# Development of Design Practices for Additively Manufactured Micro-Mix Hydrogen Fueled Turbine Combustors with High-Fidelity Simulation Analysis, Reduced Modeling and Testing

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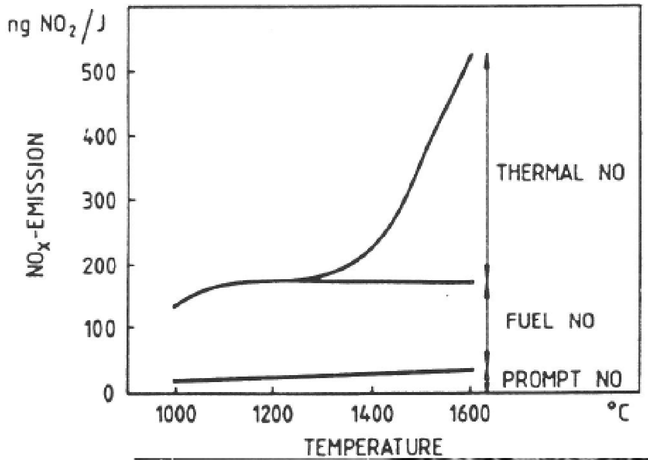
**(DE-FOA-0002397)**

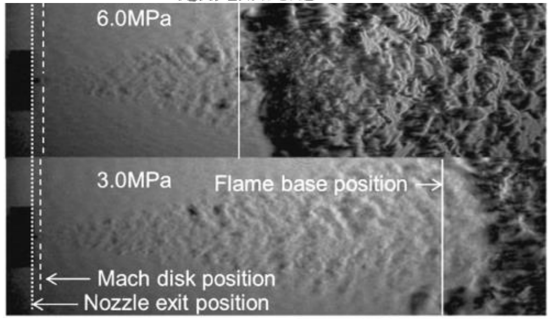
# Outline

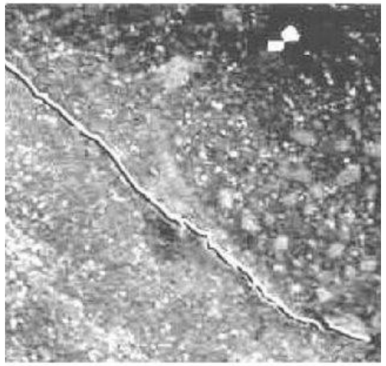
- Motivation and Objectives
- Models and Codes
  - LES and FDF
  - DG and FD
  - Semi-Lagrangian vs. Particle Methods
- Simulations
  - LES of Injector in cross stream and dump combustor
  - Cold Flow  and Reacting Flow
  - Wall roughness and additive manufacturing
- Reduced Modeling
  - Input-Output Design Maps
  - Reduced dynamic modeling for QoIs
- Testing
- Timeline

# Challenges in Hydrogen Combustion

- High temperature of combustion of $H_2$
  - higher heat flux to the combustor's structure
  - increased $NO_x$ emissions
- High laminar flame speeds of $H_2$
  - flashback
  - flameout for lean fuel mixtures
  - highly strained subgrid scales
- Metal embrittlement



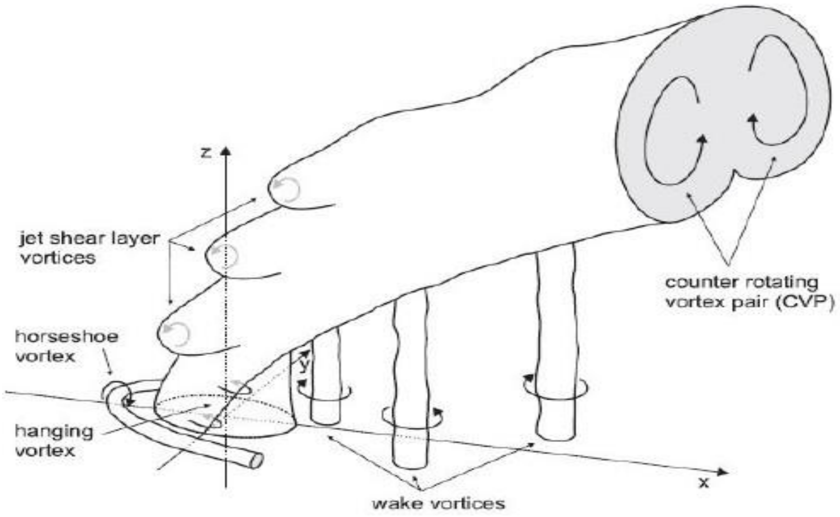



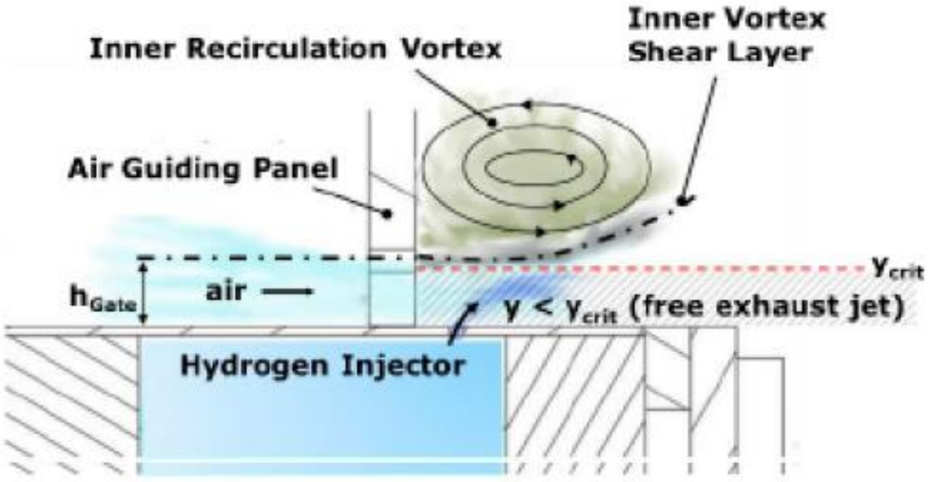
# Injector Design

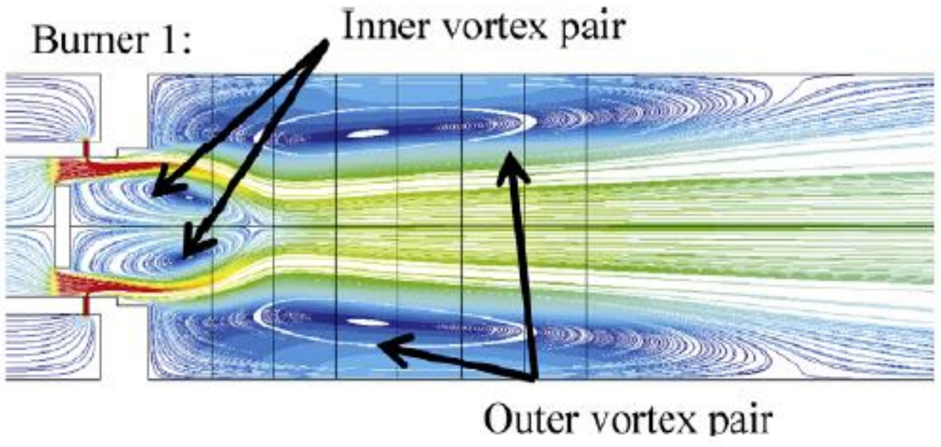
- Mitigating of hydrogen issues using micro-mixers
  - optimal positioning of the ignition plugs
  - miniaturization decreases residence times of the reactants because reaction zones are small, which significantly reduces $NO_x$

- Considerations
  - ignition
  - a stable flameholding
  - a drag overhead
  - penetration of the fuel into the flow



# Open Questions




- What is the effect of the geometric design and the location and configuration of injector arrays?
- What are the optimal flow conditions for a hydrogen fuel injector that produce a good quality of
- combustion?
- What is the effect of additive manufacturing on the mixing characteristics and combustion?
- What is good practice for combustion design in terms of air guides and flame holding?
- What is the best practice for simulation of these flows? Which models are suited to simulate hydrogen mixing and combustion?

