Bayesian Inference for the Calibration of DSMC Parameters

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Motivation

Benefits of the current work include:

- DSMC will provide PECOS with useful insight about the shock-tube problem, and about re-entry flowfields in general.
- Bayesian statistical methods will be introduced to a field where they have seen little if any prior use.
- Calibrated parameters obtained from this work will be of use to the DSMC community.

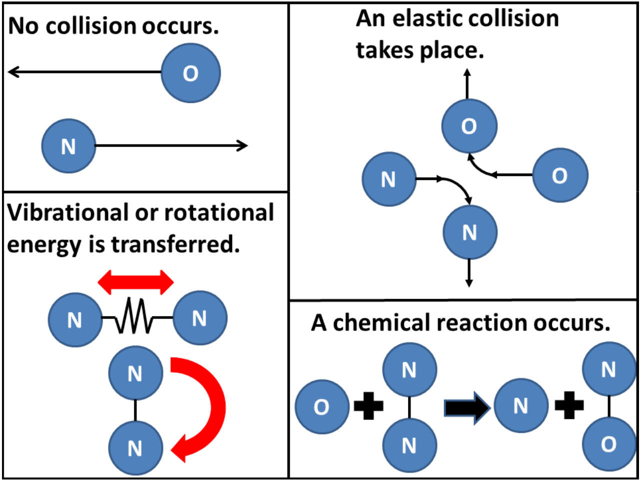
Introduction: DSMC

Direct Simulation Monte Carlo (DSMC) is a particle based simulation technique.

- Simulated particles represent large numbers of real particles.
- Particles move and undergo collisions with other particles.
- Can be used in highly non-equilibrium flowfields (such as strong shock waves).
- Can model thermochemistry on a more detailed level than most CFD codes.

DSMC Collisions

DSMC collisions are performed between molecules which are randomly selected from within a cell. Possible outcomes include:



DSMC Parameters

The DSMC model includes many parameters which govern the probability of each possible outcome for a given pair of molecules. Some examples common to most DSMC codes include:

- Elastic collision cross-sections: $(\sigma_{E_{N_2-N_2}}, \sigma_{E_{N-N_2}}, \sigma_{E_{O_2-N_2}}, ...)$.
- Vibrational and rotational excitation probabilities: $(Z_{V_{N_2-N_2}}, Z_{V_{N_2-NO}}, Z_{R_{O_2-N_2}}, Z_{R_{O_2-NO}}, ...)$.
- Reaction cross-sections: $(\sigma_{R_{N_2+N_2->N_2+N+N}}, \sigma_{R_{N_2+O_2->N_2+O+O}}, \sigma_{R_{N_2+NO->N_2+N+O}}, ...)$.

DSMC Parameters

- In many cases the precise values of some of these parameters are not known.
- Parameter values often cannot be directly measured, instead they must be inferred from experimental results.
- By necessity, parameters must often be used in regimes far from where their values were determined.
- More precise values for important parameters would lead to better predictive capability for DSMC.

Solving the inverse problem via Bayesian inference would allow multiple types and sets of data (potentially from NASA EAST, CUBRC, plasma torches, etc.) to be used simultaneously in order to provide the best possible parameters for the given model. If done properly, this could be of great use to the DSMC community.

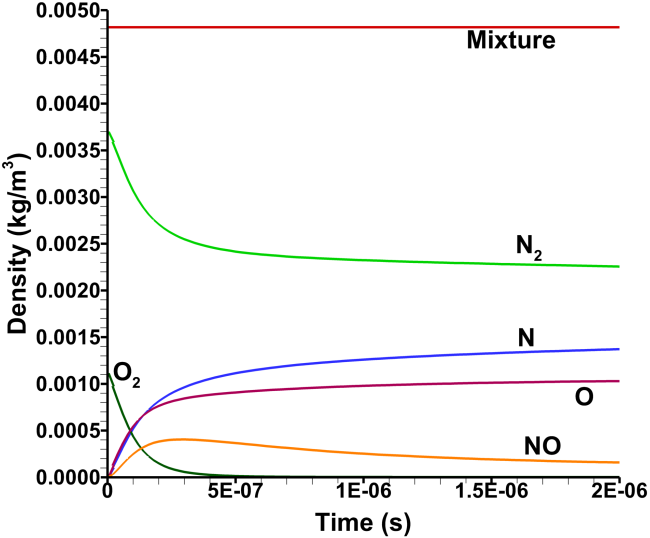
Scenario - 0-D Relaxation

Scenario examined in this work is a 0-D relaxation from an initial high-temperature state. A 0-D box is initialized with $79\% N_2, 21\% O_2$, with initial conditions:

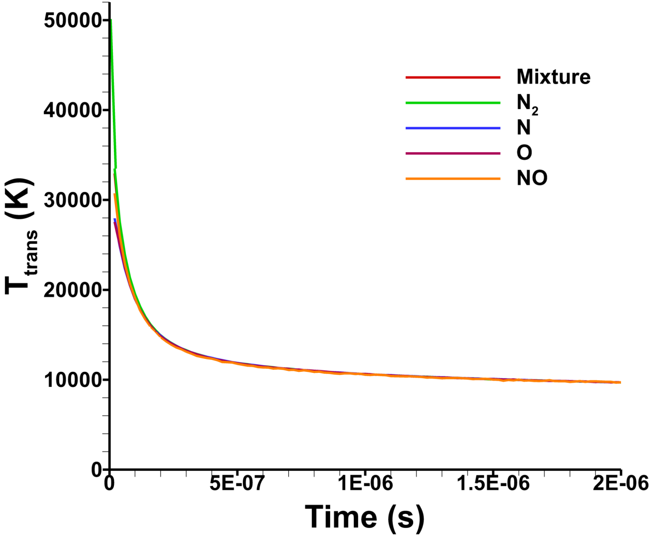
- Bulk number density = $1.0 \times 10^{23} \# / m^3$.
- Bulk translational temperature = 50,000 K.
- Bulk rotational and vibrational temperatures are both 300 K.

Scenario is a 0-D substitute which is in some ways similar to a hypersonic shock at ˜8 km/s, with the assumption that the translational mode equilibrates much faster than the internal modes.

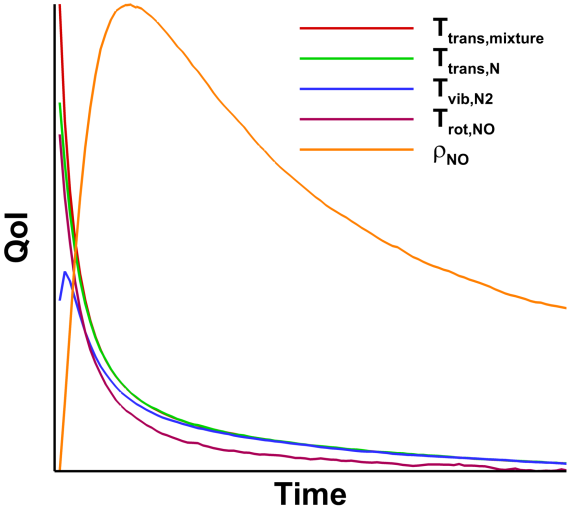
0-D Relaxation - Densities



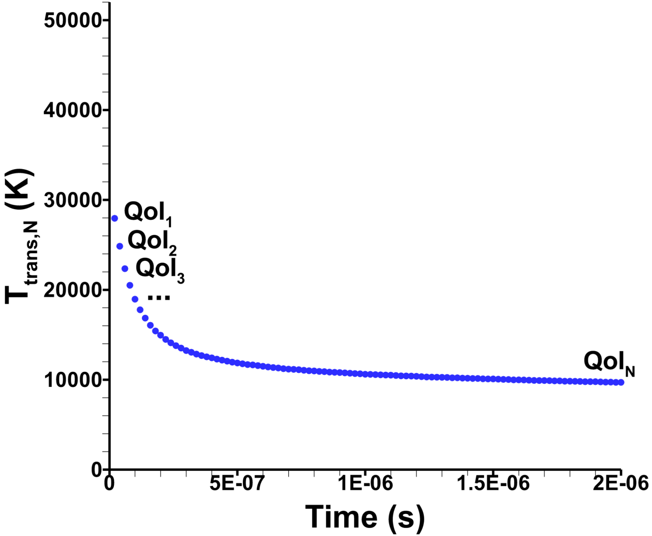
0-D Relaxation - Temperatures



0-D Relaxation - QoI Possibilities



0-D Relaxation - Our QoI



0-D Relaxation - Parameters

The parameters to be calibrated here are the pre-exponential constants in the Arrhenius rate equations for the 17 reaction mechanisms included for 5-species air in the current work.

