Center for Predictive Engineering and Computational Science

The PECOS Center

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PECOS Team

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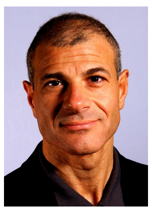
Director, PECOS



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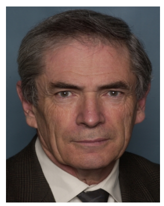
Software Architect



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V&V – UQ Team Chair

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Greg Rodin	**Philip Varghese**

Sub-Awardees

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Marvin Adams **Jim Morel**
Bani Mallick

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Raul Tempone

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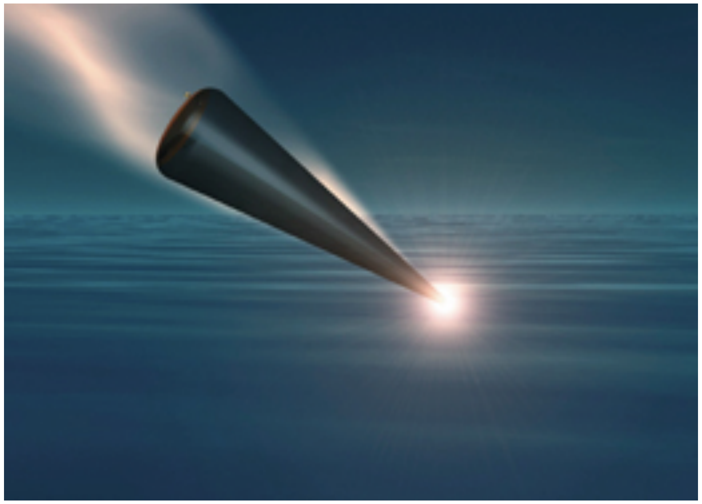
Partners at NASA

- NASA JSC
  - Development of the new Orion space craft
  - Driving extensive experimental program for validation
- NASA AMES
  - Development of the Orion TPS
  - Extensive modeling & validation
  - Development of the DPLR Hypersonic Code

Atmospheric Reentry

- Hypersonic reentry produces an extreme thermal environment
- Aerodynamic heating requires thermal protection
  - Failure can be catastrophic
- Design and operation of reentry vehicles requires reliable predictions



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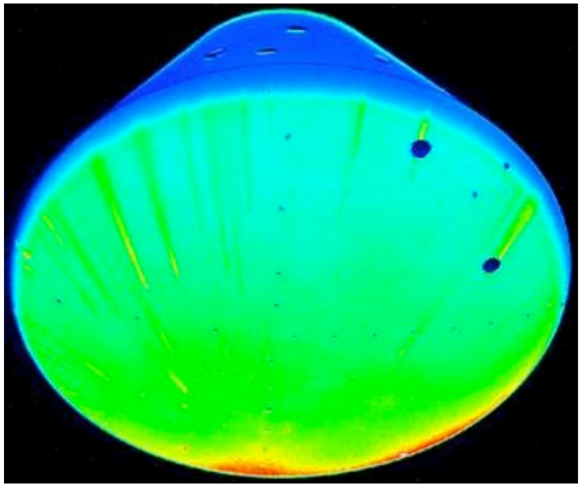
For an Earth Reentry

- M=20 to 45(depends on mission)
- Maximum energy flux occurs at ~60km
  - Flux on order 100 MW / m^2 *(9 km/s)*
  - About 60s duration
- Shock layer temperature: 6,000-20,000K
  - Dissociation and possible ionization of nitrogen and oxygen



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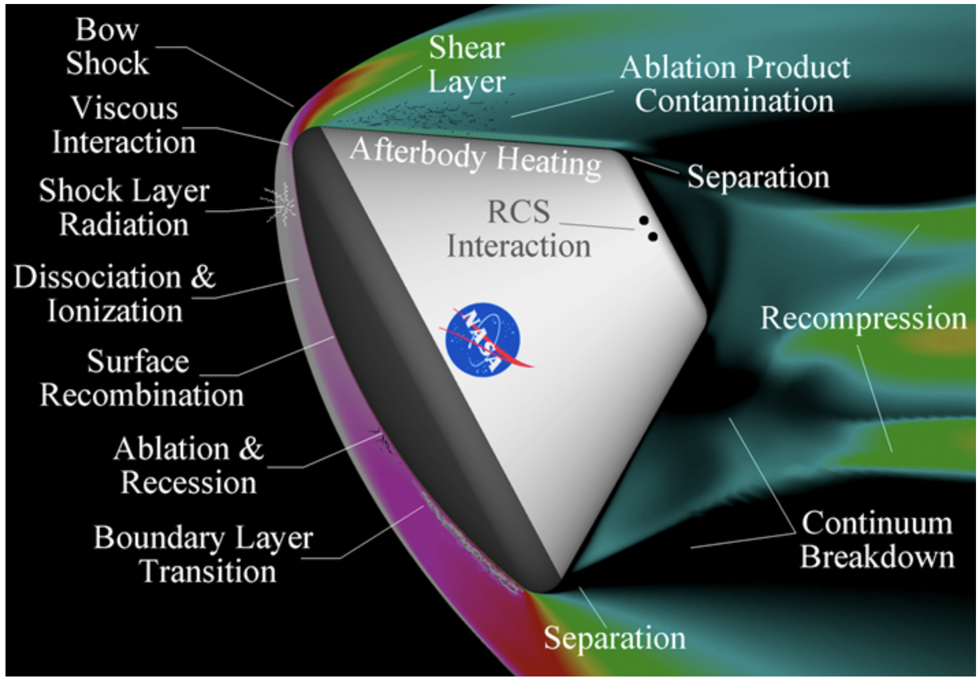
Reentry Vehicle Physics



- RV problem presents numerous physical modeling challenges at multiple scales
- Models involve numerous uncertain parameters

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Uncertainty Quantification is Valuable for RVs

- Provide information with quantified reliability to decision makers
  - Design decisions
  - Operational decisions
- Reentry vehicle flights are dangerous and failures are expensive
- Flight data is sparse

Example: Gap-fillers on shuttle “return to flight” mission

Surviving the Thermal Environment

- Central design and operational issue
- We are focused on:
  - Adequacy of ablative TPS
  - Peak heating period
    - When most of the TPS is consumed
    - When vehicle is most at risk
  - Localized heating due to RCS firing

