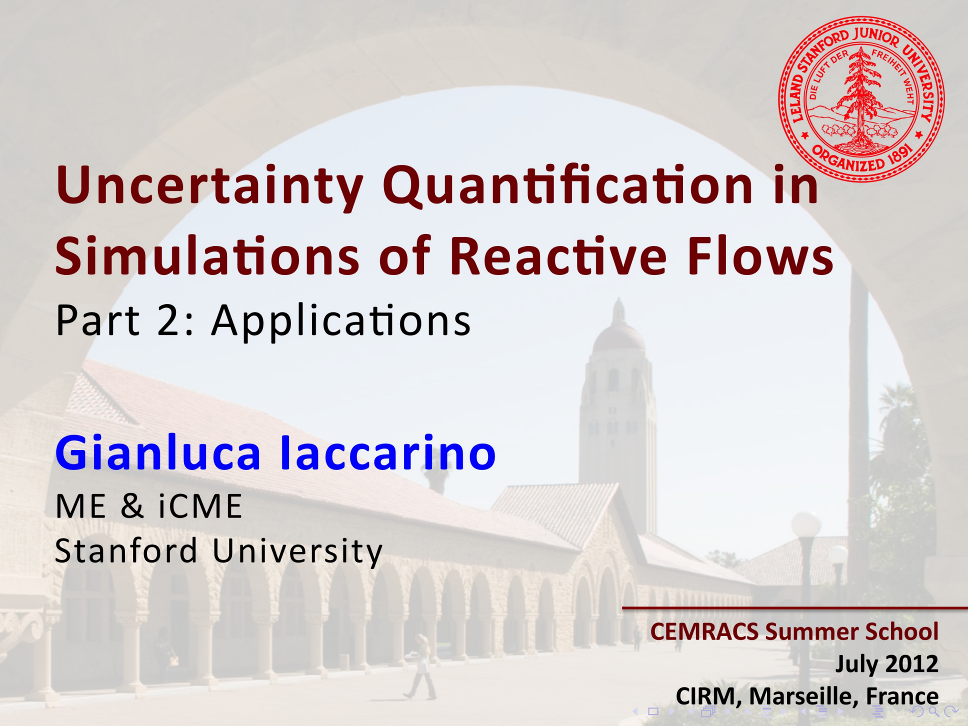

Uncertainty Quantification in Simulations of Reactive Flows

Part 2: Applications

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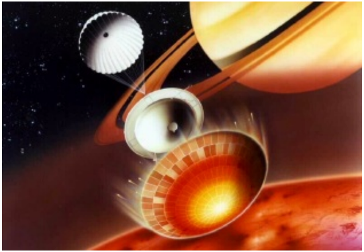
CEMRACS Summer School
July 2012
CIRM, Marseille, France

UQ in Reacting Flows

Planetary Entry Simulations

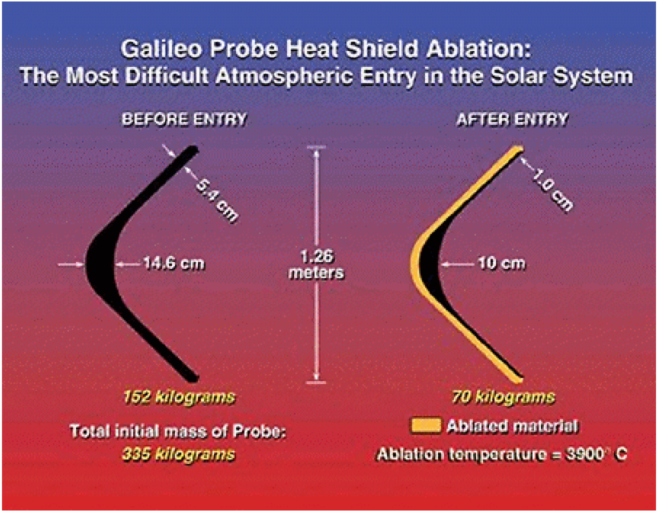
High-Temperature Reactive Flow

- During descent in the atmosphere vehicles experience extreme heating loads



- The design of the thermal protection system (TPS) is the most critical component of every planetary entry mission
- TPS design is fundamentally computation-based because no ground-test can reproduce all the aspects of flight
- Safety (and reliability) requires rigorous evaluation of the uncertainties present

Jupiter Entry Probe - Galieo



Source: NASA

Titan Entry Simulations

High-Temperature Reactive Flow

Predictions of TPS heating loads re-entry are challenging

- Physics Components
  - Chemistry
  - Radiation
  - Turbulence
  - etc.
- Computational issues
  - Strong shocks
  - Thin boundary layers
  - Flow separation
  - etc.

We focus on the uncertainties in the chemical kinetics, and their impact on the heat transfer at the stagnation point...

