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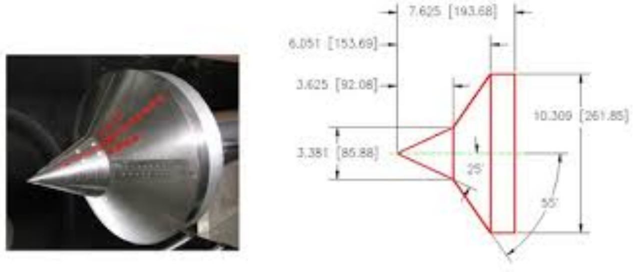

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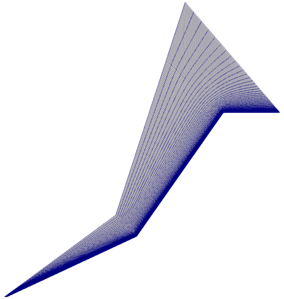

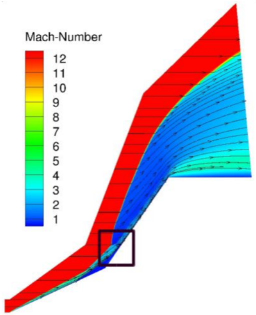

Estimation of inflow uncertainties in laminar hypersonic double-cone experiments

J. Ray, S. Kieweg, B. Carnes, V. G. Weirs, B. Freno, M. Howard, T. Smith, I. Nompelis & G. V. Candler

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What is this talk about?

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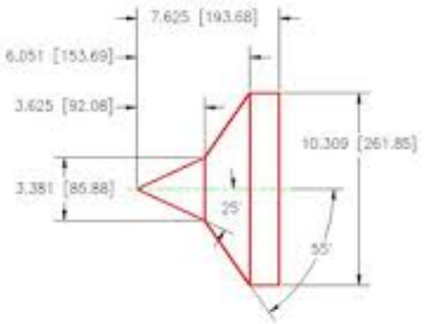
- When we validate simulations with experimental data, we assume that the data is trustworthy and the model is not
  - What happens if you suspect that the situation is flipped? Prove it?
- In the previous talk, you saw some of our difficulties in reproducing LENS-XX experiments with SPARC
- We'll discuss a statistical framework that can be used 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

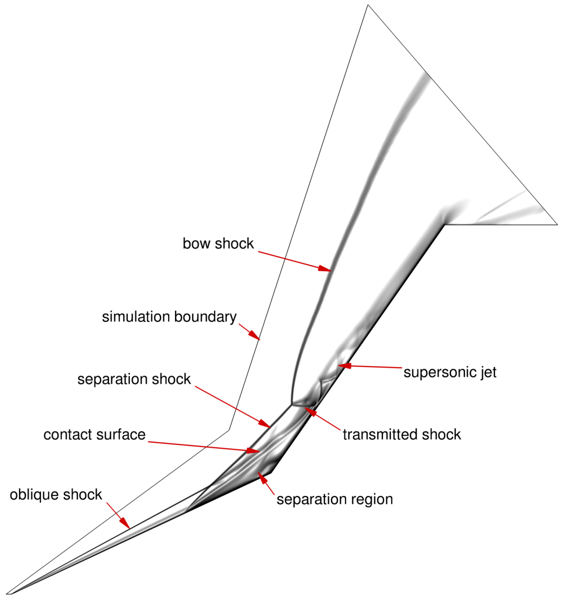
Introduction

- **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?

