Uncertainty and Parameter Sensitivity in Multiphysics Reentry Flows

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PECOS and Uncertainty Quantification

**Calibration**
- Collect data in low level experimental scenarios
- Determine uncertain model parameter Probability Distribution Functions (PDFs)

**Validation**
- Exercise models in higher level scenarios
- Compare to experimental data
- Determine confidence in calibrated models

**Prediction**
- Exercise models in scenario of interest
- Evaluate Quantity of Interest (QoI) functionals
- Propagate uncertainty to output PDFs
PECOS and Atmospheric Entry

- Multiphysics submodels: Flow, Aerothermochemistry, Ablation, Surface chemistry, Radiation, Turbulence
- Data sources: Thermogravimetrics, Shock tube, Wind tunnel, DNS
## Challenges

### Uncertainty Quantification
- High individual forward solve cost
- High parameter count

### Verification
- Code complexity
- Lacking analytical solutions to complex physics
- Sole interest: Quantity of Interest functionals

### Validation
- Validation processes are cyclical
  - Modeling informs experiment informs modeling
  - Full System Simulation results inform model research, data collection
Modeling for Quantity of Interest

Peak Ablation Rate Scenario

- CEV-based axisymmetric capsule
- Peak heating point from ISS return trajectory
  - Mach 21.7
  - 19° Angle of Attack
  - Altitude ≈ 60 km
  - 239 K freestream temperature
  - $0.282 \frac{g}{m^3}$ freestream density

Peak Ablation Rate Ignores

- Wake domain
- Integration over trajectory
Uncertain Parameters

Submodel Uncertainties

- Hypersonic Flow
  - Chemical reaction rates
  - Diffusive flux model coefficients
  - Turbulent mixing augmentation
- Radiation
  - Absorptivity/Model Error
- Ablation
  - Virgin, char densities
  - Reaction rate, equilibrium constants

\[\sim 300 \text{ independent parameters}\]
### Uncertain Priors

<table>
<thead>
<tr>
<th>Flow and Transport</th>
<th>Ablation</th>
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<tbody>
<tr>
<td>• Gupta transport curves ±10%</td>
<td>• Virgin, char densities ±10%</td>
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<tr>
<td>• Reaction rates ±1 OOM</td>
<td>• Enthalpy of formation (\approx \pm 10 - 15%)</td>
</tr>
<tr>
<td>• Turbulent augmentation model error: +50% − −100%</td>
<td>• Elemental mass fractions (\approx \pm 10 - 15%)</td>
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<td>• Activation energies (\approx \pm 10 - 15%)</td>
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<tr>
<td></td>
<td>• Sublimation, oxidation coefficients (\approx \pm 10 - 15%)</td>
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<tr>
<td></td>
<td>• Nitridation coefficient (\approx \pm 1 \text{OOM})</td>
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### Radiation

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Acknowledgements

- Flow based on DPLR, NASA/Ames
- Two temperature thermochemical nonequilibrium
- 13 species, 18 reaction classes
- Algebraic turbulence model, fully laminar through fully turbulent
- Ablation, Radiation in-house

DPLR++ Core
- Paul Bauman
- Karl Schulz
- Roy Stogner

Data Parallel Line Relaxation
- Michael Wright
- Todd White
- Mike Barnhardt

Radiation, Ablation
- Andre Maurente
- Rochan Upadhyay
Quasi-steady Ablation

- Assumes ablation timescale $<<$ trajectory timescale
- Assumes negligible substructure conduction
Ablation Interface Conditions

Recession:

\[ \rho v_w = \dot{m}_c'' + \dot{m}_g'' \]  

\[ J_i \big|_{gas} + \rho v_w C_i = \tilde{N}_i(C_i, T) + \dot{m}_g'' C_{i,g} ; (i : 1..N_s) \]

Energy:

\[ -k \frac{\partial T}{\partial y} \bigg|_{gas} - \sum_{i=1}^{N_s} h_i(T_w) J_i \big|_{gas} + \dot{m}_c'' h_c(T) - \rho v_w h_w(T) \]

\[ +\alpha \dot{q}_r'' - \sigma \epsilon T_w^4 + \sum_{i=1}^{N_s} \dot{m}_g C_{i,g} h_i(T_w) + k_s \frac{\partial T}{\partial y} \big|_{solid,w} = 0 \]

- Nonlinear Robin Boundary Conditions
- Enables quasi-steady solves, restarts
• MUTATION precalculates equilibrium chemistry for a given temperature, pressure, elemental mass fraction set