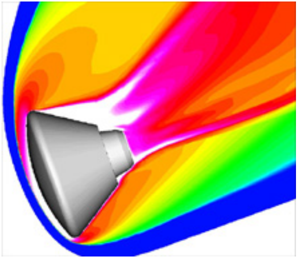
Titan Entry Simulations

Aero-thermodynamic model

We consider *nominal* conditions for the Titan entry:

Table: Freestream conditions

N_2	CH_4	$\rho_\infty (kg/m^3)$	$V_\infty (km/s)$	$T_\infty (K)$
95%	5%	1.49×10^{-4}	5.76	152.7



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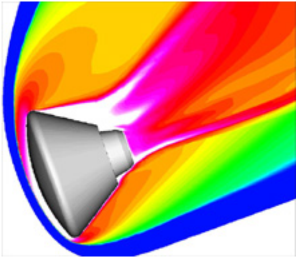


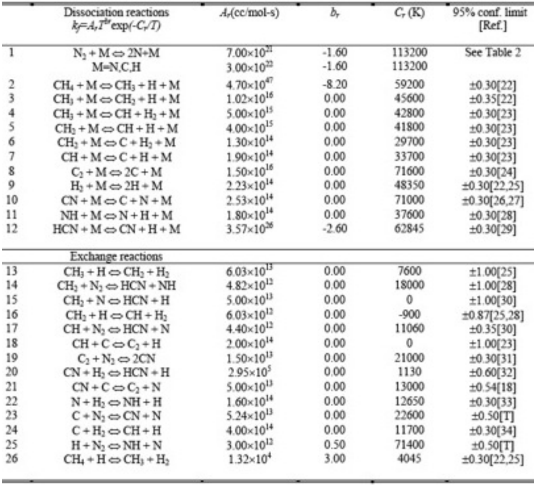
The strong bow shock induced strong non-equilibrium effects and dissociation/ionization

- We assumed a 13-species mechanism:
- C, H, N, C_2, CH_4, CH_3, CH_2, CH, CN, H_2, HCN, N_2, NH
- 26 reactions: 12 dissociation & 14 exchange

Probabilistic approach

Reaction rates in ionization/dissociation models

- Uncertainty in the reactions rates, gathered from
  - theory
  - experiments
  - engineering judgment
- Uncertainty in the reaction rates is described using independent u.r.v.s



	Dissociation reactions $k_f=A_r T^{b_r}\exp(-C_r/T)$	A_r(cc/mol-s)	b_r	C_r (K)	95% conf. limit [Ref.]
1	$N_2 + M \Leftrightarrow 2N + M$	7.00×10^{21}	-1.60	113200	See Table 2
	M=N,C,H	3.00×10^{22}	-1.60	113200	
2	$CH_4 + M \Leftrightarrow CH_3 + H + M$	4.70×10^{47}	-8.20	59200	±0.30[22]
3	$CH_3 + M \Leftrightarrow CH_2 + H + M$	1.02×10^{16}	0.00	45600	±0.35[22]
4	$CH_3 + M \Leftrightarrow CH + H_2 + M$	5.00×10^{15}	0.00	42800	±0.30[23]
5	$CH_2 + M \Leftrightarrow CH + H + M$	4.00×10^{15}	0.00	41800	±0.30[23]
6	$CH_2 + M \Leftrightarrow C + H_2 + M$	1.30×10^{14}	0.00	29700	±0.30[23]
7	$CH + M \Leftrightarrow C + H + M$	1.90×10^{14}	0.00	33700	±0.30[23]
8	$C_2 + M \Leftrightarrow 2C + M$	1.50×10^{16}	0.00	71600	±0.30[24]
9	$H_2 + M \Leftrightarrow 2H + M$	2.23×10^{14}	0.00	48350	±0.30[22,25]
10	$CN + M \Leftrightarrow C + N + M$	2.53×10^{14}	0.00	71000	±0.30[26,27]
11	$NH + M \Leftrightarrow N + H + M$	1.80×10^{14}	0.00	37600	±0.30[28]
12	$HCN + M \Leftrightarrow CN + H + M$	3.57×10^{26}	-2.60	62845	±0.30[29]
	Exchange reactions				
13	$CH_3 + H \Leftrightarrow CH_2 + H_2$	6.03×10^{13}	0.00	7600	±1.00[25]
14	$CH_3 + N_2 \Leftrightarrow HCN + NH$	4.82×10^{12}	0.00	18000	±1.00[28]
15	$CH_2 + N \Leftrightarrow HCN + H$	5.00×10^{13}	0.00	0	±1.00[30]
16	$CH_2 + H \Leftrightarrow CH + H_2$	6.03×10^{12}	0.00	-900	±0.87[25,28]
17	$CH + N_2 \Leftrightarrow HCN + N$	4.40×10^{12}	0.00	11060	±0.35[30]
18	$CH + C \Leftrightarrow C_2 + H$	2.00×10^{14}	0.00	0	±1.00[23]
19	$C_2 + N_2 \Leftrightarrow 2CN$	1.50×10^{13}	0.00	21000	±0.30[31]
20	$CN + H_2 \Leftrightarrow HCN + H$	2.95×10^{5}	0.00	1130	±0.60[32]
21	$CN + C \Leftrightarrow C_2 + N$	5.00×10^{13}	0.00	13000	±0.54[18]
22	$N + H_2 \Leftrightarrow NH + H$	1.60×10^{14}	0.00	12650	±0.30[33]
23	$C + N_2 \Leftrightarrow CN + N$	5.24×10^{13}	0.00	22600	±0.50[T]
24	$C + H_2 \Leftrightarrow CH + H$	4.00×10^{14}	0.00	11700	±0.30[34]
25	$H + N_2 \Leftrightarrow NH + N$	3.00×10^{12}	0.50	71400	±0.50[T]
26	$CH_4 + H \Leftrightarrow CH_3 + H_2$	1.32×10^{4}	3.00	4045	±0.30[22,25]