# Goals

1. Determination of foundational design rules for hydrogen micromixer injectors in industrial gas turbine combustors using high-fidelity analysis and testing

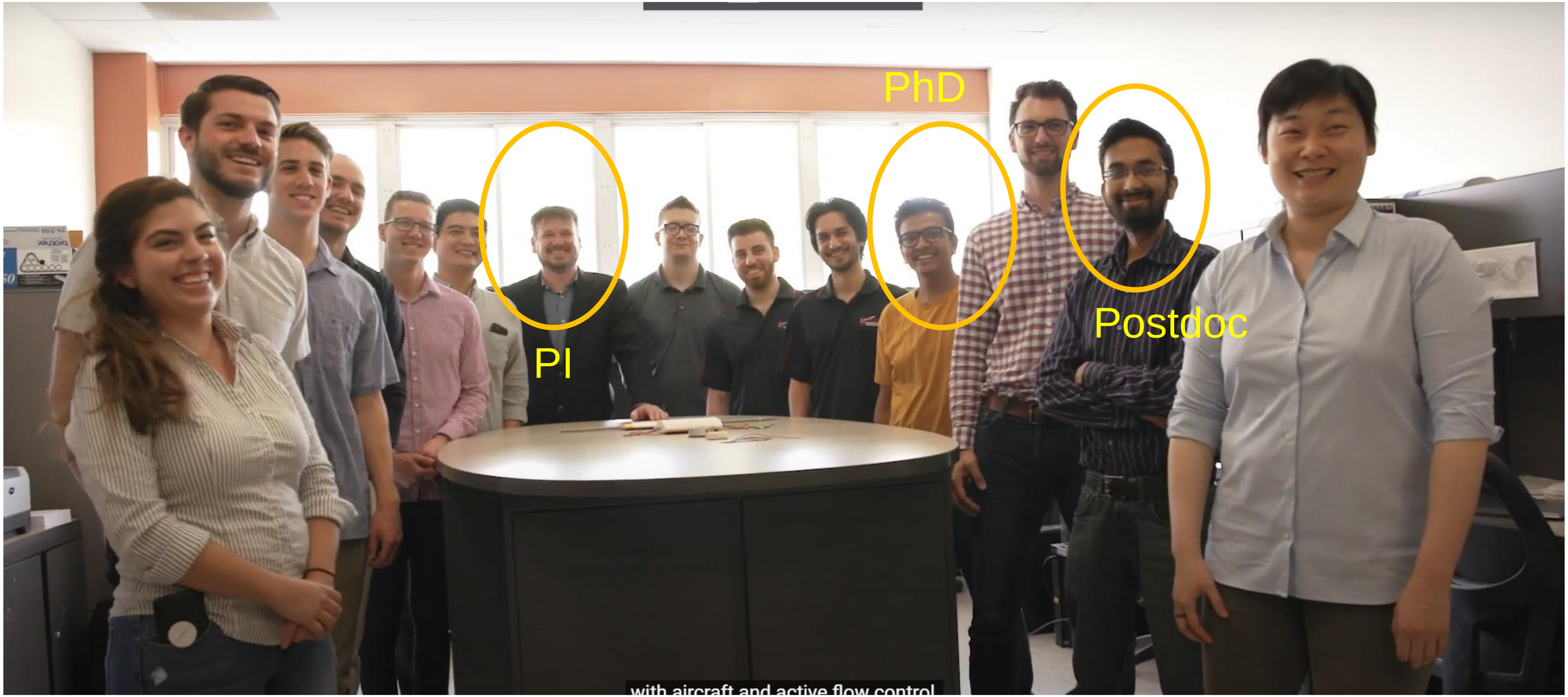
2. Assessment of the impact of additive manufacturing on the roughness topography including its anistropy in and around injectors on cold flow and combustion characteristics

3. Development of design tools through reduced models that predict flow mixing, pressure losses, heat transfer and flame stability as a function of geometric and flow design parameters in a computationally efficient manner

# Approach

- High-Fidelity simulation of cold flow and reacting
  - Canonical injector arrays and combustor geometries with parametric dependencies
  - Development of  stochastic models for AM geometries
  - Systematic study of the  effect of geometric design
  - Systematical study of the effect of flow conditions
- Reduced dynamic modeling for combustion characteristics
- Testing in Solar Turbine’s rigs

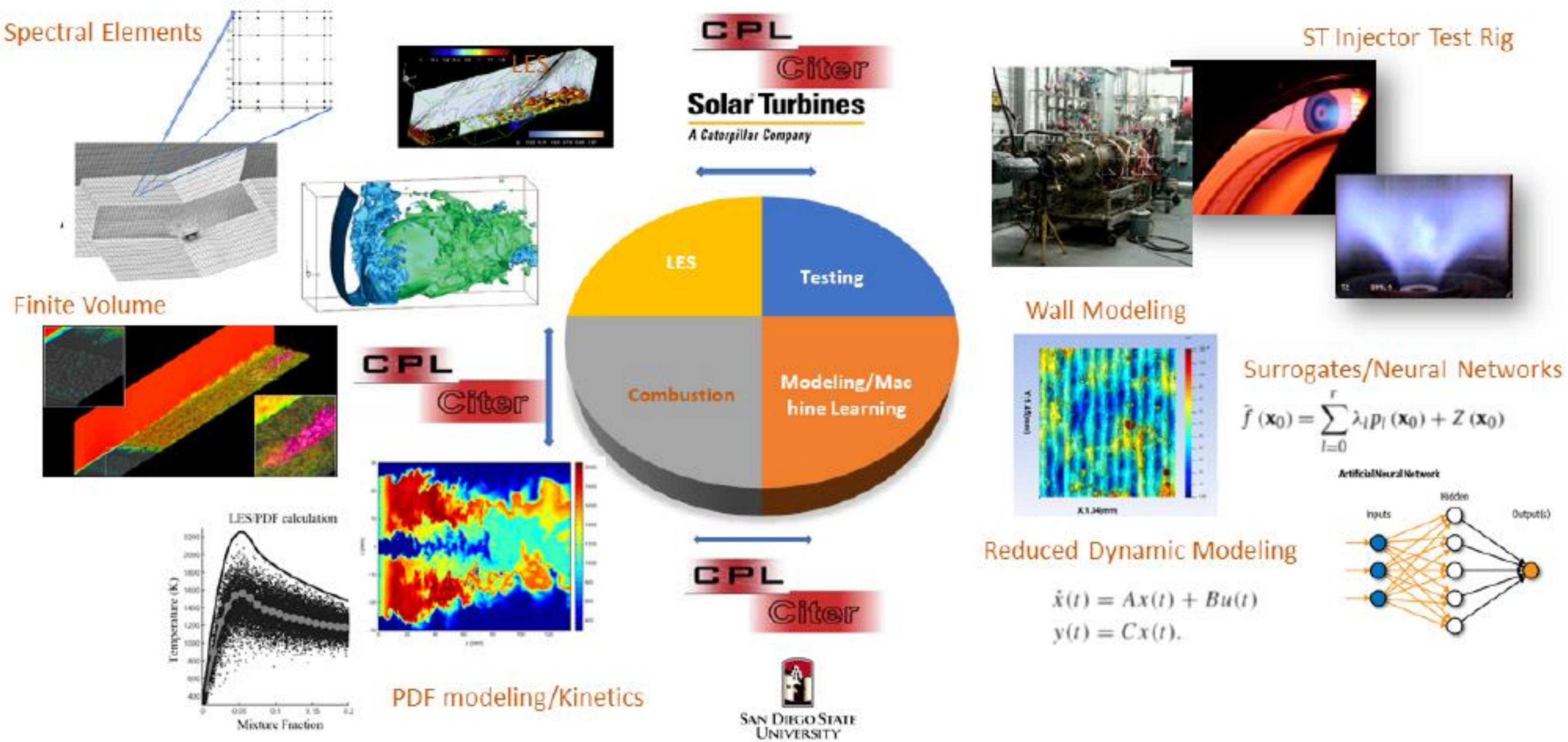
# Computational Physics Lab



# Solar Core Team

- **Dave Voss** – Manager of University & Government Programs
- **Mike Ramotowski** – H2 NPI Program Manager for TMP Engineering
- **Luke Cowell** – Manager, Combustion NPI & Strategy
- **Rajeshriben “Raj” Patel** – H2 Combustion Project Lead
- **Gareth Oskam** – Combustion Senior SME
- **Yonduck Sung** – Combustion Methods, CFD/LES analysis SME
- **Daniel Ryan** – Materials and Additive Manufacturing SME