• SPECAIR precalculates line-by-line intensities for a shock layer of given thickness, chemistry

• Grey gas model integrates through spectrum and shock layer, gives mean absorption coefficient
Tangent Slab Radiation Transfer Model

Decomposition

- Independent solution in each column of “slabs”
- Radiative heat transfer becomes locally 1D
- Accurate where flow field is locally 1D
Multiphysics Coupling

- Full (Multi-way) Coupling
  - Changes in radiation, ablation feed back to flow solver
  - Every parameter change requires full re-solve
- Loose vs Tight Coupling
- Uncertainty Quantification
  - Submodel sensitivities amplified or damped
  - Sensitivities to parameters missing in base models
Methodology

Forward UQ Propagation Setup

- Off-baseline perturbations resume from hand-converged baseline
- Dakota ILHS study generation, modified preprocessor builds input workspaces
- Input samples run on Hera
  - 80 processors per sample
  - 1024 total samples
  - 5 hours runtime per sample
- Automatic detection/resumption of failed runs

Postprocessing

- Quantities of interest from DPLR++, coupled models, postflow
- “make summarize” - extraction, collection, calculations
- Makefile-based job submission, lonestar/hera options
Parameter Sensitivity Triage

Deterministic Perturbations
- One parameter at a time
- Identifies insensitivities

Limitations
- Nonlinearities
- Multiparameter effects
Significant Parameters

**Flow and Transport**
- Turbulent augmentation!
- Transport: $N_2$, $O$, $C$, $CO$
- Reactions:
  \[ N_2 + C \leftrightarrow CN + N, \]
  \[ CO + N \leftrightarrow CN + O, \]
  \[ N_2 + M \leftrightarrow N + N + M, \]
  \[ N_2 + O \leftrightarrow NO + N \]

**Radiation**
- Reradiation emissivity

**Ablation**
- Nitridation coefficient!
- Virgin, char densities
- Enthalpy of formation
- Pyrolysis temperature
Monte Carlo Integration

Errors

- $\bar{q}^{MC} - \bar{q}$ variance: $\sigma^2_{e[\bar{q}]} = \frac{\sigma^2}{N_s}$
- $(\sigma^2_q^{MC})^2 - \sigma^2_q$ variance: $\sigma^2_{e[\sigma^2]} = \sigma^4 \left( \frac{2}{N_s-1} + \frac{\kappa}{N_s} \right)$
- $P_{MC}^C - P_C$ variance: $\sigma^2_{e[P_C]} = \frac{P_C - P_C^2}{N_s}$

- Sampling-based scheme errors are PDFs
- Errors based on variance $\sigma^2$ of sampled entity
- Error “bound” width: $\sigma_e \propto N^{-1/2}$
Incremental Latin Hypercube Sampling

**Algorithm**
- Form quantile bins in each parameter
- Permute samples to empty bins
  - Reducing correlations
- Randomly place each sample within its bins

**Uses**
- Reduce variance from additive functions
- Higher order convergence for separable functions
Results: Monte Carlo Outputs

Accuracy

• \( \sim 2 \) significant figures on mean
• \( \sim 1 \) significant figure on standard deviation
• Higher order statistics: worse
• \( \sim 0.5 \) million CPU-hours on Hera, LLNL
Results: Output PDFs

- Correlations in output sample set estimate sensitivities
- (In)sensitivities consistent with deterministic perturbation results
  - Subject to Monte Carlo error...
- Top uncertainties
  - Turbulent transport augmentation
  - Nitridation reaction rate
- Data mining possible: e.g. surrogate QoI choice analysis
Results: Parameter Sensitivities

- Forward UQ depends on input parameter PDFs!
  - Priors update with every new literature result
  - Calibrated PDFs update with new experiments
- Updating knowledge (e.g. $\beta_N$ priors) changes, requires repetition of the problem
Results: Submodel Sensitivities

Submodel Updates
- Enlarged nitridation prior
- Chemistry/radiation coupling

Top Priorities
- Nitridation validation
- Turbulence model validation
Development Directions

Uncertainty Quantification

- Accelerated Stochastic Techniques
- Accelerated Full System Simulations

Verification

- Code verification - Method of Manufactured Solutions
  - Submodels independently verified
  - Combined code requires verification
  - Standardized in MMS library “MASA”
- A posteriori error estimation
  - Goal-oriented error estimates

Validation

- Submodel calibration experiments
- Multilevel model comparisons
Thank you!

Questions?