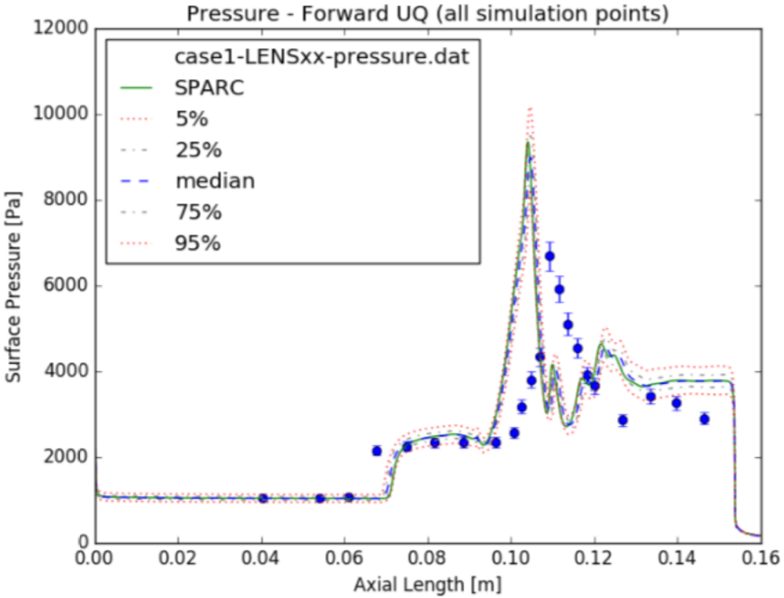
Recap – The experiments

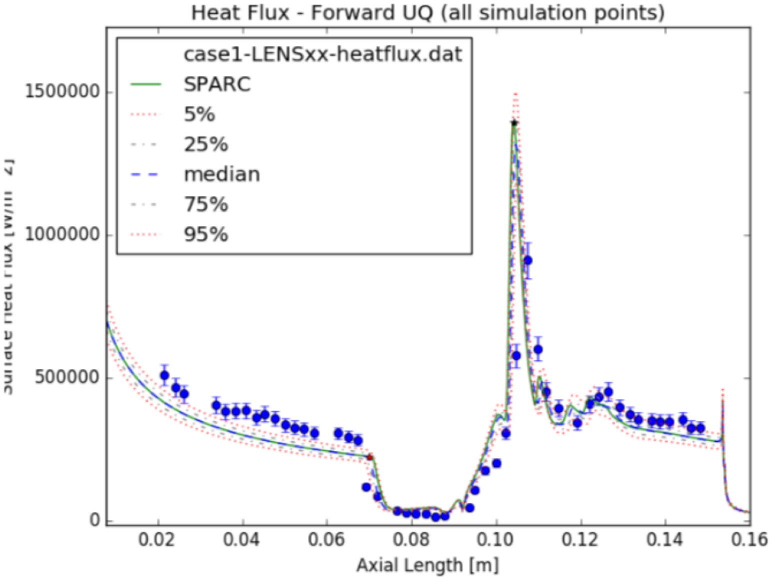
- We have a double-cone in hypersonic flow
  - Expansion tunnel, low temperatures, thermochemical equilibrium freestream
  - Freestream errors: 3 % (U, T); 7% (ρ)
  - 6 experiments, H_0 = [5.4, 21.8] MJ/kg
  - Mild vibrational non-equilibrium to widespread dissociation
- Laminar, attached flow on the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

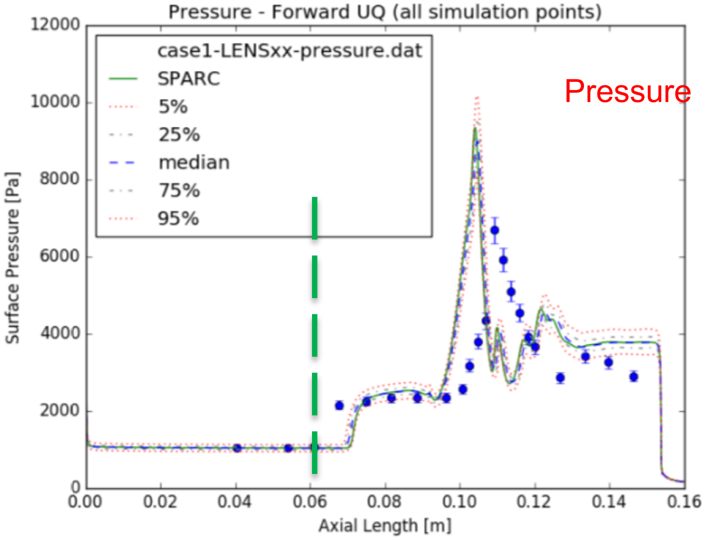
Hypotheses

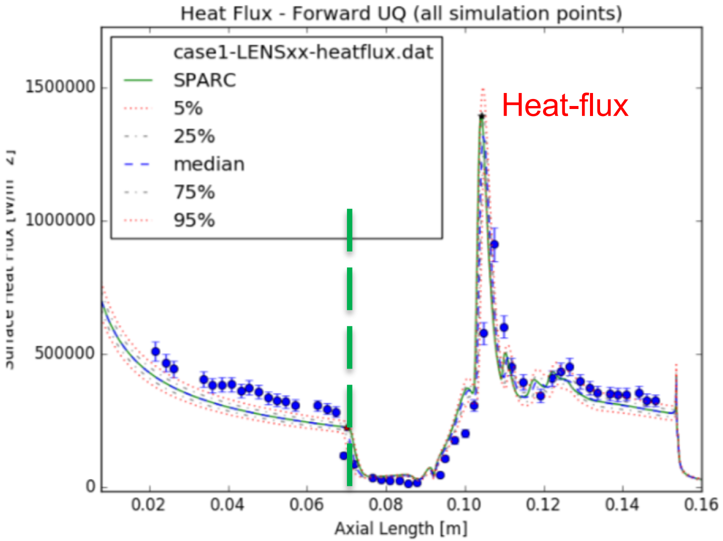
- The causes of the model – experiment mismatch could be:
  - **Cause I** – the experimental environment, specifically freestream conditions, could be inconsistent with measurements of flow processes
    - **Test:** Infer "true" freestream from direct measurements and compare with stated conditions
  - **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

