SENSITIVITY ANALYSIS FOR DSMC SIMULATIONS OF A HYPERSONIC SHOCK

PECOS
Predictive Engineering and Computational Sciences

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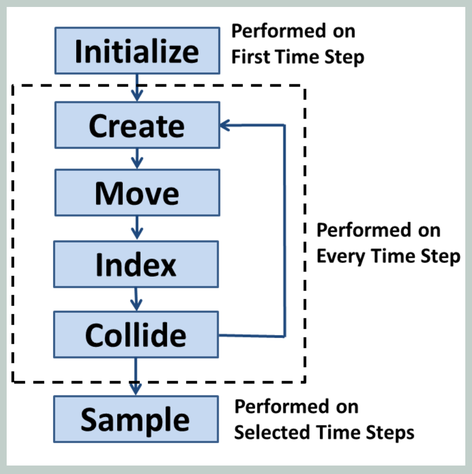
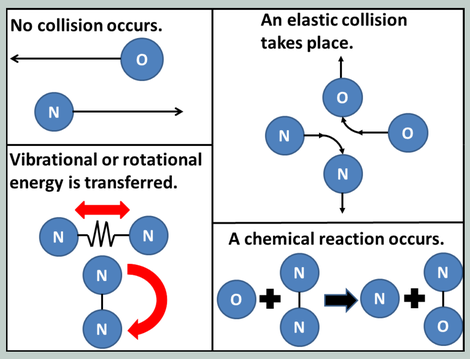
DSMC Method

Direct Simulation Monte Carlo (DSMC) is a particle based method for the simulation of gas flows.

- 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.

Our DSMC code can model flows with rotational and vibrational excitation and relaxation, as well as five-species air chemistry, including dissociation, exchange, and recombination reactions.





DSMC Parameters

The DSMC model includes many parameters related to gas dynamics at the molecular level:

- Elastic collision cross-sections.
- Vibrational and rotational excitation probabilities.
- Reaction cross-sections.
- ...etc.

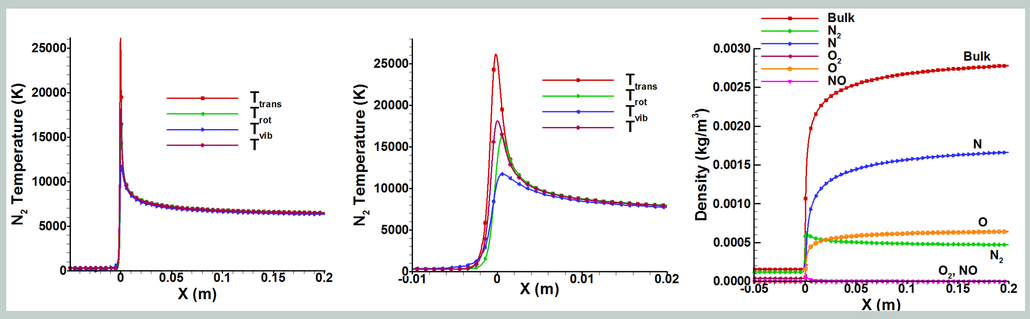
In many cases the values of some of these parameters must be inferred from experimental results. More precise values for important parameters would lead to better simulation of the physics, and thus to better predictive capability for the DSMC method. The ultimate goal of this work is to use experimental data and Bayesian statistical methods to calibrate important DSMC parameters.

Sensitivity Analysis - Overview

In the current context, the goal of sensitivity analysis is to determine which parameters most strongly affect a given quantity of interest (QoI). Only parameters to which a given QoI is sensitive will be informed by calibrations based on data for that QoI.

Scenario:

- 1-D, steady shock.
- Upstream speed $\approx 8000\ m/s$.
- Upstream number density $= 3.22 \times 10^{21}\ \#/m^3$.
- Upstream composition by volume: $79\%\ N_2$, $21\%\ O_2$.
- Upstream temperature $= 300\ K$.



