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An Assessment of the Laminar Hypersonic Double-Cone Experiments in the LENS-XX Tunnel

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AIAA SCITECH 2023, NATIONAL HARBOR, MD

January 24, 2023

U.S. DEPARTMENT OF ENERGY NNSA

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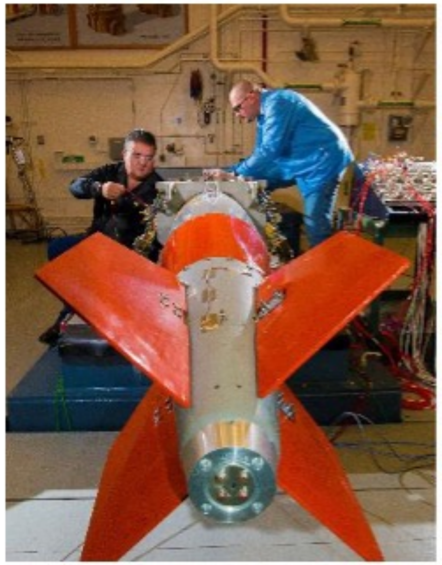
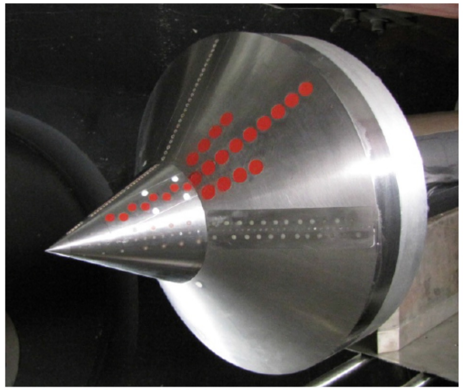


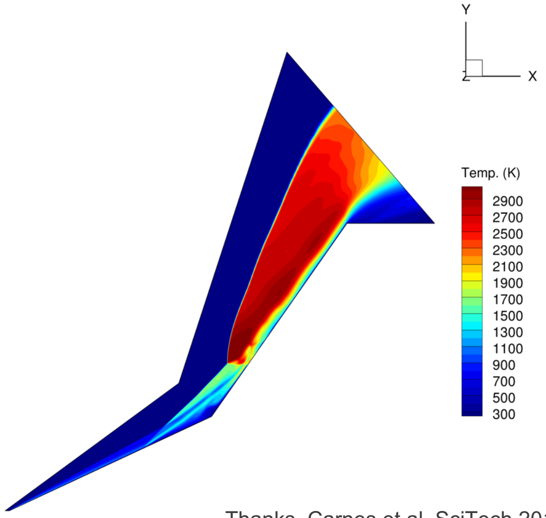
What is this talk about?

- A cautionary tale on decision-making using surrogate models
- Surrogate models: Data-driven, fast running proxies of CFD solvers
  - Widely used in UQ and Bayesian inverse problems – but they *are* approximate
    - Results e.g., point estimates from inverse problems can be wrong
    - Ditto, wrong decisions based on *point* estimates
- Application: Checking the consistency of experimental datasets from LENS-XX expansion tunnel
  - Laminar flow over double cone. Never modeled successfully
    - Questions about inaccurate inlet boundary conditions (BCs)
- Basic idea: Infer inlet BC by inverting measurements on the cone
  - To be safe, Bayesian inference; BCs as probability density functions (PDFs)
  - But what if the surrogate models of the Navier-Stokes simulator are approximate?



Thanks, Kieweg et al, SciTech 2019

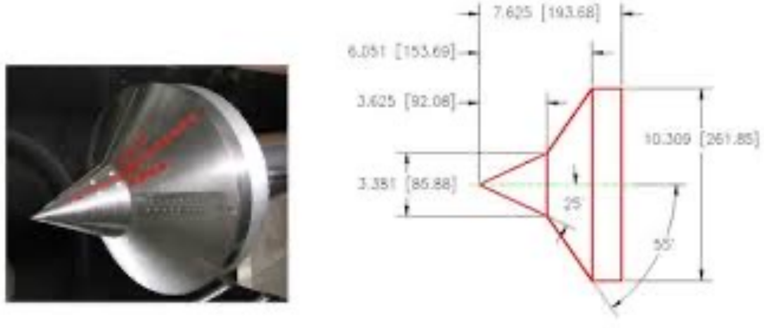
(a)



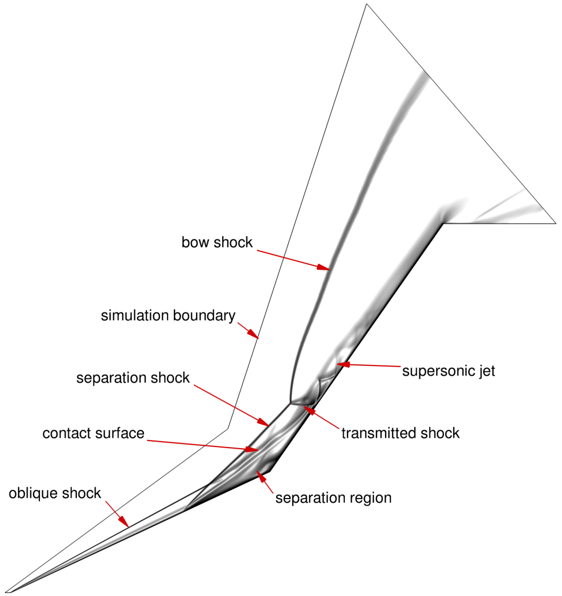
Thanks, Carnes et al, SciTech 2019

Recap – the experiments

- We have a double-cone in hypersonic flow
  - LENS-XX expansion tunnel, low temperatures, thermochemical equilibrium in freestream (in principle)
  - 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 on the aft cone
- Experiments of interest
  - Case 1: H_0 = 5.4 MJ/kg; mild vibrational non-equilibrium
  - Case 4: H_0 = 21.8 MJ/kg; vibrational & chemical non-equilibrium