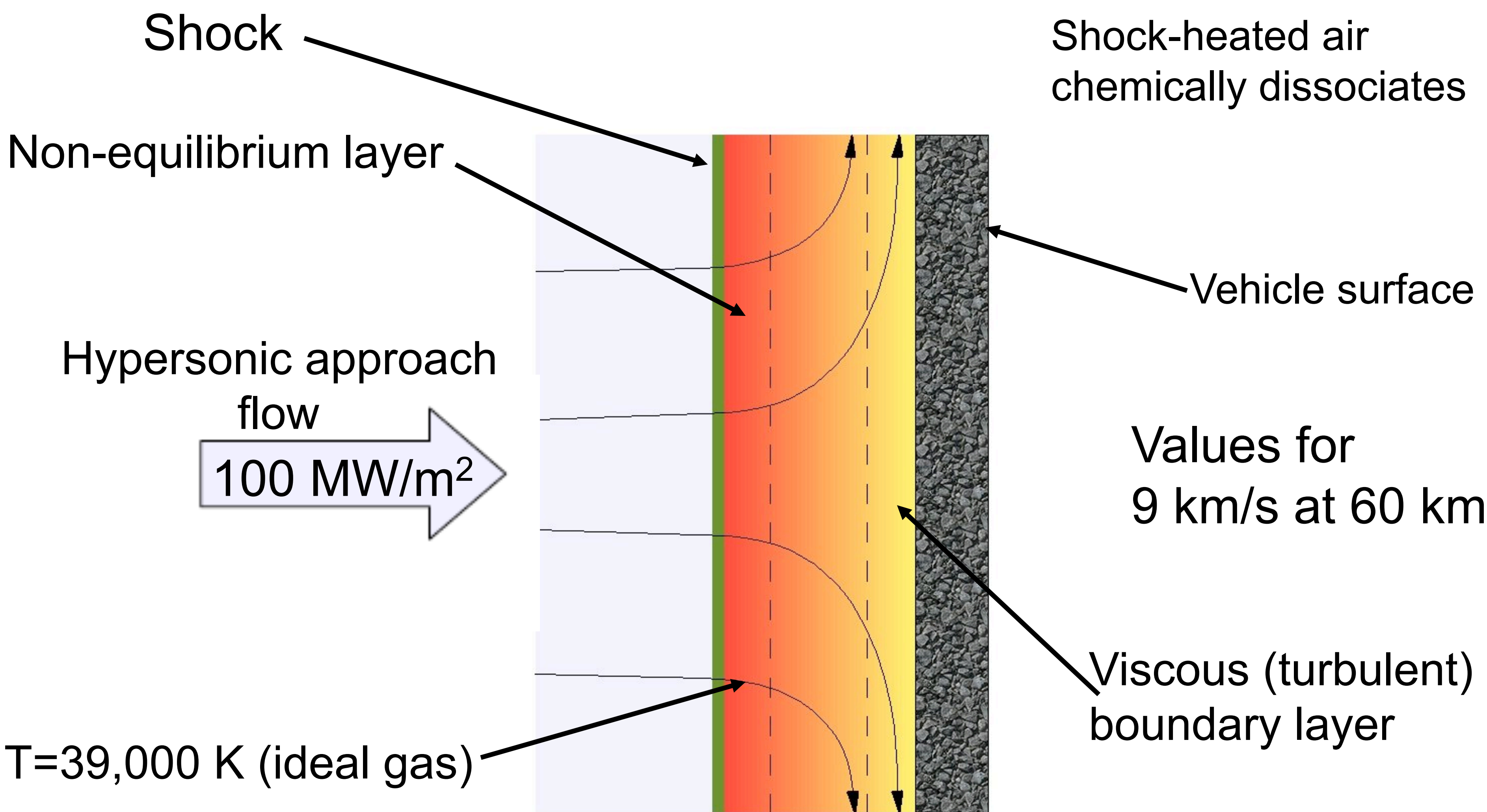
We will simulate

- Reentry vehicle with ablative TPS
  - Earth reentry to start
- The thermal environment
  - Radiative
  - Convective
  - Chemical
- The heat loads on the vehicle
- The consumption of ablative TPS
- During the peak heating regime

Quantities of Interest

- V&V - UQ must be done in the context of specific quantities of interest (QoI)
- Quantities to be predicted
- To assess survival of a vehicle, two key quantities:
  - Rate of recession of TPS (throughout peak heating regime)
  - Local peak heat flux to after-body
    - Enhanced heat flux due to RCS jets
- Validation and uncertainty quantification will be pursued for these QoI

