

# DEPARTMENT OF MECHANICAL ENGINEERING

## WILLIAM MAXWELL REED SEMINAR SERIES

### “Next-Generation Chemical Kinetics for Hypersonic Flows”

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University of Colorado Boulder

**Abstract:** Hypersonic vehicles can cause shocks yielding temperatures in excess of 10,000 K. At these conditions, air begins to chemically decompose. The rate and manner of this decomposition must be accurately predicted, for example to determine the amount of reactive atomic oxygen near the surface. However, the extreme nature of these phenomena makes them difficult to study experimentally. Instead, molecular interactions can be simulated using the quasiclassical trajectory (QCT) method, using accurate descriptions of atomic forces from quantum chemistry. QCT calculations are performed for 5 reactions that are relevant for air chemistry, and the results are presented in the context of the inputs necessary for CFD. Emphasis is placed on linking the microscopic behavior of these interactions to the bulk effects that are relevant for vehicle-scale calculations. A new model is proposed, that captures the dominant mechanisms while remaining computationally tractable for vehicle design. Results with this new model are compared to existing methods for several configurations.

**Bio:** Ross Chaudhry received his Ph.D from the University of Minnesota in 2018. His dissertation work used quantum chemistry data to design reduced-order thermochemical kinetics models for CFD, designed to study the airflow around vehicles at hypersonic conditions. His new model is now implemented in two hypersonic CFD codes and is being used by authors at several institutions. He has also investigated the freestream disturbance content in hypersonic wind tunnel facilities, for which he received a NATO AVT panel excellence award as part of the "Hypersonic Boundary-Layer Transition Prediction" team. He is currently a postdoctoral associate at the University of Colorado Boulder.

**Date:** Friday, Nov. 13<sup>th</sup>

**Place:** <https://uky.zoom.us/j/92940732923>

**Time:** 3:00PM EST

**Contact:** Dr. Alexandre Martin 257-4462

Attendance open to all interested persons