

JULY
11-14
2017

6th International Workshop on Model Reduction in Reactive Flow

Topics

Theoretical Foundations

Theoretical foundations of model reduction techniques, definitions of slow, fast, invariant manifolds and related subjects.

Mechanism Simplification

Chemical kinetic mechanisms simplification.

Model Reduction in ODE's, DAE's and PDE's

Computational Tools

Computational tools to compute and analyze reacting flows.

Applied Engineering

WWW.MODELREDUCTION.NET



**PRINCETON
UNIVERSITY**

Day 1 – Tuesday 11/7

05:00 pm – 08:00 pm	Registration
06:00 pm – 08:00 pm	Welcome Reception

Day 2 – Wednesday 12/7		
08:00 am – 08:30 am	Breakfast	
08:30 am – 08:45 am	Welcome – Y. Ju, T. Grenga	
08:45 am – 09:30 am	Invited Talk Chair: TBD	TBD - Prof. Y.G. Kevrekidis
09:30 am – 09:55 am	Reaction Diffusion System 1 Chair: U. Mass	Evolution in the State Space and Model Reduction of a Reactive Flow System – U. Mass, V. Bykov
09:55 am – 10:20 am		Physically-Derived Reduced-Order Manifolds for Multi-Modal Turbulent Combustion – M.E. Mueller, B.A. Perry, A.C. Nunno
10:20 am – 10:50 am	Coffee Break	
10:50 am – 11:15 am	Attractive Manifold 1 Chair: J.M. Powers	Reduced Manifolds and Trajectory Curvature – J.M. Powers
11:15 am – 11:40 am		An Online Slow Manifold Approach for Efficient Optimal of Multiple Time-Scale Kinetics – M. Heitel, D. Lebiecz
11:40 am – 12:05 am		Revealing Approximative Low Dimensional Manifold for Accelerating Atomistic Simulations – E. Chiavazzo, J.M. Bello-Rivas, C.W. Gear, I.G. Kevrekidis
12:05 am – 01:35 pm	Lunch Break	
01:35 pm – 02:00 pm	Mechanism Simplification 1 Chair: D.A. Goussis	Asymptotic Analysis of a Pharmacokinetics Model – L.Y. Michalaki, D.A. Goussis
02:00 pm – 02:25 pm		ASVDADD Algorithm for Automatic Selection of RCCE Constraints – G.P. Beretta, M. Janbozorgi
02:25 pm – 02:50 pm		Computational Identification of Quasi-Steady State and Partial Equilibrium in Chemical Kinetics – P. Zhao, T. Lu, C.K. Law, S.H. Lam
02:50 pm – 03:20 pm	Coffee Break	
03:20 pm – 03:45 pm	Mechanism Analysis 1 Chair: H.N. Najm	Computational Singular Perturbation Analysis of Stochastic Chemical System with Stiffness – X. Han, L. Wang, Y. Cao, H.N. Najm
03:45 pm – 04:10 pm		Ignition Delay Control through Additives in DME/Air and EtOH/Air Mixtures – E.A. Tingas, D.C. Kyritsis, D.A. Goussis
04:10 pm – 04:35 pm		Extinction and Re-ignition Predictions of a Time-Evolving Turbulent Non-Premixed Flame: Sensitivity to Chemical Kinetics Models – S. Yang, R. Ranjan, V. Yang, W. Sun, S. Menon
04:35 pm – 05:00 pm		Machine Learning to Predict Combustion Chemistry Phenomenon – V. van Oudenhoven, S. Mani Sarathy
06:30 pm – 08:30 pm	Banquet	

Day 3 – Thursday 13/7		
08:00 am – 08:30 am	Breakfast	
08:30 am – 09:15 am	Invited Talk Chair: C.K. Law	Prof. S.H.Lam
09:15 am – 09:40 am	Attractive Manifold 2 Chair: D. Lebiez	Covariant Geometric Characterization of Slow Invariant Manifolds: New Concepts and Viewpoints – D. Lebiez
09:40 am – 10:05 am		TBD – D. Frezzato
10:05 am – 10:35 am	Coffee Break	
10:35 am – 11:00 am	Reaction Diffusion System 2 Chair: T. Lu	Reduced Models for Mixture-Averaged Diffusion – Y. Gao, J.-W. Park, T. Lu
11:00 am – 11:25 am		Identification of Low-Order Dynamics in Turbulent Premixed Flames with Dynamic Mode Decomposition – T. Grenga, J.F. MacArt, M.E. Mueller
11:25 am – 11:50 am		Multi-scale Adaptive Reduced Chemistry Solver (MARCS) for High-Dimensional Combustion Modeling with Detailed Chemical Kinetics – W. Sun, L. Wang, T. Grenga, Y. Ju
11:50 am – 12:15 am		Computation of supersonic reacting mixing layers with detailed and reduced kinetic mechanisms – C Qian, Z. Huiqiang, Z. Weijiang, B. Peng, Y. Yunjun
12:15 am – 01:45 pm	Lunch Break	
01:45 pm – 02:10 pm	Mechanism Simplification 2 Chair: M. Valorani	A Novel Strategy for Analysis and Reduction of Uncertain Chemical Kinetic Models – R. Malpica Galassi, M. Valorani, H.N. Najm, C. Safta
02:10 pm – 02:35 pm		LES for Turbulent Non-Premixed Jet Flame with CODAC Reduction – Z. Liu, W. Han, W. Kong, Y. Ju
02:35 pm – 03:00 pm		Automated Construction, Reduction, and Optimization of Chemistry for Reactive Flow Modelling – X. Gou, Z. Chen, W. Sun, Y. Ju
03:00 pm – 03:25 pm		Propagation of Kinetic Uncertainty through Surrogate Subspace in Combustion Simulations – W. Ji, J. Wang, B. Yang, Z. Ren, C.K. Law
04:00 pm – 06:00 pm	Social	
06:00 pm – 09:00 pm	Social Dinner	

Day 4 – Friday 12/7		
08:00 am – 08:30 am	Breakfast	
08:30 am – 08:55 am	Mechanism Analysis 2 Chair: H.G. Im	Dynamics of n-Heptane/Air Low Temperature Autoignition – E.A. Tingas, Z. Wang, S. Mani Sarathy, H.G. Im, D.A. Goussis
08:55 am – 09:20 am		Enhancements of the G-Scheme Framework – M. Valorani, P.P. Ciottoli, R. Malpica Galassi, S. Paolucci, T. Grenga, E. Martelli
09:20 am – 09:45 am		Using Global Pathway to Understand Chemical Kinetics – X. Gao, S. Yang, W. Sun
09:45 am – 10:15 am	Coffee Break	
10:15 am – 10:40 am	Mechanism Simplification 3 Chair: F. Mauss	Horizontal Species Lumping Using Structural Information from a Mechanism Generator – M. Hilbig, L. Seidel, F. Mauss
10:40 am – 11:05 am		Reduced High-Temperature Combustion Chemistry Models of Jet Fuels – Y. Gao, R. Xu, H. Wang, T. Lu
11:05 am – 11:45 am	Open Discussion Chair: Y. Ju	Challenges on Model Reduction Research
11:45 am – 12:00 am	Adjourn – Y. Ju, T. Grenga	