Aerospace Seminar

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Reduced-Order Model Framework for Thermochemical Non-equilibrium Hypersonic Flows

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Abstract: The study of vehicles traveling at hypersonic speeds is extremely complex and involves many non-equilibrium physical phenomena occurring on broad time and length scales. For gas flow around a hypersonic vehicle, non-equilibrium energy transfer and chemistry of the gas particles directly affects heat transfer to the vehicle. Work focused on modeling this type of flowfield has been hindered by inaccurate physical and chemical models. For example, the conventional approach widely used today was developed nearly 40 years ago and relies heavily on calibration with heritage data. Recent advances in computational chemistry and computational resources have enabled the construction of extremely detailed models for the chemical non-equilibrium effects based on *ab initio* quantum chemistry data, called the state-to-state (StS) approach. Unfortunately, due to enormous cost, StS calculations can only be used in highly simplified test cases. This motivates the development of reduced order models for chemical non-equilibrium which can capture the essential physics at a massively lower cost. The model reduction framework proposed is based on the maximum-entropy principle, and leverages quasi-classical trajectory (i.e., atomistic) calculations to compute n-moment kinetic data for a reduced set of molecular states, thus providing the crucial link between the *ab initio* quantum chemistry data and computational fluid dynamics (CFD). The talk covers the key aspects involved in model development, namely: the model reduction framework, the use of scattering calculations to integrate the *ab initio* data, and application of the model to CFD. Key findings and their implication on vehicle design are discussed.

Bio: Dr. Robyn Macdonald received her BS in Aerospace Engineering from the University of Illinois at Urbana-Champaign (UIUC) in 2013. In December 2018, she successfully defended her PhD thesis “Reduced-order model framework for thermochemical non-equilibrium hypersonic flows.” Her PhD research focused on development of quantum chemistry informed reduced order models for thermochemical non-equilibrium hypersonic flows. She is currently a post-doctoral research fellow at the Computational Hypersonics Research Lab at the University of Minnesota studying turbulence in hypersonic flows. Dr. Macdonald is recipient of a National Defense Science and Engineering Graduate (NDSEG) Fellowship, and her post-doctoral research is supported by the President’s Postdoctoral Fellowship Program. During her PhD she received a number of awards: including the NASA Space Technology Research Fellowship (declined to accept NDSEG), Zonta Amelia Earhart Fellowship (declined to accept NDSEG), and AE Faculty Outstanding Graduate Student Award from the Dept. of Aerospace Engineering at UIUC. Her work on reduced order models for thermochemical non-equilibrium was awarded the Weaver Thermophysics Best Student Paper Award from AIAA and was selected as Editor’s Pick when published in the Journal of Chemical Physics.