# Characterization of an Adaptive Technique to Reduce Combustion Thermochemistry

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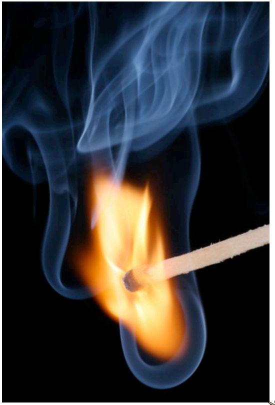
# Outline

# The Combustion Phenomena

- Physicochemical phenomena characterized by a sequence of chemical reactions which convert reagents in products of combustion.
- Application in several industrial devices (e.g. gas turbines, process furnaces, etc.).
- The processes of energy production based on combustion represent a significant share of the global ($> 90\%$) and of the Brazilian ($> 80\%$) energy matrix.



# Computational Model for Chemically Reacting Flows

A computational model to predict the behavior of chemically reacting flows must include a detailed reaction mechanism to describe the combustion thermochemistry and solve the following equations:

- Continuity
- Momentum
- Energy
- Transport for the Chemical Species
- State Variables Relations
- Constitutive Relations

It is necessary to solve $(\#\ species + 5)$ partial differential equations.

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# Objectives of this Work

This work objetives to characterize the *In Situ* Adaptive Tabulation, a technique for efficient computation of the chemically reactive flows models, in terms of:

- Accuracy
- Performance
- Memory Usage

# Governing Equation

The thermodynamical state of a reactive mixture in a homogeneous transient reactor is determined by *composition* vector

$$\phi \equiv (h, p, Y_1, \cdots, Y_{n_s})^{\mathrm{T}},$$

which evolves according

$$\frac{d\phi}{dt} = -\boldsymbol{\Gamma}(t) + \mathbf{S}(\phi, t),$$

being

- $\boldsymbol{\Gamma}$ the rate of change due to micromixing transport
- $\mathbf{S}$ the rate of change due to the chemical reactions

# Pairwise Mixing Stirred Reactor (PMSR)

- Even number $n_p$ of particles
- Types of events: *inflow*, *outflow* and *pairing*,
- Time scales: $\tau_r$, $\tau_p$ and $\tau_m$
- System of evolution equations:

$$\frac{d\phi^{(j_1)}}{dt} = -\frac{\phi^{(j_1)} - \phi^{(j_2)}}{\tau_m} + \mathbf{S}(\phi^{(j_1)}, t),$$

$$\frac{d\phi^{(j_2)}}{dt} = -\frac{\phi^{(j_2)} - \phi^{(j_1)}}{\tau_m} + \mathbf{S}(\phi^{(j_2)}, t).$$

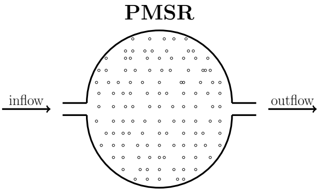


Figure: Sketch of a PMSR reactor.

# In Situ Adaptive Tabulation (ISAT)

- Requires less memory than a traditional look-up table method since the tabulation is done *in situ*.
- Allow a conservative error control.
- It is extremely flexible to couple with other reduction techniques.
- Pope (1997) reports speed-ups of up to three orders of magnitude in the simulation time compared with the direct integration of the governing equations.

Pope (1997) Computationally efficient implementation of combustion chemistry using *in situ* adaptive tabulation. Combustion Theory and Modelling, v.1 p. 41-63

# ISAT Algorithm Overview

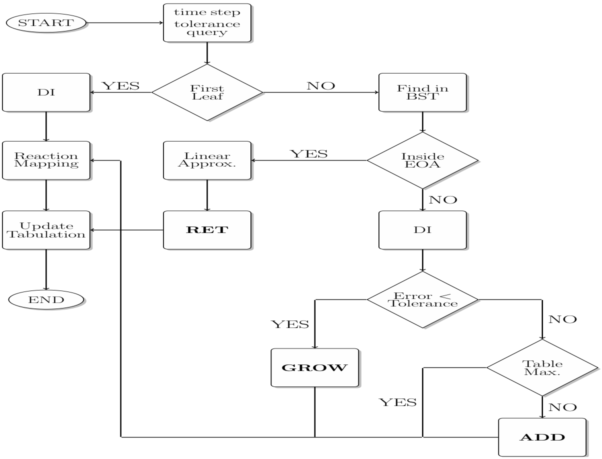


Figure: ISAT algorithm flowchart.

# Description of the Cases of Study

- binary search tree with a maximum of 50,000 entries
- $\Delta t = 10\ \mu\mathrm{s}$ and $\varepsilon_{tol} = 10^{-3}$
- Mixture of $CO/O_2$ (4 species and 3 reactions)

  Gardiner Mechanism (2000)
- initial mixture: $\Phi = 0.7,\ T = 2948.5\ \mathrm{K}$ and $p = 1\ \mathrm{atm}$
- inflow mixture: $\Phi = 0.7,\ T = 300\ \mathrm{K}$ and $p = 1\ \mathrm{atm}$
- time scales (Case 1): $\tau_m/\tau_r = 1/2$ and $\tau_p/\tau_r = 1/2$
- time scales (Case 2): $\tau_m/\tau_r = 1/10$ and $\tau_p/\tau_r = 1/10$

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# Evolution of $\langle T \rangle^*$

$$\tau^* \equiv \frac{t}{\tau_r} \qquad \langle T \rangle^* \equiv \frac{1}{n_p} \sum_{j=1}^{n_p} [T^*]^{(j)}$$

There is a good agreement between ISAT and DI results for $\langle T \rangle^*$.