# Teams and Connectivity



# MODELS and CODES

# Cold Flow LES Model

Filtered Navier-Stokes equations

$$\frac{\partial \langle \rho \rangle_l}{\partial t} + \frac{\partial \langle \rho \rangle_l \langle u_i \rangle_L}{\partial x_i} = 0$$

$$\frac{\partial \langle \rho \rangle_l \langle u_j \rangle_L}{\partial t} + \frac{\partial \langle \rho \rangle_l \langle u_i \rangle_L \langle u_j \rangle_L}{\partial x_i} = -\frac{\partial \langle p \rangle_L}{\partial x_j} + \frac{\partial \langle \tau_{ij} \rangle_l}{\partial x_i} - \frac{\partial T_{ij}}{\partial x_i}$$

$$\frac{\partial \langle \rho \rangle_l \langle \phi_\alpha \rangle_L}{\partial t} + \frac{\partial \langle \rho \rangle_l \langle u_i \rangle_L \langle \phi_\alpha \rangle_L}{\partial x_i} = -\frac{\partial \langle J_i^\alpha \rangle_l}{\partial x_i} + \langle \rho \rangle_l \langle S_\alpha \rangle_L - \frac{\partial M_i^\alpha}{\partial x_i}$$

We use a computationally efficient numerical filter => implicit LES

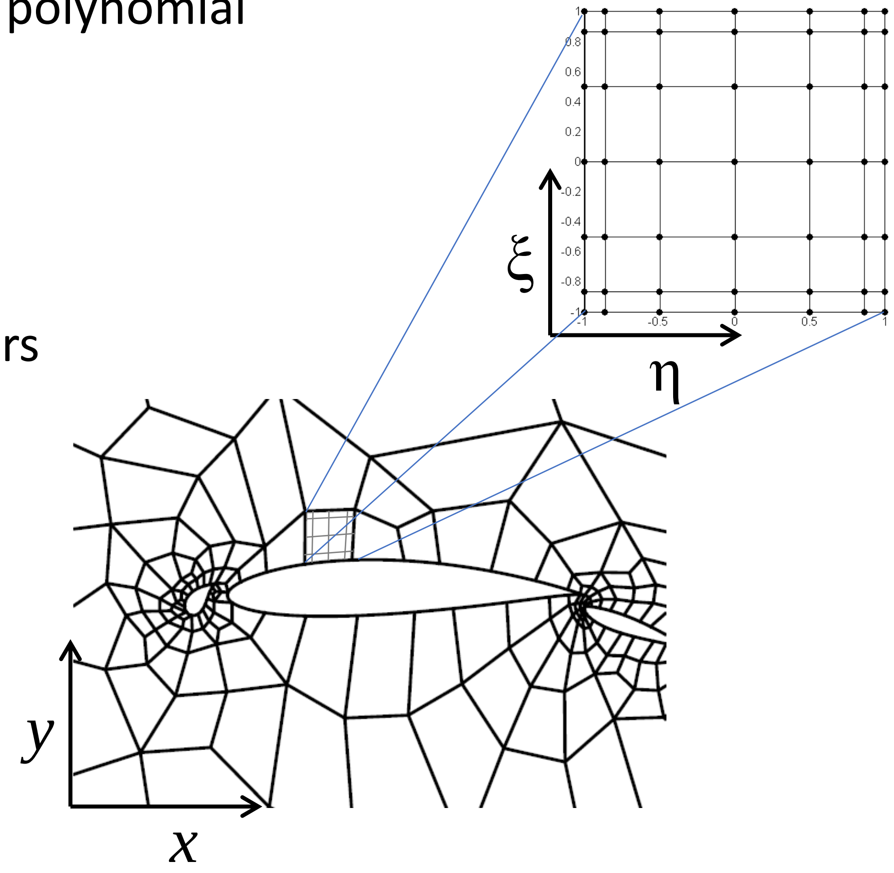
[Chaudhuri, Jacobs et al. , JCP, 2017]

# LES with Discontinuous Galerkin Spectral Element Method

- Divide computational domain into elements
- Map each physical element onto a master element
- Approximate solution with higher-order (Jacobi) polynomial

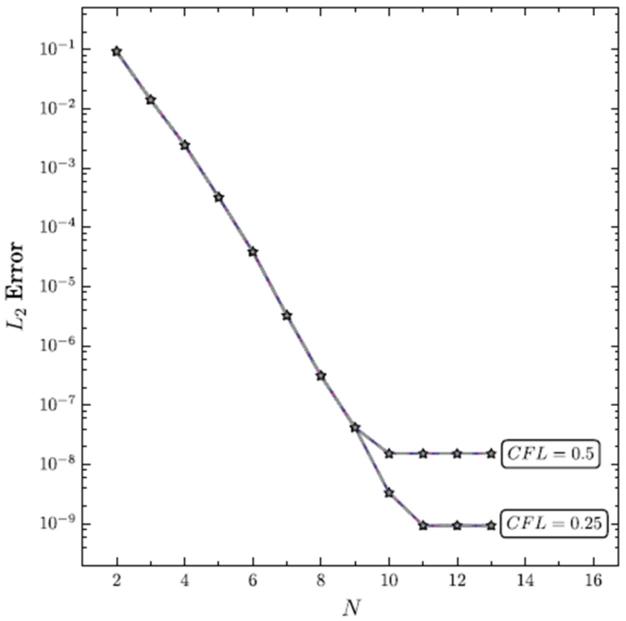
$$f(x_i) \approx \sum_{j=0}^{N} \hat{f}_j L_j(x_i) = \sum_{j=0}^{N} f_j \ell_j(x_i) \qquad f'(x_i) \approx \sum_{j=0}^{N} f_j \ell'_j(x_i)$$

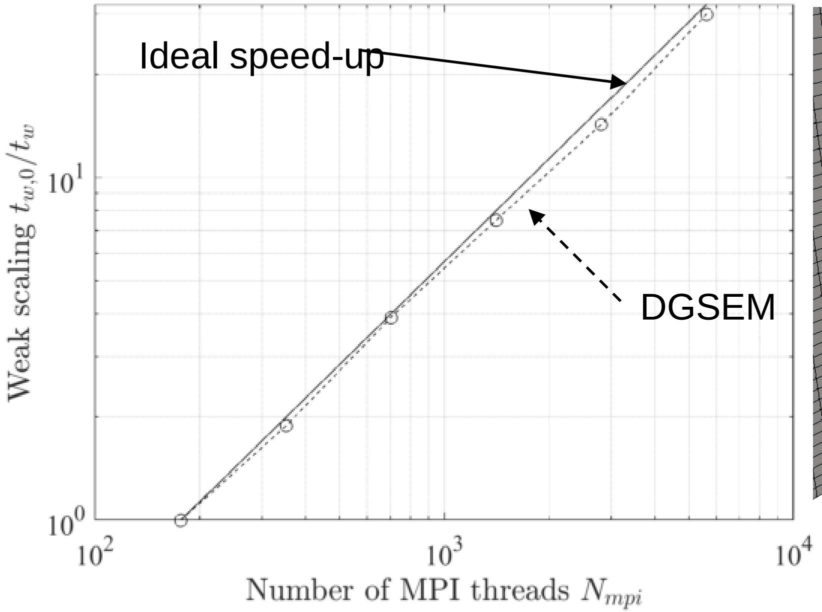
- Based on Method of Weighted Residuals
- Elements are connected through Riemann solvers

