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

A. Matynia, P. Sambou, E. El Rassy

Sorbonne Université, Centre National de la Recherche Scientifique, UMR 7190, Institut Jean Le Rond d'Alembert, F-75005 Paris, France

alexis.matynia@sorbonne-universite.fr

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

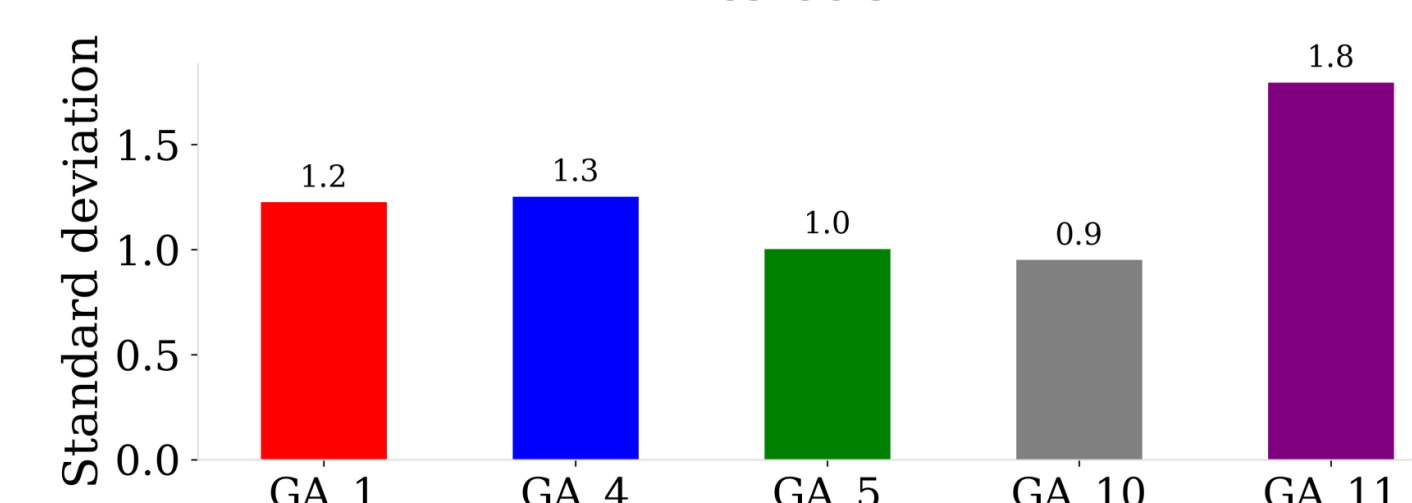
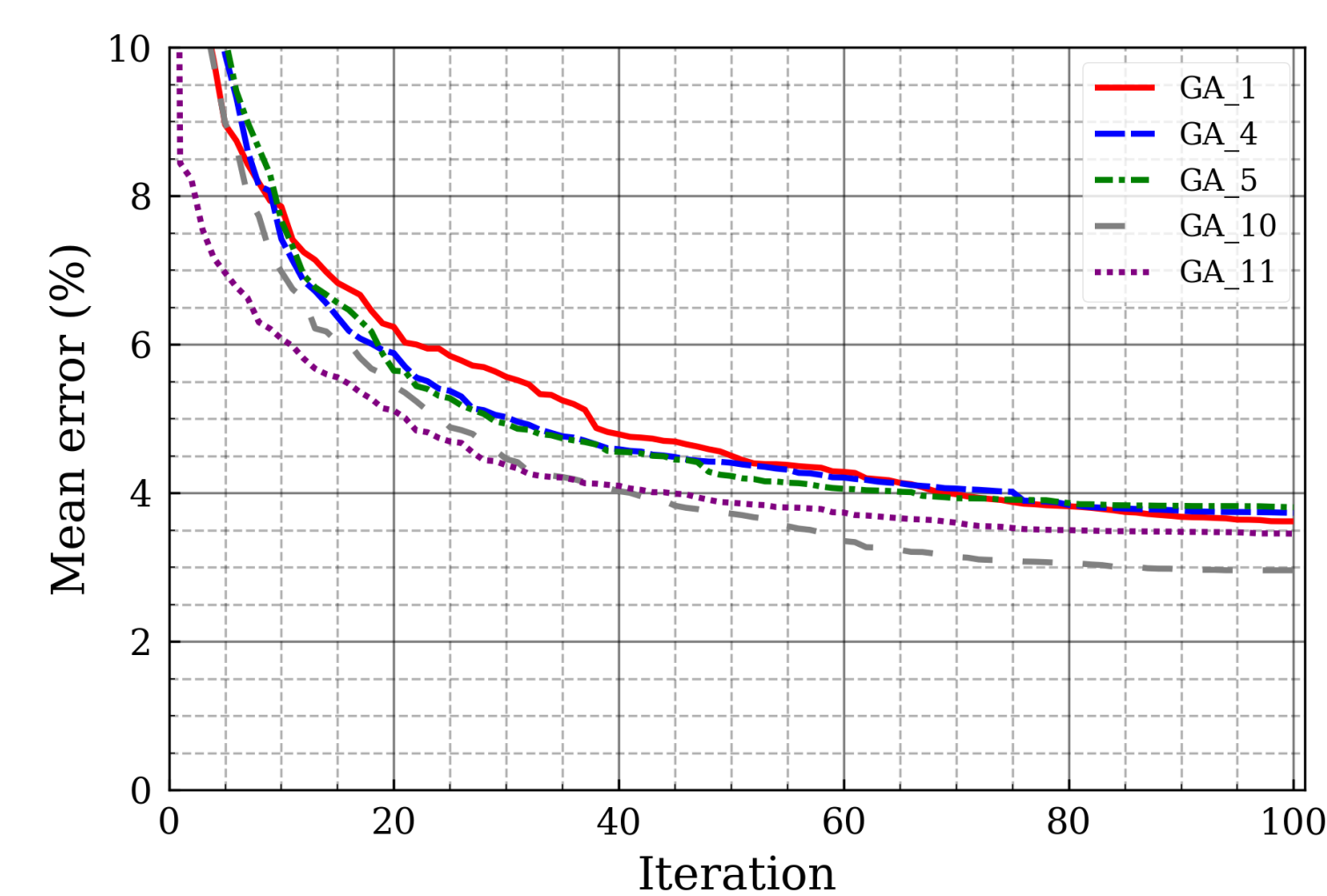
• Comments

