Estimation of inflow uncertainties in laminar hypersonic double-cone experiments


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What is this talk about?

- When we validate simulations with experimental data, we assume that the data is trustworthy and the model is not trusted.
  - What happens if you suspect that the situation is flipped? Prove it?
- In the previous talk, you saw some of our difficulties in reproducing LENS-XX experiments with SPARC.
- We’ll discuss a statistical framework that can be used to check whether an experimental dataset is consistent.
  - Hypothesize causes behind the mismatch of predictions & experimental data; gather evidence for/against in a quantifiable manner.
- We’ll demonstrate this framework with the double-cone problem.
Introduction

- **Problem:** Our model (SPARC) and others cannot reproduce LENS-XX double cone experiments
  - Even when stated experimental errors are accommodated in model predictions
- **Aim:** Could it be that stated experimental settings are inconsistent with measurements? Can you prove it?

**Process:**
- Propose experimental settings that may be in error, and ones that are not
- Infer the true values of the experimental variables deemed wrong
- Compare inferred (“true”) and stated (“wrong”) values. Are they outside their respective uncertainty bounds?
Recap – The experiments

- We have a double-cone in hypersonic flow
  - Expansion tunnel, low temperatures, thermochemical equilibrium freestream
  - Freestream errors: 3 % (U, T); 7% (ρ)
  - 6 experiments, \( H_0 = [5.4, 21.8] \) MJ/kg
  - Mild vibrational non-equilibrium to widespread dissociation
- Laminar, attached flow on the fore-cone; simple physics
  - Shock interactions, separation bubble
Recap – Our difficulties

- Case I – lowest $H_0$. Pressure ($p(x)$) prediction fine but under-predict heat flux ($q(x)$) on the forecone. After separation, agreement is bad
- Adding in uncertainty due to freestream conditions doesn’t help (no overlap)
A bit about experimental datasets ...

- Most experimental datasets have two parts:
  - The data that specifies the experimental environment (IC & BC for models)
  - The data that describes the physical processes that occur in the experiment

- Not all data in an experimental dataset are measurements
  - Some are inferred using models, and have assumptions built into them

- Uncertainties in actual measurements are usually known
  - Uncertainties in inferred quantities are harder to quantify

- In LENS-XX / double-cone datasets:
  - Flow processes on the double-cone are actually measured (direct quantities)
  - Experimental settings e.g. axisymmetry, freestream etc. are often inferred from more fundamental measurements (derived quantities)
The causes of the model – experiment mismatch could be:

- **Cause I** – the experimental environment, specifically *freestream conditions*, could be *inconsistent* with measurements of flow processes
  - **Test**: Infer “true” freestream from direct measurements and compare with stated conditions

- **Cause II** – The *thermochemical models* e.g., reactions, models of viscosity etc. are *not suitable* for high enthalpy flows
  - **Test**: Prediction errors using “true” freestream for low enthalpy flows should be smaller than for higher enthalpy flows

- **Cause III** – the incoming freestream is *not axisymmetric*
  - **Test**: Do the flow processes satisfy self-similar collapses?
Investigating Cause I

- **Claim:** The true freestream conditions $(\rho_\infty, U_\infty, T_{rot,\infty}, T_{vib,\infty})$ lie outside the stated uncertainty bounds.

- **Test:** Estimate $\theta = (\rho_\infty, U_\infty, T_{rot,\infty}, T_{vib,\infty})$ consistent with measurements $Y = (p(x), q(x), H_0, P_0)$
  - Use data from 3 $p(x)$ and 17 $q(x)$ sensors.
Bounding & Global Sensitivity Analysis

- Can a $\pm 15\%$ uncertainty bound about the nominal freestream bracket experimental data? Yes
- Does variation of $\theta$ affect $Y$? Global Sensitivity Analysis!
  - Compute the Sobol indices of $p(x)$ and $q(x)$ as $X$ is varied over the +/- 15% uncertainty bounds
  - Only $\rho$ and $U$ have any impact on pressure and heat flux
A self-similarity collapse

