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# Empirical evaluation of the efficiency of Genetic and Particle Swarm algorithms for kinetic mechanism optimization.

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## Context and Objective

- Genetic Algorithm (GA) and Particle Swarm Optimization (PSO) are two evolutionary algorithm widely used for optimization
- GA is well known and used for detailed kinetic mechanisms optimization [1] but, so far, PSO is not
- Objective: compare the performances with the open-source tool Brookesia [2]

## 2. Error computation

- Ignition delay**
- $T$  and species profiles**

$$Er(\delta) = 1 - \frac{\delta_{\text{opt}}}{\delta_{\text{ref}}} \quad Er(i) \approx \frac{|A_{\text{ref}} - A_{\text{opt}}|}{A_{\text{ref}}}$$

with:  $Er$ : relative error     $\delta$ : ignition delay time     $A$ : area below the profile  
ref / opt: simulation from reference / optimized mechanism

## 3. a. Optimization by Genetic Algorithm

### • Concept

- from randomly modified kinetic mechanisms a series of simulation is performed
- based on the result analysis, the best mechanisms (individuals) are retained (**Selection** operator)
- individuals will share parameters (**Cross-Over** operator) to generate new mechanisms (childs)
- some individuals will be partially randomly modified (**Mutation** operator)
- a new series of simulation is performed and the cycle is repeated

### • Strategies

number of individuals: 20

| Strategies | Selection     | Crossover (*)  | Mutation (*)  |
|------------|---------------|----------------|---------------|
|            | Roulette Rank | Geometric norm | Elitism       |
|            |               | Simple         | Multiple      |
|            |               | Arithmetic     | Heuristic     |
|            |               | Uniform        | Non-uniform   |
|            |               |                | Boundary      |
| 1          | x             |                | 2 2 4 4 3 3 2 |
| 2          | x             |                | 2 2 4 4 3 3 2 |
| 3          |               | x              | 2 2 4 4 3 3 2 |
| 4          |               | x              | 2 2 4 4 3 3 2 |
| 5          |               | x              | 6 2 2 2 3 3 2 |
| 6          |               | x              | 2 6 2 2 3 3 2 |
| 7          |               | x              | 2 2 6 2 3 3 2 |
| 8          |               | x              | 2 2 2 6 3 3 2 |
| 9          |               | x              | 2 2 4 4 6 1 1 |
| 10         |               | x              | 2 2 4 4 1 6 1 |
| 11         |               | x              | 2 2 4 4 1 1 6 |

