Reduced Basis and Stochastic Modeling of Liquid Propellant Rocket Engine as a Complex System

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The treatment of combustion and flow processes in a liquid-propellant rocket engine as a complex system using a confluence of advanced mathematical methods is aimed to understand and characterize nonlinear triggering, transient oscillations, and limit-cycle oscillations at supercritical pressures.

- Complex systems involve stochastic behaviors of semi-autonomous components networked in a way that allows emergent behavior to develop.
- Our complex system components will include combustion chamber, convergent nozzle, propellant injectors, and all flow and thermal structures.
- Uncertainties that justify stochastic approach relate to magnitude, duration, and location of triggering disturbances; property values in supercritical domain.
- Stochastic processes may apply to fluctuations in propellant flow rates, fluctuations in fluid properties, and flow turbulence.
- Emergent structures of interest include large-amplitude acoustic oscillation.
- Stochastic terms may enter analysis as initial conditions, boundary conditions, or directly into differential equations as forcing functions or coefficients.
- Reduced Basis Modeling (RBM) coupled with LES will provide a rapid, efficient, and accurate analysis for the intensive stochastic computations.

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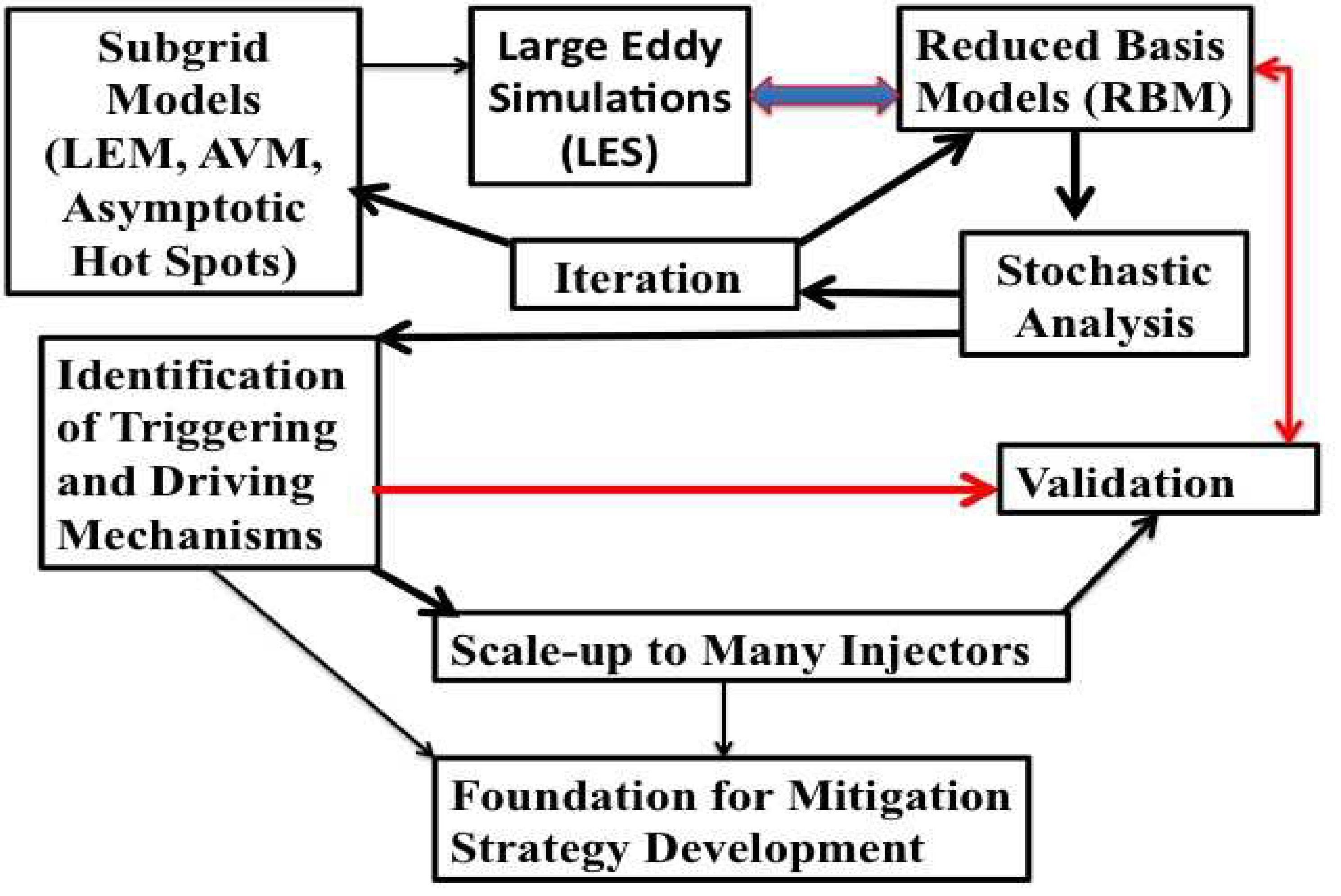
Program Flow Chart