Another uncertainty source

Radiation modeling

NASA has identified the *heating from shock layer radiation due to the CN radical formed in the* N_2/CH_4 *atmosphere as a primary uncertainty*

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Radiation modeling

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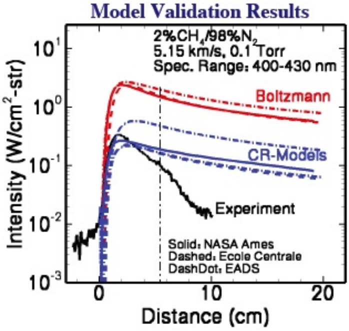
Can we predict the *CN* radical?

- State-of-the art knowledge during the design of the Huygen's probe was the Boltzmann model
- This led to overprediction of the heating rates - conservative design
- Recent work has lead to collisional-radiative (CR) models


Model Validation Results

TPS Heating load uncertainty

- We used Monte Carlo sampling (10,000 runs) to study the effect of the kinetics uncertainties
- We employed the CR model but compared to NASA earlier work (with Boltzmann model) in an attempt to characterize the epistemic uncertainty

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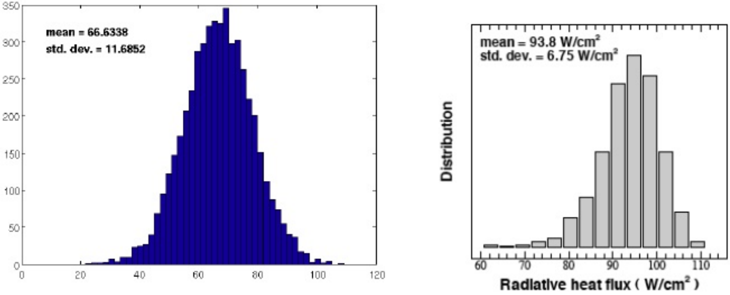
Stagnation point heat flux (W/cm^2)



CR Model: Ghaffari, Iaccarino, Magin, 2009

Boltzmann model: Bose & Wright, 2004

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Correlation: based on cross-plots of output (amount of *CN*) vs. input (uncertainty in the reaction rates)

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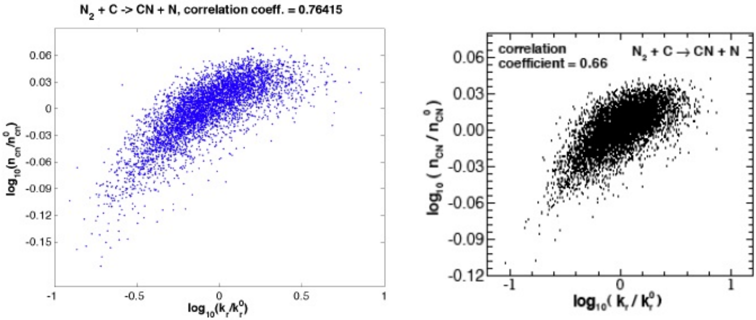
Correlation plot for $N_2 + C \rightarrow CN + N_2$



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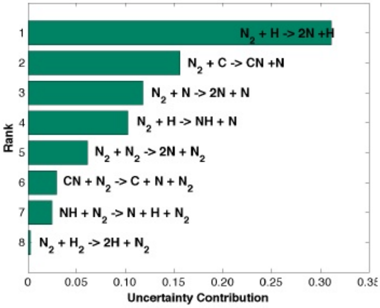
TPS Heating load uncertainty

ANOVA ANalysis Of Variance: separate the variance in factors contributed by each input uncertainty