The Shock Region



Values for
9 km/s at 60 km

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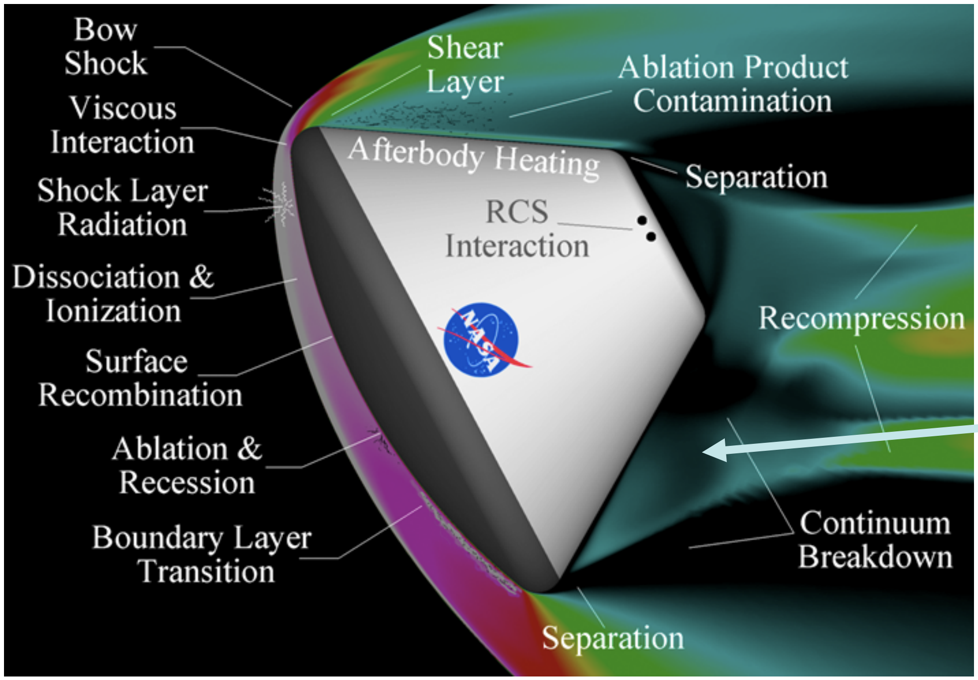
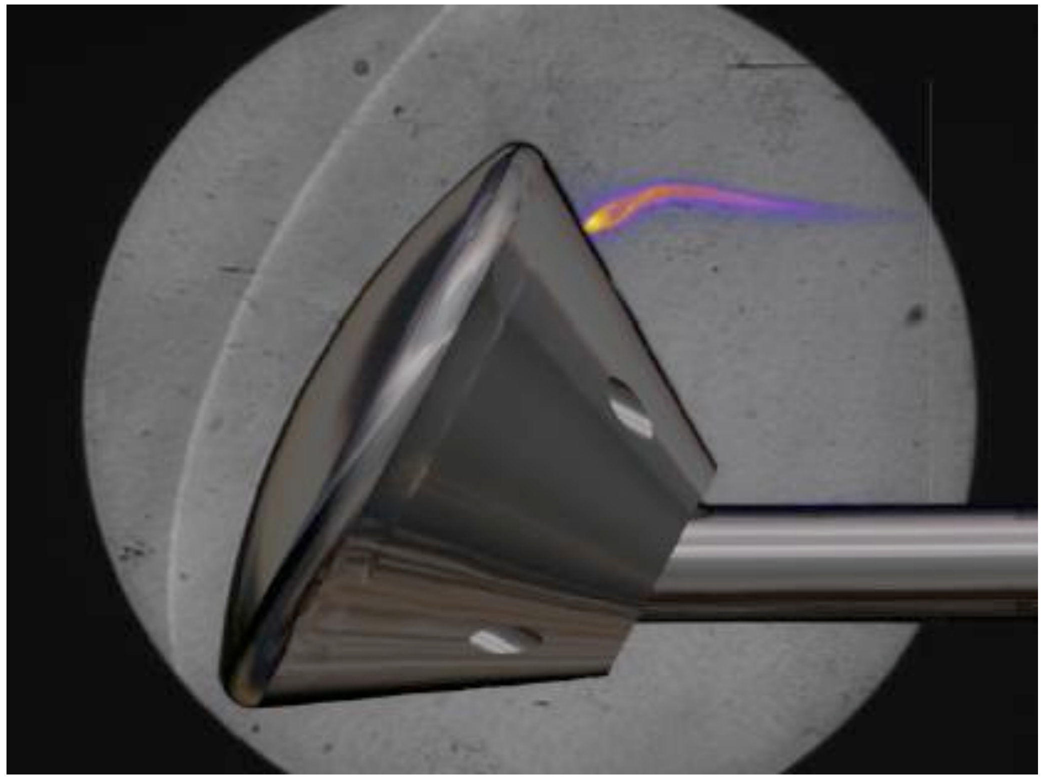
After-Body and Wake



- Flow expands around body into (turbulent) wake
  - Cooling & recombination
  - Continuum breakdown?
  - Convective & radiation on after-body
- Reaction Control System (RCS) thrusters used for attitude control
- Interact with boundary layer (M~5) and wake
- Generate up-stream transient shock

Reaction Control Jets

- Short duration pulses (10s of msec)
- Transient up-stream shock enhances surface heat transfer



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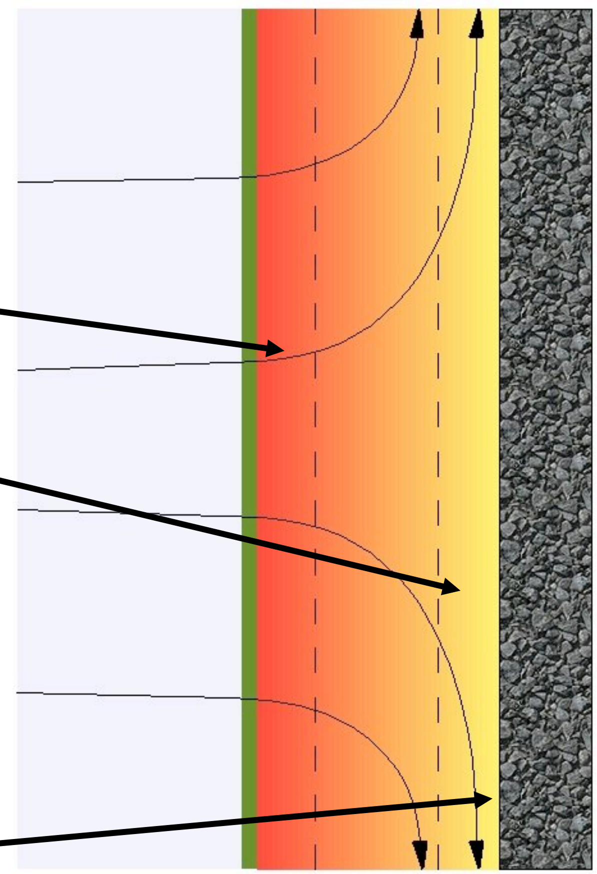
High Temperature Air Chemistry

- Shock heated air dissociates
  - Lowers gas temperature
  - Chemical and thermal non-equilibrium
- Reactions in boundary layer
  - Cooling
  - Reaction with ablation products
  - Turbulent mixing and transport
- Surface catalyzed recombination