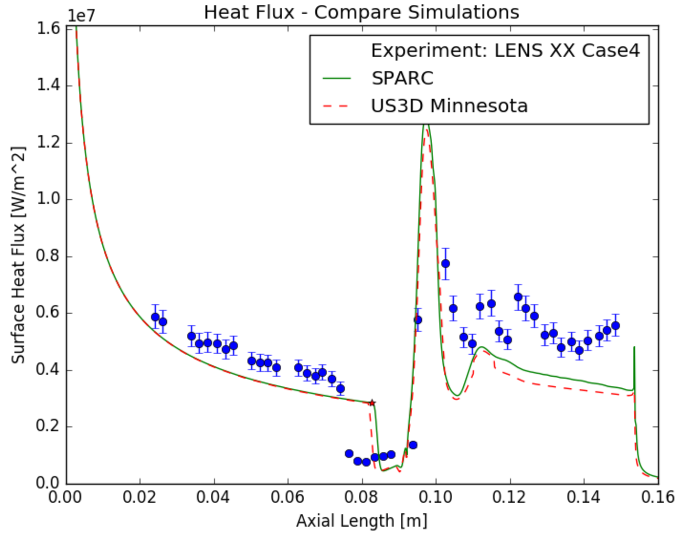
(a) (b)

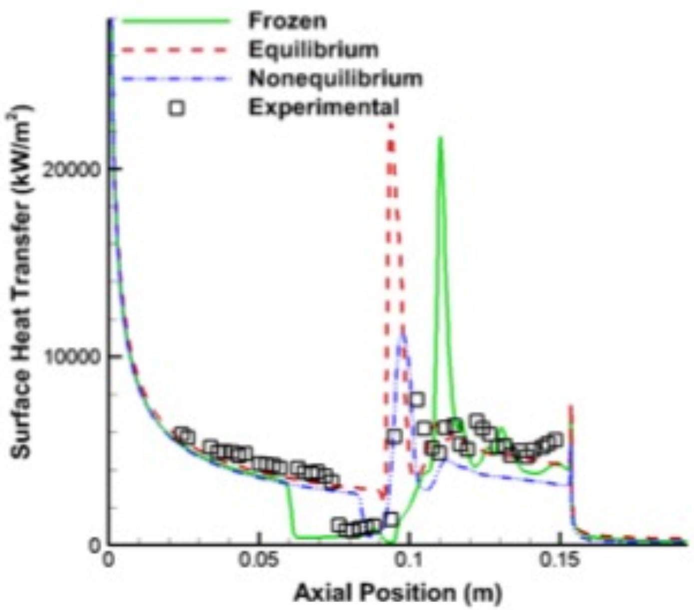


Recap – validation studies

- LENS-XX experiments never modeled successfully. Symptoms
  - Models underpredict heating on the fore cone
  - Ditto, the size of the separation zone
- Two potential causes investigated
  - Cause 1: Thermochemical models are inaccurate
    - Many thermochemical models & assumptions tried; changed the size of separation but not enough, or too much
  - Cause 2: The inlet BC is mis-specified (outside expt. error bounds)
    - Bayesian inference of (ρ, U, T, T_v) from measurements on fore-cone (laminar, attached flow)
    - Case 1 (low enthalpy): BCs barely within experimental error bounds i.e., OK
    - Case 4 (high enthalpy): BCs well outside error bounds; possibly mis-specified

Thanks, Kieweg et al, SciTech 2019

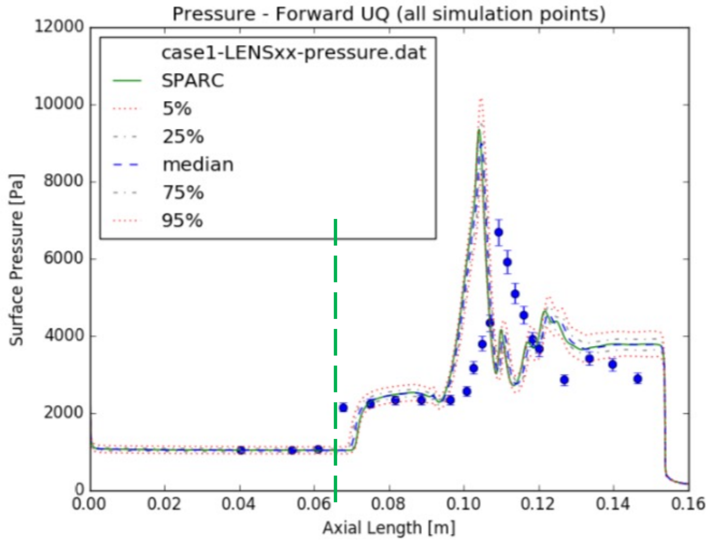


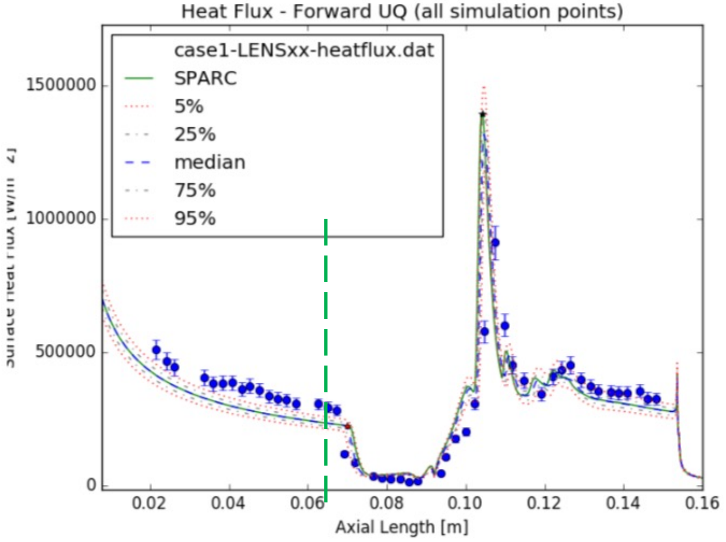


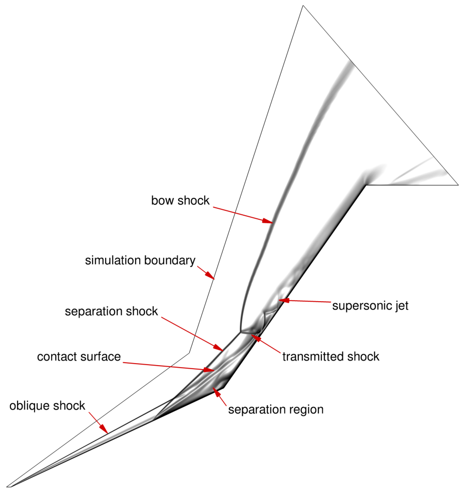
Thanks, Holloway et al, JSR, 2022. Case 4