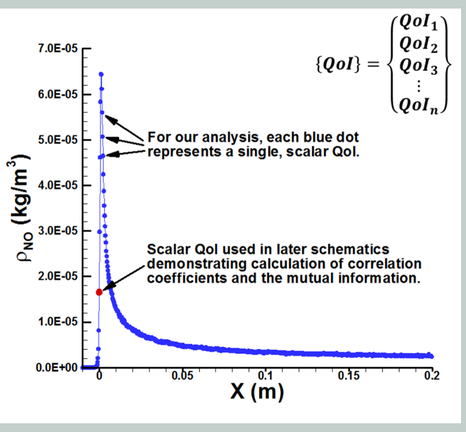
Parameters:

Our current sensitivity analysis focused on the rate constants for reactions which take place in five-species air.

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

#	Reaction	α_{min}	α_{nom}	α_{max}	Nominal Forward Rate Constants Λ	η	E_A
1	$N_2 + N_2 <--> N_2 + N + N$	-13.099	-12.099	-11.099	7.968E-13	-0.5	1.561E-18
2	$N + N_2 <--> N + N + N$	-8.161	-7.161	-6.161	6.9E-8	-1.5	1.561E-18
3	$O_2 + N_2 <--> O_2 + N + N$	-13.497	-12.497	-11.497	3.187E-13	-0.5	1.561E-18
4	$O + N_2 <--> O + N + N$	-13.497	-12.497	-11.497	3.187E-13	-0.5	1.561E-18
5	$NO + N_2 <--> NO + N + N$	-13.497	-12.497	-11.497	3.187E-13	-0.5	1.561E-18
6	$N_2 + O_2 <--> N_2 + O + O$	-11.922	-10.922	-9.922	1.198E-11	-1.0	8.197E-19
7	$N + O_2 <--> N + O + O$	-12.222	-11.222	-10.222	5.993E-12	-1.0	8.197E-19
8	$O_2 + O_2 <--> O_2 + O + O$	-11.268	-10.268	-9.268	5.393E-11	-1.0	8.197E-19
9	$O + O_2 <--> O + O + O$	-10.824	-9.824	-8.824	1.498E-10	-1.0	8.197E-19
10	$NO + O_2 <--> NO + O + O$	-12.222	-11.222	-10.222	5.993E-12	-1.0	8.197E-19
11	$N_2 + NO <--> N_2 + N + O$	-10.181	-9.181	-8.181	6.59E-10	-1.5	1.043E-18
12	$N + NO <--> N + N + O$	-8.880	-7.880	-6.880	1.318E-8	-1.5	1.043E-18
13	$O_2 + NO <--> O_2 + N + O$	-10.181	-9.181	-8.181	6.59E-10	-1.5	1.043E-18
14	$O + NO <--> O + N + O$	-8.880	-7.880	-6.880	1.318E-8	-1.5	1.043E-18
15	$NO + NO <--> NO + N + O$	-8.880	-7.880	-6.880	1.318E-8	-1.5	1.043E-18
16	$N_2 + O <--> NO + N$	-16.951	-15.951	-14.951	1.12E-16	0.0	5.175E-19
17	$NO + O <--> O_2 + N$	-21.277	-20.277	-19.277	5.279E-21	1.0	2.719E-19

Throughout the sensitivity analysis, the ratio of forward to backward rate for a given reaction is kept constant, since these ratios should be fixed by the equilibrium constant.



$$\{QoI\} = \begin{Bmatrix} QoI_1 \\ QoI_2 \\ QoI_3 \\ \vdots \\ QoI_n \end{Bmatrix}$$

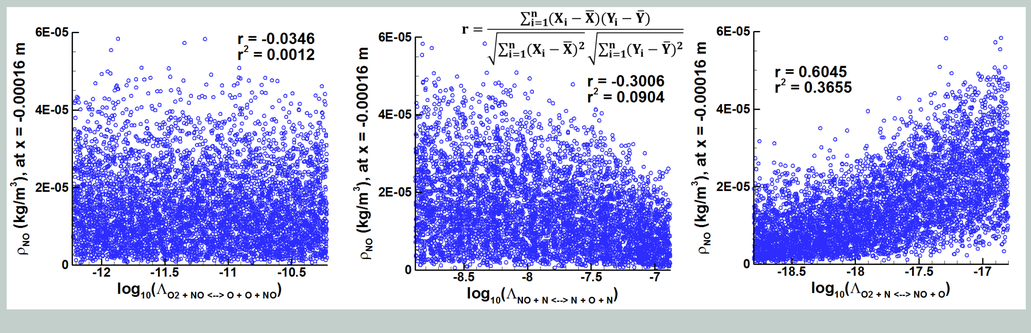
QoI:

