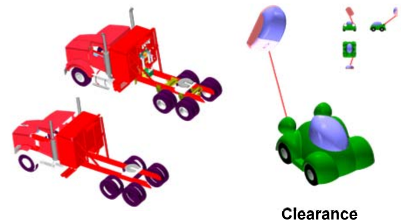
## Modeling and Computational Resources


6

## Computer Aided Modeling and Design

### Application Focus Areas

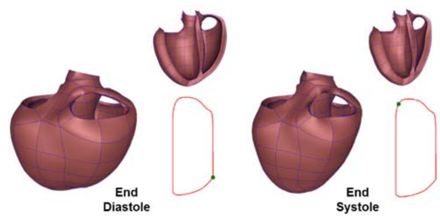
- GPU-accelerated CAD
- Geometric Modeling
- Biomechanics
- Cardiac Modeling
- Volume Rendering and Visualization



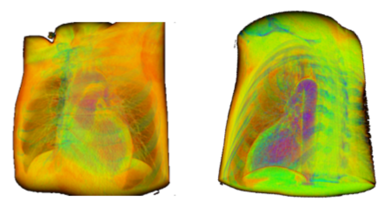
Model Simplification

Clearance Computations

GPU-Accelerated CAD



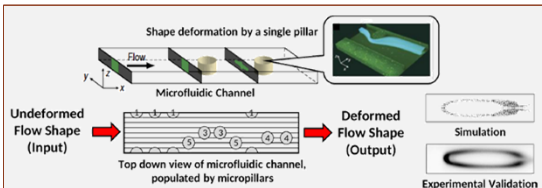

Cardiac Modeling



Volume Rendering

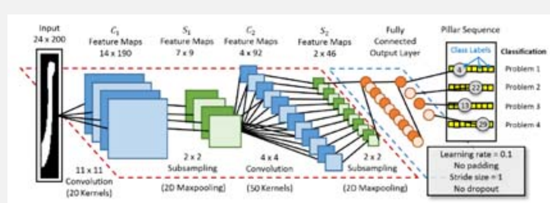
7

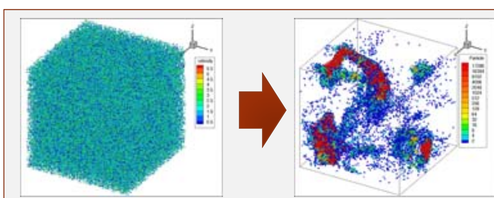
## Machine Learning for Thermo-Fluid Applications




**Forward simulation is tractable, while solving inverse problem (design of microfluidic channels) is significantly harder**

**Using Deep Convolutional Neural Network to extract features to generate pillar sequence**



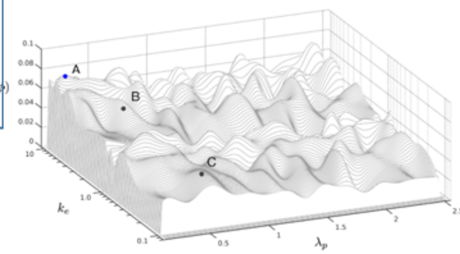


**Prediction of particle clustering using 3D Deep Convolutional Neural Networks**

8

## Multiscale Modeling and Optimization


**Multiscale modeling of morphology evolution of multi-component systems** as function of processing conditions in complex geometries
- Crystallization vs Phase separation
- Multiple solvents
- Various evaporation rates
- Flow conditions




*Rapid exploration of a two processing conditions effect on morphology*

**Tools for adaptive exploration and optimization**
Given multiscale models that account for processing conditions and molecular architecture, rapid and autonomous exploration of the design space to identify promising configurations. Uses ideas from surrogate modeling and machine learning.

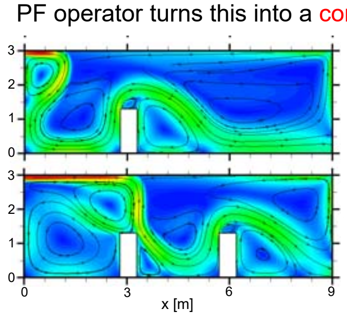
9

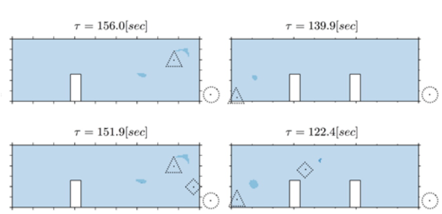
## Optimal Sensor Placement Under Uncertainty

Rapid detection, and localization of contaminants/components

- nonlinear evolution under complex, **uncertain** flow fields can be replaced by linear evolution of density propagated by Perron-Frobenious (PF) operator
- Opens up development of fast and efficient prediction, estimation, and control strategies
- Linear nature of framework allows use of intuition from linear system to nonlinear analysis