Problem statement

- Aim: Decide if the BC mis-specification is dependent on flow enthalpy
  - Or was that an artefact of using surrogate models?
- Consequence: Did thermochemical non-equilibrium (inside and upstream of LENS-XX test-section) play a role in BC (mis-) specification?
- How to address the problem?
  - Pose and solve an inverse problem for inlet BC.
  - Use Navier-Stokes CFD solver, not surrogates
  - Data: p(x), q(x), H_0 and P_{pitot} , but only on the fore-cone, before separation

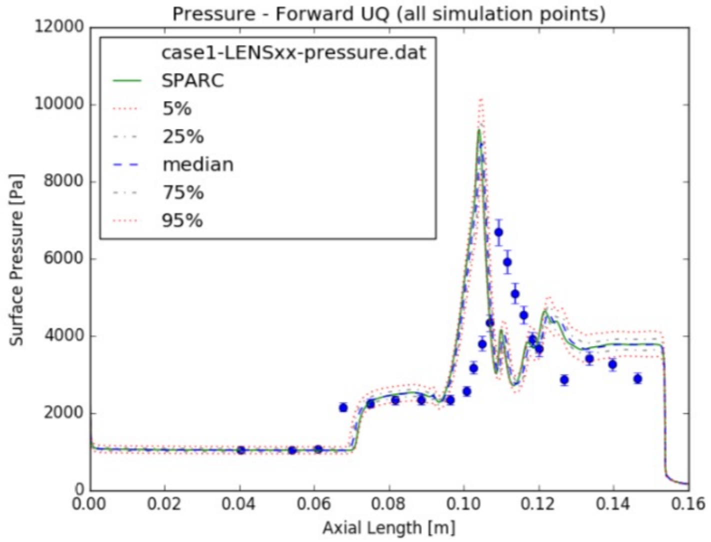


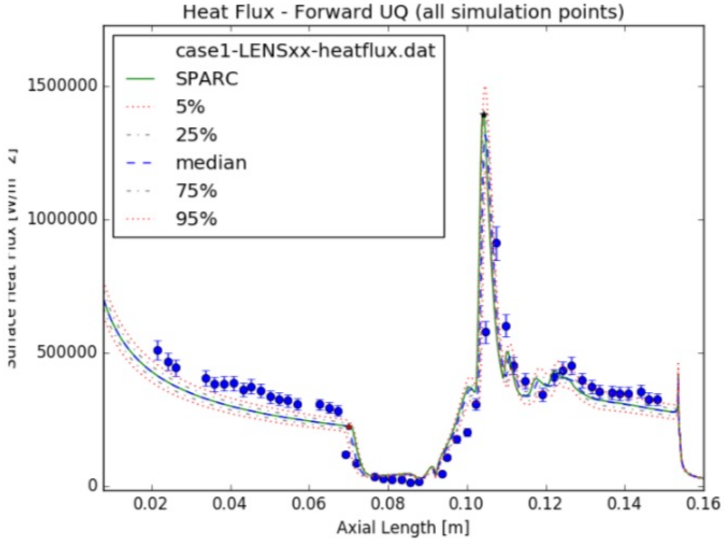




Technical approach

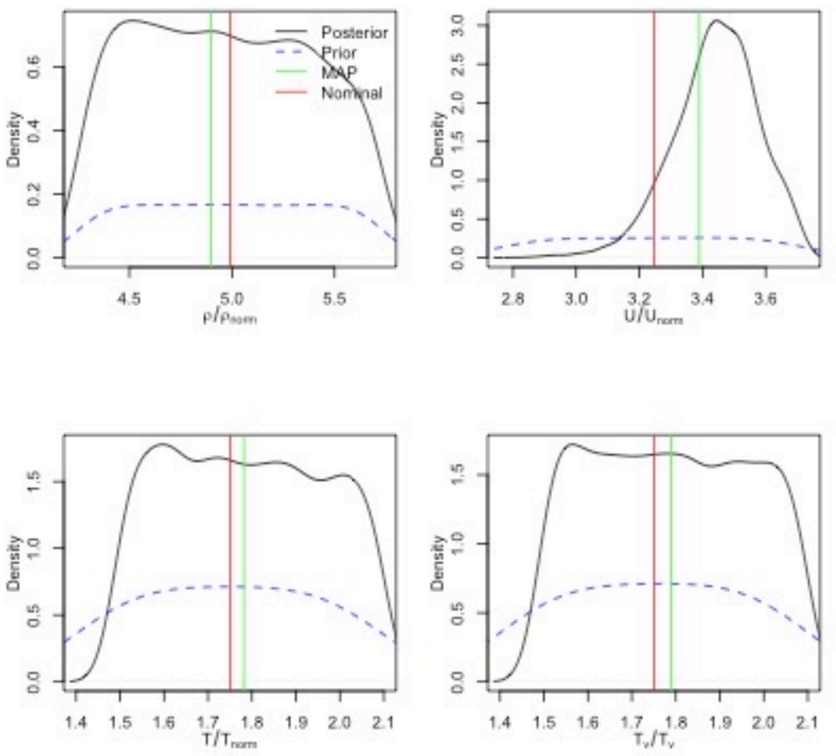
- Formulation: Deterministic inversion – optimization of a cost function J
  - Gradients (sensitivities w.r.t. optimization variables) computed using adjoints
- $\min_{\Theta} J = \alpha \left\|q^{(obs)} - q(\Theta)\right\|_2^2 + \beta \left\|p^{(obs)} - p(\Theta)\right\|_2^2 + \gamma \left\|H_o^{(obs)} - H(\Theta)\right\|_2^2 + \delta \left\|P_{Pitot}^{(obs)} - P(\Theta)_{Pitot}\right\|_2^2$
- Uncertainty bounds on Θ* under assumed Gaussian posterior distribution
  - $\Theta \sim N(\Theta^*, \Gamma), \Gamma = H^{-1}, H = \left|{\partial^2 J}/{\partial\theta_i \partial\theta_j}\right|$
- Outstanding questions:
  - Θ = {density, velocity, …..?}
  - Is the Gaussian assumption for the posterior distribution valid?





