37th International Symposium on Combustion
2nd August 2018, Dublin, Ireland

Development of a Coupling between OpenSMOKE++ and Dakota for Optimization of Chemical Kinetics

Magnus Fürst[1,2,3,*], Alberto Cuoci[2], Alessio Frassoldati[2] and Alessandro Parente[1,3]
[1]Université Libre de Bruxelles, Ecole Polytechnique de Bruxelles, Aero-Thermo-Mechanics Laboratory
[2]Politecnico di Milano, Department of Chemistry, Materials, and Chemical Engineering
[3]comBUstion and Robust optimizatioN group (BURN), Université Libre de Bruxelles and Vrije Universiteit Brussel
[*]Contact: magnus.furst@ulb.ac.be

Background

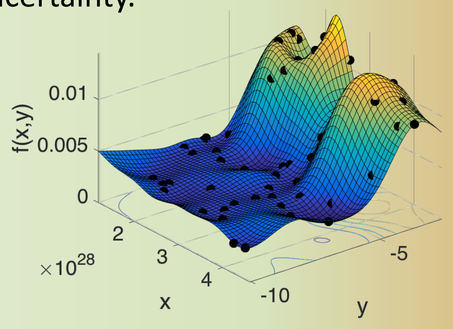
The use of detailed kinetics in large scale simulations are becoming more realizable as computational power increases. However, there are many inherent **uncertainties** in kinetic mechanisms, as each kinetic parameter (A, β, and E) has an uncertainty. Furthermore, detailed mechanisms consists of thousands of reactions, and therefore also **thousands of uncertain parameters**. The use of Uncertainty Quantification (UQ)/Optimization tools are therefore promising as they can be used to improve the performance of existing mechanism. The focus of this work is therefore to create an efficient coupling between the two software OpenSMOKE++ [1] and Dakota [2], which together can be used towards **optimizing** kinetic mechanisms.

DAKOTA
Explore and predict with confidence.

Developed and distributed at Sandia National Laboratories as an open-source toolkit for interfacing analysis codes with iterative analysis methods. Dakota includes algorithms for:

- Local and Global optimization, with gradient and non-gradient based methods
- Uncertainty Quantification
- Parameter estimation with nonlinear least squares methods
- Sensitivity analysis with design of experiments and parameter study methods

These capabilities may be used on their own or as components within advanced strategies such as surrogate-based optimization, mixed integer nonlinear programming, or optimization under uncertainty.



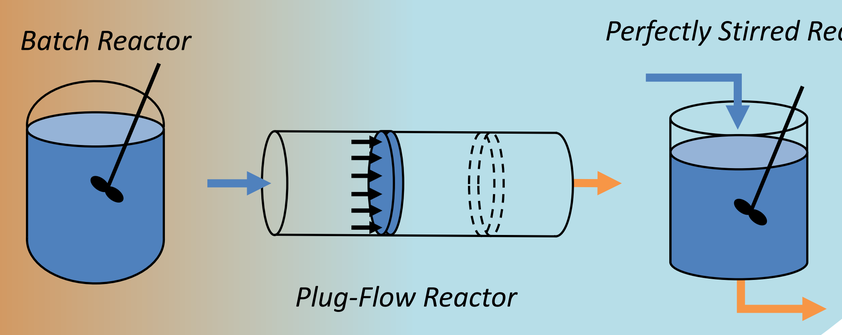
Response surface of an objective function

OpenSMOKE++

Developed at Politecnico di Milano to solve reacting systems, using detailed kinetic mechanisms, with thousands of species and reactions. The software can solve:

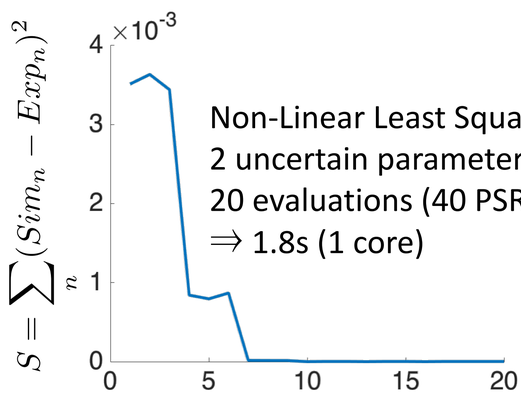
- Batch Reactors
- Plug-Flow Reactors
- Perfectly Stirred Reactors
- Shock-Tube Reactors
- Rapid Compression Machines
- Laminar Flamelets
- Counter Flow Diffusion Flames
- Etc …

Since these simulations (with detailed kinetic mechanisms) are very time consuming, OpenSMOKE++ adopts advanced numerical techniques able to reduce the computational cost, without sacrificing the accuracy and the robustness of the calculations.