8 major contributors to uncertainty



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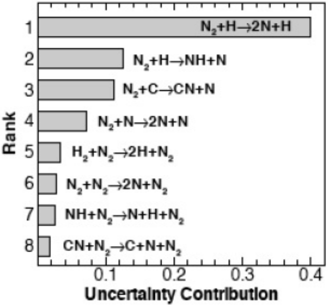
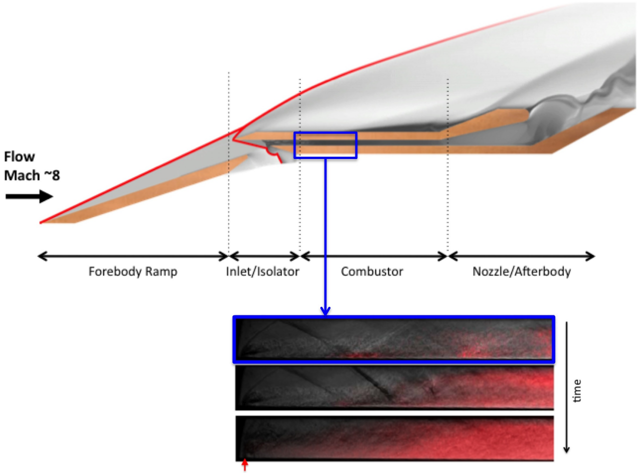


Boltzmann model: Bose & Wright, 2004

Uncertainty in Ignition Delay Time

Determination of Ignition Delay Time is an important design consideration, for example in air-breathing hypersonic propulsion systems



Uncertainty in Ignition Delay Time

In scramjet there are two competing mechanism causing sudden ignition of mixture:

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  - Hydrogen chemistry (9 species, 25 elementary reactions)

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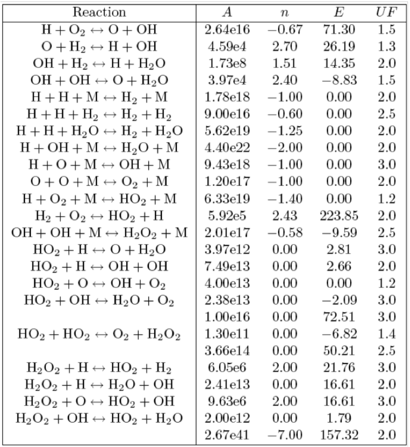
- Simplified Problem:
  - Integrate evolution of reacting mixture in homogeneous isochoric (constant volume) reactor
  - Hydrogen chemistry (9 species, 25 elementary reactions)
  - What is the uncertainty?

Hydrogen Chemistry

Reaction Rate Uncertainties

- Rate (and their uncertainties) are available in the literature
- Modified Arrhenius form $k = AT^n exp(-E/RT)$
- The uncertainty factor *UF* is such that $[k/UF : k \times UF]$ provide *probable* bounds!
- *Assume* that the reaction rate are independent, lognormally distributed r.v.



Reaction	A	n	E	UF
$H + O_2 \leftrightarrow O + OH$	2.64e16	−0.67	71.30	1.5
$O + H_2 \leftrightarrow H + OH$	4.59e4	2.70	26.19	1.3
$OH + H_2 \leftrightarrow H + H_2O$	1.73e8	1.51	14.35	2.0
$OH + OH \leftrightarrow O + H_2O$	3.97e4	2.40	−8.83	1.5
$H + H + M \leftrightarrow H_2 + M$	1.78e18	−1.00	0.00	2.0
$H + H + H_2 \leftrightarrow H_2 + H_2$	9.00e16	−0.60	0.00	2.5
$H + H + H_2O \leftrightarrow H_2 + H_2O$	5.62e19	−1.25	0.00	2.0
$H + OH + M \leftrightarrow H_2O + M$	4.40e22	−2.00	0.00	2.0
$H + O + M \leftrightarrow OH + M$	9.43e18	−1.00	0.00	3.0
$O + O + M \leftrightarrow O_2 + M$	1.20e17	−1.00	0.00	2.0
$H + O_2 + M \leftrightarrow HO_2 + M$	6.33e19	−1.40	0.00	1.2
$H_2 + O_2 \leftrightarrow HO_2 + H$	5.92e5	2.43	223.85	2.0
$OH + OH + M \leftrightarrow H_2O_2 + M$	2.01e17	−0.58	−9.59	2.5
$HO_2 + H \leftrightarrow O + H_2O$	3.97e12	0.00	2.81	3.0
$HO_2 + H \leftrightarrow OH + OH$	7.49e13	0.00	2.66	2.0
$HO_2 + O \leftrightarrow OH + O_2$	4.00e13	0.00	0.00	1.2
$HO_2 + OH \leftrightarrow H_2O + O_2$	2.38e13	0.00	−2.09	3.0
	1.00e16	0.00	72.51	3.0
$HO_2 + HO_2 \leftrightarrow O_2 + H_2O_2$	1.30e11	0.00	−6.82	1.4
	3.66e14	0.00	50.21	2.5
$H_2O_2 + H \leftrightarrow HO_2 + H_2$	6.05e6	2.00	21.76	3.0
$H_2O_2 + H \leftrightarrow H_2O + OH$	2.41e13	0.00	16.61	2.0
$H_2O_2 + O \leftrightarrow HO_2 + OH$	9.63e6	2.00	16.61	3.0
$H_2O_2 + OH \leftrightarrow HO_2 + H_2O$	2.00e12	0.00	1.79	2.0
	2.67e41	−7.00	157.32	2.0