Bayesian comparison

- BC estimation done via Bayesian inversion and surrogate models
  - Data: Used the same measurements on the fore-cone
  - Method: MCMC
    - Exact posterior PDFs for (ρ, U, T, T_v); quantified the uncertainty in the estimates
    - Also MAP values (most probable or maximum a posteriori)
- Findings:
  - PDFs for T, T_v too wide – can't be estimated from data
  - Case 1's BC (MAP values) barely inside experimental error bounds
  - Case 4's BC (MAP values) outside experimental error bounds
- Reliance on MAP values and surrogate models to make decisions is a deadly combination
  - So check it – remove surrogates, for starters

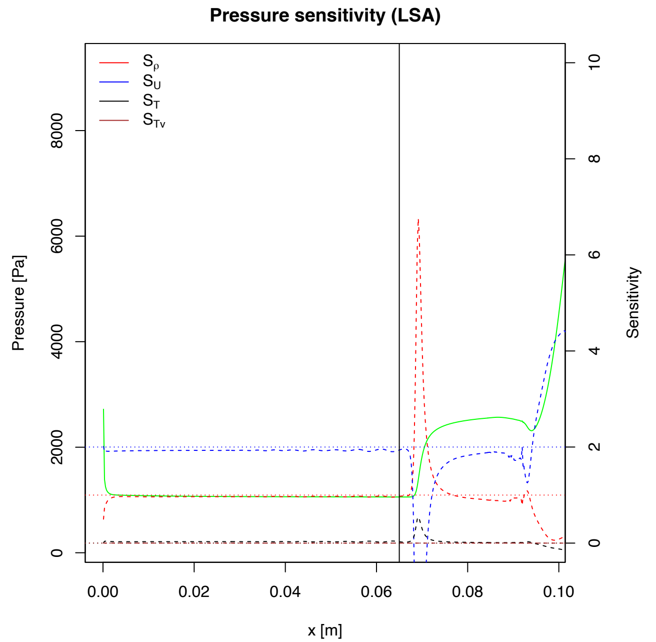


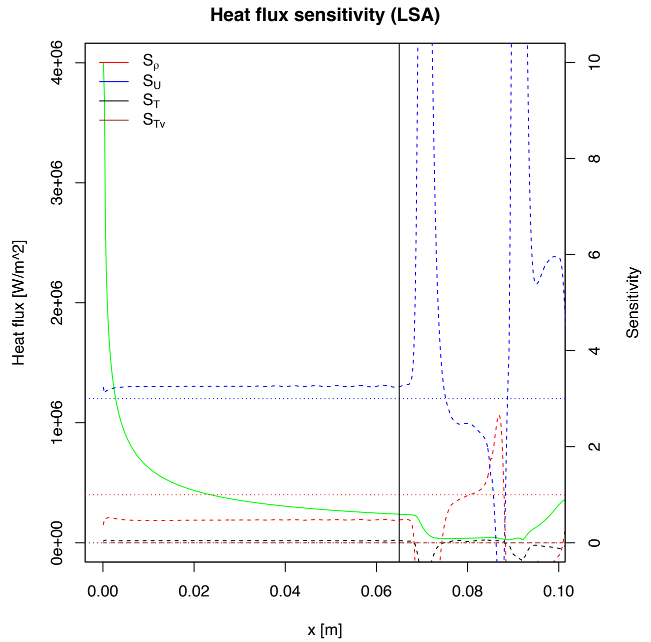
Case 4

Local sensitivity analysis

- Sensitivity = $\partial A / \partial B$ at the nominal inlet conditions
  - A = {surface pressure, surface heat flux} on double cone
  - B = {ρ, U, T, T_v}
- Findings:
  - Sensitivity w.r.t. {T, T_v} too small – won't be able to estimate from data
    - Expected – hypersonic flow energies are kinetic, not thermal
  - So, Θ = {ρ, U}
    - Hold T, T_v at the values specified in the experimental dataset

