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Large Scale Optimization Algorithms

UTC for Computational Engineering

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INTRODUCTION

The aim of this research is to develop ***large scale*** global optimization algorithms in the framework of expensive ***black-box*** functions, that produce reasonably good solutions with a limited number of function evaluations. We have used some of the current surrogate optimization approaches in order to suggest possible ways of combining and extending them to increase their efficiency. Our numerical simulations are based on a set of benchmark problems which acts as virtual black-box function, characterised by specific mathematical properties (i.e. non-linearity, multi-modality, convexity, etc.), that allow conclusions to be drawn about the search history and the convergence behaviour of the tested optimization strategies. Table 1 gives an overview of the surrogate models and update strategies (we have 12 different search strategies, most of them implemented in **OPTIMAT**). The numerical results for each search strategy are based on 5 different Design of Experiments (DoEs), generated via a *Spacefill* approach. The dimension of the DoE is computed considering $nDoE = PD \times \mathrm{D}$, where PD is the point density equal to 1, 2, 5 and D is the dimension of the problem (40 or 50). The simulation budget is equal to $2 \times nDoE$, where one-half is for the initial sampling plan and one-half for the infill points (i.e. number of iterations). In Figure 1 the objective functions are represented in 2 dimensions, however all the analyses are done in 50 and 40 dimension. Table 2 summarises the statistical results for all the search strategies taking into account only the final iteration. The ranking is based only on the mean value obtained from the final iteration.

Surrogate Model	Update strategy	Line plot color
Krig EI	Expected Improvement	----------------
Krig Optimum	Optimum	----------------
UKrig EI	Expected Improvement	----------------
UKrig Optimum	Optimum	----------------
Gaussian	Optimum	----------------
Cubic	Optimum	----------------
Cubic+Poly2Order	Optimum	----------------
Linear	Optimum	----------------
ThinPlate	Optimum	----------------
InvMultiquadratic	Optimum	----------------
Cubic+Poly1Order	Optimum	----------------
Best	Optimum	----------------

Table 1: Surrogate models, update strategies and line plot colours used in the history graph. Krig, Ukrig, CubicPoly1 and CubicPoly2 are Kriging, Universal Kriging and Cubic spline coupled with first and second order polynomial trend respectively. Best is based on a set of RBFs and uses a leave-one-out cross validation procedure for the tuning process.