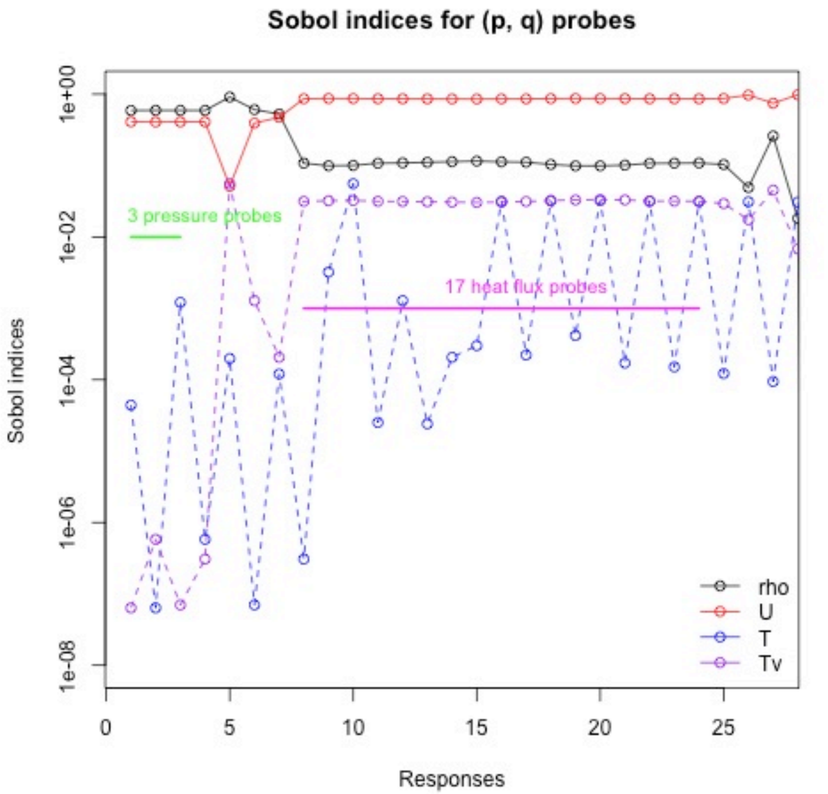
- **Test:** Estimate $\theta = (\rho_\infty, U_\infty, T_{rot,\infty}, T_{vib,\infty})$ consistent with measurements $Y = (p(x), q(x), H_0, P_o)$
  - Use data from 3 p(x) and 17 q(x) sensors