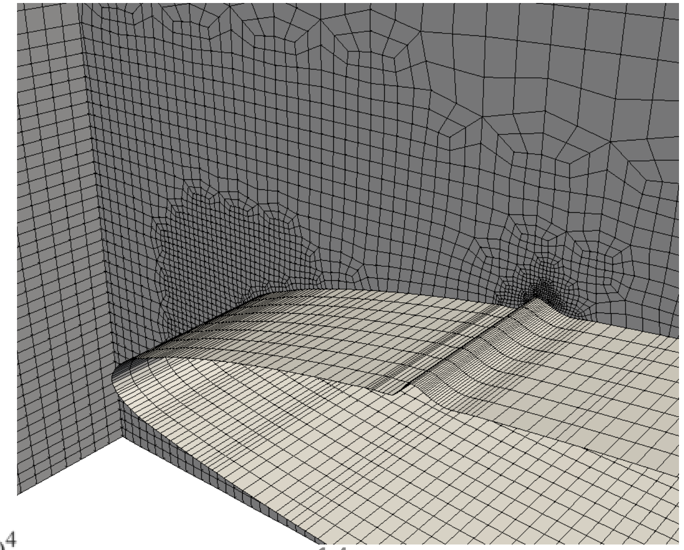


# Why use a Discontinuous Spectral Element Method (DSEM)?

- Complex geometries: unstructured grids
- Accurate wall modeling: boundary fitted elements to accurately model roughness element
  - no weird oscillation or reduced accuracy near the wall
- Accurate simulation of time-dependent flows: high-order accuracy with exponential convergence for
- Computational efficiency: highly parallelizable because of non-overlapping elements
- Numerically robust (entropy preserving methods)



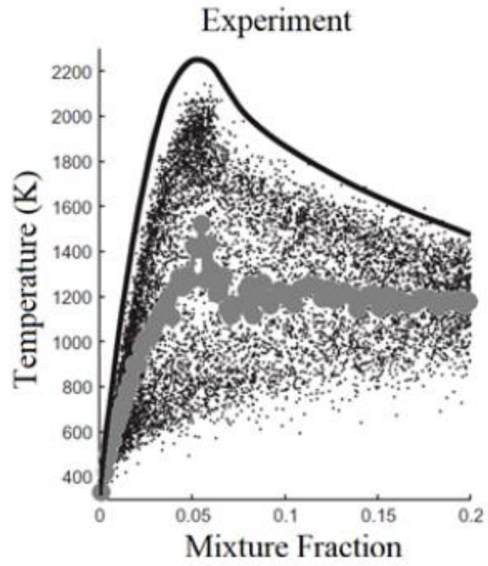



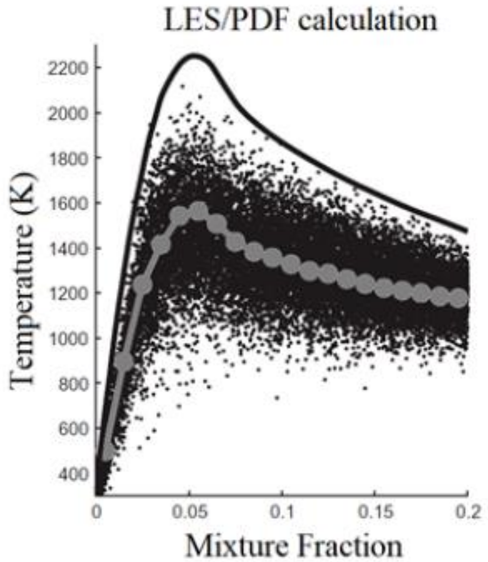
# Chemically Reacting Flows: FDF Model

- FDF approach
  - Solve for the filtered density function, $f(\boldsymbol{\psi}; \boldsymbol{x}, t)$
  - $f$ is a PDF of the composition $\boldsymbol{\psi}$ over a filter centered at $\boldsymbol{x}$

- Motivation
  - Need full temperature PDF to account for changes in reaction rate is $k = Ae^{-\frac{E_a}{RT}}$ with exponential temperature dependence challenges models like $\widetilde{k(T)} = k(\tilde{T})$
  - NOx emissions in hydrogen combustors are strongly affected by the residence time in high-temperature regions => benefits from a knowledge of the complete PDF

- FDF evolution equation
  - $\frac{\partial}{\partial t}[\rho(\boldsymbol{\psi})f] + \frac{\partial}{\partial x_i}[\rho(\boldsymbol{\psi})\langle u_i|\boldsymbol{\psi}\rangle f] + \frac{\partial}{\partial \psi_\alpha}[\rho(\boldsymbol{\psi})k(\boldsymbol{\psi})f] = \frac{\partial}{\partial \psi_\alpha}\left[\left\langle \frac{\partial J_i^\alpha}{\partial x_i}|\boldsymbol{\psi}\right\rangle f\right]$
  - Conditional terms, $\langle \cdot \mid \cdot \rangle$, require turbulence modeling



# LES-FDF

With turbulence models evolution equation is

$$\frac{\partial F_L}{\partial t} + \frac{\partial \langle u_i \rangle_L F_L}{\partial x_i} = \frac{\partial}{\partial x_i}\left[(\gamma + \gamma_t)\frac{\partial F_L/\langle \rho \rangle_l}{\partial x_i}\right] + \frac{\partial}{\partial \psi_\alpha}[\Omega_m(\psi_\alpha - \langle \phi_\alpha \rangle_L)F_L] \boxed{- \frac{\partial [S_\alpha(\phi)F_L]}{\partial \psi_\alpha}}$$

Chemical source terms in closed form
=>
unique to FDF approach

where, $\phi$ is the chemical species

$\langle u_i \rangle_L$ Filtered velocity

$\psi_\alpha$ is the species and energy domain;

$\gamma, \gamma_t$ are the molecular and thermal diffusivity;

$\Omega_m$ SGS mixing frequency term due to hydrodynamic closure

$\alpha = 1, .., N_s$; $N_s$: Number of species ~ 100

- High dimensional Fokker-Plank type equation computationally expensive to solve.
- Solve an equivalent stochastic differential equation using a Monte Carlo particle approach

# FMDF Monte-Carlo Coupled with LES

Equivalent stochastic differential equation to find the PDF of species concentration

$$dX_i(t) = u_i(X(t), t)dt + E(X(t), t)dW_i(t)$$

$$\frac{d\phi_\alpha^+}{dt} = -\Omega_m(\phi_\alpha^+ - \langle\phi_\alpha\rangle_L) + S_\alpha(\phi^+)$$

$X_i$ MonteCarlo particle position, $u_i$ drift coef, $E$ diffusion coef and $W_i$ Weiner-Levy process

Not so parallel, sample convergence is slow in Monte-Carlo approach
possible but still very expensive

$$\text{Coupled system ussually solved with particle} - \text{mesh methods}$$

# LES Monte-Carlo FDF Method

Monte-Carlo particle method that preserves accuracy and boundary fitted properties of DGSEM is very, very challenging

Dynamic particle grid requires establishing connectivity between elements and processor every time step.

Non-local distribution, not consistent with DSEM

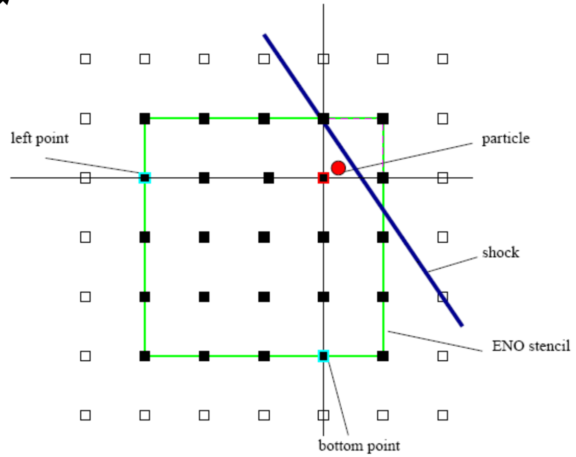
Requires computationally intensive determination of Lagrangian interpolant every time step.

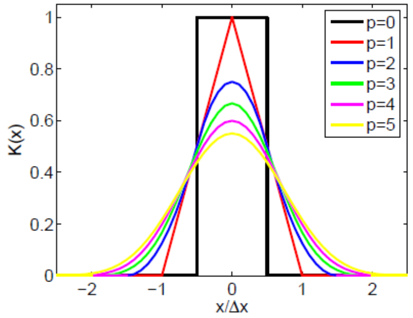
Higher-Order TVD-RK time integration of particles

Weigh particle to grid through a smooth spline/polynomial deposition function

Solve Euler eq. with high-order DSEM

Use high-order interpolation to determine field at particle position.