NUMERICAL RESULTS

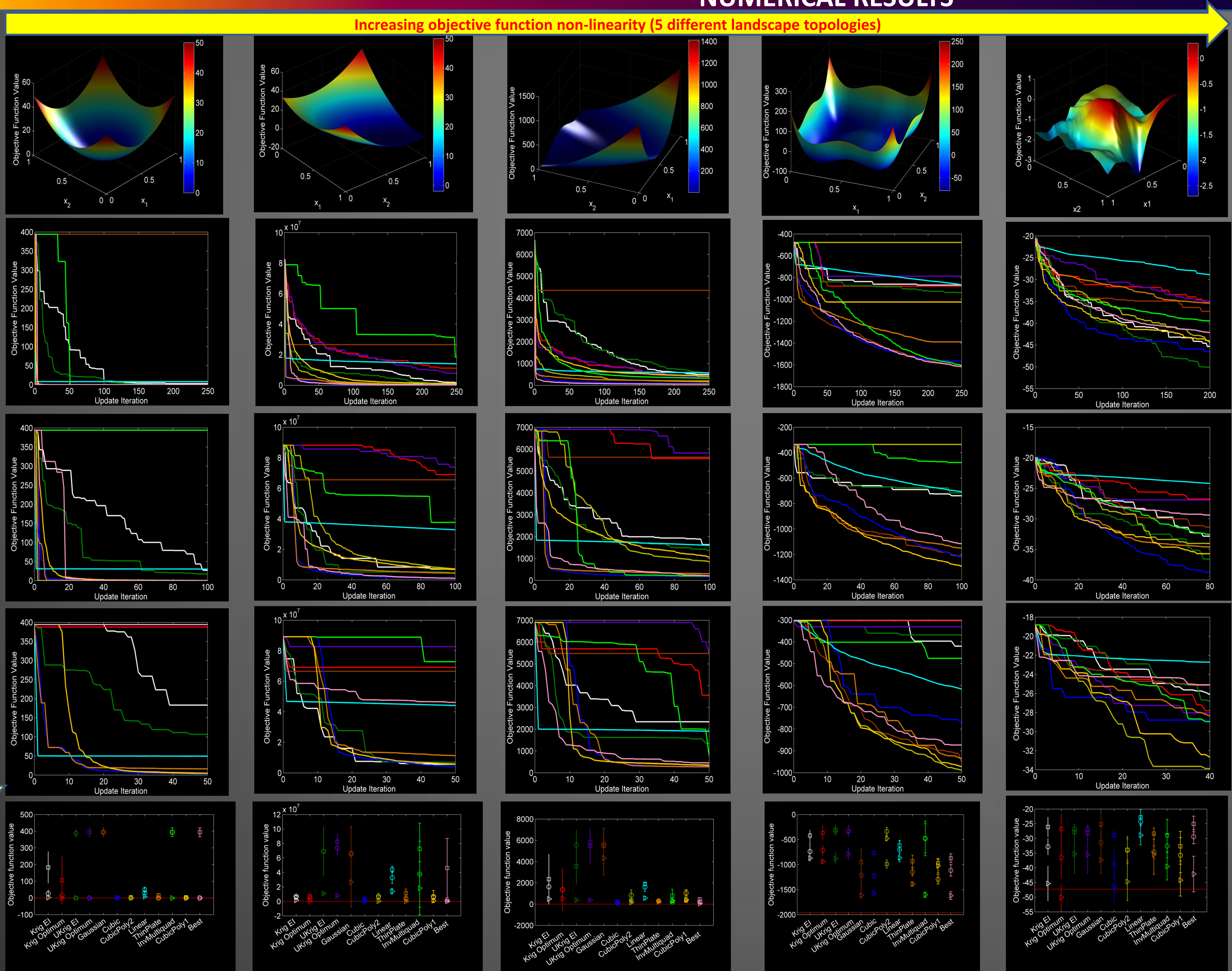

Figure 1: First row from left to right perspective view in 2 dimensions of the objective functions analysed, 4 analytical functions (Sphere, Trid, Rosenbrock, Styblinski-Tang), and one engineering function (Truss, maximisation of the vibration attenuation of a truss structure discretised with finite element Eulero-Bernoulli beams). Optimal values ($f_{Sphere} = f_{Rosenbrock} = 0, f_{Trid} = -22050, f_{Styblinski-Tang} = -1958,30, f_{Truss} = -47,28$), the Sphere, Trid, Rosenbrock and Styblinski-Tang functions are optimised in 50 dimensions while the truss is optimised in 40 dimensions. Second, third and fourth row, history plots of the 12 search strategies (with $PD = 5, 2, 1$ respectively). Fifth row, mean and standard deviation of the final iteration taking into account 5 different DoEs (triangle, circle and square markers are for $PD = 5, 2, 1$ respectively).

Sphere

	PD = 5			PD = 2			PD = 1		
RSM	Mean	Std. Dev.	Rank	Mean	Std. Dev.	Rank	Mean	Std. Dev.	Rank
Krig EI	2,81E+00	2,22E+00	10	2,71E+01	2,13E+01	9	1,83E+02	9,40E+01	7
Krig Optimum	3,08E-02	8,72E-03	7	1,74E+01	1,18E+01	8	1,07E+02	1,40E+02	6
UKrig EI	2,35E-12	9,34E-13	1	1,68E-11	3,15E-11	3	3,87E+02	2,23E+01	8
Ukrig Optimum	2,80E-12	8,53E-13	2	1,55E-11	2,79E-11	2	3,94E+02	2,62E+01	9
Gaussian	3,94E+02	2,62E+01	12	3,94E+02	2,62E+01	11	3,94E+02	2,62E+01	9
Cubic	5,63E-03	1,43E-03	6	1,23E-01	8,83E-02	4	3,18E+00	1,51E+00	1
CubicPoly2	1,02E-11	1,58E-11	3	7,94E-12	5,84E-12	1	4,89E+00	4,31E+00	3
Linear	7,89E+00	1,39E+00	11	3,04E+01	7,90E+00	10	4,94E+01	1,56E+01	5
ThinPlate	4,81E-03	1,82E-03	5	3,52E-01	1,95E-01	7	1,59E+01	9,42E+00	4
InvMultiquadratic	4,29E-02	1,11E-02	8	3,94E+02	2,62E+01	11	3,94E+02	2,62E+01	9
CubicPoly1	4,44E-04	1,69E-04	4	2,63E-01	1,29E-01	5	4,33E+00	3,18E+00	2
Best	5,80E-02	1,73E-02	9	3,49E-01	1,06E-01	6	3,94E+02	2,62E+01	9