Case 1

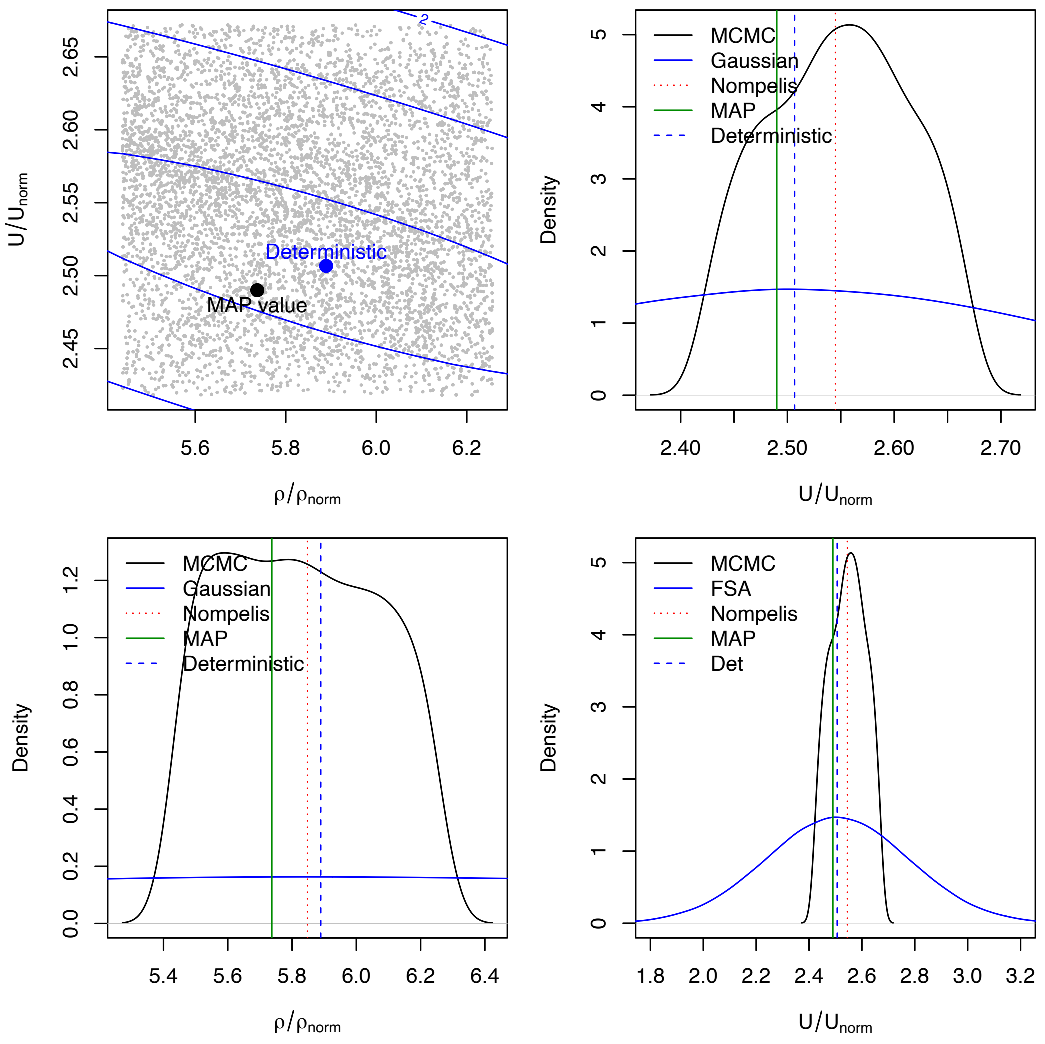




Validation with Run 35

- Low enthalpy (3.71 MJ/kg) flow; LENS-I shock tunnel
- Modeled successfully by Nompelis in 2003
  - Bayesian inference (Ray et al, 2020) established that inferred (ρ, U) lay within experimental error bounds
- Findings: Deterministic & Bayesian agree
  - Θ^* is close to $\Theta^{(MAP)}$ and $\Theta^{(Nom)}$ (experimental data)
  - Gaussian posterior is too wide
  - Conclusion: Method works

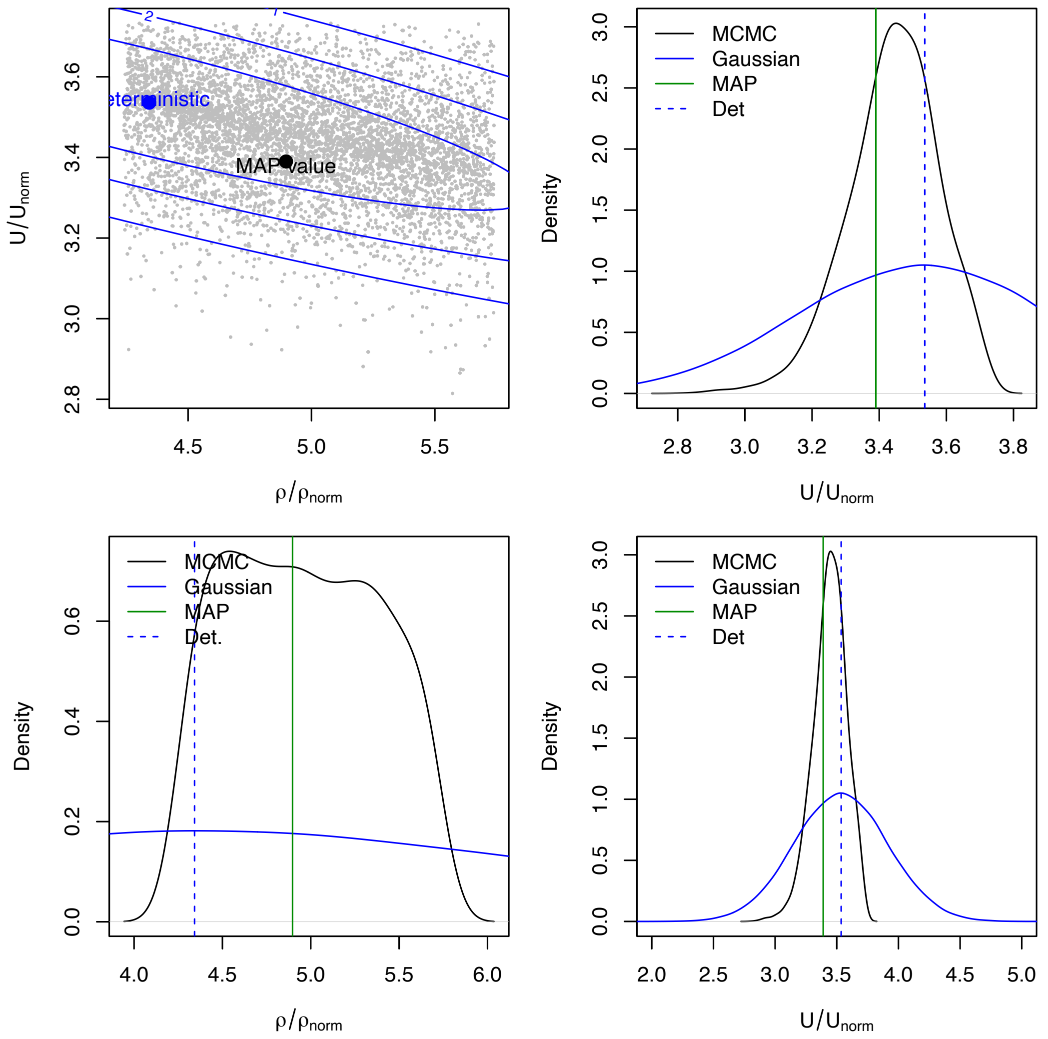
	$\Theta^{(Nom)}$ (uncertainty limits)	Θ^*	$\Theta^{(MAP)}$
ρ [g/m^3]	0.5848 (0.5429, 0.6257)	0.589	0.5737
U [m/s]	2545.0 (2468.6, 2621.4)	2506	2490.0



