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Development of an Adaptive Technique to Reduce Combustion Thermochemistry

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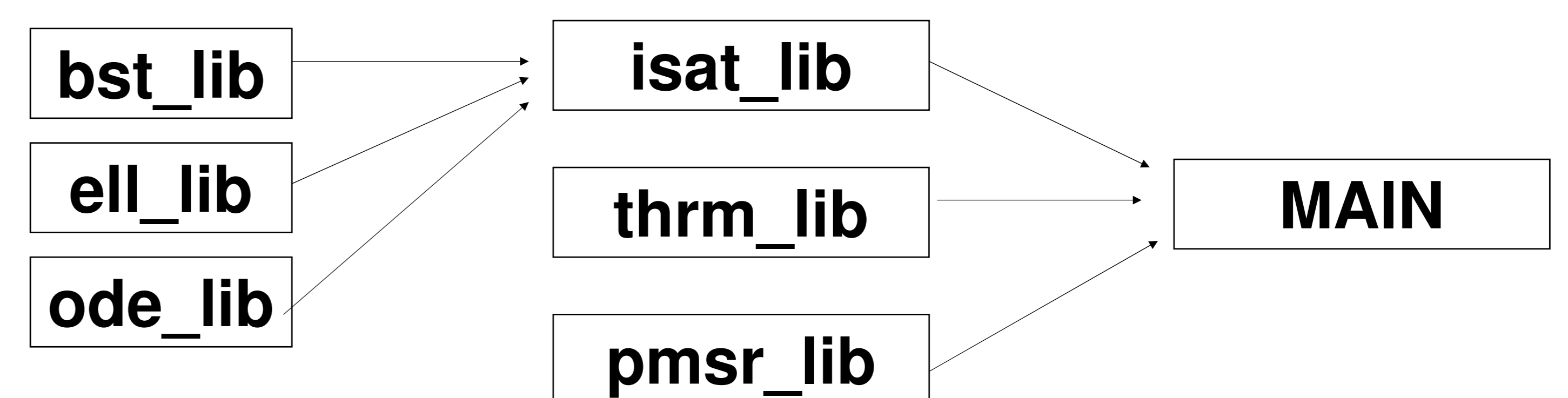
Introduction

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.

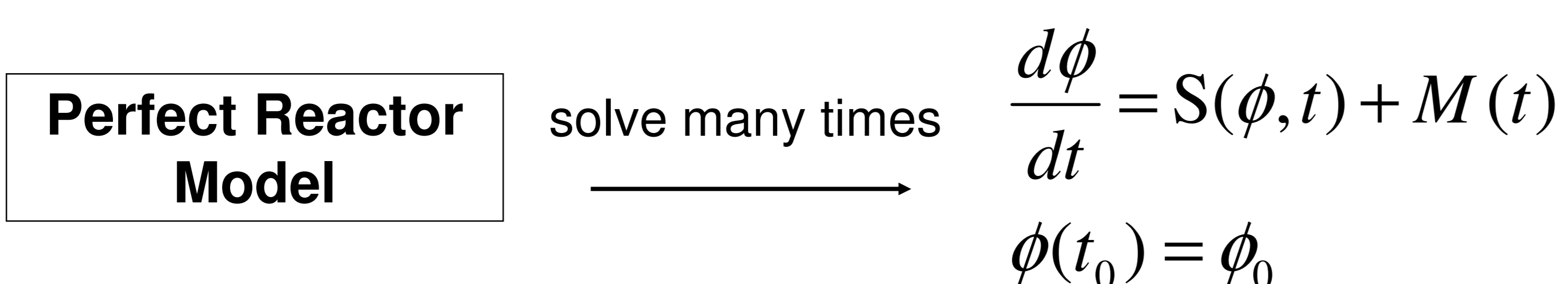
The solution of a detailed reaction mechanism is computationally demanding. This leads to the development of techniques that allow the reduction of the computational cost of the problem. A methodology that may allow to decrease the computational time by three orders of magnitude is the *in situ* adaptive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

