Comments, Jonathan Goodman, July, 2014

ElasticConstants.pdf: Miguel A. Aguilo Laura Swiler, Angel Urbina, "AN OVERVIEW OF INVERSE MATERIAL IDENTIFICATION WITHIN THE FRAMEWORKS OF DETERMINISTIC AND STOCHASTIC PARAMETER ESTIMATION", International Journal for Uncertainty Quantification, 3 (4): 289319 (2013)

1. Specific problem: recover spatially varying elastic modulus from measurements.

2. Two kinds of parameter estimation: deterministic and stochastic. Stochastic gives uncertainty estimates. Bayesian: "... multiple solutions of the unknown may be consistent with the observations."

3. References for elliptic inverse problems.

4. Likelihood function takes into account *ECE*, "error in the constitutive equation".

5. Represent the spatially varying elastic modulus using radial basis functions with unknown centers and length parameters and coefficients. Ill conditioned in radial basis coefficients $\longrightarrow$ regularize.

6. Kaipio, J. and Somersalo, E., *Statistical and Computational Inverse Problems*, Springer, NewYork, 2005.

7. Numerics: fake data, 1D, multiplicitive Gaussian observation noise, small, known variance.

8. MCMC, delayed rejection adaptive algorithm http://www.helsinki.fi/?mjlaine/dram/

9. Haario, H., Laine, M., Mira, A., and Saksman, E., DRAM:EfficientadaptiveMCMC, Stat.Comput., 16(4):339354, 2006.

10. Estimated auto-correlation function from MCMC data. Standard likelihood gives auto-correlation time in the thousands. The ECE likelihood τ is only 100 or so. Run length 20,000 samples, first 5,000 discarded (burn in).

11. 15 observation values, 5 radial basis functions (common length scale, uniformly spaced centers?) Some of the results seem to accurate to be represented with 5 radial basis functions of any kind.

TemponeAbstract.pdf: Daesang Kim, Fabrizio Bisetti, Quan Long, Raul Tempone, and Omar Knio, *Spectral Uncertainty Quantification and Optimal Bayesian Experimental Design of Combustion Reaction Systems using Sparse Adaptive Polynomial Chaos Expansion*, conference abstract, 2014

1. Polynomial chaos

2. Hydrogen flame parameters, then methane system parameters

AIAA.pdf: Paul G. Constantine, Alireza Doostan, Qiqi Wang, Gianluca Iaccarino, *A Surrogate Accelerated Bayesian Inverse Analysis of the HyShot II Flight Data*, AIAA 2011-2037, 52nd AIAA/ASME/ASCE/AHS/ASC Structures, Structural Dynamics and Materials Conference 19th AIAA 2011-2037 4 - 7 April 2011, Denver, Colorado

1. Hypersonic RANS viscous flow with combustion, model of a scramjet, 11 pressure measurements, 6 estimated parameters: speed, angle of attack, altitude, top wall temperature, bottom wall temperature, one turbulence variable, fake data.

2. Full fluid (RANS) solve for a likelihood call, or a surrogate m.odel. 1800 fluid solves.

3. Silva, D. and Skilling, J., Data Analysis: A Bayesian Tutorial, Oxford University Press, 2006.

4. Compared surrogate models, polynomial chaos, Gaussian process, Beylkin low rank approx – about the same. Crummy numerics.

BramanOliverRaman.pdf: Kalen Braman, Todd A. Oliver, Venkat Raman, *Bayesian analysis of syngas chemistry models*, Combustion Theory and Modelling, 2013 Vol. 17, No. 5, 858887

1. Full Bayesian posterior sampling for combustion chemical kinetics parameters.

2. Lots of references for UQ in chemical reaction fitting.

3. "It is important to note that the different parameters are correlated, and that varying one without adjusting the rest is not meaningful."

4. T. Russi, A. Packard, R. Feeley, and M. Frenklach, "Sensitivity analysis of uncertainty in model prediction", J. Phys. Chem. A 112 (2008), pp. 25792588. Available at http://dx.doi.org/10.1021/jp076861c.

5. Adaptive multi-level sampling algorithm, refs [28,29], related to sequential sampling? QUESO library.

6. Uses our Davis mechanism, and two others.

7. Only pre-exponential factors included in Bayesian parameter sets, not activation energies.

8. Calibrates to flame speed data, 18 measurements in all.

9. Select parameters based on some kind of a-priori sensitivity analysis.

10. Simulations done with CHEMKIN and PREMIX

11. 15,000 processor hours, ... the majority of the computational time is spent computing the flame speed.