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Development of an Adaptive Technique to Reduce Combustion Thermochemistry

Introduction

The numerical study of combustion requires description of chemical kinetic mechanisms of the reactions involved in the process. Typically, a detailed chemical kinetic mechanism for description of hydro-carbons reaction with air involves tenths of species, hundreds of elementary reactions and timescales that vary up to nine orders of magnitude.

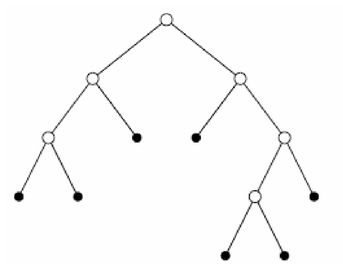
The solution of a detailed reaction mechanism is computationally demanding. This leads to the development of techniques that allow the reduction of the computational cost of the problem. A methodology that may allow to decrease the computational time by three orders of magnitude is the *in situ* adaptive tabulation (ISAT), proposed by Pope (1997). The objective of this work is the development of such a technique.

Methodology

Perfect Reactor Model $\xrightarrow{\text{solve many times}}$

$$\frac{d\phi}{dt} = S(\phi, t) + M(t)$$
$$\phi(t_0) = \phi_0$$

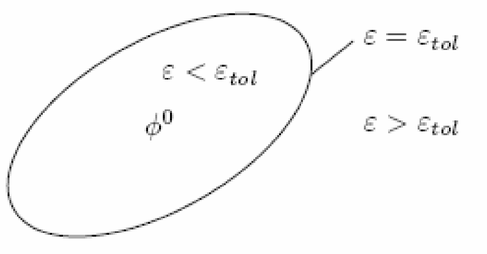
Binary Search Tree



ISAT algorithm outputs:

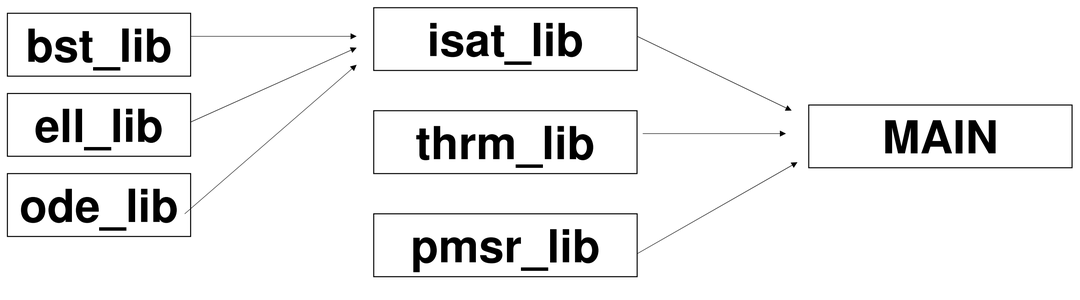
- Linear Approximation
- Growth the Ellipsoid
- Addition to the Tree

Region of Accuracy



Computational Code

The ISAT technique was implemented in a structurade modular ANSI C computational code. Currently this code is being submited to a series of functional verification tests to check if the algorithm was implemented correctly.



Final Remarks

In the near future its expected to test the ISAT method in the modelling of a transient one-dimensional perfect reactor, which is a stringent than situation than the current one.

This technique should be coupled to an existing Lardy Eddy Simulation (LES) code in a combustion modelling approach which would allow to combine detailed information about thermochemistry and large scale flow fields.

Acknowledgement

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References

Pope, S. B. **Computationally efficient implementation of combustion chemistry using *in situ* adaptive tabulation**, Combustion Theory Modelling, Vol. 1, No. 1, pp 41-63, 1997