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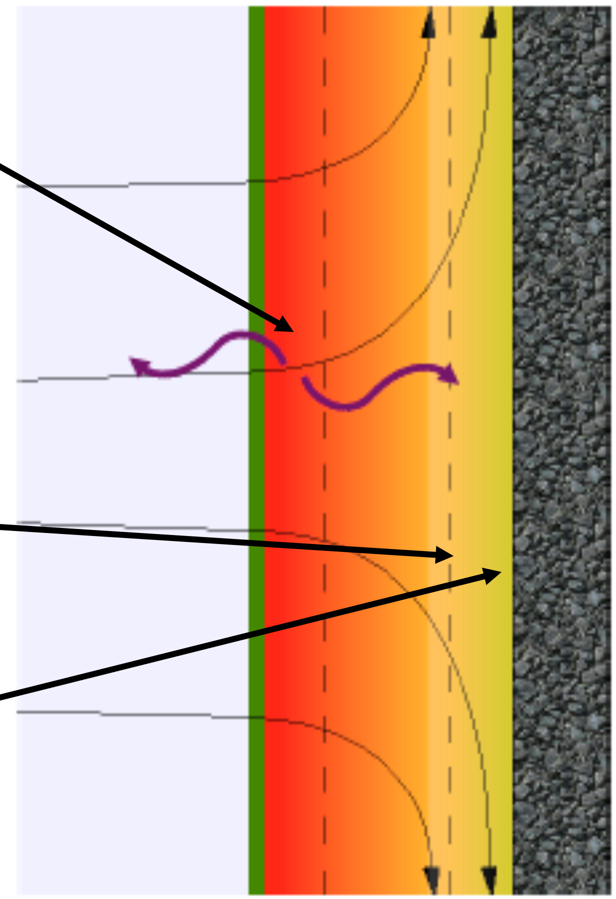
High Temperature Air Chemistry

- Current modeling practice:
  - Chemical non-equilibrium treated with Arrhenius rate models
  - Multi-temperature models for thermodynamic non -equilibrium (*ad hoc* and often inconsistent)
- Anticipated model development:
  - Context specific representation of non-equilibrium from the Boltzmann equation
  - Evaluate importance of non-equilibrium surface / ablation product chemistry

Radiative Heat Transfer

- High temperature gas radiates
  - Both line and continuum components
  - Cools gas in shock layer
- Radiation interacts with gas & particles
  - Absorption and scattering
- Radiative heating of TPS



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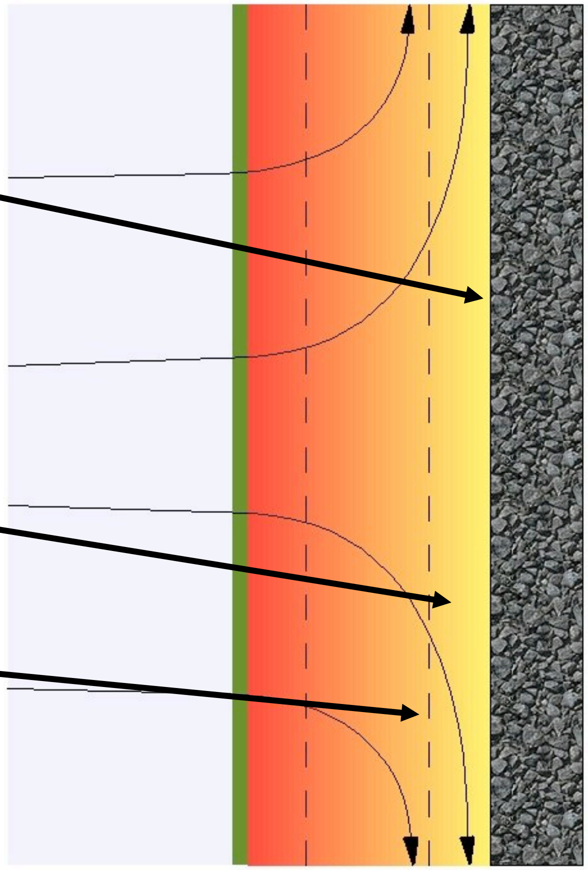
Radiation Modeling

- Current modeling practice:
  - Radiation model 1-way coupled with gas phase
  - Thermal equilibrium is often assumed
  - Range of possible approximations to transport equations
- Anticipated modeling developments:
  - Coupled / integrated with gas and ablation models
  - Coupling to thermal non-equilibrium model
  - Investigate approximation to transport and frequency representations

Boundary Layer and Turbulence

- Complex boundary layer
  - Roughness & transpiration
- Transport of species & heat
  - Enables surface catalysis
  - Enhances heat transfer
- Mixing of air and ablation products
- Transition from laminar to turbulent

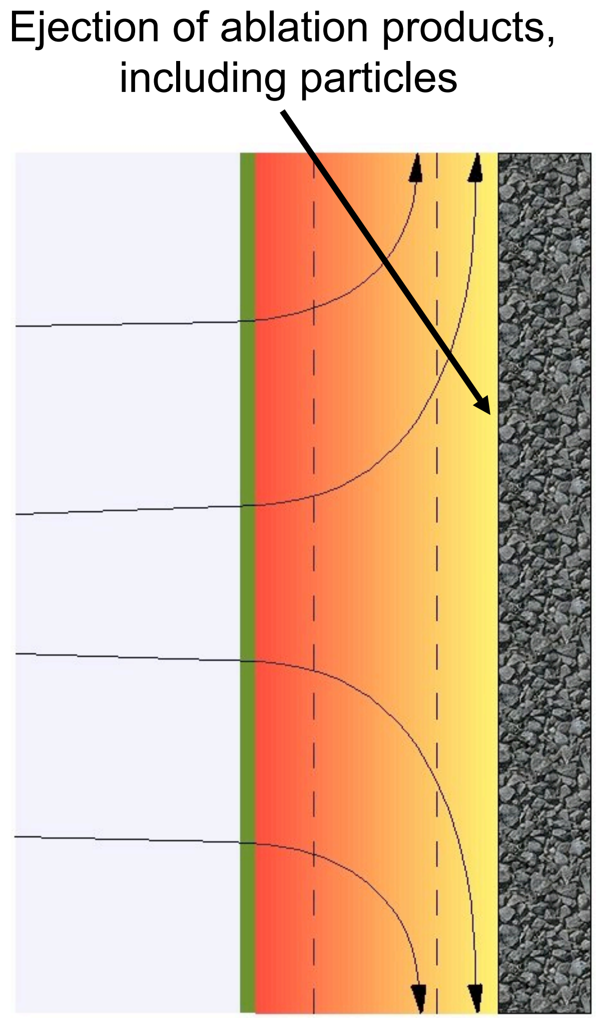


Turbulence Modeling

- Standard turbulence and transition models known to be inaccurate
  - Lead to significant model uncertainties
  - Comprehensive treatment of errors in turbulence modeling needed
- Turbulence modeling
  - Develop models for model-form uncertainty
  - Use calibration / validation / UQ process to characterize modeling inadequacies
- Transition modeling
  - Transition on a “noisy” ablator
  - Characterize condition for bypass transition (from DNS)