- While we have 3 p(x) probes and 17 q(x) probes, the information content in the measurements is meager
  - Pressure: $K_1 = \frac{P}{\rho U_\infty^2}$
  - Heat-flux self-similar. $K_2 = \frac{q(x)\sqrt{x}}{\rho U_\infty^3}$

- Implications:
  - Estimating $\theta$ not possible with much certainty – use Bayesian inference
  - 3D effects should be small, but *not* non-existent!
    - See scatter in heat-flux plot
Inverse problem for freestream conditions

- We have to infer 4 quantities $\theta = (\rho_\infty, U_\infty, T_{rot,\infty}, T_{vib,\infty})$ from 4 measurements $Y = (K_1, K_2, H_0, P_0)$ – very uncertain
  - So estimate $\theta = (\rho_\infty, U_\infty, T_{rot,\infty}, T_{vib,\infty})$ as a 4-dimensional joint probability density function (JPDF) and capture the uncertainty in the estimate
- Done using Bayesian calibration

Bayesian calibration

- Formulation: $\mathbf{y}^{(obs)} = \mathcal{M}(\theta) + \epsilon$, $\epsilon = \{\epsilon_i\}, \epsilon_i \sim \mathcal{N}(0, \sigma^2)$
- Likelihood: $\mathcal{L}(\mathbf{y}^{(obs)}|\theta) \propto \prod_{i \in S} \exp \left( - \frac{(y_i^{(obs)} - y_i^{(pred)}(\theta))^2}{2\sigma^2} \right), S = \text{sensors}$
Bayesian calibration

- Suppose we have a prior belief (a PDF) on $\theta, \pi_1(\theta)$ and one on $\sigma, \pi_2(\sigma)$
- Then by Bayes law, the posterior PDF of $\theta$

$$P(\theta, \sigma^2 | y^{(obs)}) \propto \prod_{i \in S} \exp \left( - \frac{(y_i^{(obs)} - y_i^{(pred)}(\theta))^2}{2\sigma^2} \right) \pi_1(\theta) \pi_2(\sigma)$$

- Provides the PDF of $(\theta, \sigma^2)$ conditioned on $y^{(obs)}$
- PDF constructed by sampling from $P(\theta, \sigma^2 | y^{(obs)})$ using MCMC
- Each sample consists of making a SPARC run $\sim 150$ CPU-hours; sampling is sequential
- Too expensive – replace SPARC with a statistical emulator
Statistical emulators

- A “curve-fit” that maps freestream $\theta$ to the SPARC prediction $y_i^{(pred)} = M_i(\theta)$ at a pressure or heat-flux sensor $i, i \in S$

- Take $N_s$ samples of $\theta_j, j = 1 \cdots N_s$, from a +/- 15% region around the nominal freestream $\theta$

- Run SPARC with them. Database the results $y_i^{(pred)}(\theta_j), y_i^{(pred)} = \{K_1, K_2, H_0, P_0\}$

- Try to fit 3rd order polynomials separately to $K_1(\theta), K_2(\theta), H_0(\theta), P_0(\theta)$
  - Use AIC to cut down on terms (prevent over-fitting)
  - Accept the polynomial curve-fit as a proxy for SPARC if its prediction error < 5% and use it in MCMC

- Result: Most of our surrogates are weak, linear functions of $(T_{rot,\infty}, T_{vib,\infty})$
Case 1

- $H_0 = 5.4 \text{ MJ/kg},$ vibrational non-equilibrium, no dissociation
- 50,000 MCMC steps
- As expected, can’t estimate $T_{rot,\infty}$ and $T_{vib,\infty};$ the PDFs are flat
- Can estimate freestream $\rho$ and $U$ and their most probable values
  - Discrepancies similar to meas. errors
- Implication: Stated and measured freestreams look consistent

<table>
<thead>
<tr>
<th>Disagreement</th>
<th>Meas. error</th>
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<tbody>
<tr>
<td>Density</td>
<td>~2%</td>
</tr>
<tr>
<td>Velocity</td>
<td>~4%</td>
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</tbody>
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Quality of a probabilistic forecast

- When check our inferred freestream as follows:
  - We take 100 \( \theta \) samples from the posterior distribution
  - We run SPARC forward & get 100 predictions per sensor
  - Our predictions are samples describing a PDF, \( P(y_i) \)