$$k(T) = AT^{\eta}e^{-E_a/kT} \qquad 10^{\alpha} = A$$

Reaction #	Equation	α_{min}	α_{nom}	α_{max}	A_{nom}	η	E_A
1	$N_2 + N_2 \to N_2 + N + N$	-6.94	-7.94	-8.94	1.16E-08	-1.6	1.56E-18
2	$N + N_2 \to N + N + N$	-6.30	-7.30	-8.30	4.98E-08	-1.6	1.56E-18
3	$O_2 + N_2 \to O_2 + N + N$	-6.30	-7.30	-8.30	4.98E-08	-1.6	1.56E-18
4	$O + N_2 \to O + N + N$	-6.30	-7.30	-8.30	4.98E-08	-1.6	1.56E-18
5	$NO + N_2 \to NO + N + N$	-6.30	-7.30	-8.30	4.98E-08	-1.6	1.56E-18
6	$N_2 + O_2 \to N_2 + O + O$	-7.48	-8.48	-9.48	3.32E-09	-1.5	8.21E-19
7	$N + O_2 \to N + O + O$	-7.48	-8.48	-9.48	3.32E-09	-1.5	8.21E-19
8	$O_2 + O_2 \to O_2 + O + O$	-7.48	-8.48	-9.48	3.32E-09	-1.5	8.21E-19
9	$O + O_2 \to O + O + O$	-7.48	-8.48	-9.48	3.32E-09	-1.5	8.21E-19
10	$NO + O_2 \to NO + O + O$	-7.48	-8.48	-9.48	3.32E-09	-1.5	8.21E-19
11	$N_2 + NO \to N_2 + N + O$	-13.08	-14.08	-15.08	8.30E-15	0	1.04E-18
12	$N + NO \to N + N + O$	-13.08	-14.08	-15.08	8.30E-15	0	1.04E-18
13	$O_2 + NO \to O_2 + N + O$	-13.08	-14.08	-15.08	8.30E-15	0	1.04E-18
14	$O + NO \to O + N + O$	-13.08	-14.08	-15.08	8.30E-15	0	1.04E-18
15	$NO + NO \to NO + N + O$	-13.08	-14.08	-15.08	8.30E-15	0	1.04E-18
16	$N_2 + O \to NO + N$	-16.02	-17.02	-18.02	9.45E-18	0.42	5.93E-19
17	$O_2 + N \to NO + O$	-19.38	-20.38	-21.38	4.13E-21	1.18	5.53E-20
18	$NO + N \to N_2 + O$		-16.69		2.02E-17	0.1	0
19	$NO + O \to O_2 + N$		-16.85		1.40E-17	0	2.65E-10

Sensitivity Analysis

Before any calibrations are performed, sensitivity analysis should be used to narrow down the list of parameters to be calibrated. Two measures for sensitivity were used in this work.

- Pearson correlation coefficients:

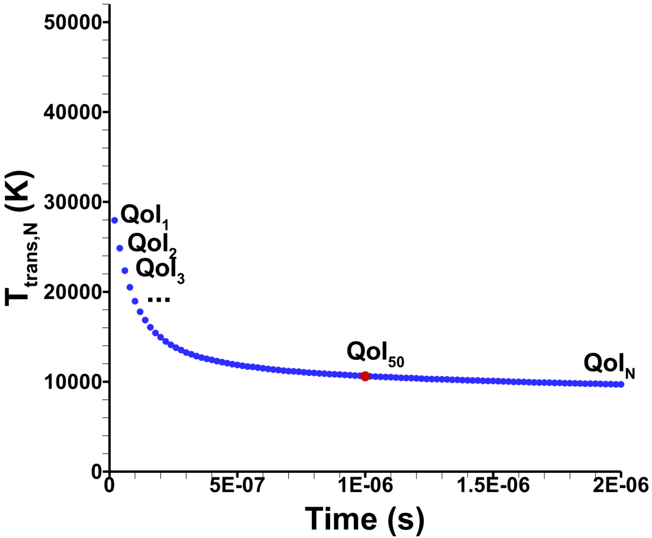
$$\boldsymbol{r} = \frac{\sum_{i=1}^{n}(X_i - \bar{X})(Y_i - \bar{Y})}{\sqrt{\sum_{i=1}^{n}(X_i - \bar{X})^2}\sqrt{\sum_{i=1}^{n}(Y_i - \bar{Y})^2}}$$