Thermal Protection is needed

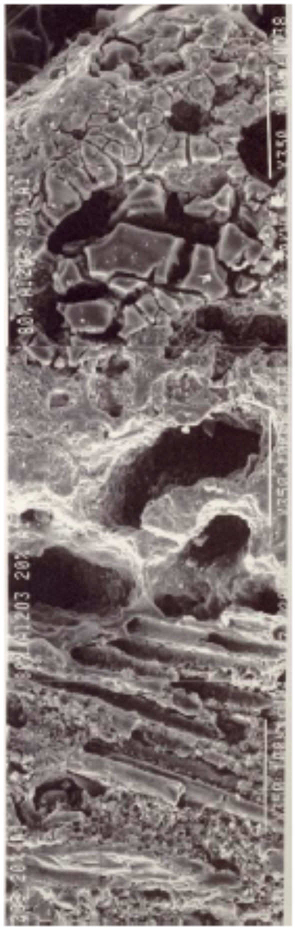
- Large heat loads (up to 10 MW/m^2) require thermal protection for the vehicle (TPS)
- Most common is an ablative TPS
  - For capsule applications (micro-structured polymer composites) are common
  - Require complex material response modeling



Ablation Process

- Leaves carbonaceous char
- Decomposition gases escape through char layer
  - Gases thicken boundary layer
- Char reradiates
- Char mechanically degraded
  - Shear and spalation

Ablative material cross section



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Ablation Modeling

- Ablation is a complex process dependent on the chemical kinetics of the ablating material and the micromechanics of the material as it ablates
- Current ablation models are inadequate
  - Include only aggregate representation of the kinetics process
  - Parameterization based on low heating rate experiments
  - Thermophysical properties of char are not well characterized
- Micromechanical models based on detailed models of kinetics and mechanical properties of the char that remains during pyrolysis
- Upscaling will result in macroscale representations of the multiscale ablation process

Modeling domains effect software design

- Coupled macroscale models of:
  - Hypersonic fluid dynamics
  - Chemistry and thermodynamics
  - Radiation
  - Ablation
  - Turbulence
  - Multiphase flow
- Must support coupling of a hierarchy of models in each domain

Simulation Modeling Infrastructure

- Build on existing hypersonic flow codes
  - DPLR (NASA AMES) and/or US3D (University of Minnesota)
  - Both include facility for chemistry and turbulence models
  - Add radiation and ablation
- Develop a generalized model software interface
  - Abstraction based on exchange of conserved quantities
  - Support Jacobians and adjoints for error estimation and uncertainty quantification
  - Scalable

High-Fidelity Stand-Alone codes

- Used to assess quality of existing macroscale models
- Used to guide development of improved macroscale models
- High-fidelity codes include:
  - DNS codes for turbulent flow (spectral and finite volume)
  - Discrete ordinates S_N radiation transport code PDT
  - Rarefied gas dynamics code DAC
  - Microscale ablation code to be developed
- All existing codes scale to 100s-1000s of processor
- Guides validation & verification

The Validation and UQ Process

- *Calibration*: determine model parameter pdfs by calibrating with experimental data (statistical inverse problem)
- *Validation*: Quantify confidence in model by misfit between pdfs of calibrated model predictions and validation data
- *Model enhancement:* Return to model development and / or data acquisition if model does not pass validation test
- *Ascend the validation pyramid* to higher level experiments
- *Predict quantities of interest* and associated uncertainties for regimes of interest using validated code
- Return to model development and/or data acquisition if uncertainties unacceptable
- **This process drives modeling research and development**

Physics models and uncertain parameters

- Component models
  - Chemistry and thermodynamics
  - Radiation
  - Ablation
  - Turbulence
  - Multiphase flow
- Uncertain model parameters
  - chemical kinetic parameters (6 x # reactions)
  - radiation coupling parameters (2 x # frequency bands)
  - ablation kinetic parameters (2 + 3 x # reactions)
  - turbulence model parameters (4 + 2 x # species)
  - ablative particle density parameters

Calibration and Bayesian Inference

- Calibration critical to validation and UQ process
  - Most model parameters not directly observable
  - essentially an inverse problem
  - what model parameters are consistent with observed data
  - often ill-posed, requiring regularization
- Bayesian inference replaces regularization
  - Given:
    - measurements and their uncertainty
    - theoretical model and its uncertainty
    - “prior” estimate of model parameters and uncertainty
  - Seek statistical characterization of family of model parameters that is consistent with data

Bayesian framework

Given:

$$\rho_M(\mathbf{m}) \;:=\; \text{prior p.d.f. for model parameters}$$

$$\rho_D(\mathbf{d}) \;:=\; \text{prior p.d.f. for the data}$$

$$\theta(\mathbf{d}|\mathbf{m}) \;:=\; \text{conditional p.d.f. relating } \mathbf{d} \text{ and } \mathbf{m}$$

Then posterior p.d.f. of model parameters given by:

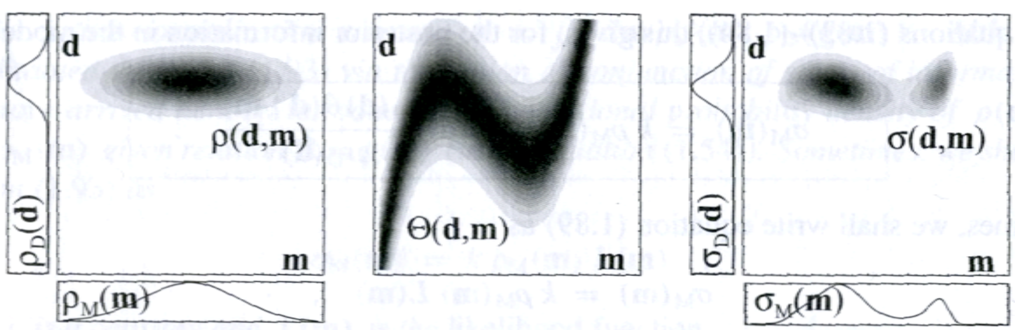
$$\sigma_M(\mathbf{m}) = k\, \rho_M(\mathbf{m}) \underbrace{\int_{\mathfrak{D}} d\mathbf{d} \frac{\rho_D(\mathbf{d})\, \theta(\mathbf{d}|\mathbf{m})}{\mu_D(\mathbf{d})}}_{L(\mathbf{m})}$$

constant for linear data space ($\mu_D(\mathbf{d})$)

normalization constant (k)

$L(\mathbf{m}) :=$ likelihood function

From Tarantola, 2005



Validation Approach

- Apply model to predict new data not used in calibration
  - Experimental observations with uncertainty
  - Model predictions with uncertainty
- Ask how likely that model prediction and experimental observations are consistent
- Does not test validity of model in predicting QoIs
- New approach: recalibrate model using validation data and calibration data
  - Issue predictions of QoI with uncertainty with original calibration and recalibration
  - Ask if two predictions are consistent
- Will pursue both approaches

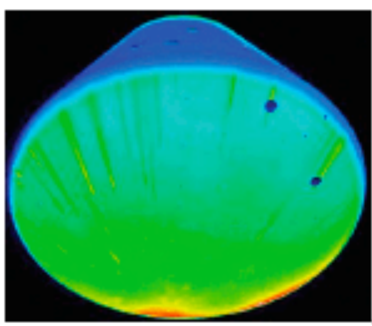
Algorithmic Challenges

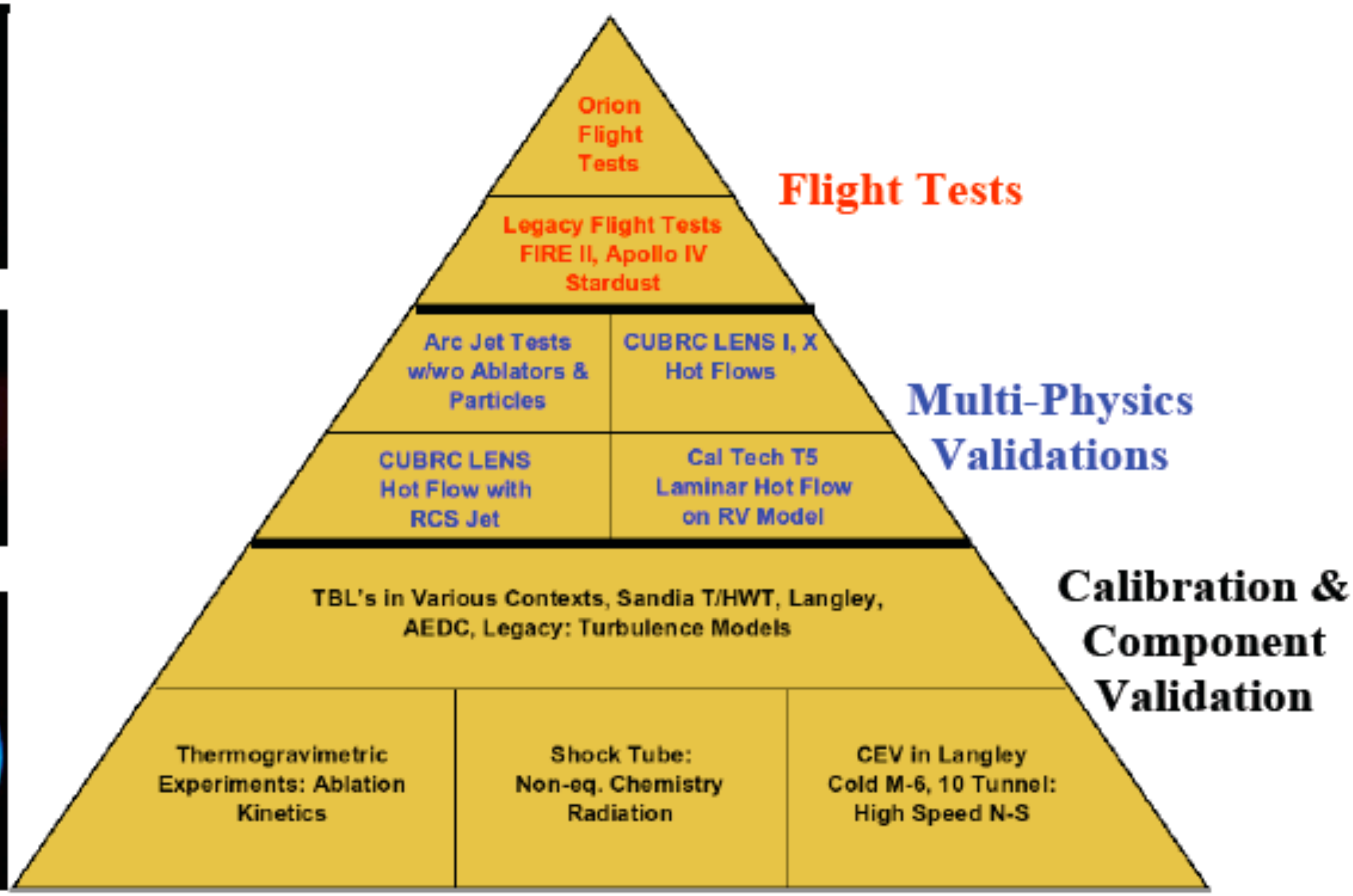
- Fundamental operation: sampling probability spaces
  - High dimensional
  - Single evaluation is costly
  - Need algorithms to reduce dimensionality, sample effectively, reduce cost of evaluations (model reduction)
  - Some algorithms benefit from adjoints, sensitivities or other embedded diagnostics
- For calibration (Bayesian)
  - Appropriate priors
  - Representation and parameterization of model uncertainty
  - More sampling
- Uncertainty propagation for validation and prediction