Test – Case 1

- LENS-XX; low enthalpy (5.44 M/kg); mild vibrational non-eq
- Bayesian method (w/ surrogates): Inferred (ρ, U) within experimental error bounds
- Finding: Deterministic & Bayesian *disagree*
  - Θ^* is *not* close to $\Theta^{(MAP)}$ and $\Theta^{(Nom)}$
  - Gaussian posterior too wide

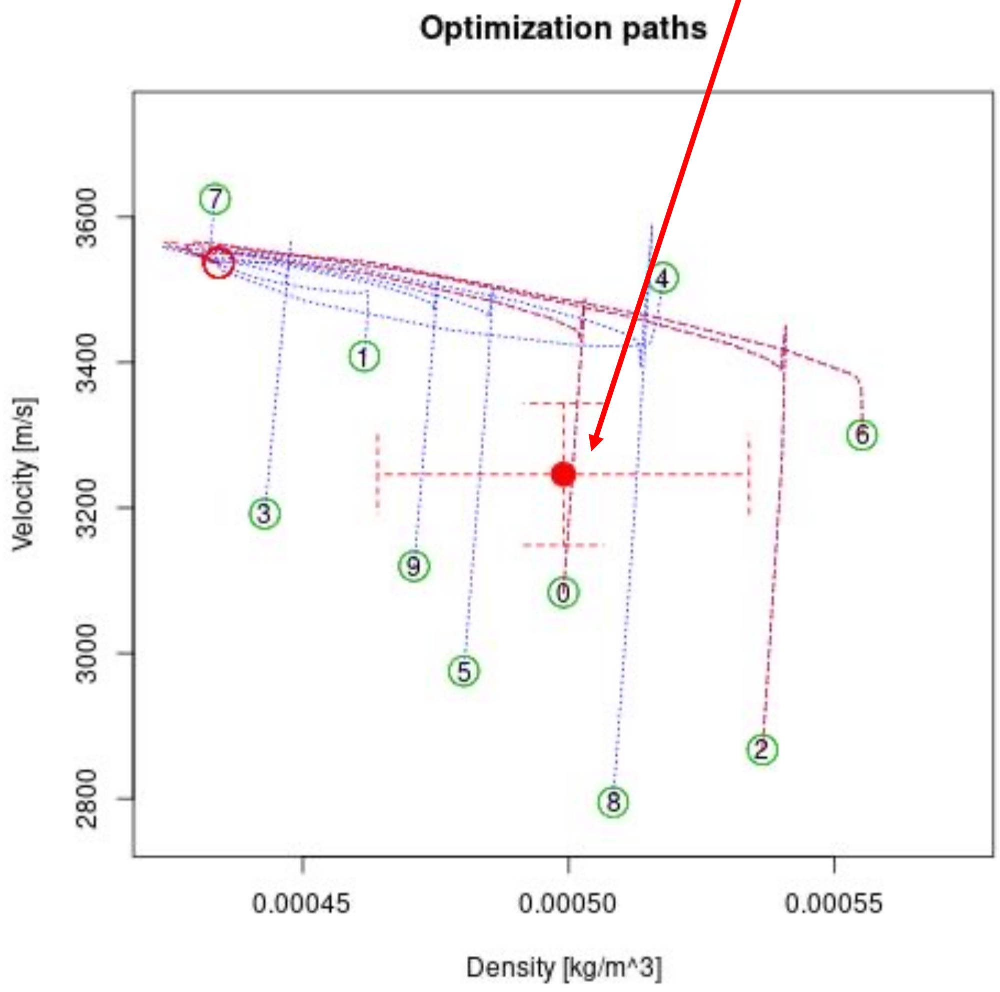
	$\Theta^{(Nom)}$ **(uncertainty limits)**	Θ^*	$\Theta^{(MAP)}$
ρ [g/m^3]	0.499 (0.4641, 0.5339)	0.433	0.4897
U [m/s]	3246 (3148.6, 3343.4)	3540	3340



