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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 evolutionnary 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**

$$Er(\delta) = 1 - \frac{\delta_{\text{opt}}}{\delta_{\text{ref}}}$$

- **T and species profiles**

$$Er(i) \approx \frac{|A_{\text{ref}} - A_{\text{opt}}|}{A_{\text{ref}}}$$

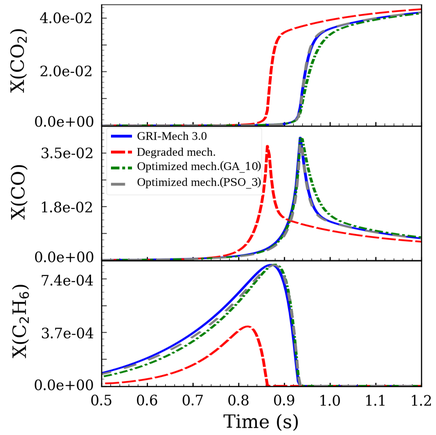
with: Er: relative error δ: ignition delay time A: area below the profile
ref / opt: simulation from reference / optimized mechanism

1. Simulations

- **6 Conditions**
  - Constant pressure & enthalpy reactor (Cantera [3])
  - composition :
    - CH_4/air
    - $\Phi = 0.5,\ 1.0,\ 1.5$
  - $p = 10^5$ Pa / $T = 1050,\ 1500$ K
- **7 Targets**
  - ignition delay time
  - temperature
  - species: CH_4, CO, CO_2, C_2H_4, C_2H_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. c. Simulation results

CH_4/air Φ=0.5 $T = 1500$ K



3. a. Optimization by Genetic Algorithm

- **Concept**

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

- **Strategies**

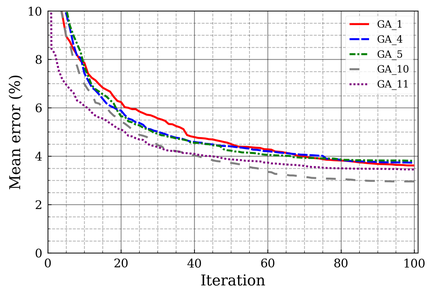
number of individuals: 20

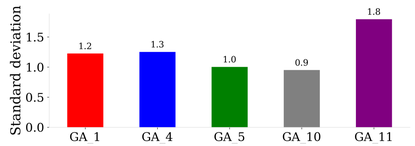
Strategies	Selection				Crossover (*)				Mutation (*)		
	Roulette	Rank	Geometric norm	Elitism	Simple	Multiple	Arithmetic	Heuristic	Uniform	Non-uniform	Boundary
1	x				2	2	4	4	3	3	2
2		x			2	2	4	4	3	3	2
3			x		2	2	4	4	3	3	2
4				x	2	2	4	4	3	3	2
5			x		**6**	**2**	**2**	**2**	3	3	2
6			x		**2**	**6**	**2**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

- **Performances**

each strategies repeated 20 times:
- Mean error is averaged over the 20 trials
- the standard deviation measured between trials is shown below





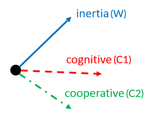
- **Comments**
  - Optimization efficiency seems **relatively insensitive to the strategy**
  - Strategies 10 and 11 show the best results indicating the importance of a good setting of the mutation rate.

3. b. Optimization by Particle Swarm Algorithm

- **Concept**

1. from randomly modified kinetic mechanisms a series of simulation is performed
2. 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
3. a new series of simulation is performed and the cycle is repeated

- **Strategies**

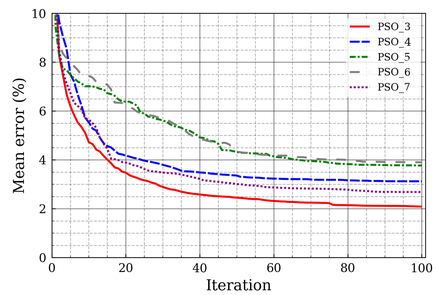


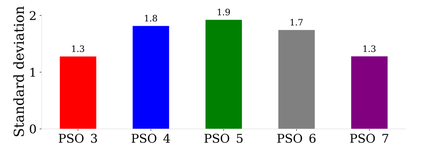
number of individuals: 20

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

- **Performances**

Each strategies repeated 20 times:
- Mean error is averaged over the 20 trials
- the standard deviation measured between trials is shown below





- **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

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

[1] Elliott L, Ingham DB, Kyne AG, Mera NS, Pourkashanian M, Wilson CW. Prog. Energy Combust. Sci. 2004;30:297–328.
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