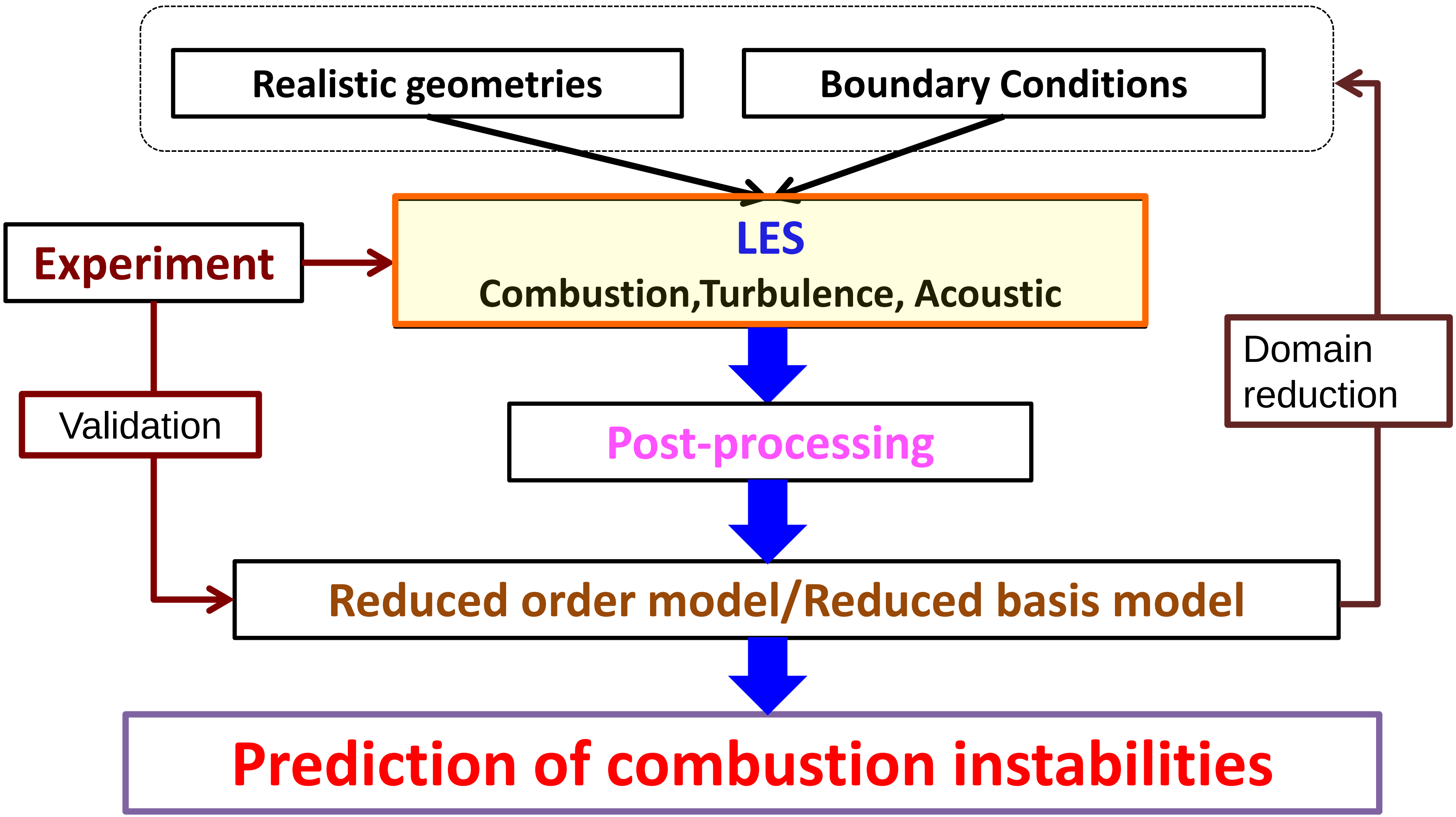
TEAM APPROACH

- UCI (Sirignano, Sideris, and Popov) will develop stochastic framework. They will formulate stochastic partial differential equations in coordination with Georgia Tech and Hypercomp.
- Georgia Tech (Menon and postdoc) will develop Large-eddy Simulation (LES) approach and make computations for specified realizations in the stochastic behavior.
- Hypercomp (Munipalli and Ota) will develop reduced basis models fitting the LES results. These RBMs will allow inexpensive computations of many realizations for the stochastic analysis.
- KISS (Kassoy) will develop and propose thermoacoustic and thermomechanical models to describe relevant combustion phenomena. Some of this modelling will also be done at UCI (Sirignano).
- Continuing communication and iteration amongst team members will occur.
- The approach and integration of contributions from team members will be tested on model equations as well as with full Navier-Stokes, multicomponent-flow based equations.
- The approach introduces and integrates various advanced mathematical and computational method: stochastic processes; asymptotic analysis; large-eddy simulation; reduced-basis modelling.

Stochastic modeling-Uncertainty quantification

- **General stochastic PDE**: $\mathcal{L}(\boldsymbol{x}, t, \omega; \boldsymbol{u}) = \boldsymbol{f}(\boldsymbol{x}, t, \omega)$ with $\boldsymbol{u}(\boldsymbol{x}, t, \omega)$ the solution, $\boldsymbol{f}(\boldsymbol{x}, t, \omega)$ a forcing function, $\mathcal{L}$ a (possibly) nonlinear differential operator, $t \in [0\ T]$ the time variable, $\boldsymbol{x} \in D$ spatial variables, and $\omega \in \Omega$ signifying dependence on random quantities.