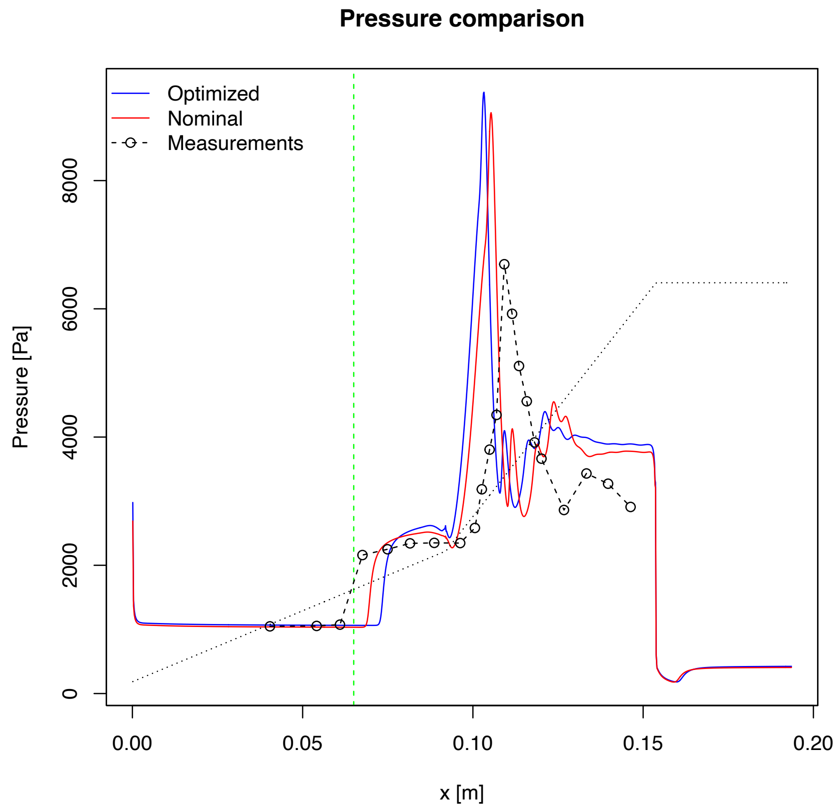
Case 1 – multi-start check

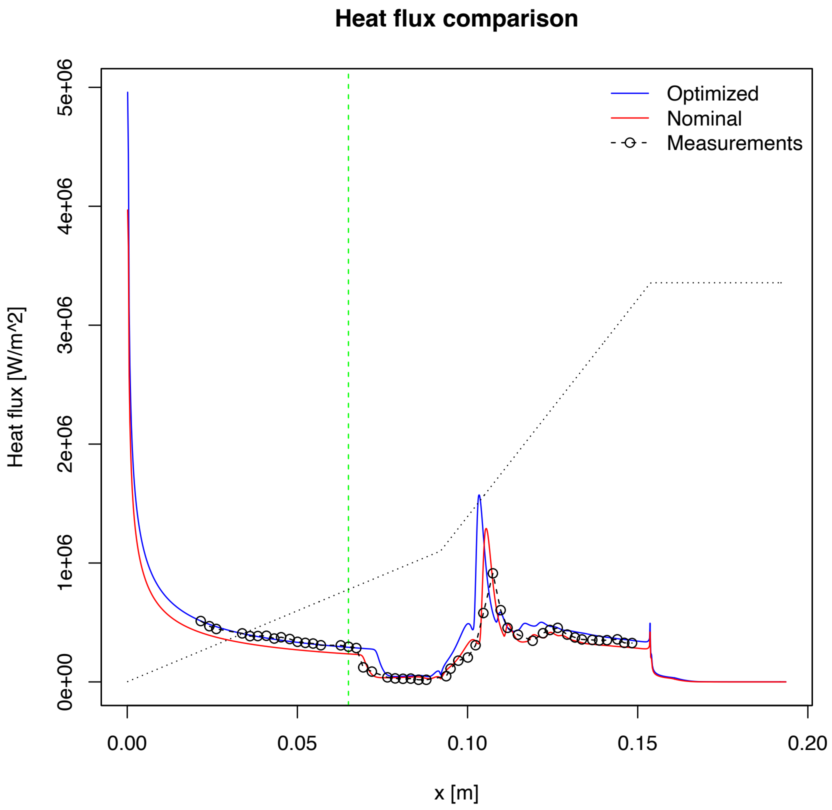
- Case 1 BC also seem to be mis-specified
  - Deterministic & Bayesian inference disagree
- Did we fall into a local minima?
  - Redo inference starting from different guesses
    - Guesses outside the experimental error bounds
    - All converge to the same estimate of (ρ, U)
- Conclusion
  - The estimate of (ρ, U) is correct
    - The approximate surrogate models & MCMC did not find the MAP estimate
  - Case 1 inlet BC may be mis-specified

Nominal/experimental inlet condition & uncertainty bounds



Did we improve predictive skill?





RMS Error

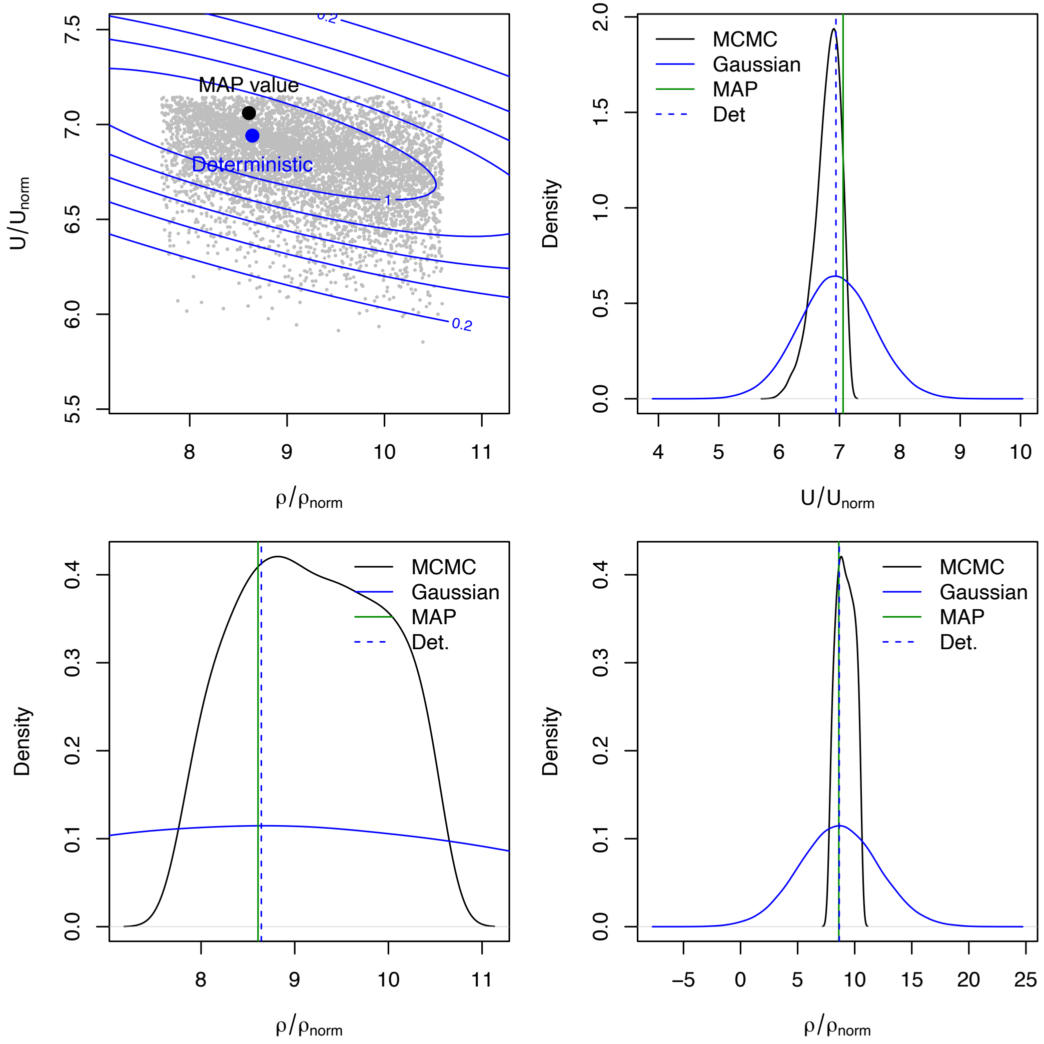
	Θ^*	$\Theta^{(Nom)}$
p(x) [N/m²]	1.9 e+3	1.8 e+3
q(x) [W/m²]	1.5 e+5	8.68 e+4