Example of using the PF operator for sensor placement: Sensors placed based on the criteria of maximizing the observability
Thus accounting for ALL possible release scenarios
PF operator turns this into a convex optimization problem



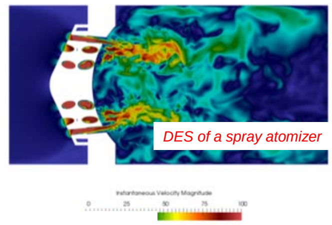

Sensor placement under geometric variations, sensing constraints, location constraints

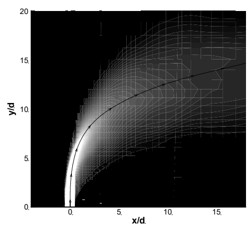
10

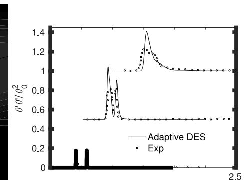
## Multiphase Turbulent Flows

- Relevant Problems
  - Separation on smooth or rough blades
  - DES/LES with heat transfer
  - mixing
- Computations
  - RANS/LES/DES
  - Inverse modeling/M.L.
- Modeling

  RANS/DES/LES, data-driven


*DES of a spray atomizer*

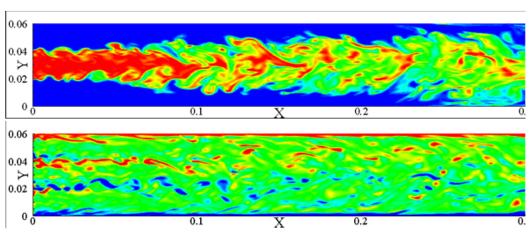


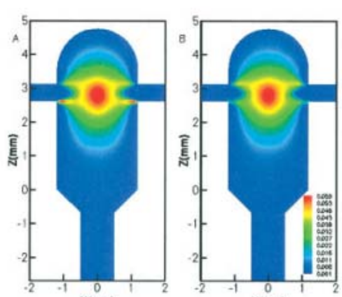



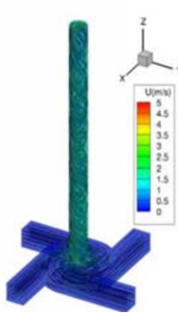
*DES of heat transport, jet in cross flow*

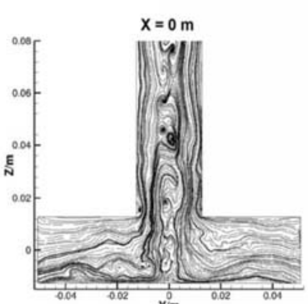
11

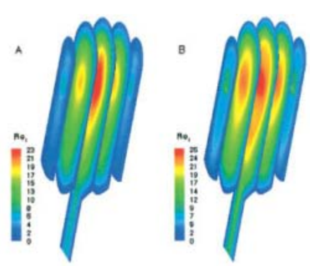
## Turbulent Mixing and Reacting Flows



12

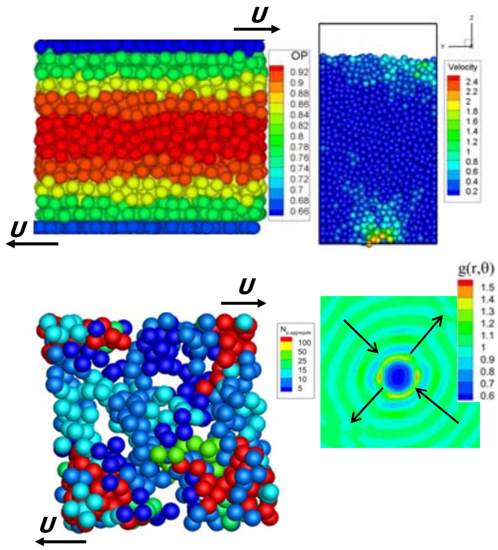
## Granular Flows

*Motivation*
Continuum models for granular materials fail in the vicinity of regime transitions

*Approach*
Close macroscopic stress using microscopic variables accounting for structure

*Accomplishments*
Stress models which perform well for canonical flows across the transition

*Significance & Impact*
- Such models are important for industrial applications
- Local kinematic variables may be insufficient to characterize stress in granular systems

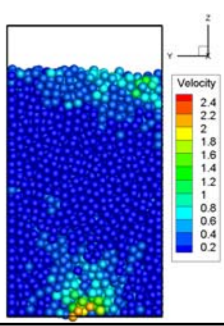


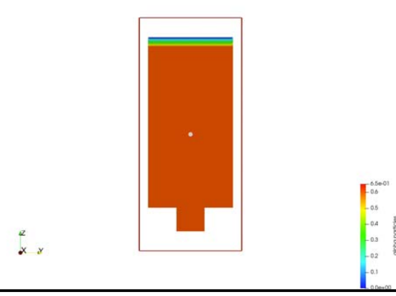

13

## Hopper Discharge

**Motivation**
- Predictable discharge of granular materials stored in silos or hoppers is critical to many industries
- Need physics-based understanding to extend to wider range of problems