Davis, Joshi, Wang, Egolfopoulos, Proc. Combust. Inst. 30, 2005

Ignition Delay Time

Uncertainty Propagation

- Conditions: Stoichiometric Hydrogen-Air Mixture (29.6% H_2; 14.8% O_2); Temperature: 1000 K; Pressure: 1 atm;
- Non-intrusive LHS Sampling (25 uncertain variables)

Ignition Delay Time

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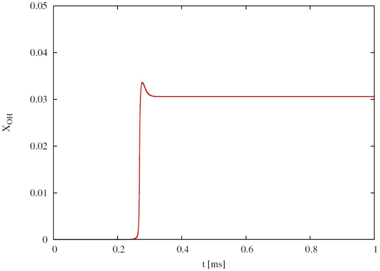
Number of Samples	Mean [ms]	UF
100	0.202060	1.7362
1000	0.201304	1.7054
10000	0.201256	1.7039
100000	0.201263	1.7075

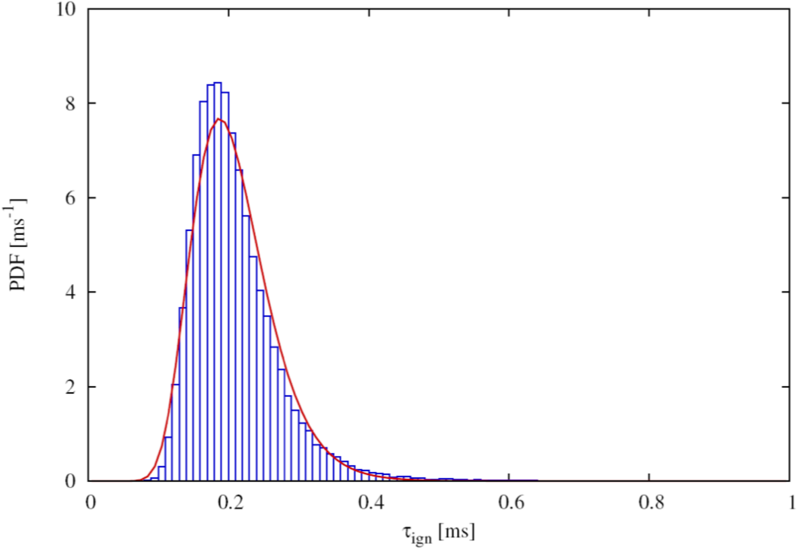
One Sample Showing Ignition at ~0.25 ms



DAKOTA UQ Suite from Sandia National Lab. used for this example

Ignition Delay Time

Uncertainty Propagation



Ignition Delay Time

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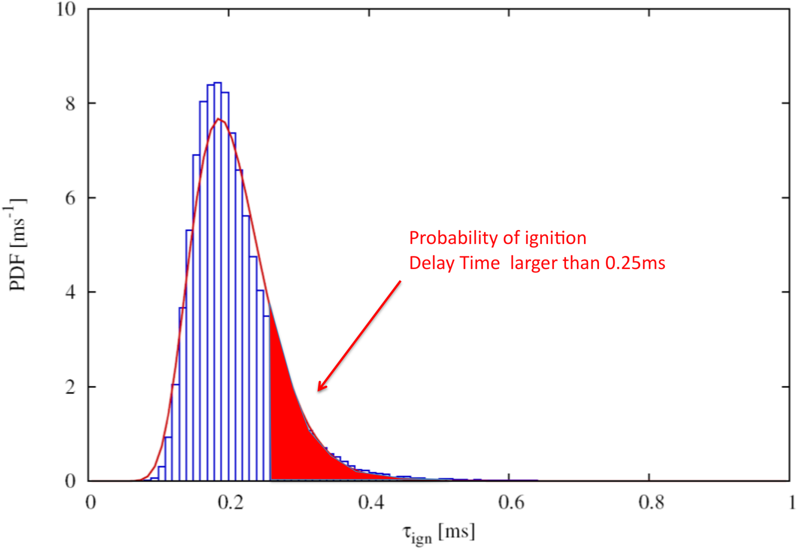

Probability of ignition
Delay Time larger than 0.25ms

Ignition Delay Time

Uncertainty Propagation

- UQ provides an effective quantification of the range (and likelihood) of the ignition delay time

Ignition Delay Time

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- Given that hydrogen chemistry is the simplest possible chose and we still need $\approx$ 5000 solutions to get an accurate answer (using LHS), two questions remain
  - Good to know, so what?
  - Can we do this faster?