- **Polynomial Chaos Expansion (PCE) approximation:** $\boldsymbol{u}(\boldsymbol{x}, t, \omega) \cong \sum_{i=0}^{N} \boldsymbol{u_i}(\boldsymbol{x}, t) \Phi_i\big(Z(\omega)\big)$, with $Z = (Z_1, \ldots, Z_d)$ orthornormal RV's, and the Φ_i 's multi-dimensional orthogonal polynomials.
- **Stochastic Galerkin (SG) approach:** $\boldsymbol{u_i}(\boldsymbol{x}, t)$, are obtained by requiring
  $$< \mathcal{L}\big(\boldsymbol{x}, t, \omega; \textstyle\sum_{i=0}^{N} \boldsymbol{u_i} \Phi_i\big), \Phi_k > = < \boldsymbol{f}(\boldsymbol{x}, t, \omega), \Phi_k >, \ k = 0,1, \ldots, N,$$
  which is a system of coupled deterministic PDE's in the $\boldsymbol{u_i}(\boldsymbol{x}, t)$'s.
- **Stochastic Collocation (SC) approach:**
  $\boldsymbol{u_i}(\boldsymbol{x}, t) = \frac{1}{\gamma_i} < \boldsymbol{u}(\boldsymbol{x}, t, \omega), \Phi_i(Z(\omega)) > \cong \frac{1}{\gamma_i} \sum_{i=1}^{N} \boldsymbol{u}\big(\boldsymbol{x}, t, \omega^{(j)}\big) \Phi_i\big(z^{(j)}\big) w^{(j)}$, (with $z^{(j)}, \ j = 1, \ldots, M$ samples (quadrature nodes)) are obtained from the deterministic PDE's: $\mathcal{L}\big(\boldsymbol{x}, t, \omega^{(j)}; \boldsymbol{u}^{(j)}\big) = \boldsymbol{f}(\boldsymbol{x}, t, \omega^{(j)})$.
- **Remarks:**
  - In both the SG and SC methods, the simulation approach of *Georgia Tech* and *HyPerComp* can essentially be used.
  - From the PCE expansion, statistics for the solution and machine learning tools for the detection of triggered instabilities will be developed.