- 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

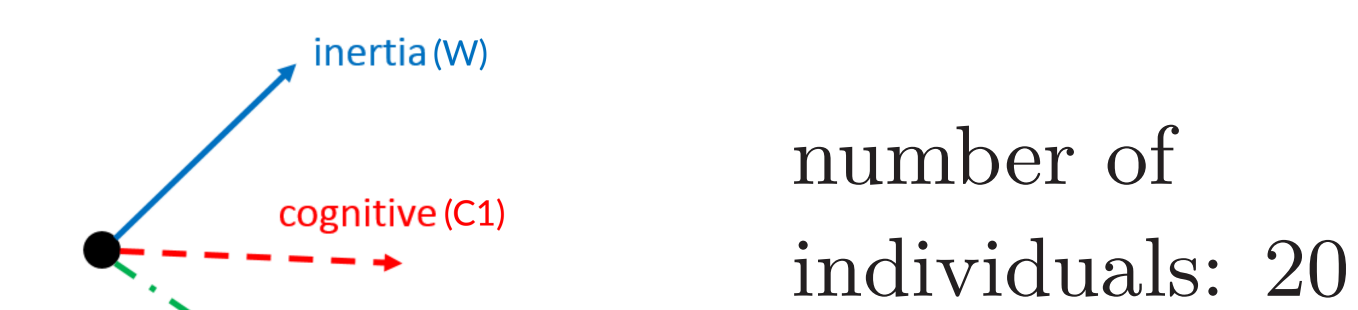
- the 7th most important reactions for each of the 7 targets randomly modified
- Importance evaluated on the basis of the direct interaction coefficients between a species A and a reaction r_i , (see ref. [5])