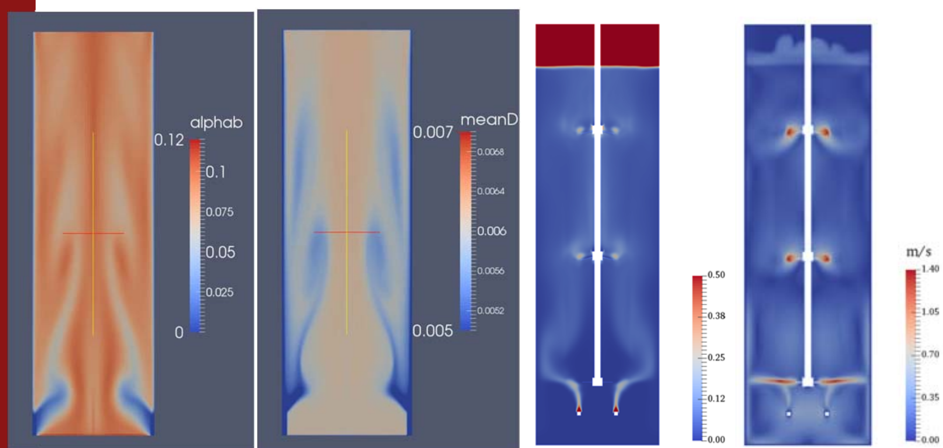
**Approach**
- Continuum model simulation is used to predict discharge
- Discrete element method (DEM) is also used for comparison
- Use DEM simulation results to inform continuum models



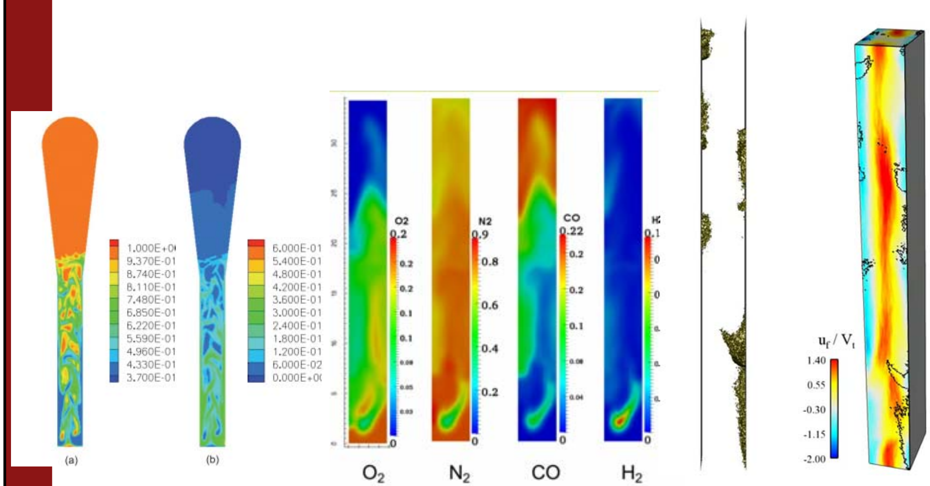
14

## Gas-Liquid and Bubbly Flows




15

## Fluidized Beds and Gas-Particle Reacting Flows



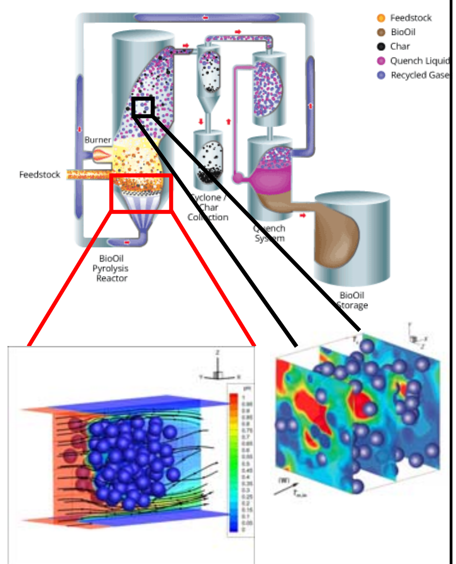

16

## Heat and Mass Transfer in Gas-Particle Flows

*Motivation*
Effects of walls and entrance on heat and mass transfer models for multiphase CFD simulations

*Accomplishments*
Simulation of heat transfer in a fixed particle bed in a duct

*Significance & Impact*
- Extension of heat and mass transfer models to account for wall effects
- Entrance effect on the computation of mean quantities such as Nusselt number and drag force