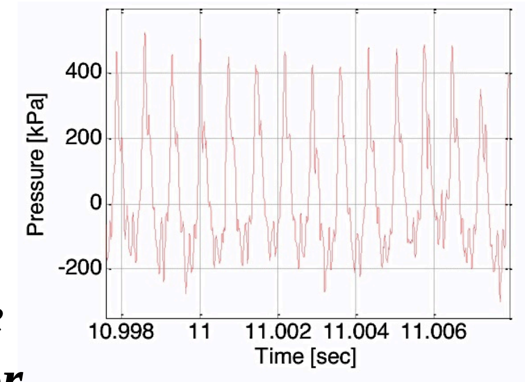
ROM/RBM-LES Strategy

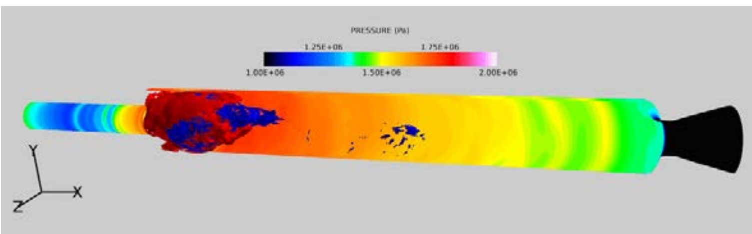


Previous Experience and Year 1 -Work Plan @ GT

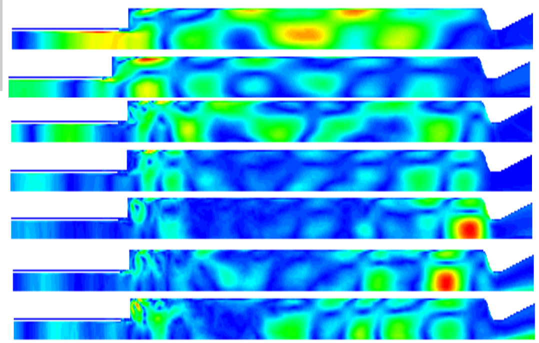
- POD/ROM analysis of existing LES data underway
  - LOX-GH2 supercritical jet mixing (PSU)
  - GH2-GOX subcritical instability (Purdue)
  - LOX-GCH4 supercritical combustion (CNRS)

Experiments (CVRC-Purdue)



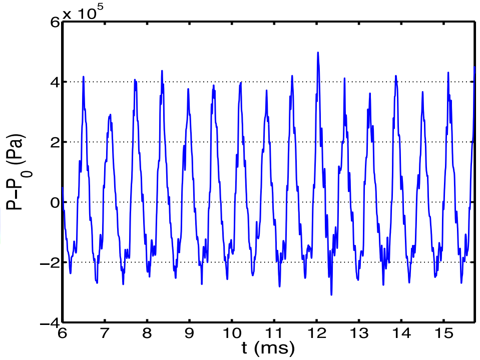


Longitudinal mode in CVRC Combustor



Some velocity POD modes for CVRC

LES



- LES test case for transverse instability to be defined.
- Injector flow field characterization for RBM analysis
- Develop post processing tools for on-line and off-line analysis of the LES data
- Team collaboration to provide inputs for stochastic and RBM modelling.