We are not yet at a point where the DSMC simulation results can be compared with experimental shock tube results from EAST, and so we must choose a surrogate QoI. For this work, we have chosen the density of NO as our QoI. We have found in past work that this QoI is sensitive to several of our parameters. We are not concerned with just one specific point downstream of the shock, instead we are interested in how changes in the rate constants affect the non-equilibrium chemistry in the post-shock region. For this reason, we need to treat our QoI as a vector, where each component of that vector represents ρ_{NO} at a specific x-location. The sensitivity analysis methods we will use, however, are intended for a scalar QoI. To overcome this problem, we treat the vector QoI as a set of scalar QoI's. We apply the full sensitivity analysis procedure to each scalar QoI and then combine the results of those individual analyses.

Sensitivity Analysis - Procedure

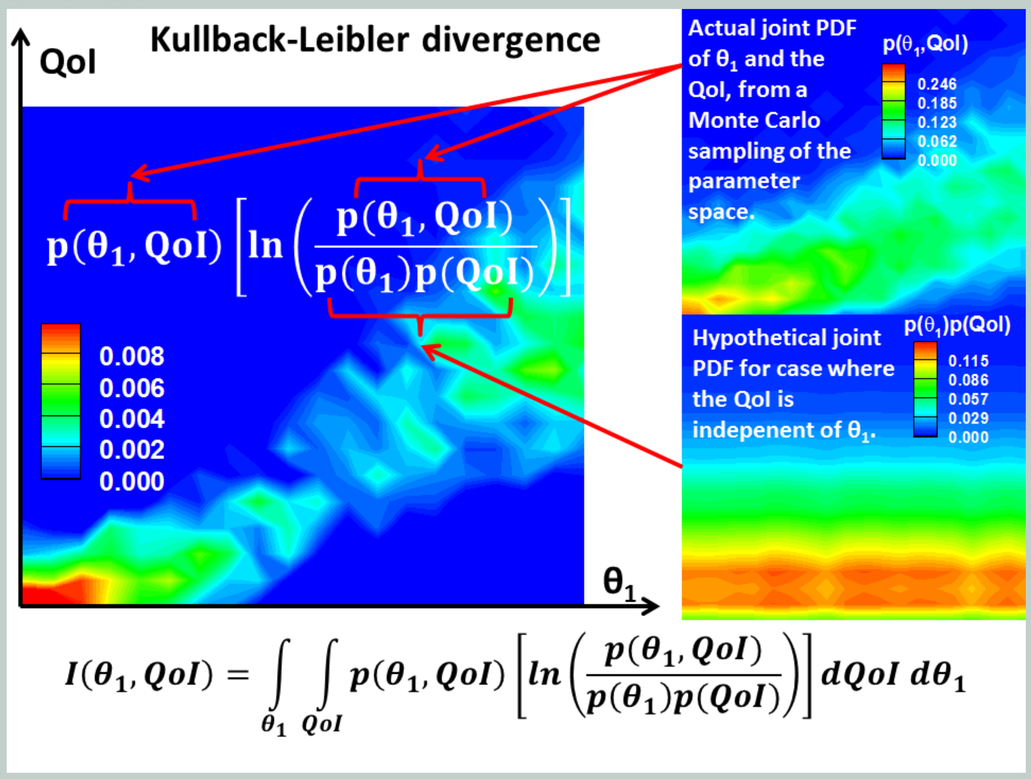
Two measures for sensitivity were used in this work. Both measures involve global sensitivity analysis based on a Monte Carlo sampling of the parameter space, and thus the same datasets can be used to obtain both measures.