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



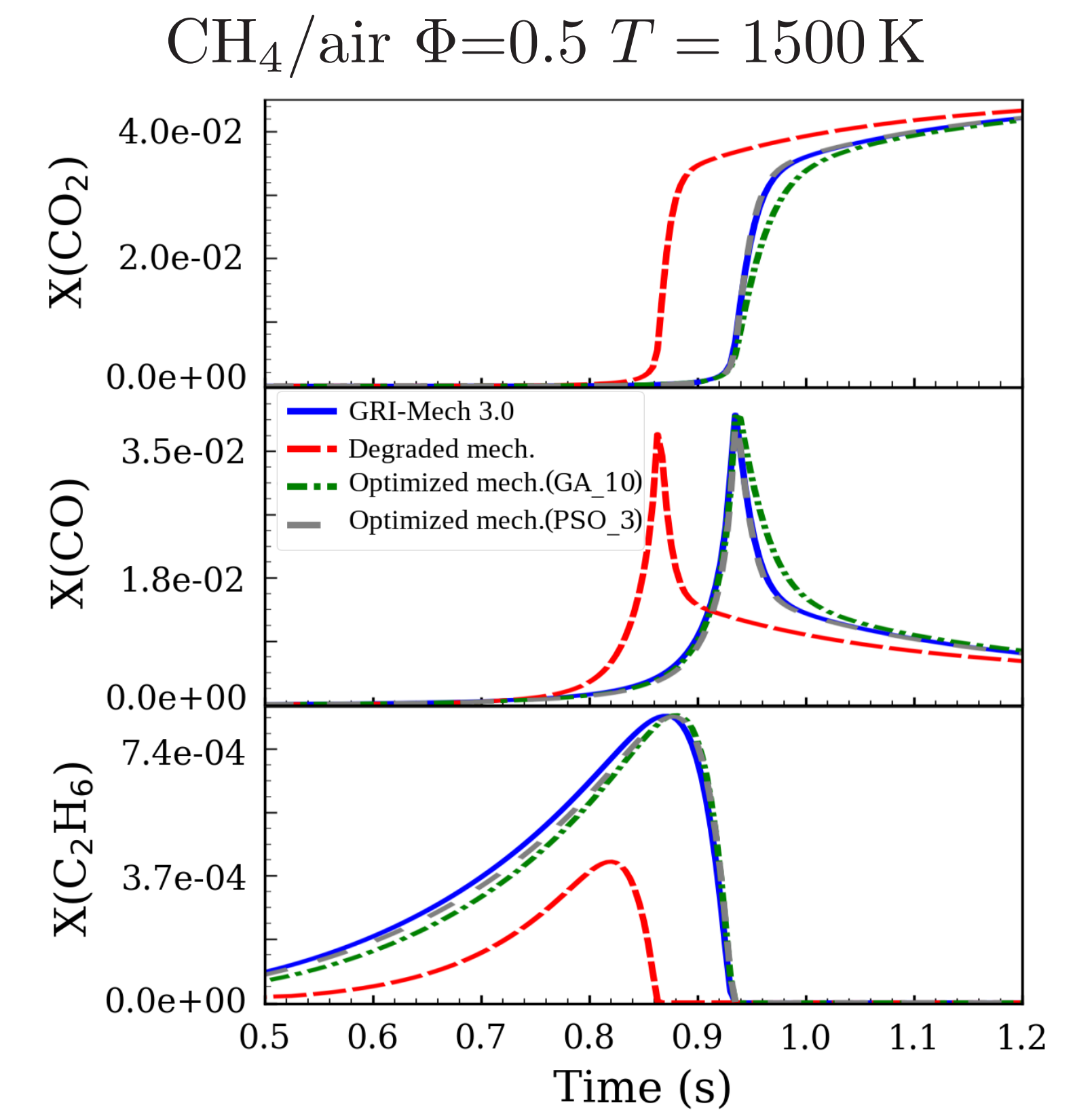
number of individuals: 20

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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