Experimental Data

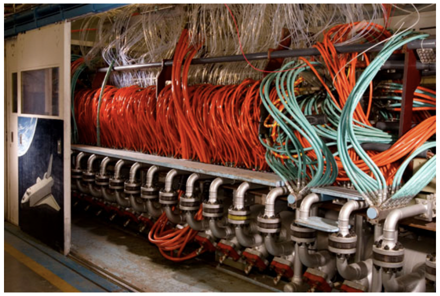
- V&V-UQ framework **requires** experimental data
- Calibration of component model parameters
  - Thermochemistry (e.g. kinetic paramters)
  - Radiation (e.g. absorbtions & emissions)
  - Turbulence (e.g. model constants)
  - Ablation (e.g. kinetic parameters)
- Validation of component models
- Validation of coupled models

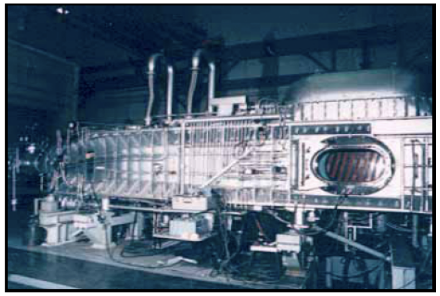
Validation is Hierarchical

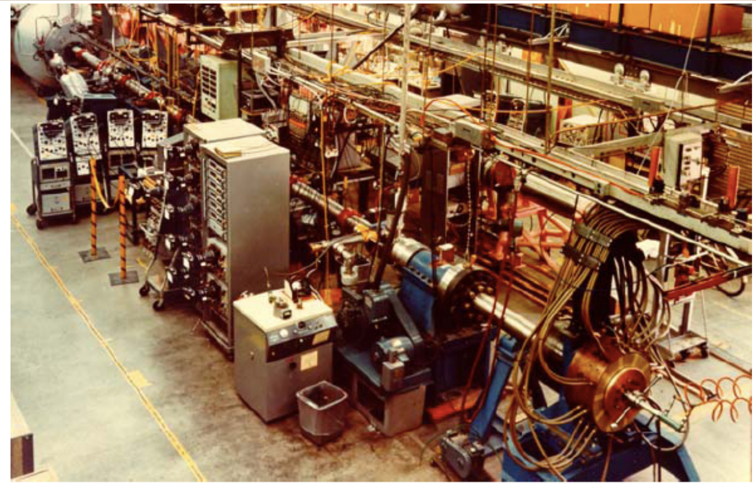


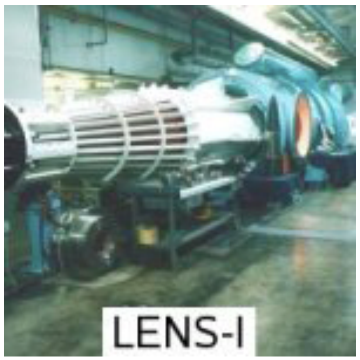


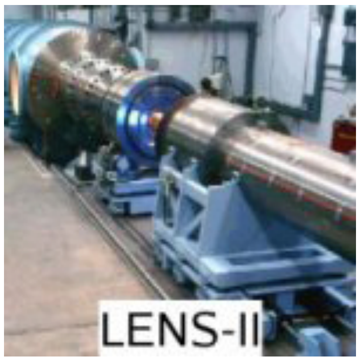
Hypersonic Experimental Facilities

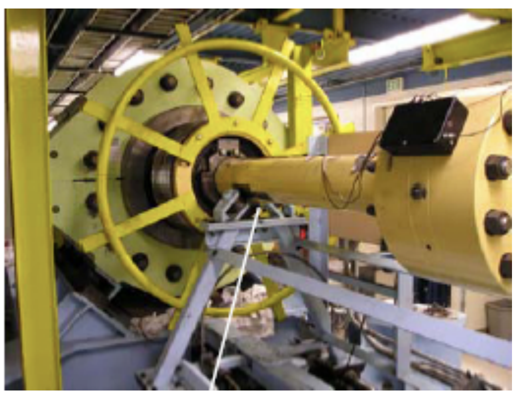


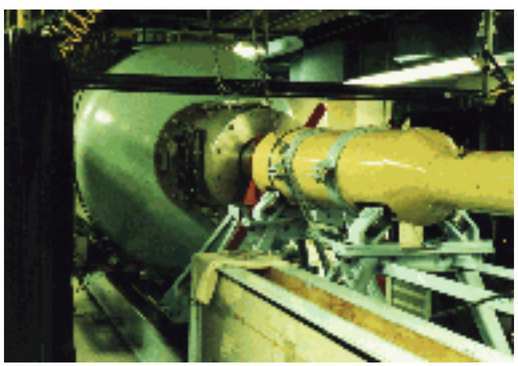










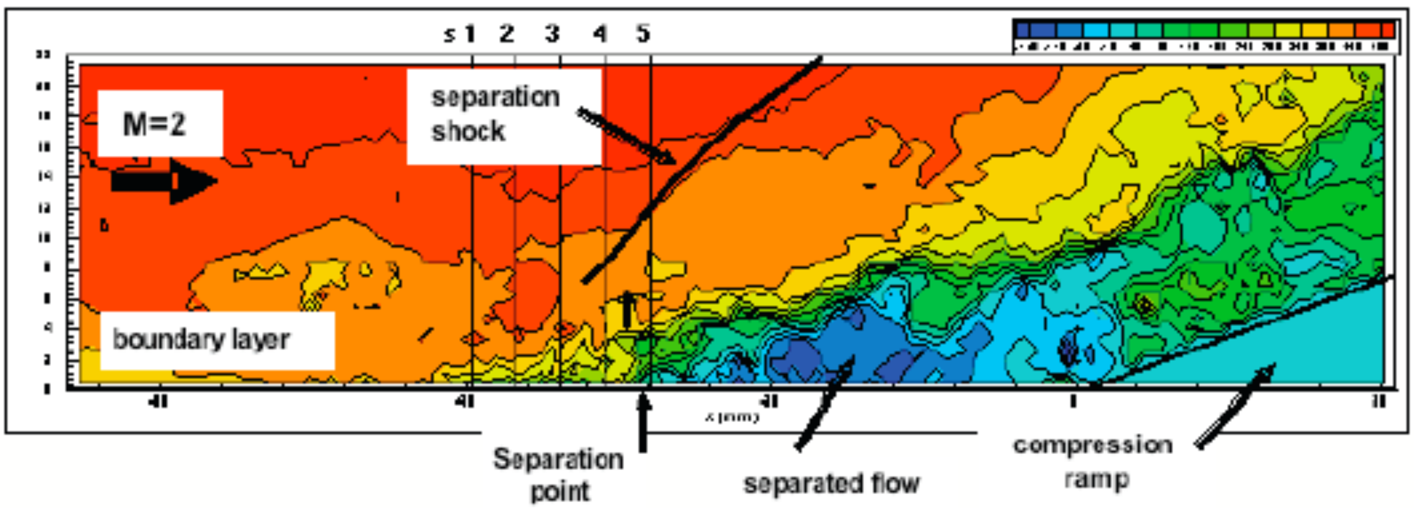


Calibration and Component Validation

- Non-equilibrium chemistry & radiation coupling
  - AMES EAST Shock tube tests at range of conditions
    - Simulate shock layer thermal & chemical profile with radiative heat losses and spectrally resolved radiative transmission to radiometer
    - Calibrate uncertain chemical & radiation coupling models
    - Validate non-equilibrium chemical and radiation coupling models
      - Cases not used for validation

Calibration and Component Validation

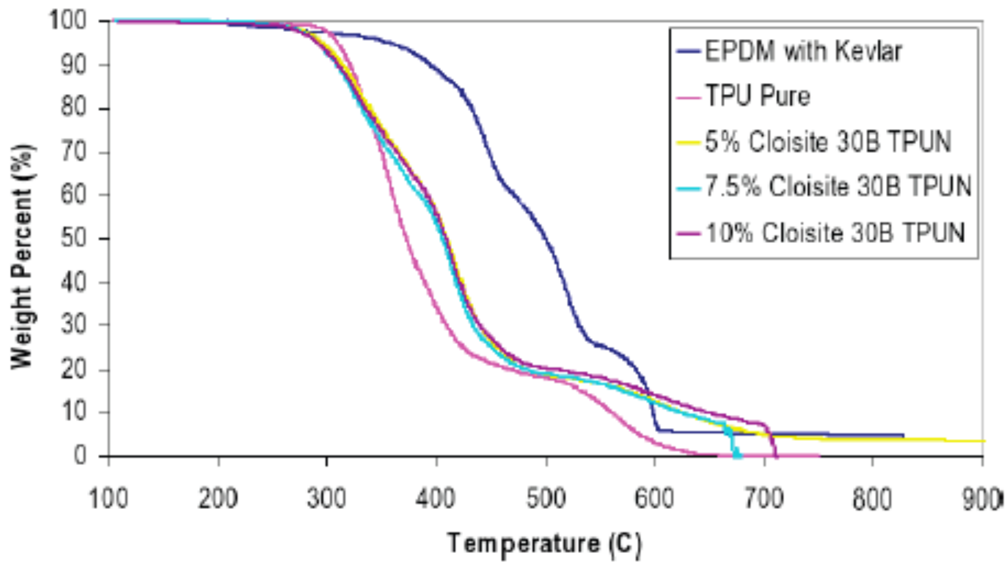
- Compressible flow turbulence models
  - High speed boundary layers on various bodies(Sandia, AEDC, legacy, DNS, UT)
    - Simulate many test configurations
    - Representation of model-form uncertainty
    - Calibrate model parameters & inlet conditions
    - Validate turbulence model & uncertainty representation



PIV measurements in a shock wave / boundary layer interaction

Calibration and Component Validation

- Ablation kinetics
  - Themogravimetric tests of ablator samples
    - Measure weight as a function of temperature
    - Simulate quasi steady heating of ablator material
    - Calibrate ablation kinetic parameters



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Example: Multi-Physics Validation

- High enthalpy M<12 flows onto ablator samples
  - Ames & JSC arc-jet tunnels, measuring recession rates, surface temperatures, and radiometry
    - Validate ablation models coupled with gas dynamics, radiation, chemistry and turbulence
  - Ames & JSC arc-jet tunnels, measuring particle densities
    - Validation data for particle generation and transport