Ignition Delay Time

Pose the UQ quest as an Inverse Problem

- What uncertainty in the reaction rates can we tolerate to ensure that the probability of ignition delay time exceeding 0.25 ms is less than 10%?

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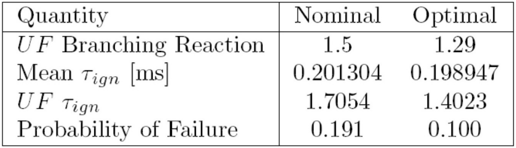
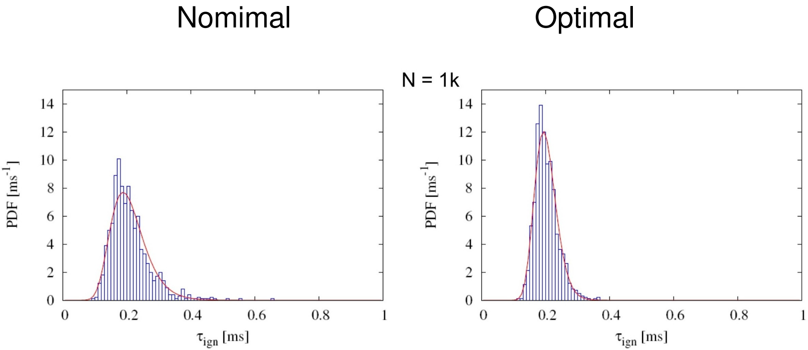


Quantity	Nominal	Optimal
UF Branching Reaction	1.5	1.29
Mean τ_{ign} [ms]	0.201304	0.198947
UF τ_{ign}	1.7054	1.4023
Probability of Failure	0.191	0.100

Ignition Delay Time

Uncertainty Propagation



Nominal

Optimal

N = 1k

- Overall uncertainty in the IDT is reduced
- Failure probability below critical requirement

Ignition Delay Time

Efficiency of UQ

The results shown so far use sampling to compute the statistics of the output of interest

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We need to use/develop algorithms that discover the true dependency of the solution

Low-Rank Approximations

High-Dimensional UQ

Extend the concept of Separation of variables to computational methodologies

Low-Rank Approximations

High-Dimensional UQ

Extend the concept of Separation of variables to computational methodologies

- Assume y_j for $j = 1, \ldots, d$ are the input uncertainties
- Define $u(y_1, \ldots y_d) \approx \sum_{k=1}^{r} u_1^{(k)}(y_1) \times u_2^{(k)}(y_2) \times \cdots \times u_d^{(k)}(y_d)$

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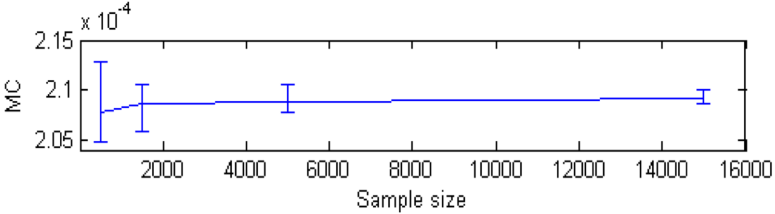
- Need to discover the functions $u^{(k)}$ and the *rank* r
- We cast it as an optimization problem: Find the lowest possible r which approximates a set of given function evaluations with $u^{(k)}$ being polynomials of fixed maximum order

Low-Rank Approximations

Mean Ignition Delay Time

Reuse the solutions computed in the autoignition example



Low-Rank Approximations

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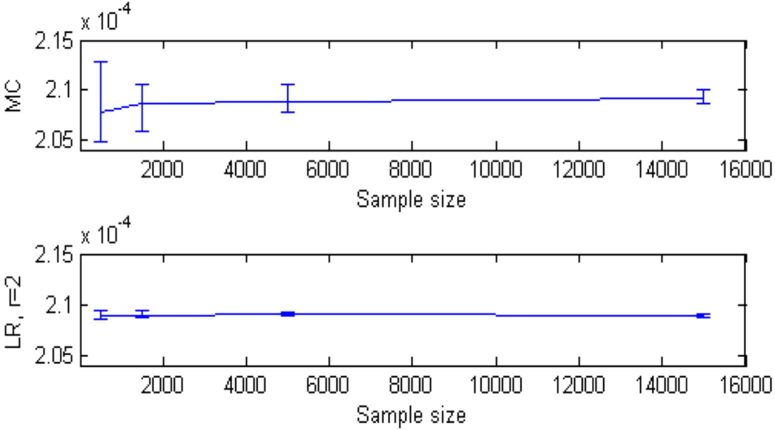
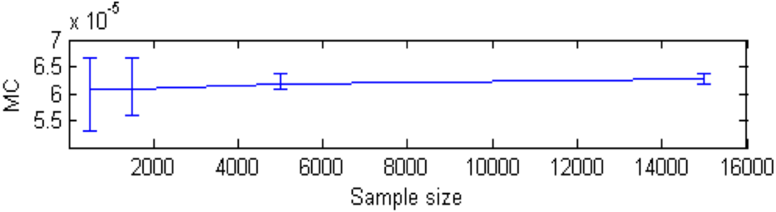