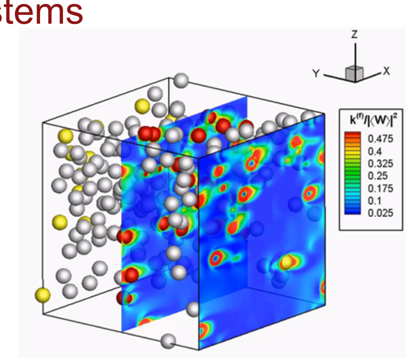


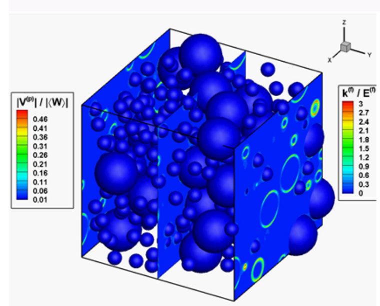

17

## PR-DNS of Gas-Particle Systems

***Theme***
- Particle-resolved direct numerical simulations to gain insight into microscale flow physics
- Use PUReIBM data in canonical gas-solid flows to quantify unclosed terms in closures for gas-solid flow

***Significant Accomplishments***
1. Pseudo-turbulence in gas-solid flow
2. Hydrodynamics and heat transfer in clustered configurations
3. Heat and mass transfer in gas-solid flow
4. Validate PR-DNS with experiments

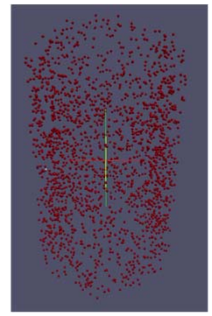


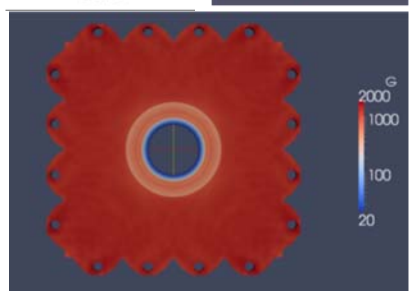



18

## Multiphase Reactors

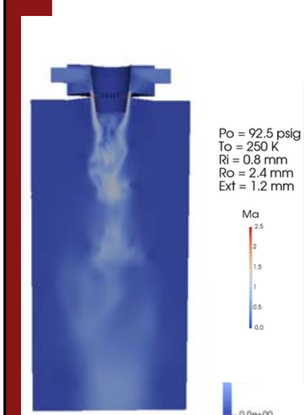
- **Eulerian-Eulerian Gas-Liquid and Liquid-Liquid CFD Simulation**
  - Taylor-Couette flow
  - Interphase mass transport
  - Yield-stress and shear thinning fluids
  - Droplet/Bubble coagulation and breakup
- **3D Spectral Radiation Transport Simulations**
  - Photobioreactors
- **Monte-Carlo/Brownian-Dynamics Simulation of Aggregation/Breakup**
  - Fractal morphology
- **Population Balance Modeling – Analytical Solutions and Scaling Analysis**
  - Self-preserving size distributions
  - Aggregation/breakup kernels characterized by homogeneity indices

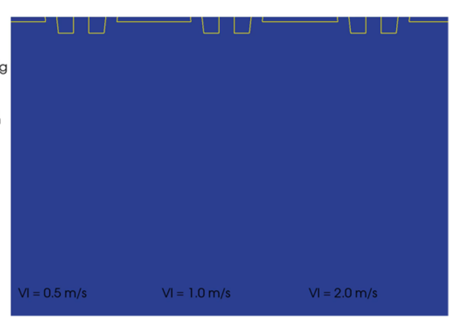


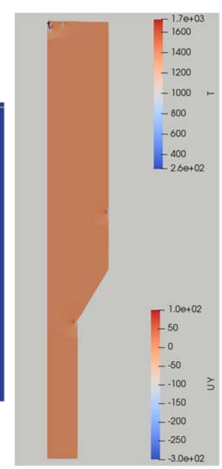



19

## Compressible Flow and Gas Atomization




20

21

## OpenQBMM – www.openqbmm.org

**What is OpenQBMM?**
A suite of libraries and solvers for OpenFOAM® to implement quadrature-based moment methods.

**Features**

- Robust
  - Automatic enforcement of moment realizability
  - Moment-preserving advection schemes
  - Realizable integration of stiff source terms
- Validated
  - Test-case provided for each core component
  - Validation cases provided as example application for solvers

**What problems can it solve?**

Nanoparticle formation
(St << 1)

Gas-liquid systems with coalescence and breakup
St = O(1)

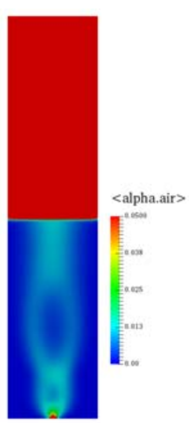
Polydisperse particulate systems (dense and dilute flows)
St >> 1