Trid

	PD = 5			PD = 2			PD = 1		
RSM	Mean	Std. Dev.	Rank	Mean	Std. Dev.	Rank	Mean	Std. Dev.	Rank
Krig EI	1,66E+06	1,41E+06	7	7,01E+06	3,27E+06	6	5,60E+06	1,72E+06	2
Krig Optimum	5,13E+05	2,38E+05	5	4,69E+06	1,18E+06	4	6,98E+06	3,73E+06	5
UKrig EI	1,11E+07	1,75E+06	9	6,90E+07	1,51E+07	11	6,92E+07	3,37E+07	10
Ukrig Optimum	7,86E+06	1,32E+06	8	7,38E+07	9,95E+06	12	8,27E+07	9,78E+06	12
Gaussian	2,66E+07	3,48E+07	12	6,56E+07	3,63E+07	10	6,66E+07	3,71E+07	9
Cubic	8,78E+04	4,02E+04	1	8,24E+05	3,28E+05	1	3,96E+06	8,45E+05	1
CubicPoly2	2,59E+05	3,10E+05	3	7,22E+06	3,48E+06	7	5,60E+06	2,33E+06	3
Linear	1,41E+07	3,56E+06	10	3,28E+07	8,00E+06	8	4,42E+07	4,23E+06	7
ThinPlate	2,68E+05	1,54E+05	4	4,35E+06	1,36E+06	3	1,13E+07	5,72E+06	6
InvMultiquadratic	1,84E+07	3,64E+07	11	3,76E+07	4,56E+07	9	7,28E+07	3,52E+07	11
CubicPoly1	1,10E+06	1,37E+06	6	6,81E+06	8,33E+06	5	5,80E+06	2,51E+06	4
Best	2,54E+05	3,97E+05	2	1,04E+06	9,57E+05	2	4,62E+07	4,08E+07	8

Rosenbrock

	PD = 5			PD = 2			PD = 1		
RSM	Mean	Std.Dev.	Rank	Mean	Std.Dev.	Rank	Mean	Std.Dev.	Rank
Krig EI	4,93E+02	1,22E+02	9	1,63E+03	1,02E+03	9	2,34E+03	2,37E+03	9
Krig Optimum	5,49E+02	2,12E+02	10	1,37E+03	7,89E+02	7	1,36E+03	1,97E+03	7
UKrig EI	3,92E+02	1,17E+02	7	5,57E+03	1,37E+03	10	3,56E+03	1,66E+03	10
Ukrig Optimum	3,84E+02	5,84E+01	6	5,82E+03	5,04E+02	12	5,46E+03	1,58E+03	11
Gaussian	4,35E+03	1,67E+03	12	5,63E+03	1,48E+03	11	5,48E+03	1,67E+03	12
Cubic	6,39E+01	8,37E+00	2	1,68E+02	1,84E+01	1	2,50E+02	2,57E+01	1
CubicPoly2	1,61E+02	6,20E+01	3	8,41E+02	4,95E+02	5	3,54E+02	7,03E+01	4
Linear	5,73E+02	1,63E+02	11	1,60E+03	4,11E+02	8	1,91E+03	1,17E+02	8
ThinPlate	2,04E+02	6,93E+01	4	3,03E+02	1,06E+02	4	2,78E+02	4,82E+01	2
InvMultiquadratic	3,27E+02	1,67E+02	5	2,01E+02	8,32E+01	2	7,93E+02	5,96E+02	6
CubicPoly1	4,17E+02	2,21E+02	8	1,06E+03	2,95E+02	6	3,38E+02	4,73E+01	3
Best	5,10E+01	1,58E+00	1	2,07E+02	8,56E+01	3	4,54E+02	1,63E+02	5