- Mutual information:

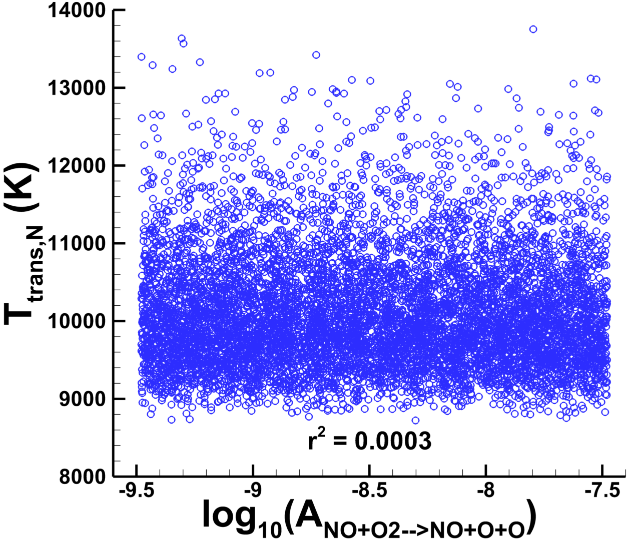
$$I(\theta_1, QoI) = \int_{\theta_1}\int_{QoI} p(\theta_1, QoI)\left[ln\left(\frac{p(\theta_1, QoI)}{p(\theta_1)p(QoI)}\right)\right] dQoI\, d\theta_1$$

Both measures involve global sensitivity analysis based on a Monte Carlo sampling of the parameter space, and the thus the same datasets can be used to obtain both measures.

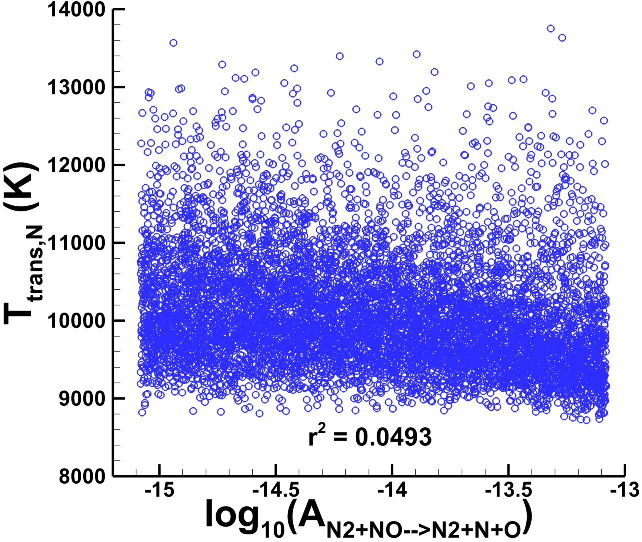
Sensitivity Analysis - Scalar vs. Vector QoI