- Fore-cone predictions are good but separation zone shortened; RMS errors increased
- Inlet BC are definitely only part of the cause

Test – Case 4

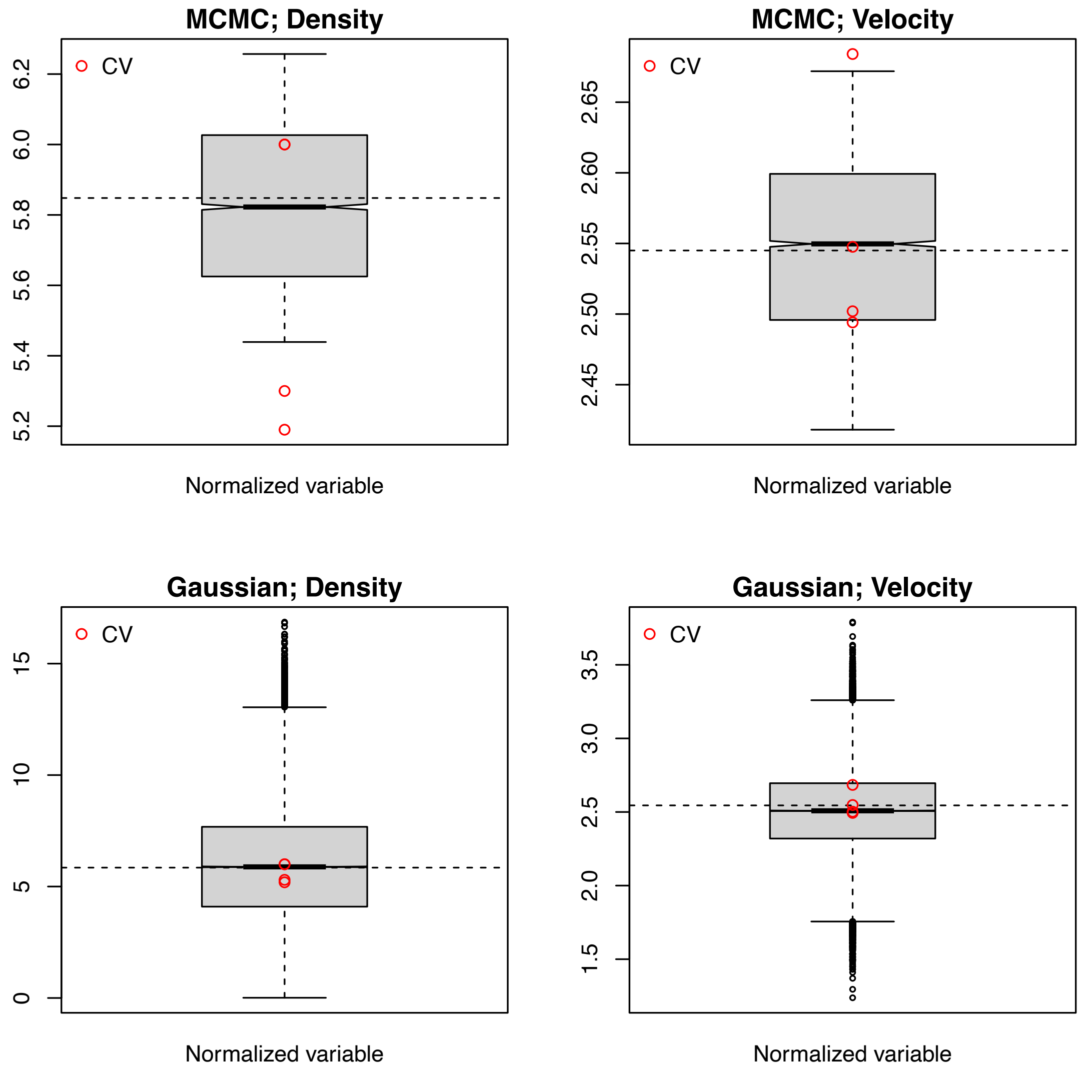
- LENS-XX; high enthalpy (21.77 MJ/kg); vibrational & chemical non-eq
- Bayesian method (w/ surrogates): Inferred (ρ, U) outside experimental error bounds
- Finding: Deterministic & Bayesian *agree*
  - Θ^* is close to $\Theta^{(MAP)}$ and far from $\Theta^{(Nom)}$
  - Gaussian posterior too wide

	$\Theta^{(Nom)}$ (uncertainty limits)	Θ^*	$\Theta^{(MAP)}$
ρ [g/m3]	0.9840 (0.9151, 1.0529)	0.8619	0.8608
U [m/s]	6479 (6284.6, 6673.4)	6950	7060.0



Cross-validation of Gaussian assumption

- The Gaussian posteriors are wrong and not useful
  - Discovered when we compared with MCMC posteriors
  - Test for Gaussian assumption?
- Cross-validation
  - Generate estimates $(\rho, U)_k$, k = 1 …K using random subsets of the observations
  - Scatter in $(\rho, U)_k$ wider than the (unknown) exact posterior
    - Because $(\rho, U)_k$ drawn on fewer data / information
    - "Upper bound" on true posterior / uncertainty
  - If scatter is narrower than Gaussian posterior, assumption not justified
- Our case (using Run 35): Not justified
  - Scatter commensurate with MCMC posterior
  - Scatter too narrow compared to Gaussian posterior



Conclusions

- Developed a deterministic inference method to check inflow BC for LENS-XX experiments
  - They have never been modeled successfully
  - Method uses the Navier-Stokes CFD solver, not surrogates
  - Also computed uncertainty bounds using a Gaussian assumption
- Findings:
  - Both LENS-XX experiments (low & high-enthalpy) have an inflow BC that is inconsistent with double-cone surface measurements
    - But correcting the BC does not fix the problem. There are other causes behind the model / experiment mismatch
  - Gaussian posterior is easy to calculate, but the Gaussian assumption may not be valid
    - Constructed cross-validation checks to test the validity of Gaussian assumption
    - Gaussian assumption inappropriate; corroborated with MCMC posterior distributions