Even with 500 samples the estimate of the mean ignition delay is acceptable (smaller than MC with 14,000)

Low-Rank Approximations

STD of Ignition Delay Time

Similar results for the variance



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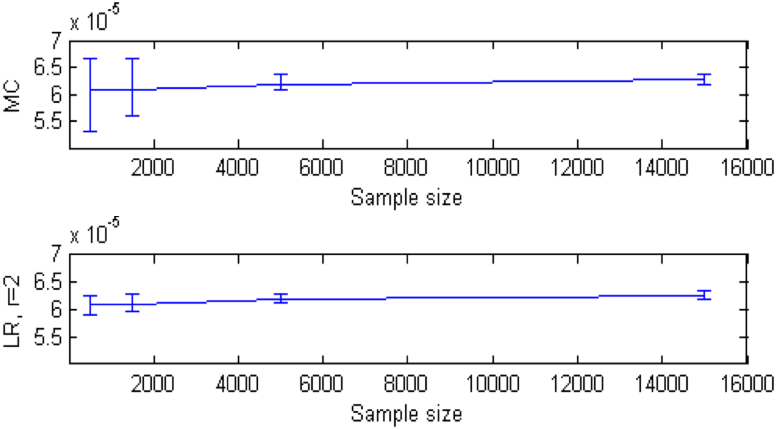
STD of Ignition Delay Time

Similar results for the variance



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...so far

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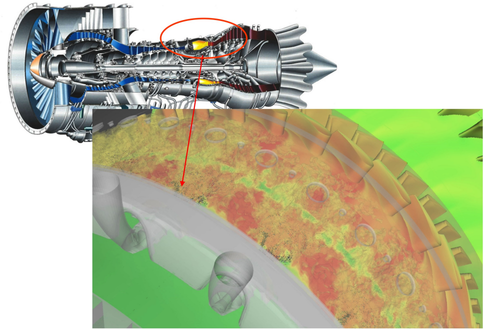
To finish, I want to give you an example of UQ combined with realistic flow simulations...

Turbulent reacting flows

Challenges

- Turbulent flow simulations in realistic geometries with detailed kinetic mechanisms are still beyond the reach of computational engineering



PW6000 simulations enabled by the flamelet modeling approach, but still requiring 1000 CPUs

Turbulent reacting flows

UQ Challenges

- Uncertainties in kinetic mechanisms might still dominate, especially for the prediction of pollutants
- It is impossible to perform more than a handful of simulation ($\mathcal{O}(5)$)
- Non-intrusive approach (even our fancy LR method) have no hope of success
- Need to be intrusive and connect the physics/mathematics/UQ

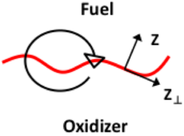
Turbulent reacting flows

Non-intrusive framework

- Perform MANY simulations and sample the outputs

Reacting Flow Modeling - Flamelet

- Basic Premise
  - Since scales of chemical reaction are much smaller than the smallest scales of turbulent, a turbulent flame is simply an ensemble of laminar ÒflameletsÓ embedded in a turbulent flow field
  - Solve for flame structure independently from the flow field
- Coordinate Transformation
  - Transform to coordinate system attached to the flame $(x, y, z) \rightarrow (Z, Z_\perp)$
  - Neglect all gradients in tangential directions



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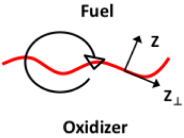

- Coordinate Transformation
  - Transform to coordinate system attached to the flame $(x, y, z) \rightarrow (Z, Z_\perp)$
  - Neglect all gradients in tangential directions
- Resulting equations are a one-dimensional set of reaction-diffusion equations parameterized by the mixture fraction Z
- Solved in advance and tabulated for a given fuel