- Our experimental data is either a number \( y_i^{(obs)} \) or a uniform distribution \( Q(y_i^{(obs)}) \)

- Comparison
  - CRPS : Continuous ranked probability score
  - Sorensen distance, \( d_s = \frac{\sum_k |P_k(y) - Q_k(y)|}{\sum_k |P_k(y) + Q_k(y)|} \)
    - \( d_s = 1 \) (no overlap); \( d_s = 0 \) (complete overlap)
Predictive skill

- **Case 1 (low enthalpy), after calibrating the freestream**
- **Pressure**
  - OK, fore-cone
  - Bad, separation zone
  - Bad, post-reattachment
- **Heat transfer**
  - OK, fore-cone
  - Bad, separation zone
  - OK after reattachment
Case 4

- $H_0 = 21.7 \text{ MJ/kg}$, extensive dissociation
- 50,000 MCMC steps
- As expected, can’t estimate $T_{rot,\infty}$ and $T_{vib,\infty}$; the PDFs are flat
- Can estimate freestream $\rho$ and $U$ and their most probable values
  - Discrepancies greater than meas. errors
- **Implication:** Stated and measured freestreams are inconsistent

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<thead>
<tr>
<th></th>
<th>Disagreement</th>
<th>Meas. error</th>
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<tbody>
<tr>
<td>Density</td>
<td>10.4%</td>
<td>7%</td>
</tr>
<tr>
<td>Velocity</td>
<td>8.45%</td>
<td>3%</td>
</tr>
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Predictive skill

- **Case 4 (high enthalpy), after calibrating the freestream**
  - **Pressure**
    - OK, fore-cone
    - Bad, separation zone
    - OK, post-reattachment
  - **Heat transfer**
    - OK, fore-cone
    - Bad, separation zone
    - So-so, after reattachment
Summarizing

<table>
<thead>
<tr>
<th>Test Case</th>
<th>Pressure ($d_s$)</th>
<th>Heat Flux ($d_s$)</th>
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<tbody>
<tr>
<td></td>
<td>Pre-calib</td>
<td>Post-calib</td>
</tr>
<tr>
<td>Case 1 ($H_0 \sim 5$ MJ/kg)</td>
<td>0.77</td>
<td>0.899</td>
</tr>
<tr>
<td>Case 4 ($H_0 \sim 21$ MJ/kg)</td>
<td>0.6756</td>
<td>0.7882</td>
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- Post-calib, Case 1 & 4 pressure predictions degrades and heat-flux improved
  - Freestream mis-specification a cause (?), but probably not the main one. [Cause # 1]
- Post-calibration $d_s$ smaller for high-enthalpy flows.
  - Thermo-chemical models not the culprit for bad predictions [Answers Cause # 2]
- The incoming flow is may be mildly axisymmetric
  - Would explain the behavior of Case 1 and 4
  - Self-similar collapse shows non-axisymmetry is small [Kind of answers Cause #3 ]
Conclusions

- Demonstrated a way of checking consistency of an experimental dataset
  - Consists of carefully demarcating between trustworthy and non-trustworthy data (e.g., derived data, which could be experimental settings)
  - Using trustworthy data and a validated model, infer the “untrustworthy” data
  - Compare the two. Requires estimation & comparison under uncertainty

- Used it to check the LENS-XX/double cone experimental dataset
  - The low-enthalpy experimental datasets seem OK (high confidence)
  - The high-enthalpy dataset has problems (medium confidence)
  - The thermo-chemical models in SPARC are not the culprit (high confidence)
  - Our model – data mismatch could be because of mild 3D effects (low confidence)
Acknowledgements

- We thank Tim Wadhams and Matthew MacLean at CUBRC for their data set files, measurement errors and help interpreting data

- Our companion papers:
BACKUP
How good is the inferred freestream PDF?

- Take 100 $\theta$ samples from JPDF
- Run SPARC and get 100 predictions @ sensors; compare with measurements
- Definite improvement, but how to quantify?
How good is the inferred freestream PDF?

- Take 100 θ samples from PDF
- Run SPARC and get 100 predictions @ sensors; compare w/ measurements
- Still, a net bias (model under-predicts)