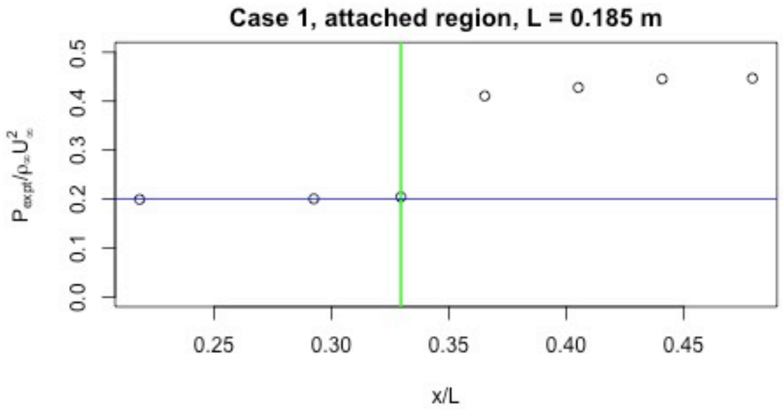
Bounding & Global Sensitivity Analysis

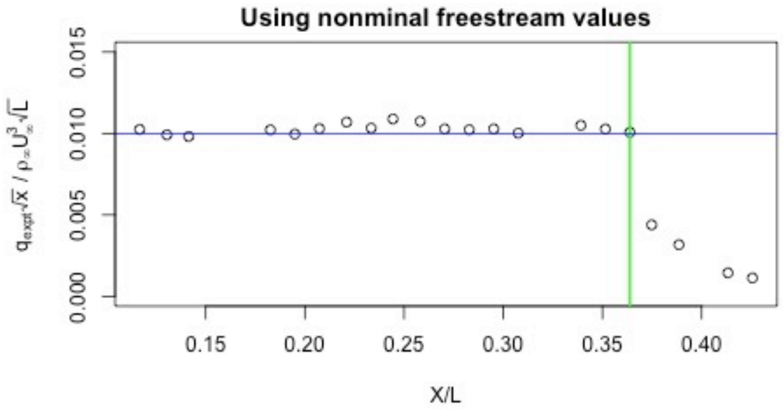
- Can a $\pm 15\%$ uncertainty bound about the nominal freestream bracket experimental data? **Yes**
- Does variation of θ affect Y? Global Sensitivity Analysis!
  - Compute the Sobol indices of p(x) and q(x) as X is varied over the +/- 15% uncertainty bounds
  - **Only ρ and U have any impact on pressure 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: $K_1 = {}^{P}/_{\rho U_\infty^2}$
  - Heat-flux self-similar. $K_2 = {}^{q(x)\sqrt{x}}/_{\rho U_\infty^3}$
- **Implications:**
  - Estimating θ 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 $\theta = \left(\rho_\infty, U_\infty, T_{rot,\infty}, T_{vib,\infty}\right)$ from 4 measurements Y = (K_1, K_2, H_0, P_0) – very uncertain
  - So estimate $\theta = \left(\rho_\infty, U_\infty, T_{rot,\infty}, T_{vib,\infty}\right)$ as a 4-dimensional joint probability density function (JPDF) and capture the uncertainty in the estimate
  - Done using Bayesian calibration
- Bayesian calibration
  - Formulation: $\boldsymbol{y}^{(obs)} = \mathcal{M}(\theta) + \boldsymbol{\epsilon}, \boldsymbol{\epsilon} = \{\epsilon_i\}, \epsilon_i \sim \mathcal{N}(0, \sigma^2)$
  - Likelihood: $\mathcal{L}\left(\boldsymbol{y}^{(obs)} \middle| \theta\right) \propto \prod_{i \in S} \exp\left(-\frac{\left(y_i^{(obs)} - y_i^{(pred)}(\theta)\right)^2}{2\sigma^2}\right), S = \text{sensors}$

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 θ

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

- Provides the PDF of (θ, σ^2) conditioned on $\mathbf{y}^{(obs)}$
- PDF constructed by sampling from $P\left(\theta, \sigma^2 \mid \boldsymbol{y}^{(obs)}\right)$ using MCMC
- Each sample consists of making a SPARC run ~ 150 CPU-hours; sampling is sequential
- Too expensive – replace SPARC with a statistical emulator

Statistical emulators

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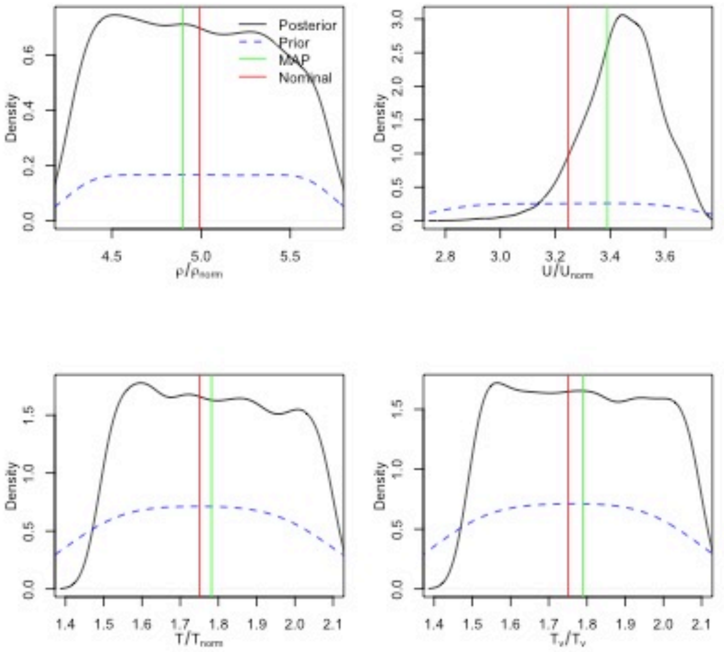
- A "curve-fit" that maps freestream θ to the SPARC prediction $y_i^{(pred)} = M_i(\theta)$at a pressure or heat-flux sensor $i, i \epsilon S$
- Take $N_s$samples of $\theta_j, j = 1 \cdots N_s$, from a +/- 15% region around the nominal freestream θ
- Run SPARC with them. Database the results $y_i^{(pred)}(\theta_j)$, $y_i^{(pred)} = \{K_1, K_2, H_0, P_0\}$
- 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

