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.
**Report Documentation Page**

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| 1. REPORT DATE | SEP 2012 |
| 2. REPORT TYPE | |
| 3. DATES COVERED | 00-00-2012 to 00-00-2012 |
| 4. TITLE AND SUBTITLE | Reduced Basis and Stochastic Modeling of Liquid Propellant Rocket Engine as a Complex System |
| 5a. CONTRACT NUMBER | |
| 5b. GRANT NUMBER | |
| 5c. PROGRAM ELEMENT NUMBER | |
| 5d. PROJECT NUMBER | |
| 5e. TASK NUMBER | |
| 5f. WORK UNIT NUMBER | |
| 6. AUTHOR(S) | |
| 7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) | University of California Irvine, Irvine, CA, 92697 |
| 8. PERFORMING ORGANIZATION REPORT NUMBER | |
| 9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES) | |
| 10. SPONSOR/MONITOR’S ACRONYM(S) | |
| 11. SPONSOR/MONITOR’S REPORT NUMBER(S) | |
| 12. DISTRIBUTION/AVAILABILITY STATEMENT | Approved for public release; distribution unlimited |
| 13. SUPPLEMENTARY NOTES | Presented at the 2012 AFOSR Space Propulsion and Power Program Review held 10-13 September in Arlington, VA. U.S. Government or Federal Rights License |
| 14. ABSTRACT | |
| 15. SUBJECT TERMS | |
| 16. SECURITY CLASSIFICATION OF: | |
| a. REPORT | unclassified |
| b. ABSTRACT | unclassified |
| c. THIS PAGE | unclassified |
| 17. LIMITATION OF ABSTRACT | Same as Report (SAR) |
| 18. NUMBER OF PAGES | 10 |
| 19a. NAME OF RESPONSIBLE PERSON | |

Standard Form 298 (Rev. 8-98)  
Prescribed by ANSI Std Z39-18
Program Flow Chart

- Subgrid Models (LEM, AVM, Asymptotic Hot Spots)
- Large Eddy Simulations (LES)
- Reduced Basis Models (RBM)
- Iteration
- Stochastic Analysis
- Identification of Triggering and Driving Mechanisms
- Scale-up to Many Injectors
- Foundation for Mitigation Strategy Development
- Validation
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: \( \mathcal{L}(x, t, \omega; u) = f(x, t, \omega) \) with \( u(x, t, \omega) \) the solution, \( f(x, t, \omega) \) a forcing function, \( \mathcal{L} \) a (possibly) nonlinear differential operator, \( t \in [0, T] \) the time variable, \( x \in D \) spatial variables, and \( \omega \in \Omega \) signifying dependence on random quantities.

- Polynomial Chaos Expansion (PCE) approximation: \( u(x, t, \omega) \cong \sum_{i=0}^{N} u_i(x, t) \Phi_i(Z(\omega)) \), with \( Z = (Z_1, \ldots, Z_d) \) orthonormal RV’s, and the \( \Phi_i \)’s multi-dimensional orthogonal polynomials.

- Stochastic Galerkin (SG) approach: \( u_i(x, t) \), are obtained by requiring
  \[ < \mathcal{L}(x, t, \omega; \sum_{i=0}^{N} u_i \Phi_i), \Phi_k > = < f(x, t, \omega), \Phi_k >, \; k = 0, 1, \ldots, N, \]
  which is a system of coupled deterministic PDE's in the \( u_i(x, t) \)’s.

- Stochastic Collocation (SC) approach:
  \[ u_i(x, t) = \frac{1}{\gamma_i} < u(x, t, \omega), \Phi_i(Z(\omega)) > \cong \frac{1}{\gamma_i} \sum_{i=1}^{N} u(x, t, \omega^{(j)}) \Phi_i(z^{(j)}) w^{(j)}, \] (with \( z^{(j)}, \; j = 1, \ldots, M \) samples (quadrature nodes)) are obtained from the deterministic PDE’s: \( \mathcal{L}(x, t, \omega^{(j)}; u^{(j)}) = f(x, t, \omega^{(j)}) \).

- 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

Realistic geometries
Boundary Conditions

LES
Combustion, Turbulence, Acoustic

Post-processing

Reduced order model/Reduced basis model

Prediction of combustion instabilities

Experiments
Validation
Domain reduction
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)

- 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 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:

\[
\frac{\partial Q}{\partial t} + F(Q) = \mathbf{w}
\]

Expand \( Q \) (Galerkin technique) in terms of modes:

\[
\psi_n \quad Q_{RBM}(x,t) = \sum_{n=1}^{N} Q_R(t)\psi_n(x)
\]

The modes \( \psi_n \) (usually orthogonal, but not necessarily) are obtained such that this approximation minimizes solution error (defined appropriately):

\[
\|Q(x,t) - Q_{RBM}(x,t)\| \leq \epsilon
\]

The coefficients \( Q_R \) are obtained as solutions to 1\textsuperscript{st} order ODEs:

\[
\frac{d Q_R(t)}{d t} = A F(P^T \psi_n(x) Q_R(t)) + \mathbf{w}(\psi_n(x) Q_R(t))
\]

(A and P are pre-computed matrices)

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.

**Model reduction implies** \( N << K \)

Challenges: Determine appropriate modes; Stable, efficient computation of nonlinear fluxes.
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 1\(^{\text{st}}\) and 2\(^{\text{nd}}\) 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 2\(^{\text{nd}}\) 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.