Computational Code

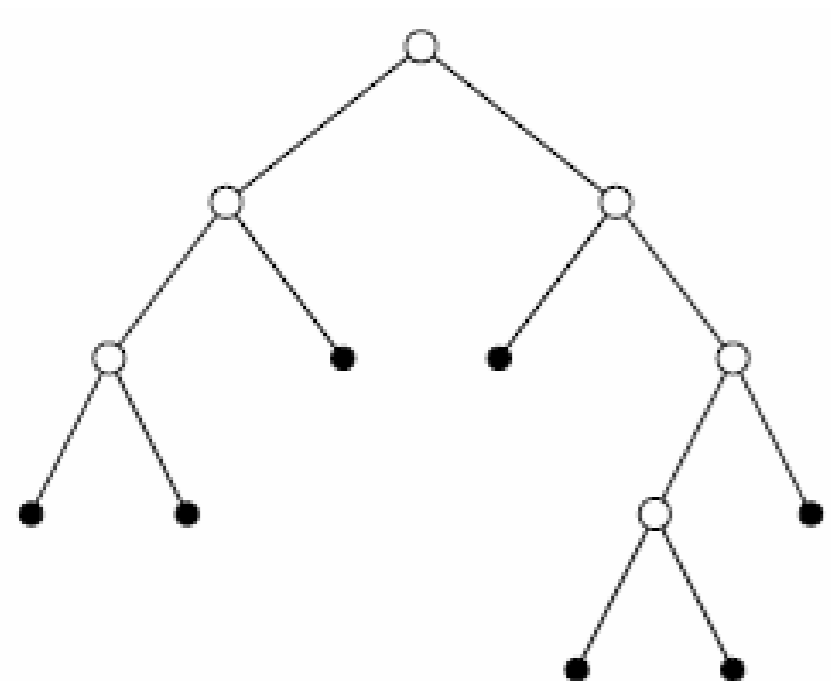
The ISAT technique was implemented in a structured modular ANSI C computational code. Currently this code is being submitted to a series of functional verification tests to check if the algorithm was implemented correctly.



Methodology



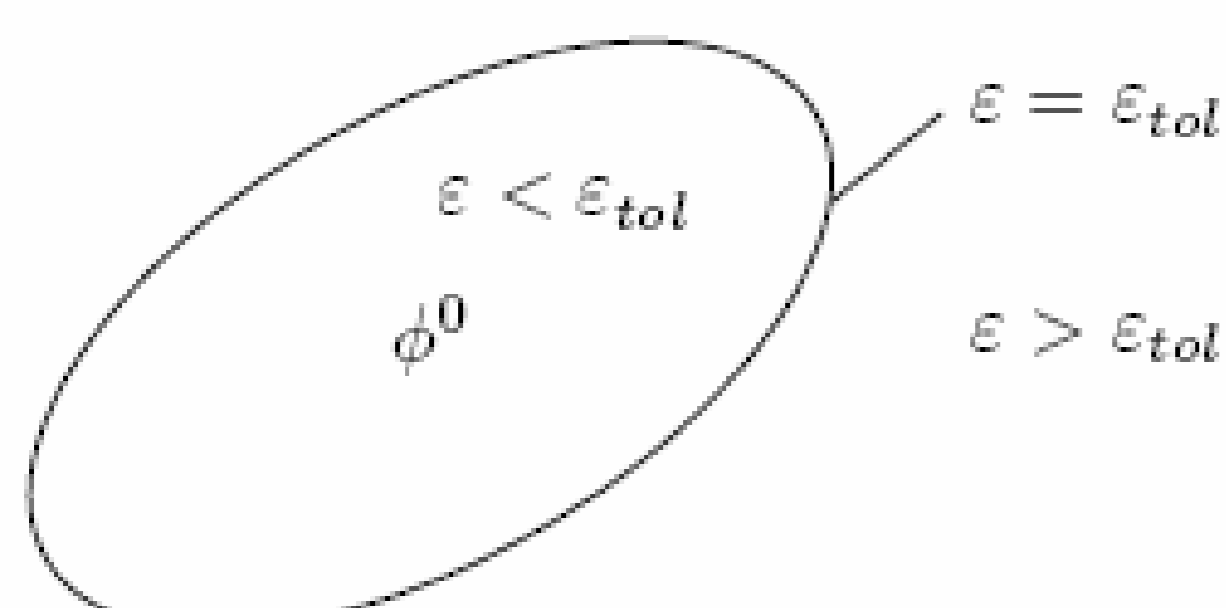
Binary Search Tree



ISAT algorithm outputs:

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

Region of Accuracy



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

To professor Guenther Carlos Krieger Filho for providing the code which serves as example to the present. The first author acknowledge CNPq and FAPERJ for the financial aid.

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