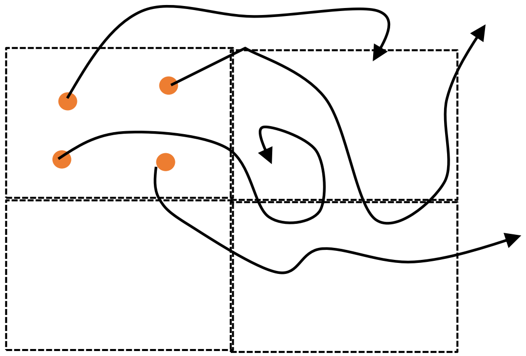




Particle mass is conserved

[Jacobs and Hesthaven, JCP, 2006][Jacobs and Don, JCP, '09][Suarez and Jacobs, SISC, 2014]

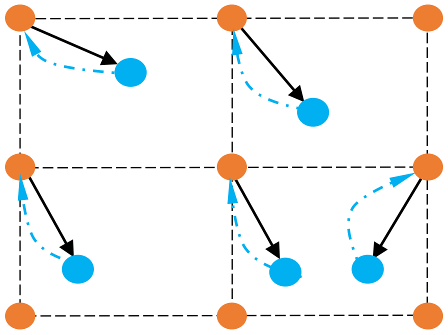
# Lagrangian vs semi-Lagrangian Methods

## Lagrangian



- Particles tracked over the entire flow field
- FDF obtained by local sampling
  - ➢ Conservative
  - ❖ Coupling with Eulerian solver, tracking particles, locality, especially HO coupling very difficult.

## Semi-Lagrangian

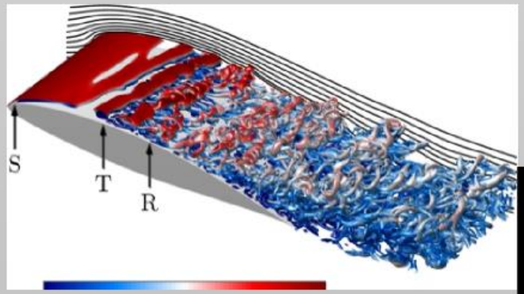


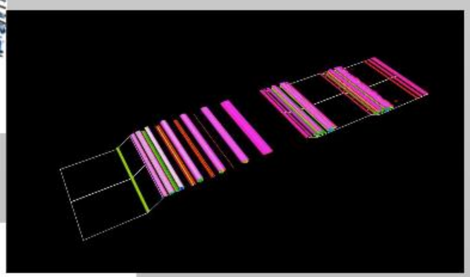
- Local, parallel, semi-fixed grid
- High-Order Accurate
- Boundary Fitted
- ❖ Conservation

[Natarajan, Popov, Jacobs, CMAME, 2021]