(\*) number of occurrence

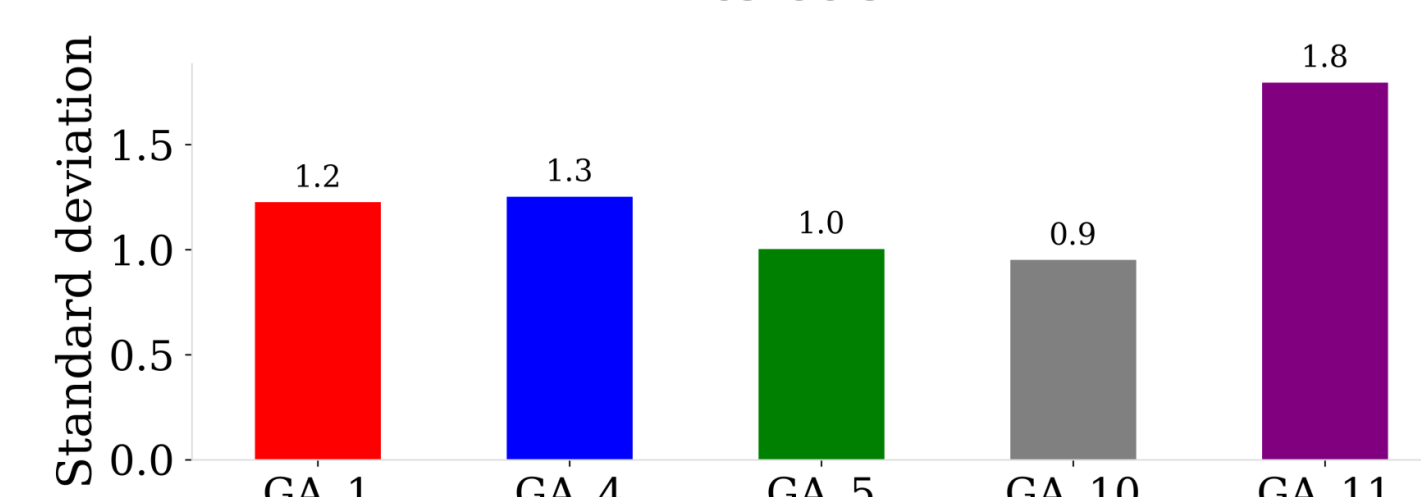
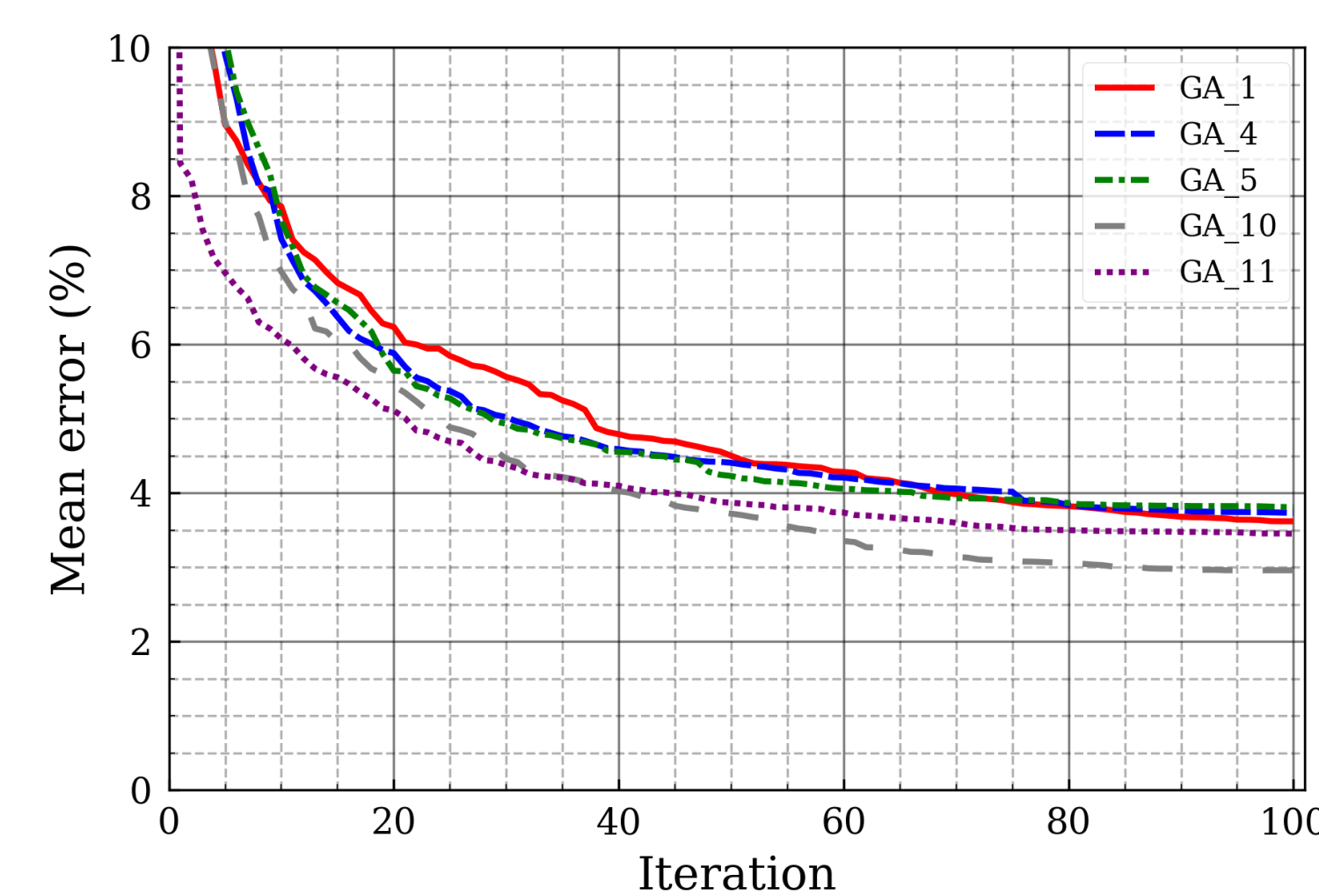
### • Comments

- Optimization efficiency seems **relatively insensitive to the strategy**
- Strategies 10 and 11 show the best results indicating the importance of a good setting of the mutation rate.