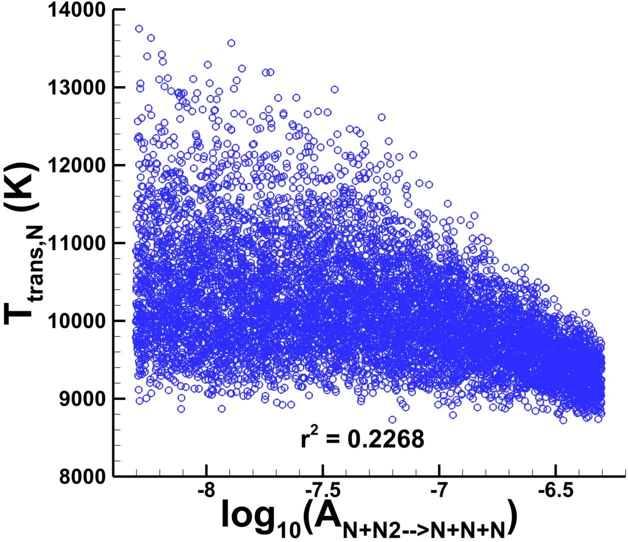
Correlation Coefficient - Scalar QoI



Correlation Coefficient - Scalar QoI

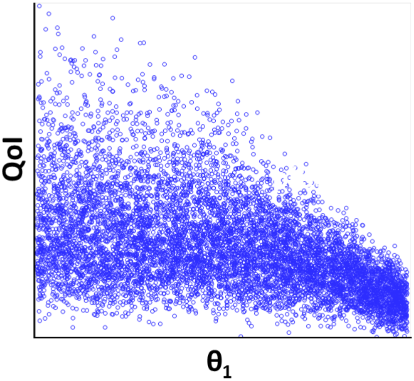


Correlation Coefficient - Scalar QoI



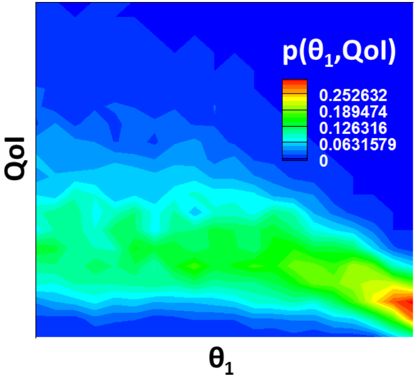
Mutual Information - Scalar QoI

To calculate the mutual information, we first normalize the data shown in the scatterplot.



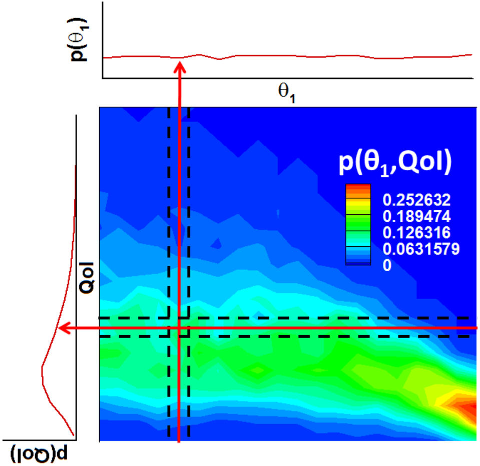
Mutual Information - Scalar QoI

Next, we obtain $p(\theta_1, QoI)$ from the scatterplot, using a histogram based method, kernel density estimation, or some other technique.



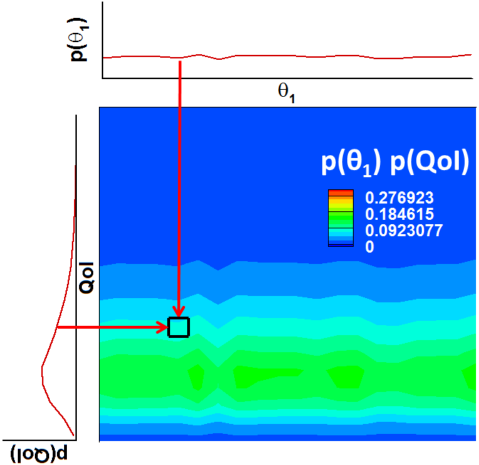
Mutual Information - Scalar QoI

We then use $p(\theta_1, QoI)$ to obtain the marginal PDFs for θ_1 and for the QoI.



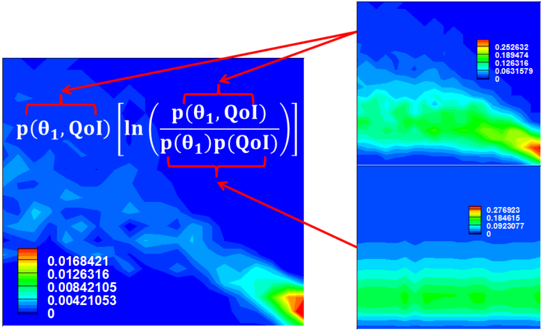
Mutual Information - Scalar QoI

Using those marginal PDFs, we then construct a hypothetical joint PDF for the case where the QoI is independent of θ_1.



