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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 algorithms 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

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

with: Er : relative error δ : 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 (children)
- 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

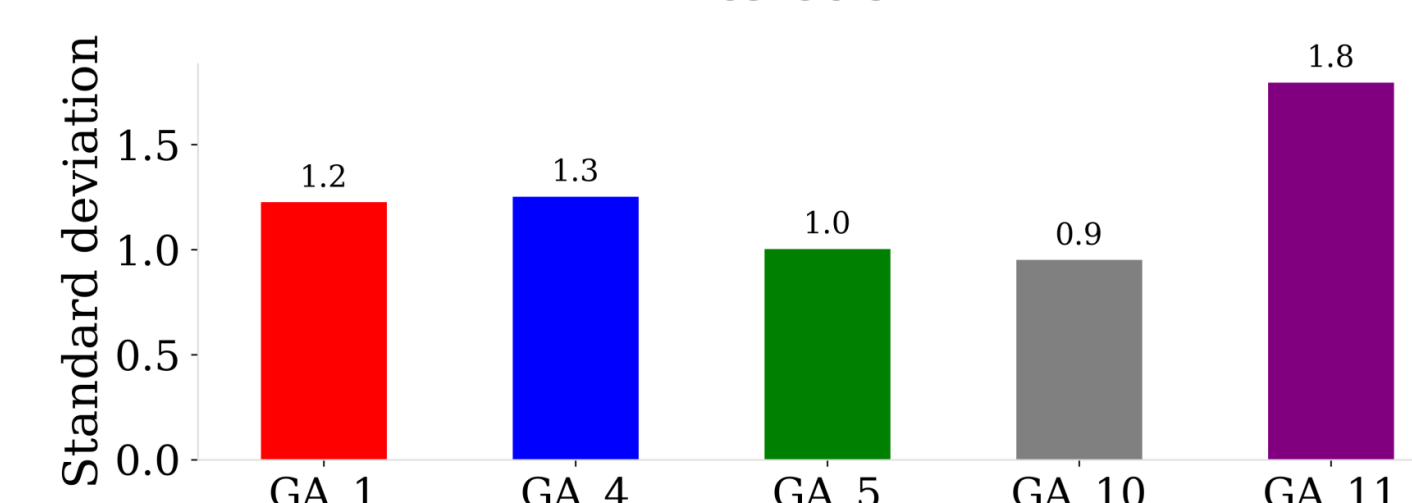
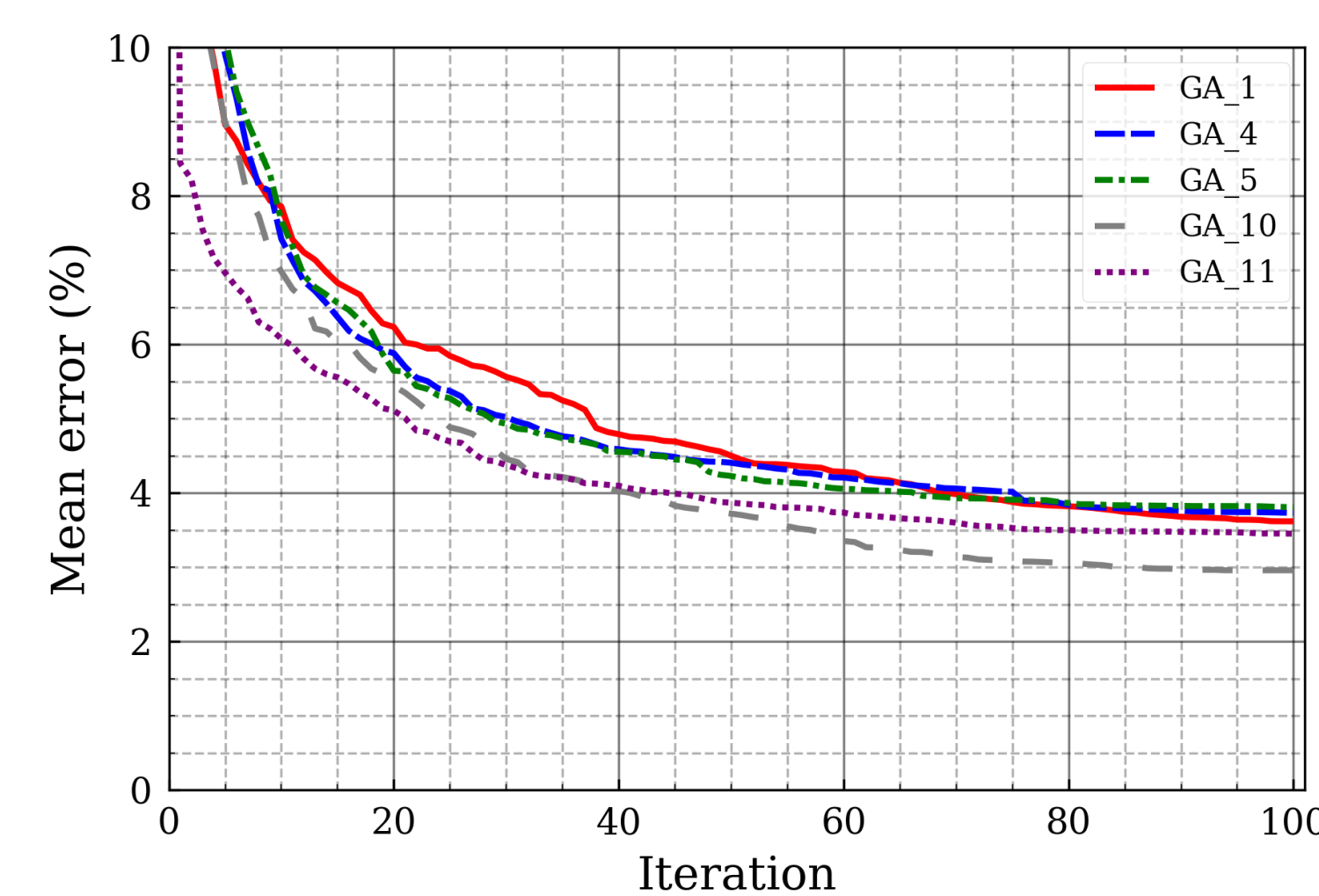
• Comments