Pearson Correlation Coefficients:



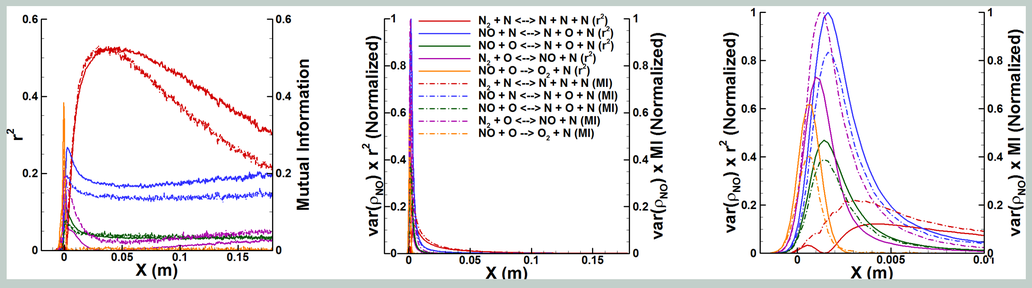
$$r = \frac{\sum_{i=1}^{n}(X_i - \bar{X})(Y_i - \bar{Y})}{\sqrt{\sum_{i=1}^{n}(X_i - \bar{X})^2}\sqrt{\sum_{i=1}^{n}(Y_i - \bar{Y})^2}}$$

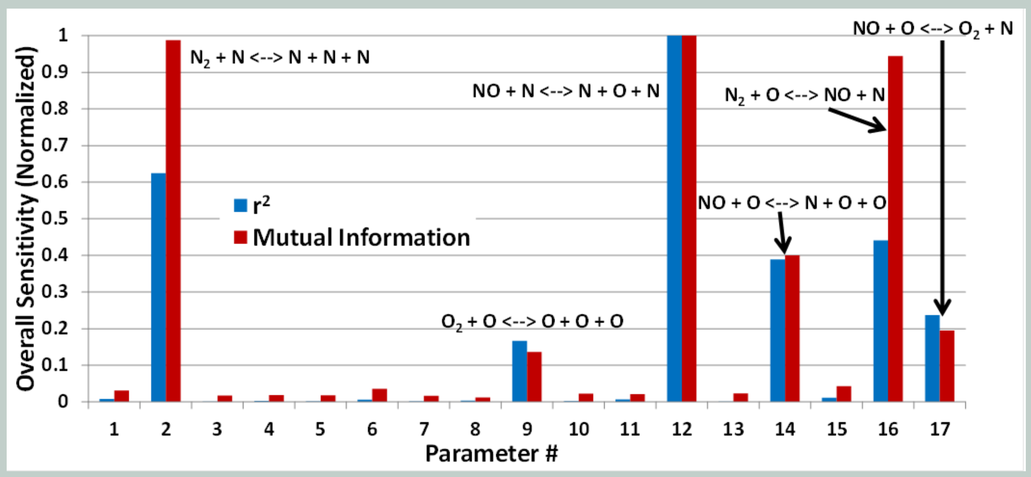
Mutual Information:



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

Sensitivity Analysis - Results





Conclusions

- Global, Monte Carlo based sensitivity analysis can provide a great deal of insight into how various parameters affect a given QoI.
- Sensitivities based on r^2 are similar to those based on the mutual information, but there are notable differences for some parameters.
- We find that our surrogate QoI, ρ_{NO}, is most strongly affected by the rates for NO dissociation reactions, the NO exchange reactions, and the dissociation of N_2 by N. These results are not unexpected, and fit with our prior understanding of the chemistry which takes place behind an 8 km/s shock.

Future Work

- Synthetic data calibrations for a 1-D shock with the current code.
- Upgrade the code to allow modelling of ionization and electronic excitation.
- Couple the code with a radiation solver.
- Sensitivity analysis for a 1-D shock with the additional physics included.
- Synthetic data calibrations with the upgraded code.
- Calibrations with experimental data from EAST or similar facility.

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