### • Performances

each strategies repeated 20 times:

- Mean error is averaged over the 20 trials
- the standard deviation measured between trials is shown below



## 1. Simulations

### • 6 Conditions

- Constant pressure & enthalpy reactor (Cantera [3])
- composition :
  - $\text{CH}_4/\text{air}$
  - $\Phi = 0.5, 1.0, 1.5$
- $p = 10^5 \text{ Pa}$  /  $T = 1050, 1500 \text{ K}$

### • 7 Targets

- ignition delay time
- temperature
- species:  $\text{CH}_4$ ,  $\text{CO}$ ,  $\text{CO}_2$ ,  $\text{C}_2\text{H}_4$ ,  $\text{C}_2\text{H}_6$

### • Kinetic mechanism

- GRI-Mech 3.0 (53 sp. 325r.) [4]

### • Degraded mechanism to be optimized

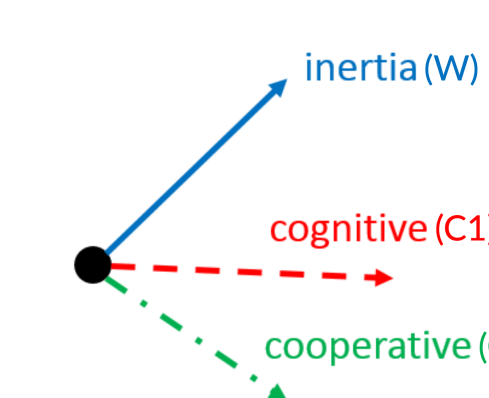
- the 7th most important reactions for each of the 7 targets randomly modified
- Importance evaluated on the basis of the direct interaction coefficients between a species  $A$  and a reaction  $r_i$ , (see ref. [5])

## 3. b. Optimization by Particle Swarm Algorithm

### • Concept

- from randomly modified kinetic mechanisms a series of simulation is performed
- each kinetic mechanism is a particle, its dynamics is governed by:
  - an **inertial** component, relative to the speed of the iteration of the previous iteration
  - a **cognitive** component based on the best solution found by the individual during the optimization process
  - a **social** component based on the best location the neighbours of the particle found up to the iteration
- a new series of simulation is performed and the cycle is repeated

### • Strategies



number of individuals: 20

| Strat | W    |       | C1   |       | C2   |       |
|-------|------|-------|------|-------|------|-------|
|       | init | final | init | final | init | final |
| 1     | 0.73 | 0.73  | 1.5  | 1.5   | 1.5  | 1.5   |
| 2     | 1.1  | 0.4   | 1.75 | 1.4   | 1.3  | 2     |
| 3     | 0.8  | 0.3   | 1.6  | 2     | 0.5  | 2     |
| 4     | 0.6  | 0.2   | 1.1  | 1.2   | 1    | 2     |
| 5     | 1    | 0.2   | 1    | 2     | 1    | 2     |
| 6     | 1    | 0.2   | 2    | 1     | 1    | 2     |
| 7     | 0.7  | 0.7   | 2    | 0.8   | 0.8  | 2     |