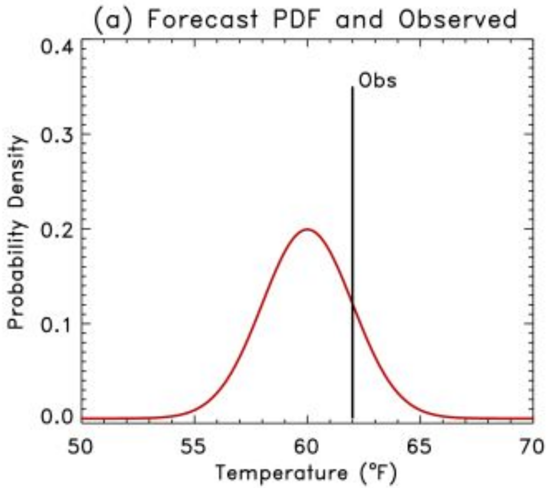
- H_0 = 5.4 MJ/kg, vibrational non-equilibrium, no dissociation
- 50,000 MCMC steps
- As expected, can't estimate $T_{rot,\infty}$ and $T_{vib,\infty}$; the PDFs are flat
- Can estimate freestream ρ and U and their most probable values
  - Discrepancies similar to meas. errors
- **Implication:** Stated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

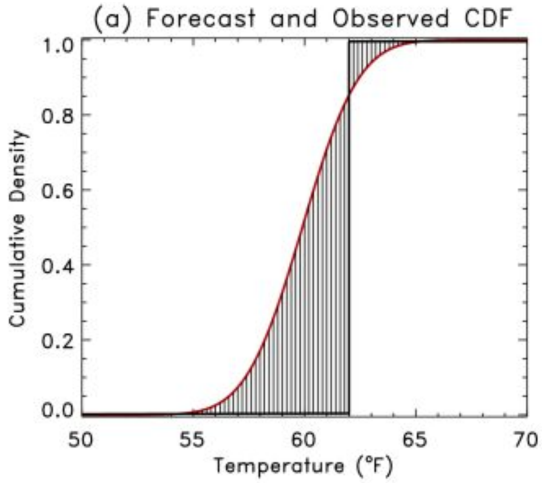


	Disagreement	Meas. error
Density	~2%	7%