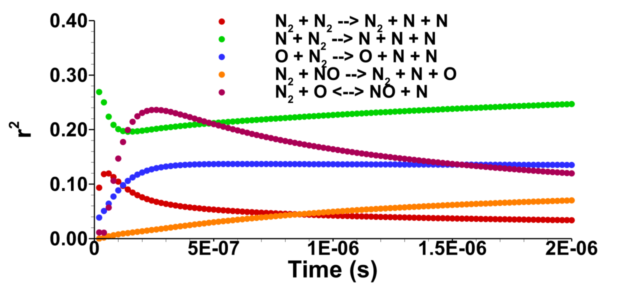
Mutual Information - Scalar QoI

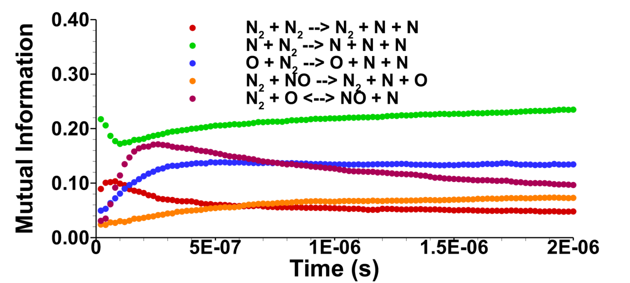
The mutual information can be thought of as the "distance" between $p(\theta_1, QoI)$, the actual joint PDF of a given parameter and the QoI, and $p(\theta_1)p(QoI)$, the hypothetical joint PDF which would result if the QoI was independent of the parameter θ_1. It provides a measure of the extent to which the QoI depends on the parameter θ_1.



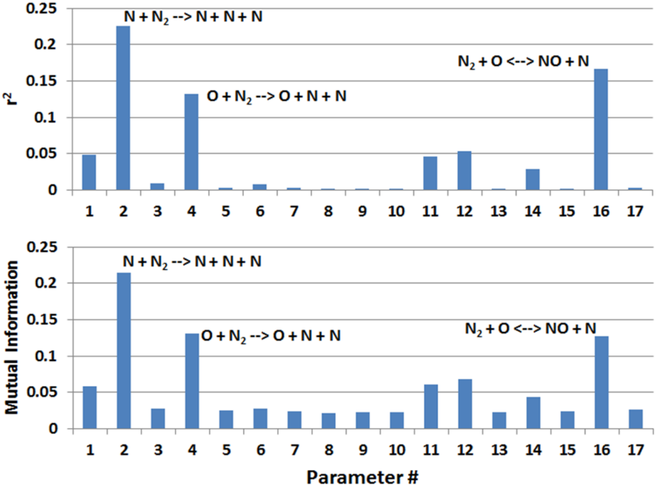
$$I(\theta_1, QoI) = \int_{\theta_1}\int_{QoI} p(\theta_1, QoI)\left[ln\left(\frac{p(\theta_1, QoI)}{p(\theta_1)p(QoI)}\right)\right] dQoI\, d\theta_1$$

Sensitivities vs. Time





Overall Sensitivities



Conclusions

- Sensitivity analysis results confirm prior physical intuition about dominant reaction mechanisms.
- For this scenario, correlation coefficients and the mutual information provide similar but not identical results.
- There are two fairly obvious tiers in sensitivity, allowing us to choose the most important three, or the most important seven reaction mechanisms for calibration.

Future Work

Me

- Perform synthetic data calibrations for the 0-D relaxation scenario.
- Use Monte Carlo sensitivity analysis to determine which parameters should be calibrated for a 1D shock scenario.
- Perform synthetic data calibrations for a 1D shock scenario.
- Complete dissertation defense by October 1st, 2011.

Someone Else

- Upgrade the DSMC code to model ionization and electronic excitation, and couple with a radiation solver.
- Perform sensitivity analysis and synthetic data calibrations at higher shock speeds such as those used in the NASA EAST experiments.
- Make use of EAST and/or other available data to calibrate as many of the relevant DSMC parameters as possible, and make the results available to the DSMC community.