Styblinski-Tang

	PD = 5			PD = 2			PD = 1		
RSM	Mean	Std. Dev.	Rank	Mean	Std. Dev.	Rank	Mean	Std. Dev.	Rank
Krig EI	-8,69E+02	3,85E+01	9	-7,39E+02	1,96E+02	6	-4,20E+02	1,06E+02	9
Krig Optimum	-9,37E+02	4,82E+01	7	-7,16E+02	1,03E+02	7	-3,69E+02	1,44E+02	10
UKrig EI	-8,78E+02	1,05E+02	8	-3,36E+02	7,94E+01	10	-3,03E+02	9,25E+01	12
Ukrig Optimum	-7,87E+02	1,16E+02	11	-3,36E+02	7,94E+01	10	-3,31E+02	1,08E+02	11
Gaussian	-1,61E+03	5,98E+01	2	-1,21E+03	3,02E+02	3	-9,53E+02	2,54E+02	3
Cubic	-1,57E+03	4,06E+01	4	-1,22E+03	4,01E+01	2	-7,71E+02	3,61E+01	6
CubicPoly2	-4,77E+02	4,93E+01	12	-3,36E+02	7,94E+01	10	-9,90E+02	8,13E+01	1
Linear	-8,66E+02	7,63E+01	10	-7,07E+02	1,88E+02	8	-6,17E+02	8,49E+01	7
ThinPlate	-1,39E+03	3,98E+01	5	-1,15E+03	7,72E+01	4	-9,35E+02	1,24E+02	4
InvMultiquadratic	-1,60E+03	5,38E+01	3	-4,78E+02	3,47E+02	9	-4,76E+02	2,91E+02	8
CubicPoly1	-1,02E+03	1,47E+02	6	-1,29E+03	9,15E+01	1	-9,72E+02	7,69E+01	2
Best	-1,62E+03	7,74E+01	1	-1,12E+03	1,15E+02	5	-8,73E+02	8,79E+01	5

Truss

	PD = 5			PD = 2			PD = 1		
RSM	Mean	Std. Dev.	Rank	Mean	Std. Dev.	Rank	Mean	Std. Dev.	Rank
Krig EI	-4,53E+01	5,91E+00	3	-3,29E+01	2,79E+00	6	-2,61E+01	3,31E+00	9
Krig Optimum	-5,01E+01	4,32E+00	1	-3,66E+01	7,09E+00	2	-2,68E+01	5,10E+00	8
UKrig EI	-3,53E+01	6,63E+00	11	-2,68E+01	1,56E+00	11	-2,78E+01	2,75E+00	7
Ukrig Optimum	-3,54E+01	6,49E+00	9	-2,69E+01	1,93E+00	10	-2,80E+01	2,44E+00	6
Gaussian	-3,73E+01	4,74E+00	8	-3,14E+01	5,40E+00	8	-2,52E+01	4,18E+00	10
Cubic	-4,65E+01	5,03E+00	2	-3,88E+01	4,53E+00	1	-2,89E+01	1,33E+00	4
CubicPoly2	-4,47E+01	6,49E+00	4	-3,40E+01	4,62E+00	5	-3,39E+01	3,70E+00	1
Linear	-2,89E+01	3,29E+00	12	-2,42E+01	1,46E+00	12	-2,27E+01	2,52E+00	12
ThinPlate	-3,54E+01	6,82E+00	10	-3,46E+01	2,05E+00	4	-2,84E+01	1,94E+00	5
InvMultiquadratic	-3,95E+01	4,62E+00	7	-3,26E+01	4,01E+00	7	-2,90E+01	5,41E+00	3
CubicPoly1	-4,42E+01	5,42E+00	5	-3,57E+01	5,98E+00	3	-3,27E+01	5,05E+00	2
Best	-4,21E+01	6,06E+00	6	-2,94E+01	2,41E+00	9	-2,51E+01	2,67E+00	11

Table 1: Numerical results for the final iteration, in terms of mean, standard deviation and search strategy ranking (best solution for the final iteration in red).

CONCLUSIONS AND FUTURE WORK

In this work we have focused our attention at the impact of problem dimensionality, size of DoE and landscape topology over 12 different search strategies, based on Kriging and Radial Basis Functions. In general the results have shown that for an unknown landscape in high dimensions and with a poor sampling plan, a good approach is to choose a simple surrogate model (e.g. Cubic spline with or without polynomial trend). Kriging methodologies are more flexible from a theoretical point of view, but they require an expensive tuning process and do not perform well in most of the cases analysed. There are four main avenues of further work required for this project: 1) a statistical study of the search strategies in order to compute the probability that one strategy performs well in comparison to the other strategies at each iteration; 2) the development of a set of guidelines for large scale black-box optimizations in the framework of surrogate models; 3) the development of new and more flexible optimization strategies; 4) test these new algorithms with real engineering problems to ensure their suitability for industrial purposes. (***FUNDING SOURCE: Clean-Sky Project***).

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