# Jacobs DSEM Code Capabilities

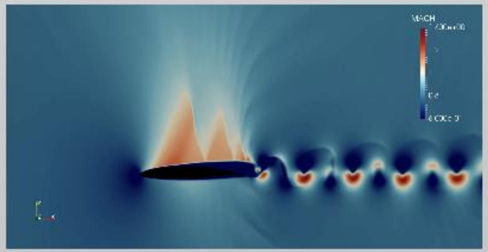
## 3D DNS and LES of complex geometries

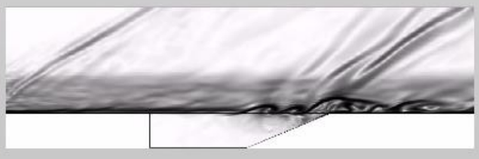


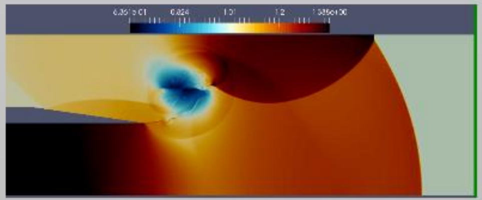



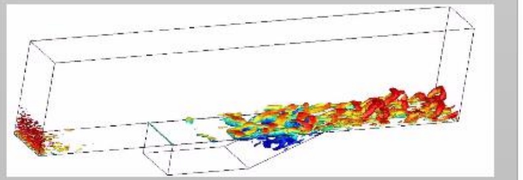
NACA 65(1)-412
at *Re* = 20,000

## 1D, 2D, 3D with Shock capturing

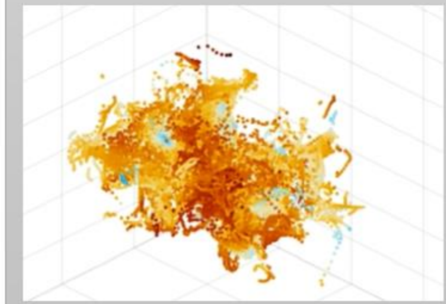


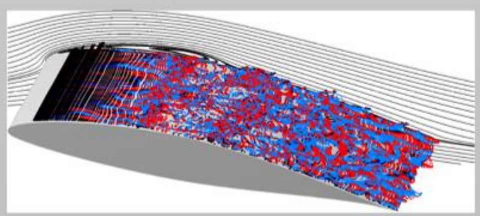




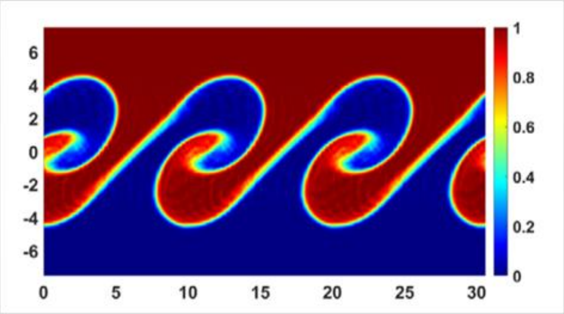


## Particle tracking (One- and two-way coupling)



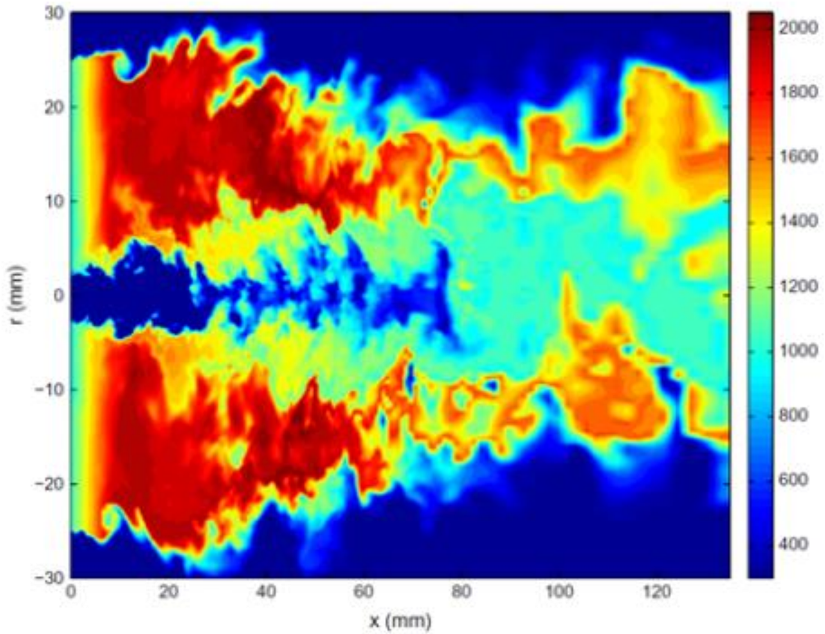



## Tracing species (transport and PDF)



# FDF-FD Popov

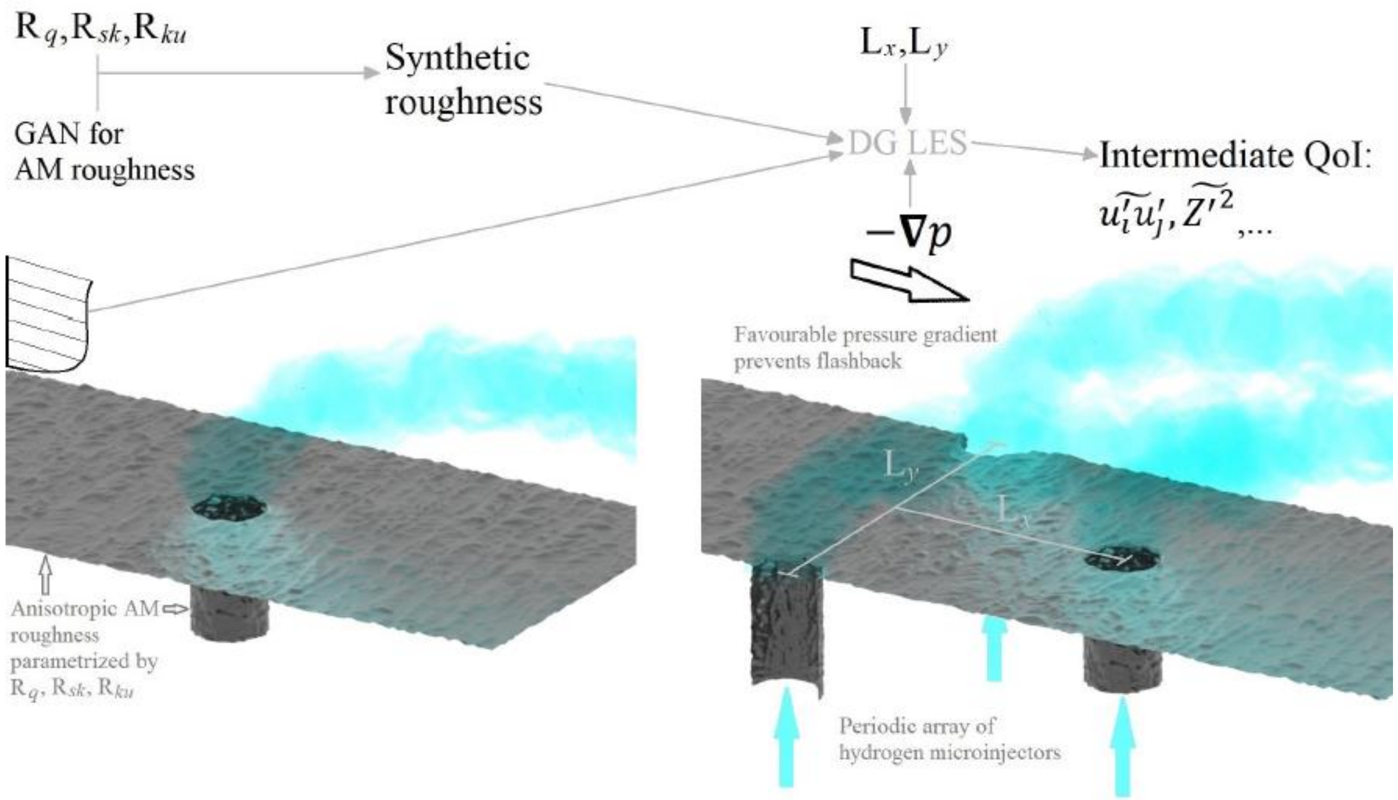
- Finite difference/filtered density function turbulent reactive flow solver
  - To be used for reactive flow simulations, and verification of the reacting version of the DSEM code
- Hybrid FD/Monte Carlo particle ensemble code
- FD handles hydrodynamics
  - Fourth order in space and time by itself
  - Provides velocity and turbulent diffusivity to particle ensemble
- Particle ensemble simulates chemical reactions, mixing and diffusion
  - Monte Carlo $N^{-1/2}$ convergence with respect to particle number, $N$
  - Weakly second-order accurate in time
  - Coupling with FD code via transported specific volume source term based on filtered particle compositions
- Demonstrated capability to predict turbulence/chemistry interactions



# SIMULATIONS

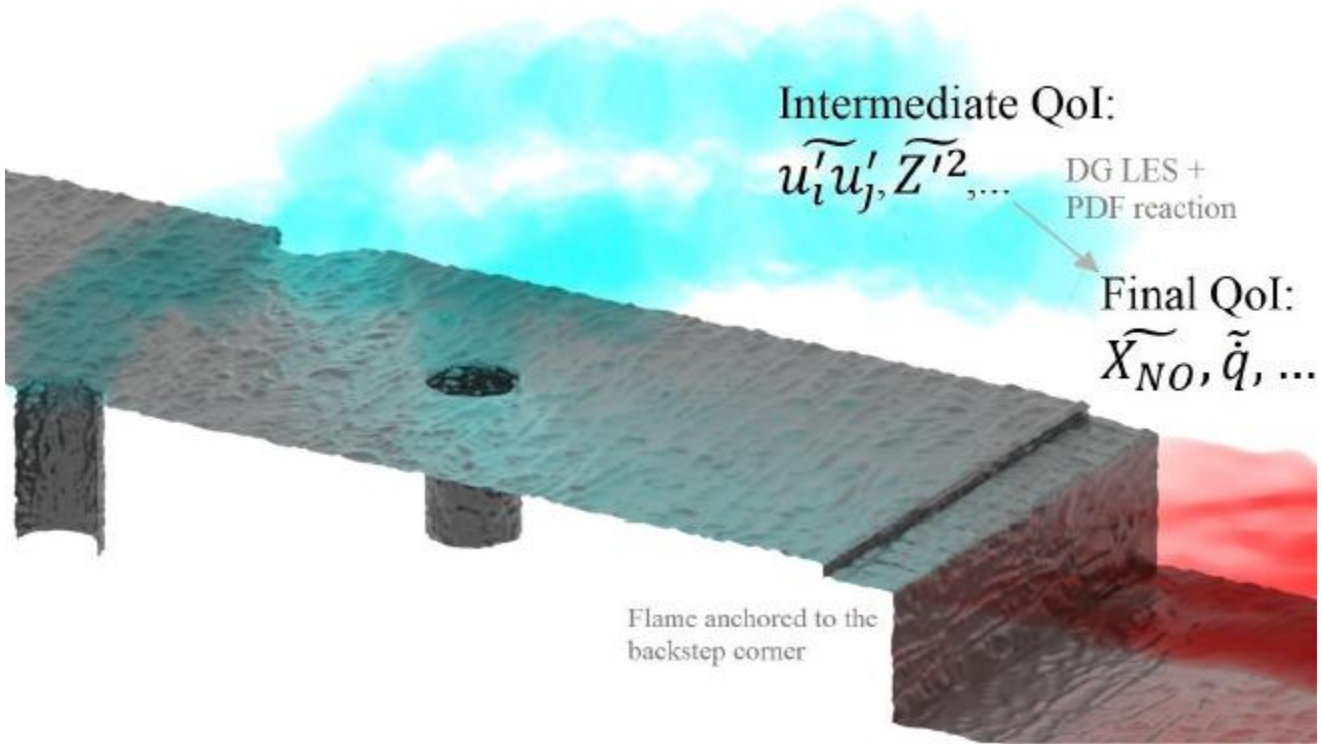
# Baseline

- Arrays of injectors in cross-stream
  - determine grid resolution and computational domain size requirements for LES.
  - provide a reference dataset for primary quantities of interest, such as mixing levels as a function of the boundary layer character and momentum flux ratio.