Full range of Stokes numbers

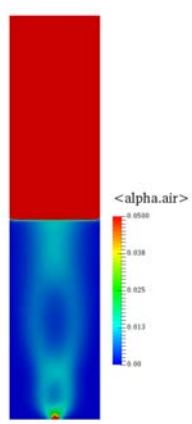
21

22

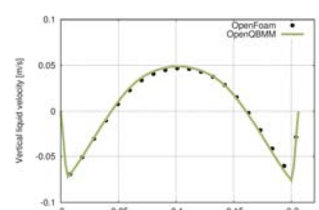
## Verification of OpenQBMM



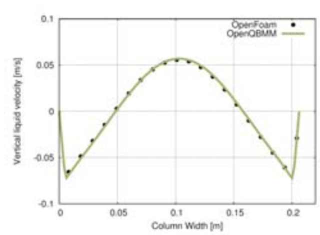

OpenQBMM




twoPhaseEulerFoam




H = 0.13 m

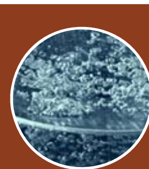



H = 0.37 m

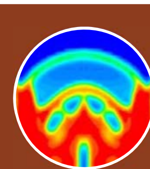
22

## Families of problems of interest

**Population balance equations**
- Non-inertial particles ($St \to 0$)
- Turbulent mixing
- Reacting flows



**Gas-liquid systems**
- Small inertia ($St < 1$)
- Coalescence, breakup
- Free surfaces



**Gas-solid systems**
- Large particle inertia ($St \gg 1$)
- Particle trajectory crossing
- Nearly packed regions

23

IOWA STATE UNIVERSITY™
**Center for Multiphase Flow Research and Education**

## Experimental Resources


24

## Experimental Ranges and Example Activities

- **Size:** Nanoscale to meters
- **Time:** fs/ps resolution to time-average
- **Reactions:** reacting and nonreacting flows
- **Recent and current activities:**
  - Biomaterial and hydrogel synthesis
  - Combustion system analysis
  - Energetic material synthesis
  - Flow through porous media
  - Gas-liquid and gas-solid hydrodynamics
  - Particle assembly
  - Particle-particle mixing
  - Spectroscopy studies
  - Spray characterization

25

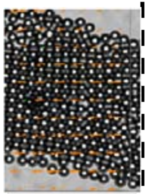
## Unique Equipment

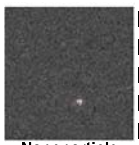
- Detonation chamber
- High-speed and stereo imaging
  - 20 kHz at full frame, faster at reduced frame size
  - Digital inline holography
  - Shadowgraphy
- Laser diagnostics
  - hybrid fs/ps coherent anti-Stokes Raman scattering
  - high-speed spectroscopy
  - PDPA/LDV
  - kHz to MHz-rate PIV and fluorescence
- 3D printing
  - energetics, hydrogels, polymers, etc.
- Video microscopy
- X-ray flow visualization
  - X-ray radiography, stereography, and computed tomography

26

## Optical Video Microscopy

**Capabilities**


Particle Image Velocimetry

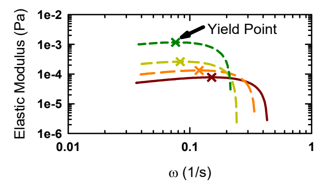

Nanoparticle Tracking

**Facilities**

- Two fluorescence microscopes
- Dedicated computers for video and image analysis
- Syringe pumps to control fluid injection
- Plasma bonding for polymer microchannels

**Applications**


Multiphase Flow in Porous Media



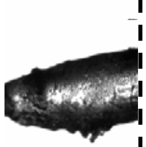
Measurements of Viscoelasticity in Biomaterials

27

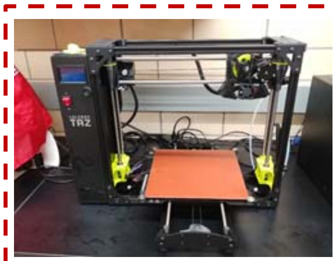
## Polymer Processing

**Capabilities**


Biocompatible Hydrogels

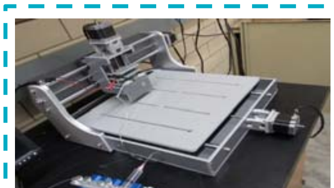

Structured Polymer Composites

**Facilities**



- Wet lab facilities for material processing
- Electrical test equipment for assembling filler particles in polymer composites
- One 3D printer for dedicated prototyping
- Second 3D printer for material deposition