Ablator sample in arc-jet

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Flight test validation

- Legacy flight tests Fire II and Apollo 4
  - Validate fully coupled multi-physics model
  - Fire II presents a fresh TPS at three altitudes
    - Initial reentry, max heating, low altitude
  - Apollo 4 was on a simulated lunar return trajectory
    - Measurements of TPS surface temperature, radiometry
    - Recovered vehicle from Apollo 4

TPS damage on recovered Apollo 4 capsule

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Flight Test Validation

- 2 Orion program flight tests planned
  - Validate fully coupled multi-physics model
    - Modern infrastructure, better spectral coverage from radiometers
    - Tests & instrumentation designed for validation
  - CEV capsule reentering from LEO (~2012)
  - 2m model capsule on simulated lunar return (~2010)
    - Measure temperature, heat flux and radiometry
    - Recovered test article, TPS analysis

Summary of V&V-UQ Challenges

- Dimensionality of parameter spaces
  - Coupled system involves 100's to 1000's of model parameters
  - Need to identify critical parameters
  - Efficiently sample high dimensional spaces
- Models and their uncertainty
  - Need to develop and validate models of model uncertainty
  - Drive model development from validation and uncertainty information

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Summary of V&V-UQ Challenges continued

- Validating coupling models challenging because relevant data are scarce
- Computational Costs
  - A single solution of these systems is expensive (100's of processors, 10's of hours)
  - Many 1000's of solutions for calibration, validation, uncertainty quantification
  - Calibration costs up to 10^6 core hours
  - Flight Validations: 10^6 to 10^7 core hours
  - Prediction with uncertainty: 10^6 - 10^7 core hours

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Questions?

Defining success

- If we have uncertainties in predicting ablation rate and local heat transfer that are significantly less than margins currently carried by NASA, then the simulations are certainly useful. NASA's margins are:

Heat Shield:	Afterbody Heat Flux
Turbulent LEO 25%	LEO 30%
Turbulent Lunar 35%	Lunar 50%
Radiative 50%	

Uncertainties better than 25% would be very useful