# LES of Chemically Reacting with Dump Combustor

- Injectors in cross-steam with dump combustor cavity and reacting flow
- To be simulated with DSEM LES/PDF solver
- Quantities of interest
  - Flame stability
  - Heat transfer to combustor structure
  - Max temperature at combustor structure
  - Pollutant (e.g., $NO, NO_2$) concentrations
- Chemical mechanisms to be used
  - Main mechanism for flame dynamics
    - Li et al., 2004
    - Shimazu et al., 2011
    - Both have 8 species and 21 reactions
  - Submechanism for $NO_x$ emissions
    - 39-reaction UCSD mechanism



# Modeling Wall-Roughness

<u>Considerations</u>

- Choosing the AM process and process parameters
- Specifying the beam path
- Orienting the particles in the powder bed
- Choosing which regions, if any, to postcondition

# Learning Geometric Roughness Models

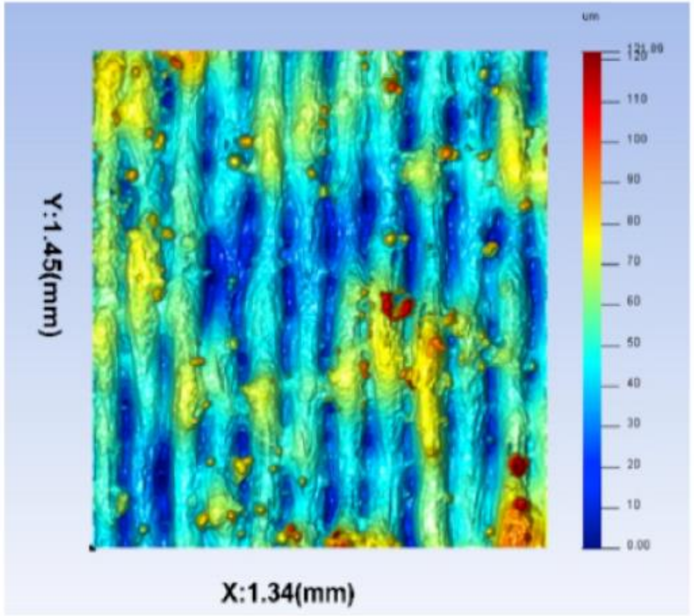
Using a generator network that uses roughness parameters and uses random factor to generate a synthetic wall roughness

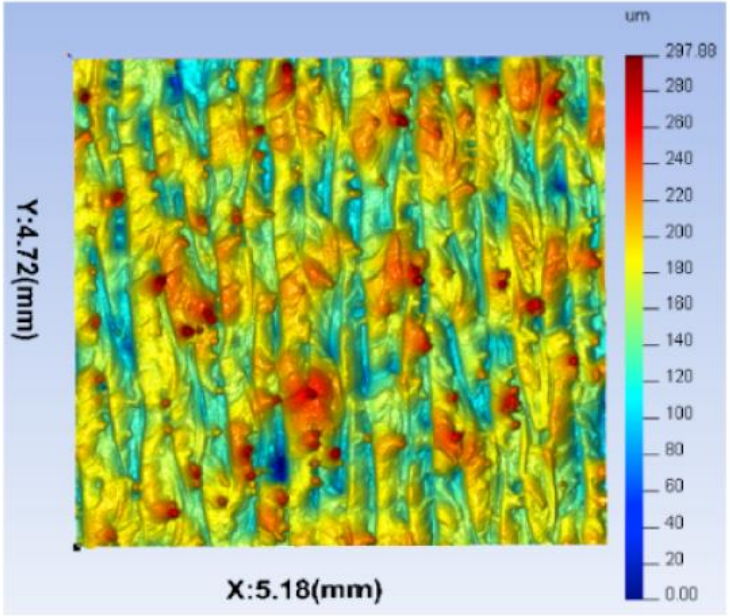
$$R^1_{i,j,k} = h^1_{act}\left(\sum_l a^1_{i,j,k,l} R^0_l\right),$$

$$R^n_{i,j,k} = h^n_{act}\left(\tau_{i,j,k}\right),$$

$$\tau_{i,j,k} = \sum_{\substack{\{q_i, r_i | i = q_i + s r_i\} \\ \{q_j, r_j | j = q_j + s r_j\}}} \sum_l a^n_{q_i, q_j, k, l} R^{n-1}_{r_i, r_j, l},$$