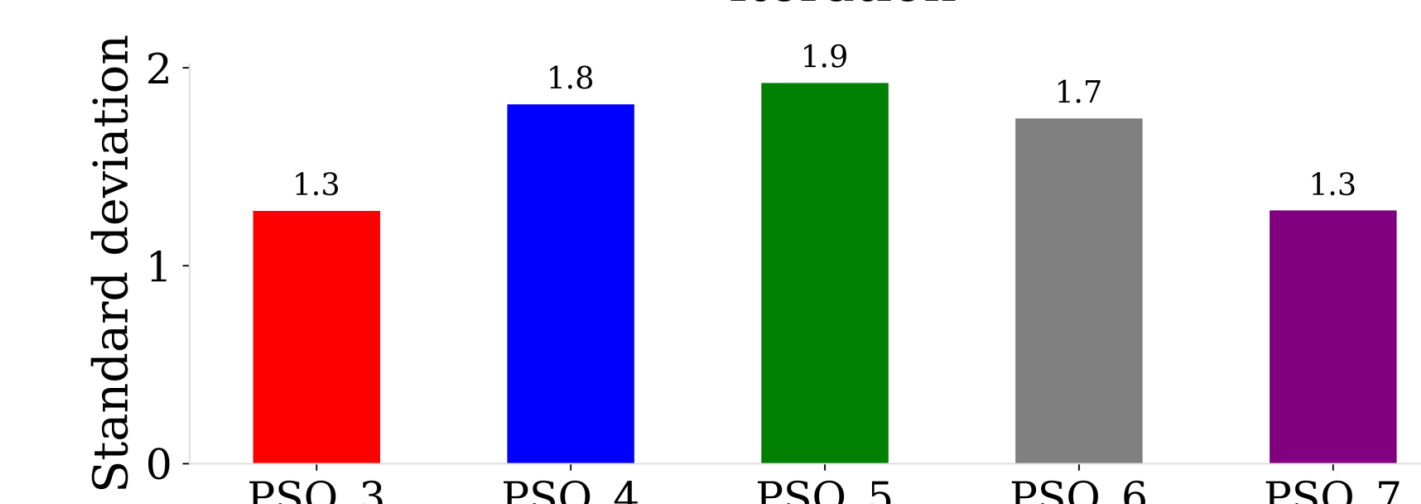
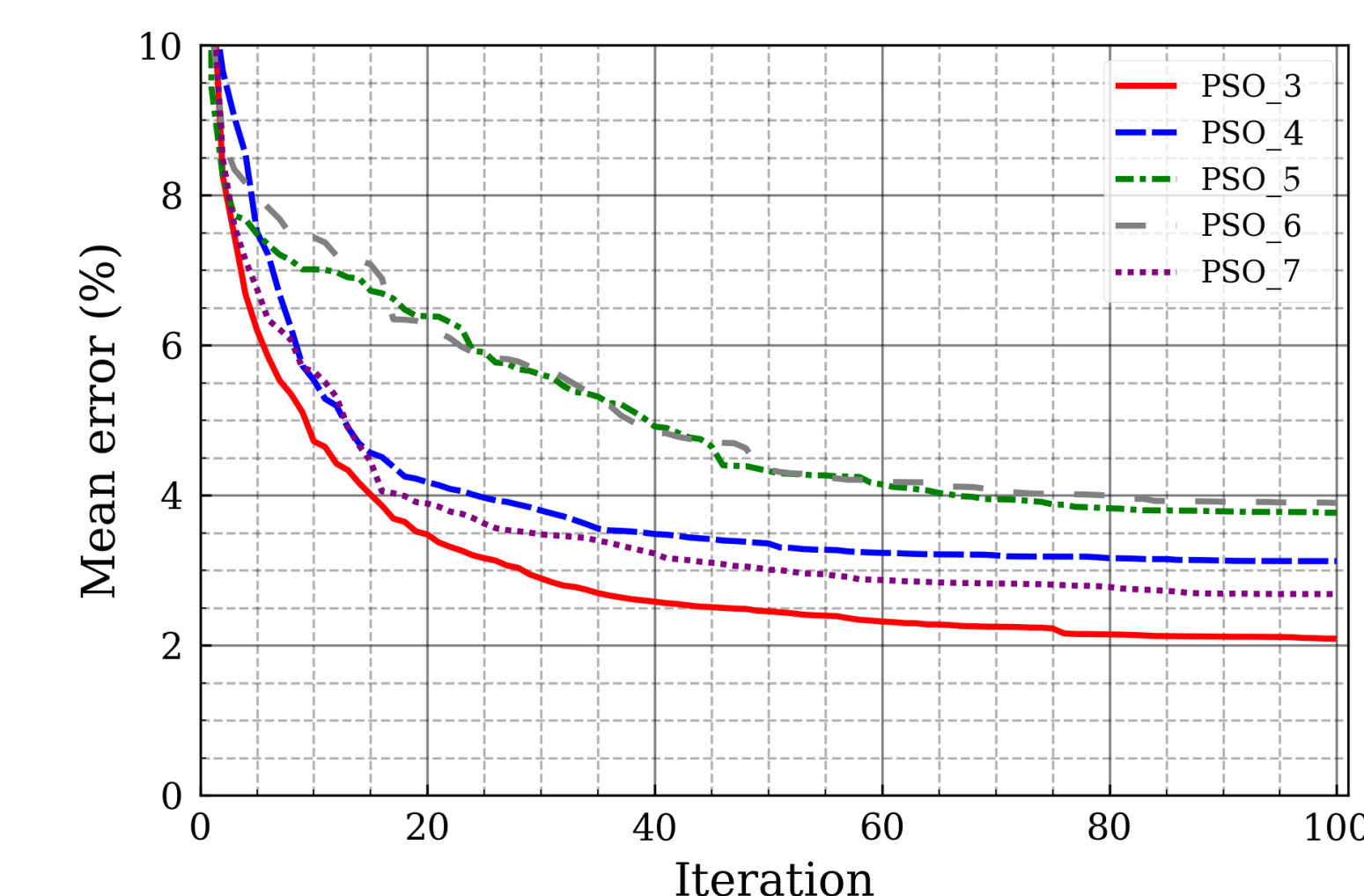
### • Comments

- Best results** for strategies 3 and 7
- Efficient strategies also present very **high convergence rate**
- Standard deviations are higher than GA indicating **lower reliability** for optimization quality