Velocity	~4%	3%

Quality of a probabilistic forecast

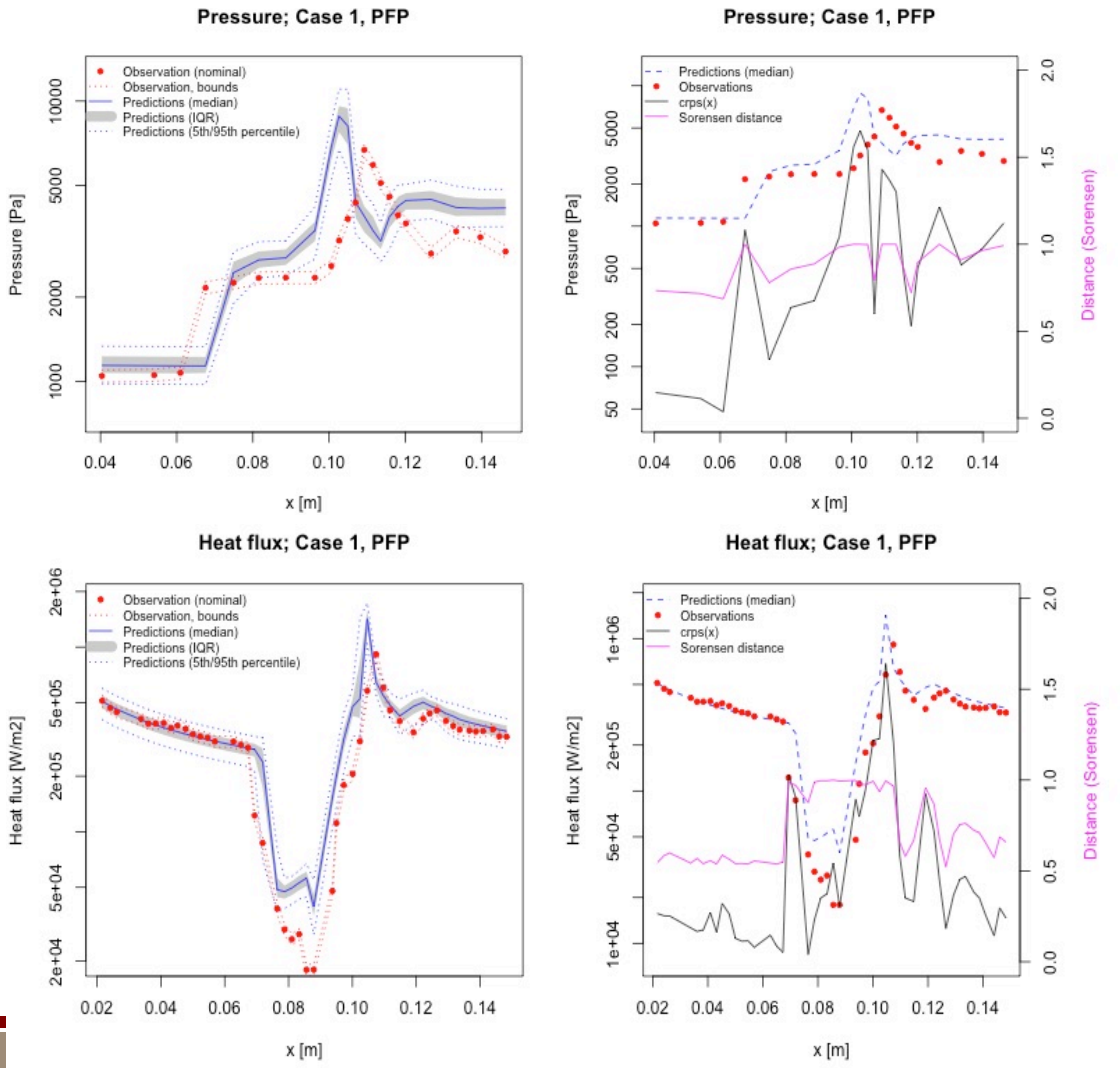
- When check our inferred freestream as follows:
  - We take 100 θ samples from the posterior distribution
  - We runs SPARC forward & get 100 predictions per sensor
  - Our predictions are samples describing a PDF, $P(y_i)$
- Our experimental data is either a number $y_i^{(obs)}$ or a uniform distribution $Q(y_i^{(obs)})$
- 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)