- Convolutional neural network learns from data



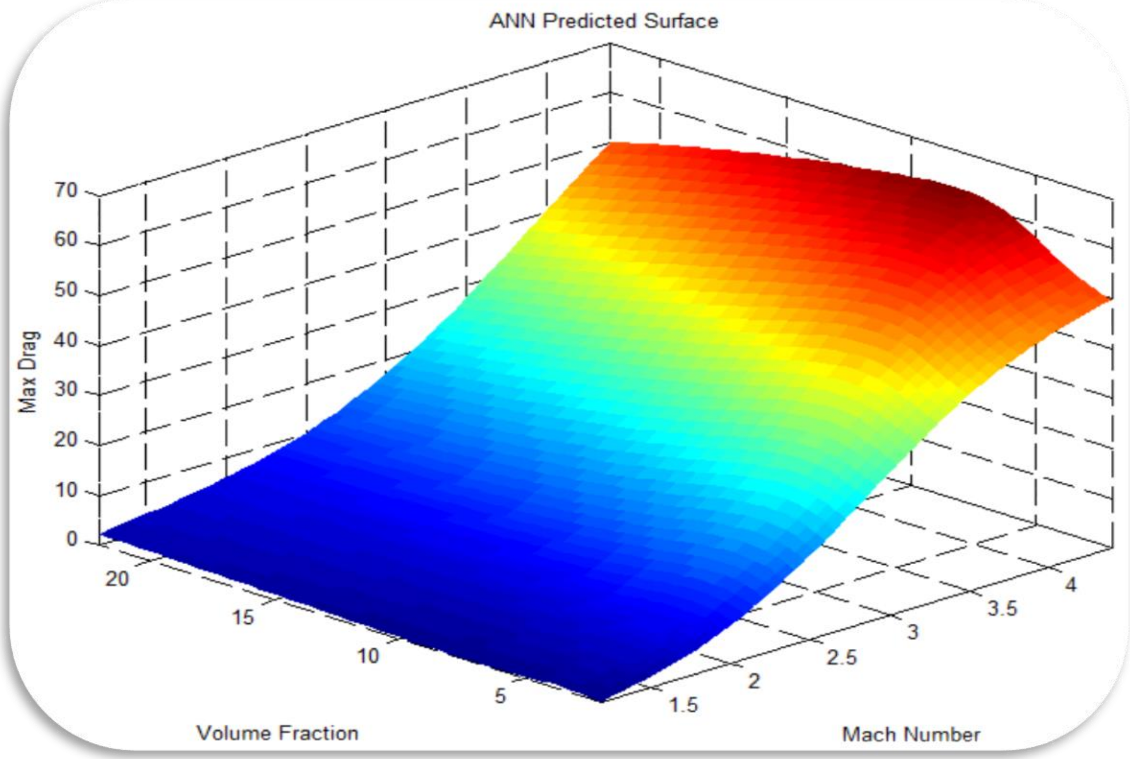



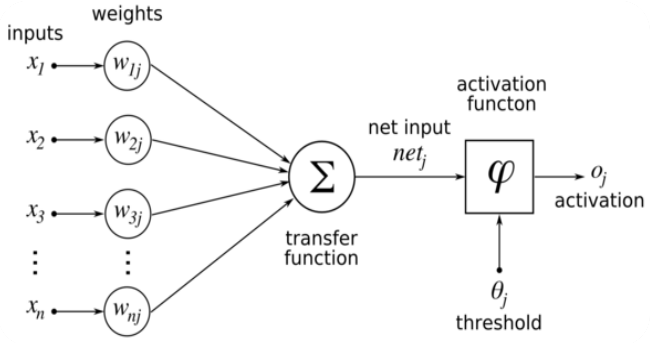

- Generator network gets trained/corrected with CNN

# REDUCED MODELING

# Input-Output Design Maps

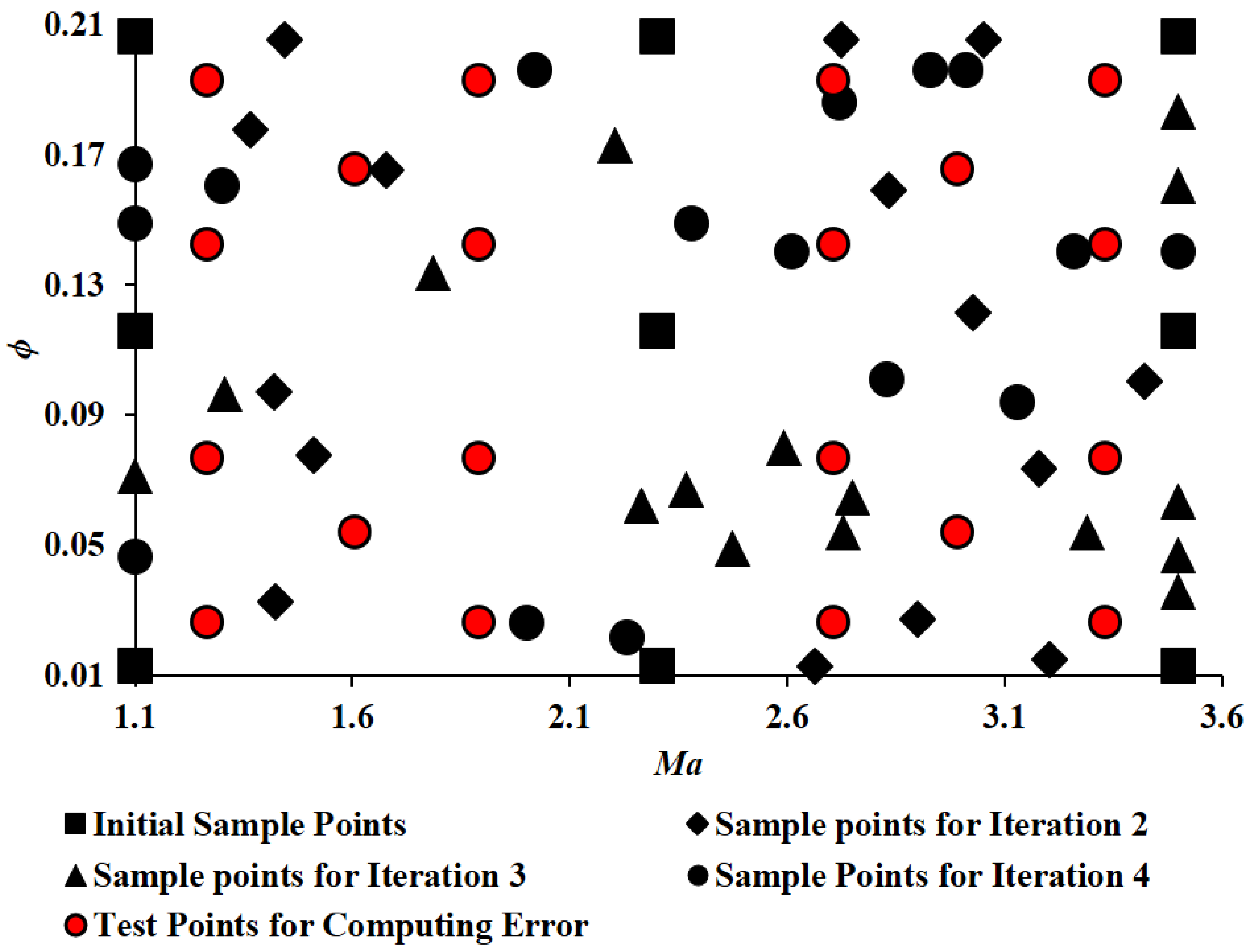
Sparse Regression with Neural Network yield Surrogate Model for Input-Output Maps



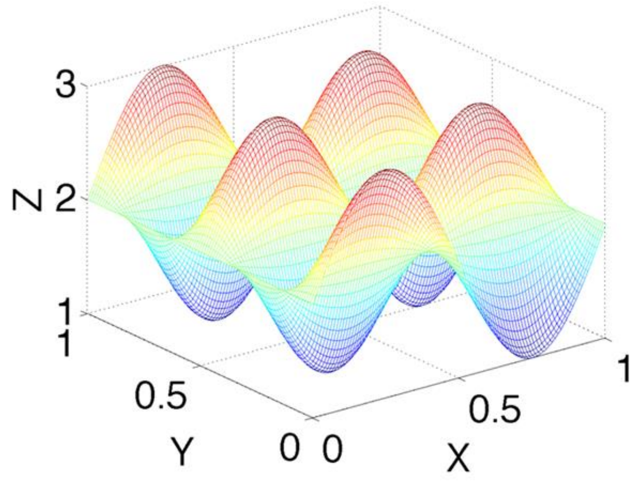

[Sen et al. *JCP*, '15]

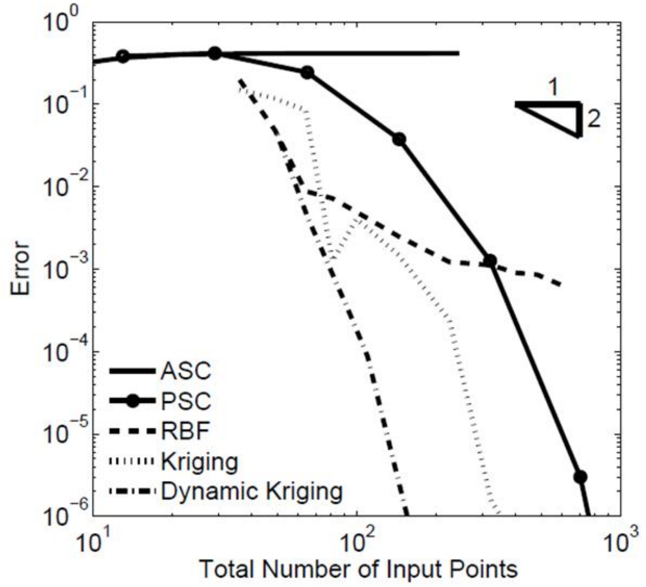
# Sparse Regression



# Experience with Sparse Regression

- Initial tests performed on smooth functions
- Gaussian fitting methods are less effective on random grids, but are much in development
- Collocation methods converge faster.
- Dynamic Kriging is a particularly effective collocation method.




[Sen, Jacobs et al. *JCP*, '15]

# Reduced Dynamic Models

**Instead of an inflow-outflow map, learn dynamical systems for state variables from data**

For each location, consider the minimum control energy problem:

minimize: $$J = \int_0^\infty u^T(\tau)u(\tau)d\tau$$

subject to
$$\dot{x}(t) = Ax(t) + Bu(t)$$
$$y(t) = Cx(t)$$
$$x(0) = x_0$$
$$x(\infty) = x_f$$

Optimal cost: $$J_{opt} = x_f^T W_c^{-1} x_f$$

Gramian: $$W_c \equiv \int_0^\infty e^{A\tau} B B^T e^{A\tau} d\tau$$

**Interpretation**:
A system with a larger controllability Gramian can reach more of state-space for a given amount of input energy (all other things being equal).

[Bhattacharjee, Jacobs et al., *TCFD*, '21]

# TESTING

# AM Problem Statement & Testing

- Develop a better understanding of the influence of AM surface roughness of the as printed part on air and fuel flow splits (Ae or effective area) & mixing

- A better understanding of modeling surface roughness is needed as the scale of roughness becomes more pronounced in micro-scale jet combustors like micromix

- Being able to reduce or eliminate post process machining of the AM micromix parts can save significant cost

- Develop a better understanding and ability to accurately simulate AM surface roughness in complex reacting flows is needed to design future DLE micromix combustors

- First steps in providing test data for model validation includes:

  - Cold flow testing to determine Ae
  - Cold flow mixing studies
  - Combustion data*

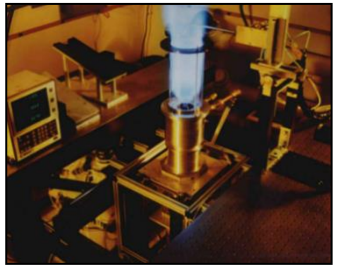
## *Combustion Data

- Solar would like to leverage the synergistic DOE program recently awarded to Solar Turbines to possibly provide AM micromix combustion data

- DE-FOA-0002400, "Development of a Retrofittable Dry Low Emissions Industrial Gas Turbine Combustion System for 100% Hydrogen and Natural Gas Blends"

- Combustion data could come from either:
  - Solar single module high pressure test rig
  - ERC (Energy Research Consultants) atmospheric pressure single module/array test rig

**Solar HP Rig**



**ERC ATM Rig**

# TIMELINE

# Plan

- Simulations
  - Baseline Injector
  - Systematic Injector Study
  - Baselin Combustor
  - Systematic Combustor Study
- Modeling
  - Wall roughness modeling
  - Sparse regression
  - Data-driven dynamics modeling
- Testing
  - Build test setup
  - Cold flow test and extract mixing characteristics
  - Hydrogen combustion tests