**Applications**

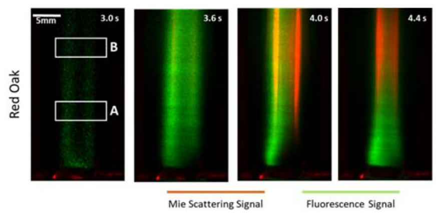

3D Printing of Multiple Materials


Separation of Biocompatible Hydrogel Materials

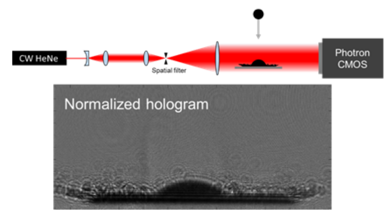
28

## Fluorescence and advanced imaging for phase discrimination and droplet measurements

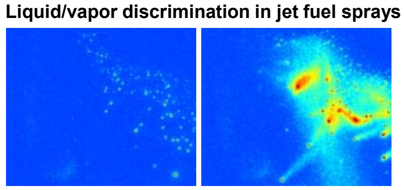
**Simultaneous imaging of condensed phase and vapor phase products of biomass pyrolysis**



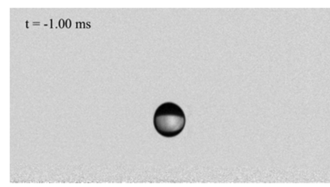

**Digital inline holography and PDPA/LDV characterization of droplet sizing of multicomponent droplet physics**




**Liquid/vapor discrimination in jet fuel sprays**



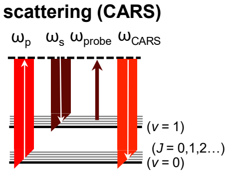
**Multi-component fuel effects at high P (50 bar), high T (800-2000 K)**



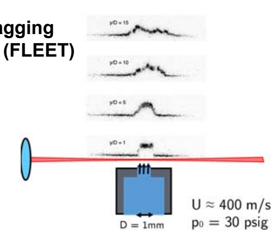

29

## Ultrafast lasers for non-equilibrium systems, precise temperature, and velocimetry

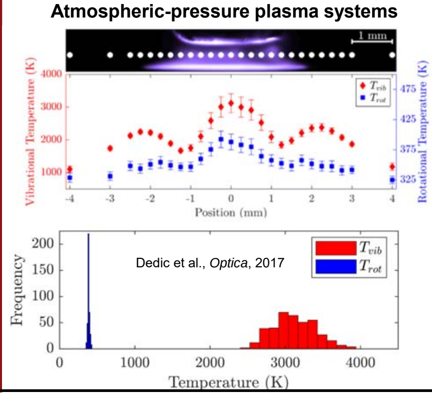
**Hybrid fs/ps coherent anti-Stokes Raman scattering (CARS)**



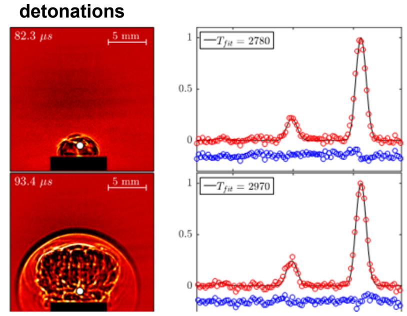

**Molecular tagging velocimetry (FLEET)**




**Atmospheric-pressure plasma systems**




**Mapping the wave structure of supersonic detonations**

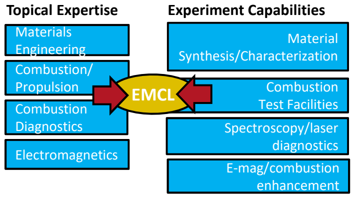



30

## Energetic Materials Combustion Lab (EMCL)

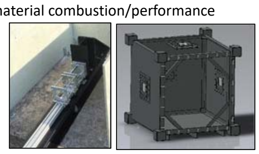
**Research Focus:** The development of energetics with unique properties that enable next generation energetic devices (propulsion systems, pyrotechnics, explosives) more favorable properties (e.g. performance, 'green' combustion, controllable combustion).

**Topical Expertise** / **Experiment Capabilities**




**Experimental Facilities Overview**

- ~1500 ft$^2$ research space, shared with combustion/diagnostics faculty (Michael)
- Material characterization (CIF, MARL, Ames Lab)
- Energetic material combustion/performance evaluation



**Left:** 500 lb$_f$ static rocket motor stand (left). **Right:** 125 ft$^3$, ~10 g TNT equivalent detonation chamber, developed for laser temperature/ speciation of detonations (Michael/Sippel)

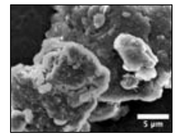
### Synthesis/Characterization

**Nanomaterial synthesis**

- Techniques: Ball milling/mechanical activation, ultrasonication, electrospray

**Energetic Fabrication**

- Propellant/explosive charge fabrication
- Safety characterization
- 3D printed energetics (current effort)