The Reduced Basis Method (RBM) – Scope

The goal of RBM is to generate accurate models of the full governing equations with far fewer unknowns – without linearization or other approximations. We are planning for the following uses for RBM in liquid rocket combustion dynamics:

- **Parametric calculations, control, optimization:** RBM can be used to span a large parameter space efficiently in large scale computations (e.g., *Re*, mass flow rate, perturbation frequency…) This can be used in designing control laws, and automatic optimization. Due to the averaging property, POD is inefficient in multiparameter systems.

- **Geometric similarity:** To use the RBM with parameterized geometries to model topologically similar domains efficiently

- **Surrogate models in complex systems:** RBMs can be used to represent subsystems such as injectors when interfacing with more complex combustor models - a network of interoperating RBMs may be used.

Brief Description of the RBM Method

The full system of Favre filtered NS equations in LES: $$\frac{\partial Q}{\partial t} + F(Q) = \mathcal{W}$$

Expand Q (Galerkin technique) in terms of modes $: \boldsymbol{\psi}_n$ $$Q_{RBM}(x,t) = \sum_{n=1}^{N} Q_R(t)\psi_n(x)$$

The modes $\boldsymbol{\psi}_n$ (usually orthogonal, but not necessarily) are obtained such that this approximation minimizes solution error (defined appropriately) : $$\left\| Q(x,t) - Q_{RBM}(x,t) \right\| \leq \varepsilon$$

The coefficients Q_R are obtained as solutions to 1st order ODEs: (A and P are pre-computed matrices) $$\frac{d\,Q_R(t)}{d\,t} = AF(P^T\psi_n(x)Q_R(t)) + \mathcal{W}(\psi_n(x)Q_R(t))$$

Calculation is done in two parts – the first, “offline” procedure constructs a set of basis functions which provide the best representation of computed data.

Next, a set of ODEs are solved “online” where the system is modeled from N unknown modal coefficients Q_R – note the full CFD solution computes O(K) unknown values where K is the number of cells.

<u>Model reduction implies $N \ll K$</u>

Challenges: Determine appropriate modes; Stable, efficient computation of nonlinear fluxes.

KISS Asymptotic Analysis

1. Thermomechanics: Spatially distributed, transient, energy deposition [Q(**x**,t)] into an isolated volume (hot spot length scale L and acoustic time scale t_A=L/a, a=local acoustic speed) at a specific rate (heating time scale t_H). When $t_H << t_A$, there must be a very low Peclet number and is not interesting here (unless radiation dominates). Much slower energy addition ($t_H >> t_A$) occurs at nearly constant pressure. Density decrease causes a small expansion Mach number driving relatively weak mechanical disturbances into the unheated environment. **Conceptual outcome**: System conversion of thermal to kinetic energy provides a source for mechanical disturbances.

2. Thermoacoustics: Linear 1st and 2nd order, 2D, nonhomogeneous wave equations describe the response of a confined gas to Q(**x**,t) when t_H=O(t_A). Longitudinal and transverse disturbances can be generated; solutions include a forced response and all the eigenmodes excited by the heat input. Potential nonlinearization can be derived analytically from the 2nd order, nonhomogeneous wave equation. Some modes can be immediately unstable. **Conceptual outcome**: Thermoacoustic modeling, describing hyperbolic phenomena is valid when the heating and the acoustic time scales are commensurate.

SUMMARY

- Innovative approach to explore the triggering mechanism of the instability and the driving mechanism for the nonlinear oscillation.
- Address the multi-injector rocket combustion chamber as a complex system with many semi-autonomous components that affect the nonlinear oscillatory macro-behavior.
- Establish key relations amongst the initiation process, nonlinear resonant oscillation growth, and transient to limit-cycle.
- The combination of new and emerging methodologies may not only aid in addressing the liquid-propellant rocket instability but can have other broader applications.