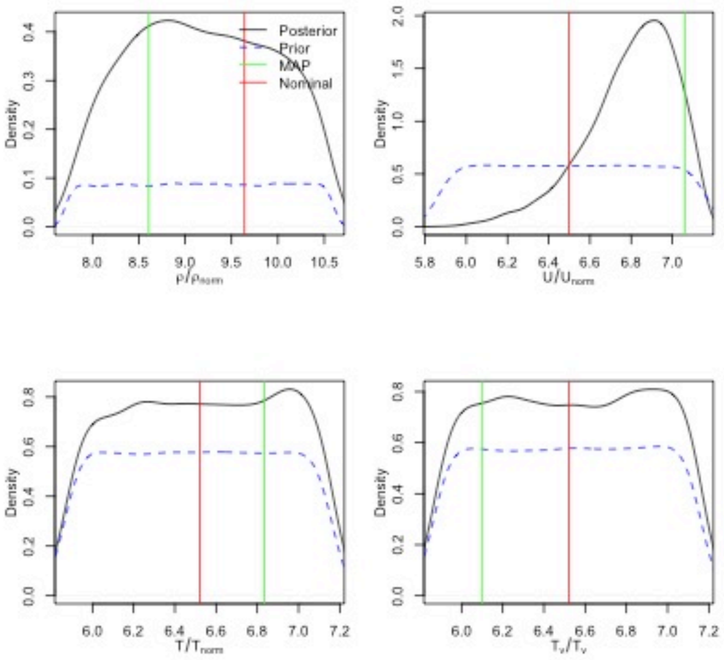
Predictive skill

- 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

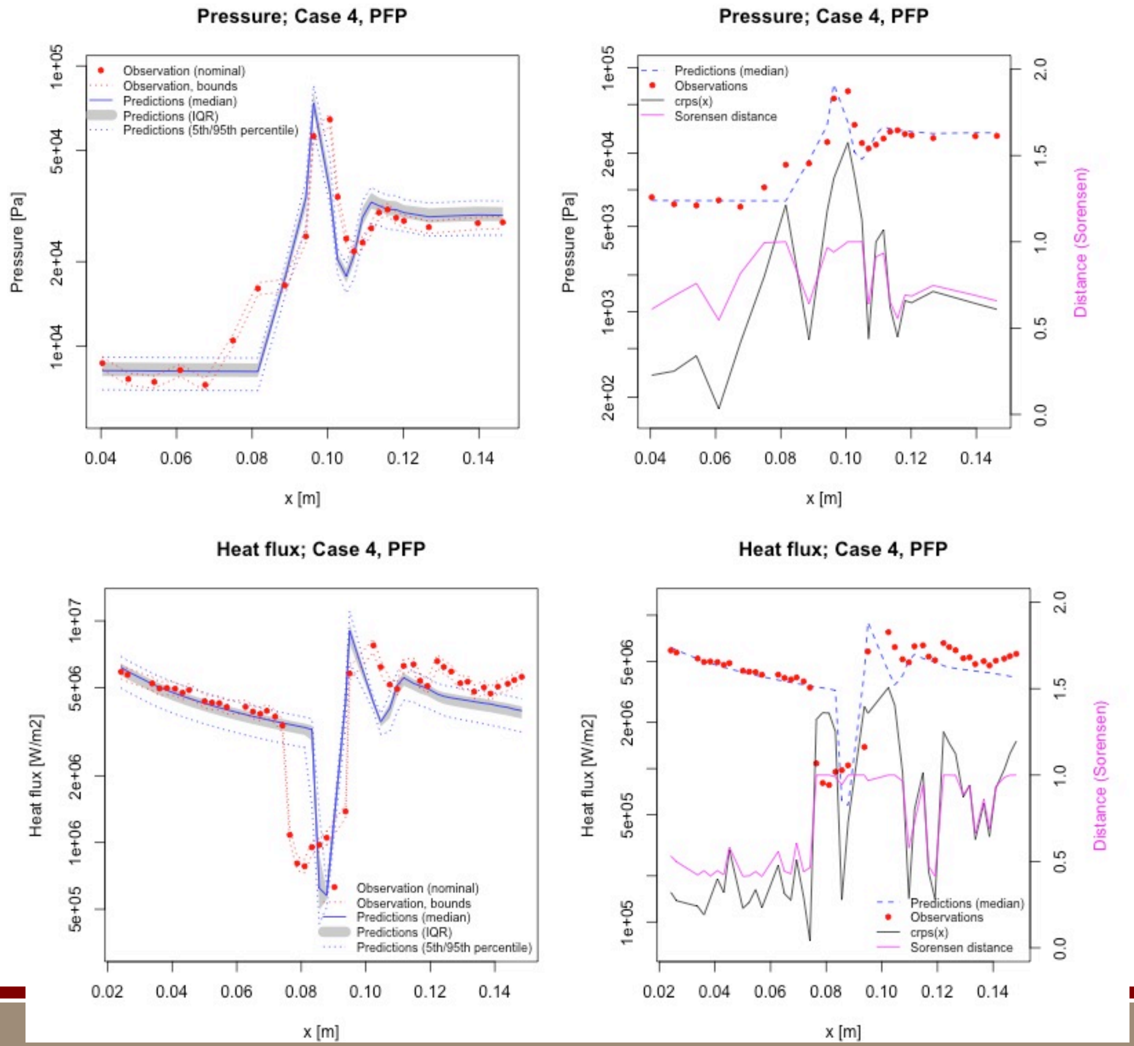
- H_0 = 21.7 MJ/kg, extensive dissociation
- 50,000 MCMC steps
- As expected, can't estimate $T_{rot,\infty}$ and $T_{vib,\infty}$; the PDFs are flat
- Can estimate freestream ρ and U and their most probable values
  - Discrepancies *greater* than meas. errors
- **Implication:** Stated and measured freestreams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



	Disagreement	Meas. error
Density	10.4%	7%
Velocity	8.45%	3%

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

Test Case	Pressure (d_S)		Heat Flux (d_S)	
	Pre-calib	Post-calib	Pre-calib	Post-calib
Case 1 (H_0 ~ 5 MJ/kg)	0.77	0.899	0.87	0.734
Case 4 (H_0 ~ 21 MJ/kg)	0.6756	0.7882	0.955	0.7248

- 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

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- 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