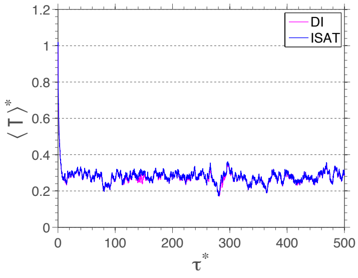


Figure: Case 1

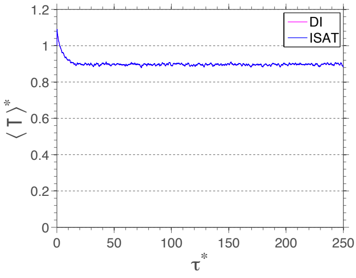


Figure: Case 2

# Evolution of Relative Local Error of $\langle T \rangle^*$

$$\varepsilon_{r,\langle T\rangle^*} \equiv \frac{\left| \langle T \rangle^*_{DI}(t) - \langle T \rangle^*_{ISAT}(t) \right|}{\left| \langle T \rangle^*_{DI}(t) \right|}$$

The statistical variation is due to the stochastic nature of the PMSR model.

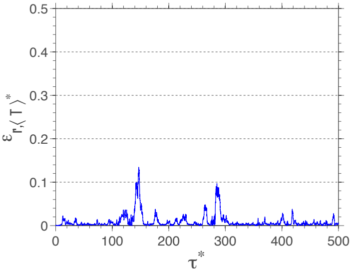


Figure: Case 1

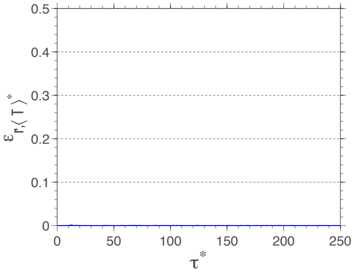


Figure: Case 2

# Absolute Global Error vs Error Tolerance

$$\varepsilon_g \equiv \frac{1}{\Delta\tau}\int_t^{t+\Delta\tau} ||\langle\phi\rangle(t')_{DI} - \langle\phi\rangle(t')_{ISAT}||dt'$$

The absolute global error decreases with $\varepsilon_{tol}$.

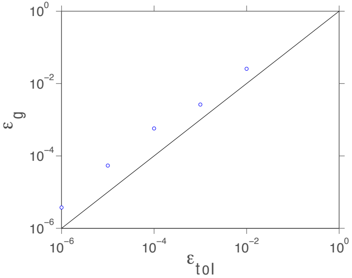


Figure: Case 1

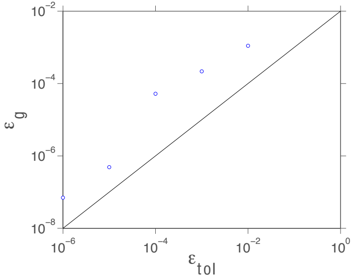


Figure: Case 2

# Evolution of ISAT Outputs

First, the binary tree is completely filled. Then retrieves exceeds additions, which ensures the efficiency of ISAT algorithm.

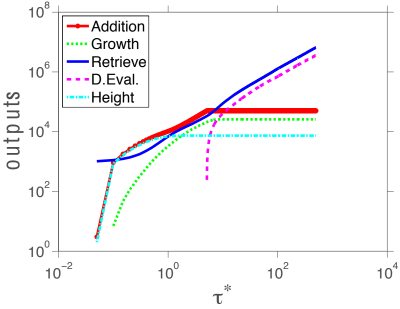


Figure: Case 1

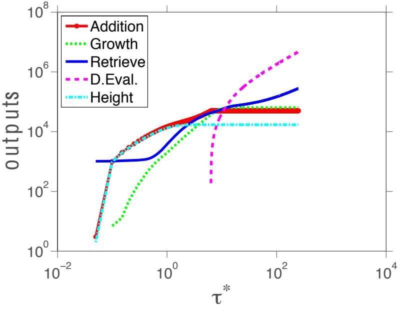


Figure: Case 2

# Computational Time Spent

Table: Comparison between the computational time spent by DI and ISAT and the corresponding speed-up factors.

| | time DI (ks) | time ISAT (ks) | speed-up | time saves |
|---|---|---|---|---|
| Case 1 | 4.3 | 2.3 | $\sim 1.9$ | $\sim 47\%$ |
| Case 2 | 3.1 | 2.1 | $\sim 1.5$ | $\sim 32\%$ |
| $CH_4$/Air | 689.3 | 454.5 | $\sim 1.5$ | $\sim 34\%$ |

# Computational Memory Spent

Table: Amount of memory used by ISAT implementation.

| | RAM Memory (Mbytes) |
|---|---|
| Case 1 | 40 |
| Case 2 | 40 |
| $CH_4$/Air | 3327 |

# Main Conclusions

- Concerning the accuracy, the ISAT shows good results from a global point of view and errors of up to 13% for the local error.
- In terms of performance, the ISAT algorithm allows to reduce the computational time of the simulations in up to 47%.
- Regarding the memory usage, the ISAT technique shows to be very demanding.

# Suggestions for Further Works

- Characterize ISAT technique in the simulation of reactors that use other reaction mechanisms.
- Incorporate the improvements of ISAT algorithm proposed by

Lu & Pope (2009)
An improved algorithm for in situ adaptive tabulation
Journal of Computational Physics,
v. 228 p. 361–386

- Coupling of a detailed reaction mechanism, using the ISAT technique, with the hybrid LES/PDF model.
- Validate the models studied in this work using data from carefully designed direct numerical simulations.

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