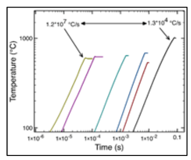



**Above:** Electron micrograph of $NaNO_3$ nano-decorated aluminum fuel

### Combustion Test Facilities

**High-Heating Rate Ignition**

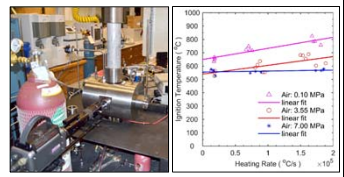
- Custom fabricated pulse mode electronics systems capable of up to 1.5 MW heating
- Linear heating up to $10^7$ C/s




**Above:** Temperature-time history of a nickel chromium ignition filament

**Windowed high-pressure combustion vessel experiments**

- Remotely operable vessels (200 bar)
- Configurable for laser ignition, high-heating rate filament ignition or electric field-flame interaction




**Left:** windowed, vessel for combustion/ignition experiments. **Right:** High-speed ignition temperature measurement of a thermite in high-pressure air

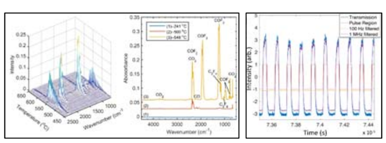


## Energetic Materials Combustion Lab (EMCL)

### Spectroscopy/Laser Diagnostics

**Time/temperature-resolved speciation**

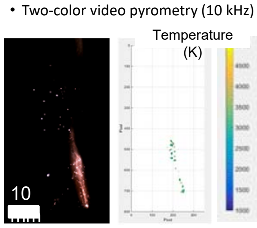
- DSC/TGA with online FTIR/MS
- High-speed (1 MHz) quantum cascade IR (9.5-10.5 μm) laser absorption
- VIS spectroscopy (300-900 nm, 10 Hz)



**Above**: Left, center: IR absorption speciation of evolved gas products from heating of a thermite. Right: Time-resolved quantum cascade IR absorption of methanol.

**Temperature/emissivity measurement**

- High-speed NIR spectroscopy (1.3 kHz, 1-4 μm)
- Two-color video pyrometry (10 kHz)

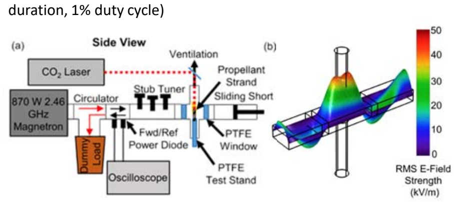



**Left:** high-speed video and phase-locked two-color video pyrometry temperature measurement of a solid propellant flame under 60 Hz microwave excitation.

### Electromagnetic Combustion Enhancement

**Microwave-Augmented Combustion Cavities**

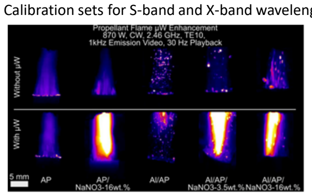
- 2.45 GHz S-band optically accessible cavities
- **Sources:** 1 kW continuous wave and 50 kW pulsed (~0.5 to 2 μs duration, 1% duty cycle)




**Above:** Diagram of microwave augmented combustion cavity (left) and electric field distribution within the cavity (right).

**Dielectric property measurement**

- Vector network analyzer (500 MHz to 30 GHz)
- Airline (broadband) and cavity insertion (narrow band) property measurement hardware
- Calibration sets for S-band and X-band wavelengths

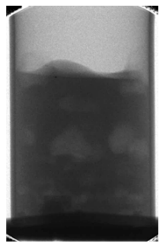



**Left:** Video of microwave-augmented combustion of composite solid propellants (several formulations), aluminized and unaluminized containing sodium nitrate dopant. 1 kHz light emission acquisition

## X-ray flow visualization of gas-solid and gas-liquid flows

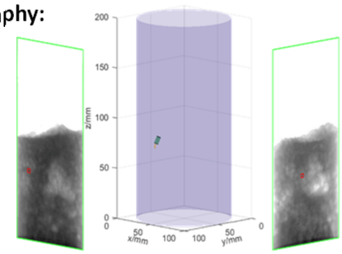
**X-ray radiography:**

Right, high-speed images of a 15.24 cm dia. fluidized bed with a single intruder particle. Images acquired at 1000 FPS and played back at 40 FPS.

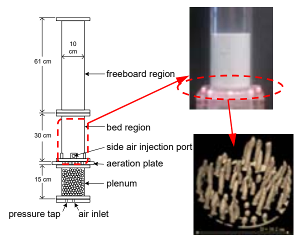


**X-ray stereography:**

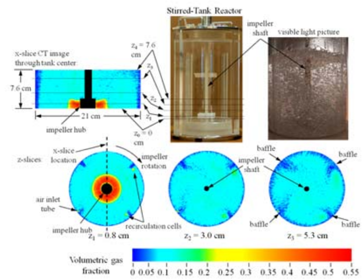
X-ray particle tracking in a binary fluidize bed. One particle is tagged to distinguish it in mutually perpendicular X-ray projections to track position AND orientation as a function of time.