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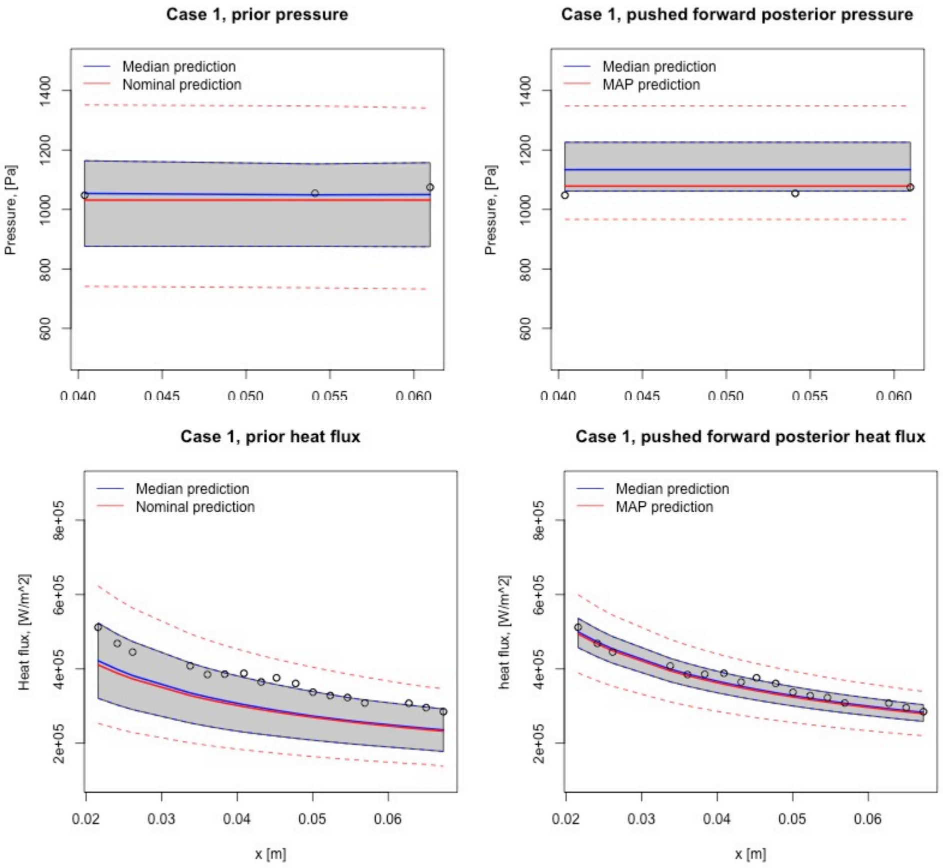
- We thank Tim Wadhams and Matthew MacLean at CUBRC for their data set files, measurement errors and help interpreting data

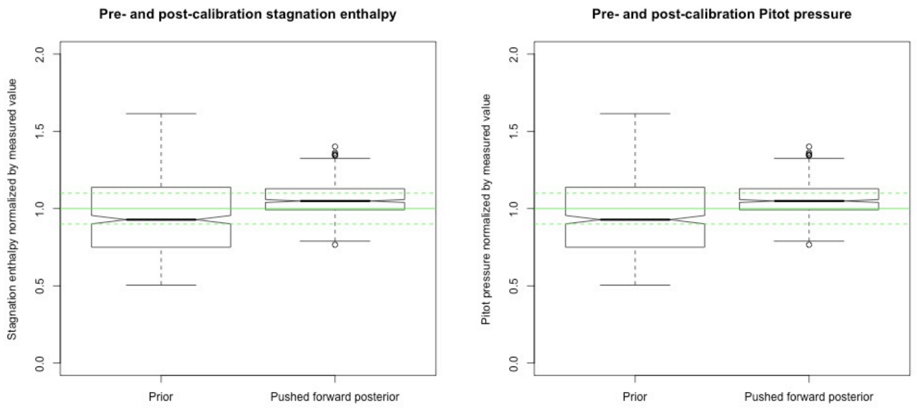
- Our companion papers:
  - **(10:30 am Gaslamp A)** Carnes, B., Weirs, V. G., Smith, T., and Dinzl, D., "Code verification and numerical error estimation with application to model validation of laminar, hypersonic flow over a double cone," AIAA 2019 Aerosciences Conference, AIAA SciTech 2019 (AIAA-2019-**2175**), 2019.
  - **(Previous talk)** Kieweg, S., Ray, J., Weirs, V. G., Carnes, B., Dinzl, D., Freno, B., Howard, M., Phipps, E., Rider, W., and Smith, T. "Validation Assessment of Hypersonic Double-Cone Flow Simulations using Uncertainty Quantification, Sensitivity Analysis, and Validation Metrics,"AIAA 2019 Aerosciences Conference, AIAA SciTech 2019 (AIAA-2019-**2278**), 2019.
  - **(This talk)** Ray, J., Kieweg, S., Dinzl, D., Carnes, B., Weirs, V. G., Freno, B., Dinzl, D., Howard, M., Smith, T., Nompelis, I., and Candler, G., "Estimation of Inflow Uncertainties in Laminar Hypersonic Double-Cone Experiments," AIAA 2019 Aerosciences Conference, AIAA SciTech 2019 (AIAA-2019-**2279**), 2019.

BACKUP

How good is the inferred freestream PDF?

- Take 100 θ 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)