- 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 :
 - CH₄/air
 - $\Phi = 0.5, 1.0, 1.5$
- $p = 10^5$ Pa / $T = 1050, 1500$ K

• 7 Targets

- ignition delay time
- temperature
- species: CH₄, CO, CO₂, C₂H₄, C₂H₆
- Kinetic mechanism**
- GRI-Mech 3.0 (53 sp. 325r.) [4]

• Degraded mechanism to be optimized

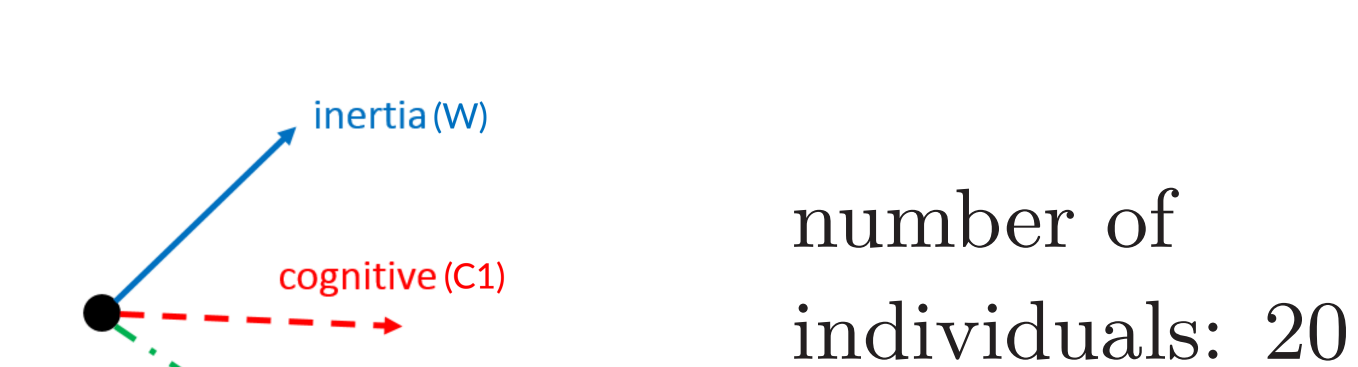
- the 7th most important reactions for each of the 7 targets randomly modified
- Importance evaluated on the basis of the direct interaction coefficients between a species A and a reaction r_i , (see ref. [5])