**X-ray computed tomography:**




X-ray CT reconstruction of the fluidized bed aeration region



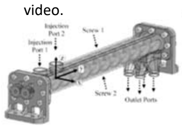

X-ray CT imaging of a 21 cm diameter gas-sparged stirred-tank reactor showing the local time-average gas holdup in a vertical slice through the STR center plane and several horizontal planes.

33

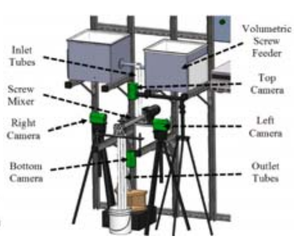
## Particle-particle mixing

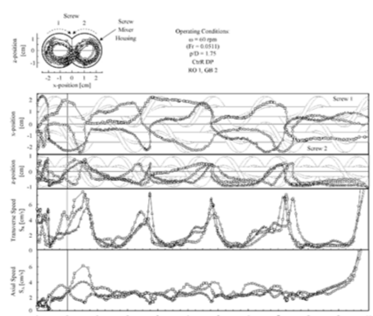
**Optical visualization:**

- 3D print mixer with post-processing to produce optically accessible mixer.
- Time-sync 4 video projections and edit into a single video.

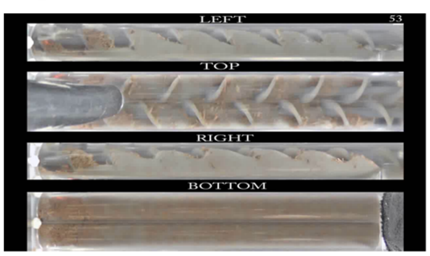


**X-ray stereography:**



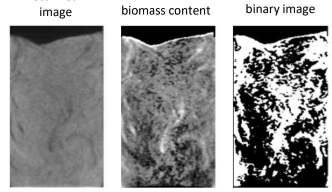
X-ray particle tracking in a double-screw mixer.




Double-screw mixer video with biomass (brown) and glass beads (gray).

**X-ray computed tomography:**

Scanned image | Converted to biomass content | Converted to binary image

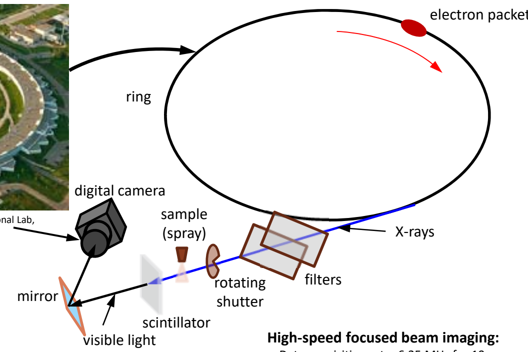


X-ray CT imaging to quantify mixing and segregation in binary (biomass-glass beads) granular systems.

34

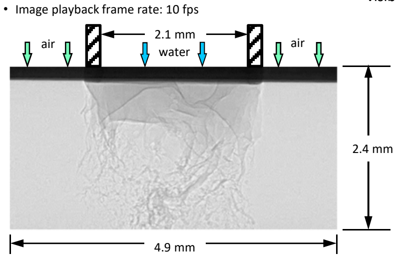
## Collaborating with Argonne National Lab: Advanced X-ray imaging using the Advanced Photon Source

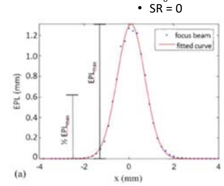
Photo acknowledgement: Advanced Photon Source, Argonne National Lab, https://www1.aps.anl.gov/sites/default/files/aerial_2010.jpg



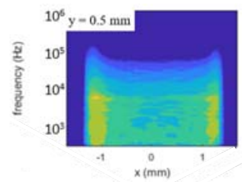

**High-speed white beam imaging:**
- $Re_l$ = 1,000
- $Re_g$ = 96,900
- SR = 1
- Image acquisition frame rate: 10,000 fps
- Image playback frame rate: 10 fps

**High-speed focused beam imaging:**
- Data acquisition rate: 6.25 MHz for 10 s
- $Re_l$ = 1,000
- $Re_g$ = 16,700
- SR = 0




Equivalent path length (EPL) measures




Frequency analysis

35

## CoMFRE Summary

- ISU has unique computational and experimental capabilities in the area of multiphase flows:
  - Range of length and time scales
  - Creeping to turbulent flow
  - Reacting and nonreacting systems

CoMFRE
Center for Multiphase Flow Research and Education

36