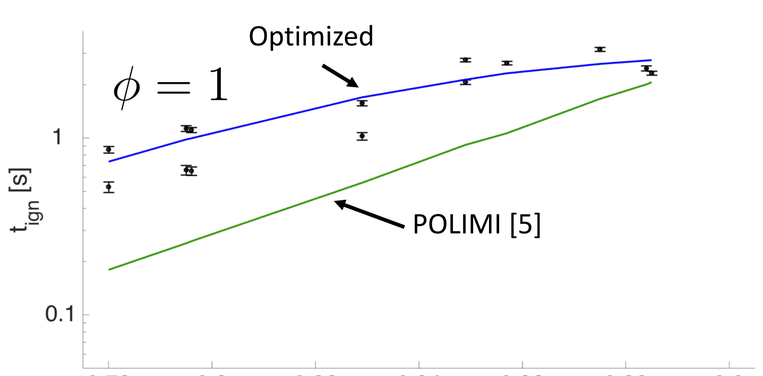
Preliminary results

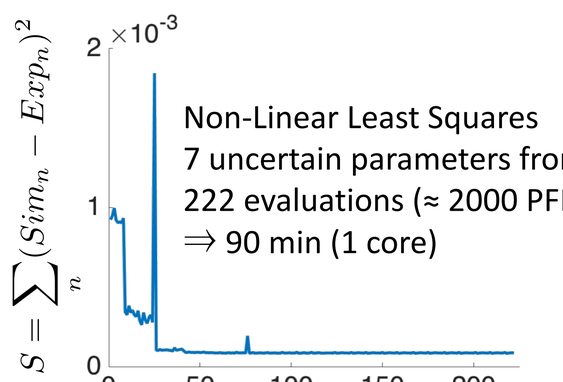
- A toy-case based on the work from Harris et al. [3], was used to evaluate the performance of the coupling. The targets were the final O_2 concentration from two PSRs.



Non-Linear Least Squares
2 uncertain parameters from 1 reaction
20 evaluations (40 PSR sim)
⇒ 1.8s (1 core)

- A second test case of ignition delay times of biomass pyrolysis gas in a PFR [4], was used. The inlet temperatures ranges from 1130-1282K, and in total 9 targets were used. Quite significant improvements can be found in the performance of the optimized mechanism.





Non-Linear Least Squares
7 uncertain parameters from 3 reactions
222 evaluations (≈ 2000 PFR sim)
⇒ 90 min (1 core)

Conclusions and Future works

The coupling between OpenSMOKE++ and Dakota shows promising results for the two test cases presented above. In the near future the usage of more than one data set will be implemented in the coupling. The coupling will also be extended to the full set of the capabilities in Dakota, as well as the combined usage of targets from several different reactor types, will be implemented. This will enable the user to account for a variety of experimental targets, and also used the method which suits the needs of the user the best. As both codes also support parallel computation, this will also be implemented in order to speed up the optimization process.

References

[1] Cuoci A, Frassoldati A, Faravelli T and Ranzi E. Comput. Phys. Commun, 192 (2015) 237-264
[2] Adams BM, Ebeida MS, Eldred MS, Geraci G, Jakeman JD, Maupin KA, et al. Dakota, A Multilevel Parallel Object-Oriented Framework for Design Optimization, Parameter Estimation, Uncertainty Quantification, and Sensitivity Analysis: Version 6.5 User's Manual 2014.
[3] S Harris, L Elliott, D Ingham, M Pourkashanian, and C Wilson, Comput. Methods Appl. Mech. Eng., 190 (2000) 1065–1090
[4] Sabia P, Lubrano Lavadera M, Sorrentino G, Giudicianni P, Ragucci R and de Joannon M. Flow, Turbulence and Combustion, 96 (2016) 433-448
[5] Ranzi E, Frassoldati A, Grana R, Cuoci A, Faravelli T, Kelley A. P and Law C. K. Prog. Energy Combust. Sci., 38 (2012) 468-501

This work has been carried out in the framework of the Short Term Scientific Mission Program of SMARTCATs COST Action (CM1404, www.smartcats.eu), supported by COST (European Cooperation in Science and Technology, www.cost.eu) as well as it has received funding from the European Union's Horizon 2020 research and innovation program under the Marie Sklodowska- Curie grant agreement No 643134, and it has been supported by the European Research Council, Starting Grant No. 714605.