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



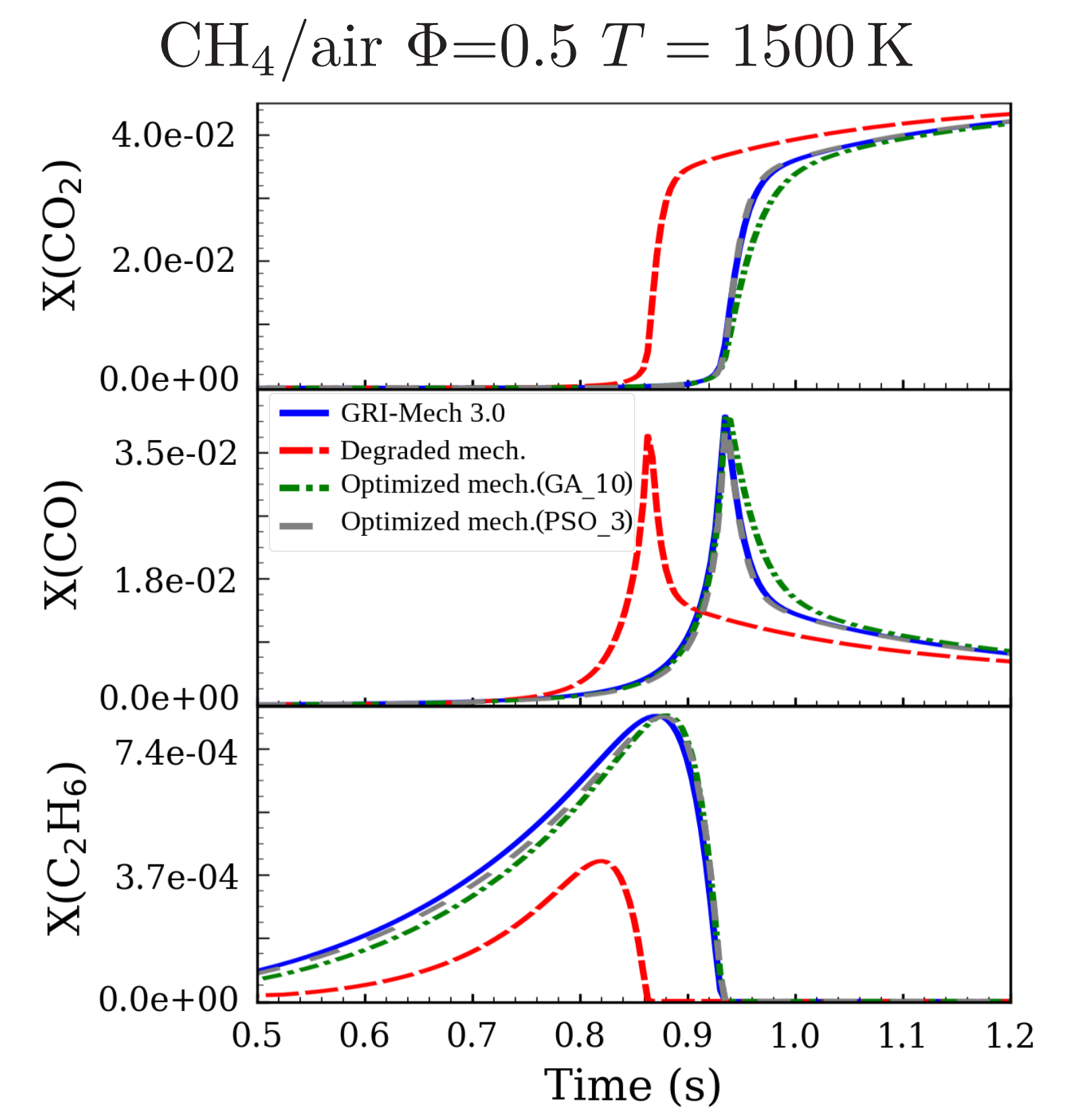
number of individuals: 20

| 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

3. c. Simulation results



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.

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