Reacting Flow Modeling - Governing Equations

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_j}{\partial x_j} = 0$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_j u_i}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j}\left[2\mu\left(S_{ij} - \frac{1}{3}\delta_{ij}\frac{\partial u_k}{\partial x_k}\right)\right]$$

$$\frac{\partial Z}{\partial t} + \frac{\partial \rho Z}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\rho D \frac{\partial Z}{\partial x_j}\right]$$

$$T = T(\rho, p, Z) \quad \rightarrow \quad \text{tabulated}$$

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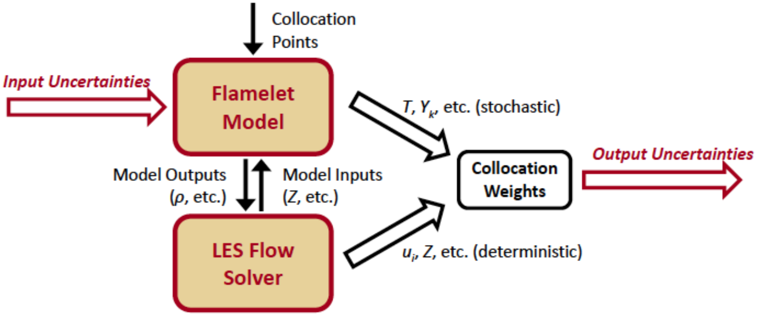
- Uncertainty in the kinetic rates appears indirectly through the density
- Use the flamelet equations to ÒconditionÓ the high-dimensional uncertainty
- Can use efficient UQ methods requiring few full system simulations

Turbulent reacting flows

Intrusive framework



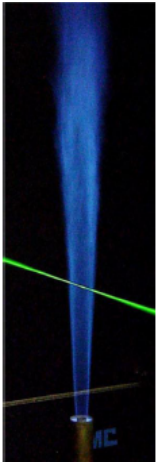
- Split the flamelet-generation part from the actual flow simulations
- Propagate the uncertainty through the flamelet
- Inject uncertainties in the link between flamelets and flow equations (via mixture fraction, density, etc.)

Turbulent reacting flows

Sandia Flame D

Piloted partially premixed methane/air flame

- Used NGA (low Mach, structured grid)
- GRI 3.0 mechanism
- Uncertainties in rates from Sheen *et al.* 2009



Simulations

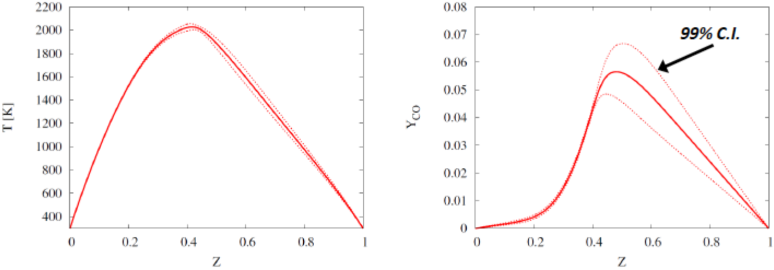
1. Used LHS sampling for flamelets (10,000 solutions)
2. Compiled tables with mean and variances of density (other uncertainties, e.g. viscosity ignored for now)
3. Performed 7 LES simulations sampling on the density distribution

Turbulent reacting flows

Sandia Flame D

Step 1

From kinetic rate uncertainties to flamelet output uncertainties



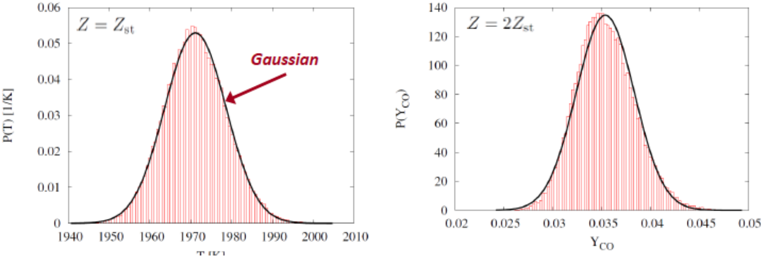
Rich part of the flame more *uncertain*

Turbulent reacting flows

Sandia Flame D

Step 2

Create a stochastic flamelet table

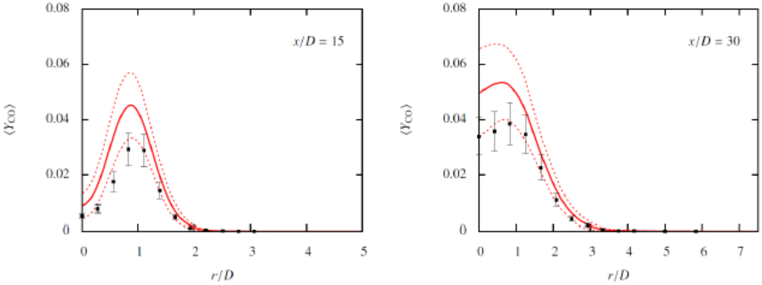


Distributions are Gaussian-like

Turbulent reacting flows

Sandia Flame D

Step 3
LES with stochastic flamelet table



Emission uncertainty is quite high, and might be comparable with other uncertainties (steady flamelet assumption, kinetic mechanism, etc.)

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CEMRACS Summer School
July 2012
CIRM, Marseille, France