### • Performances

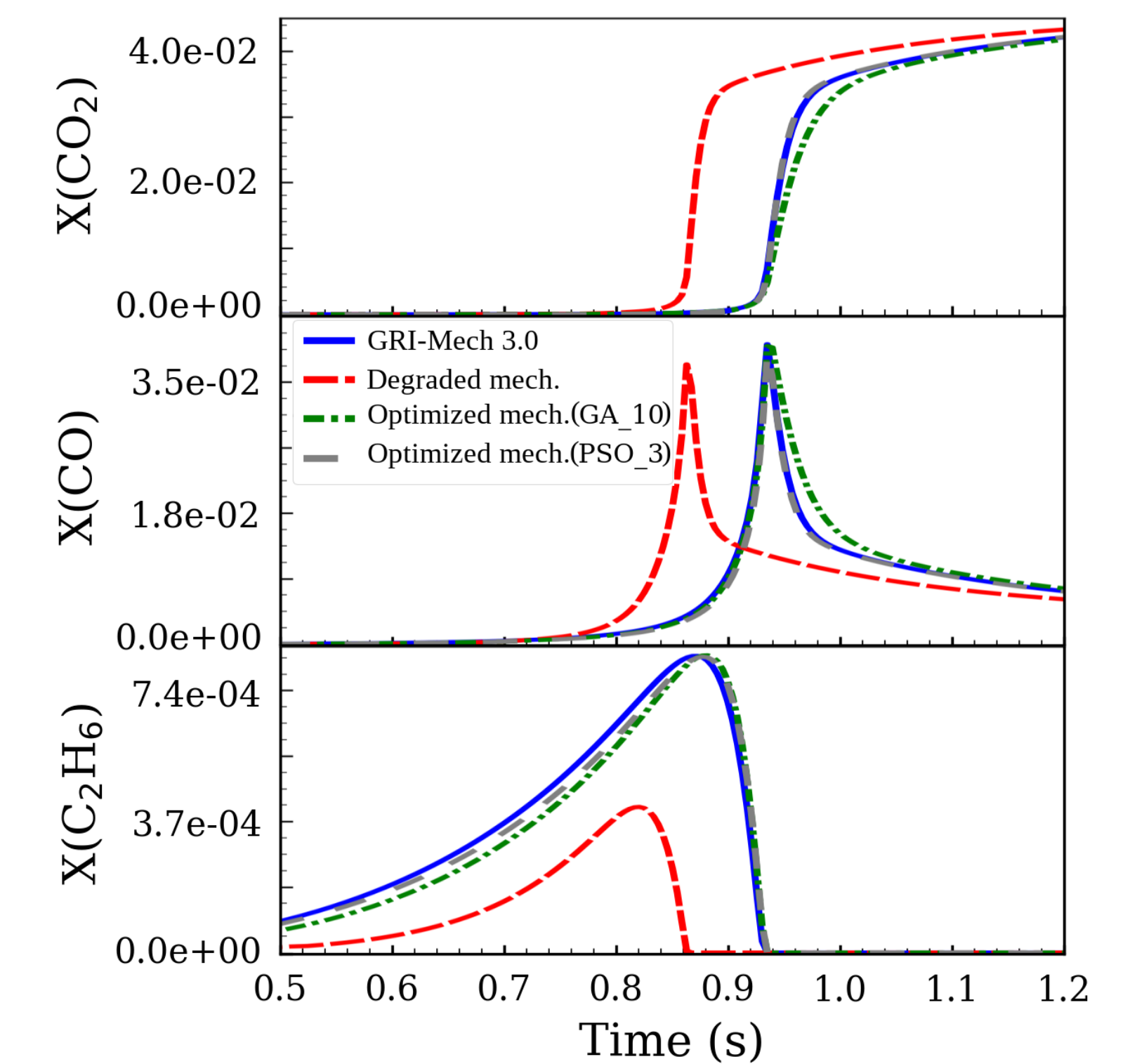
Each strategies repeated 20 times:

- Mean error is averaged over the 20 trials
- the standard deviation measured between trials is shown below



## 3. c. Simulation results

$\text{CH}_4/\text{air}$   $\Phi=0.5$   $T = 1500 \text{ K}$



## Conclusions

The comparison of the PSO to GA optimization approach led to the following observations:

- some strategies are **more efficient than GA**.
- those strategies come along with **very high convergence rates**
- high sensitivity** to the choice of parameters
- lower reliability** to the success of an optimization

Given the simplicity of the PSO approach, this work demonstrates the interest in considering PSO optimization as a good alternative to GA.

## References

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- [5] Pepiot-Desjardins P, Pitsch H. Combust. Flame 2008;154:67–81.