Very Large Scale Global Optimization with Randomised Optimisation Algorithms in DAPHNE

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Globalna optimizacija zelo velikih dimenzij z naključenimi optimizacijskimi algoritmi v DAPHNE

Povzetek — Ta članek predstavlja globalno optimizacijo zelo velikih dimenzij (GOZVD) z naključenimi optimizacijskimi algoritmi (NOA) v DAPHNE (Integracija kanalov za analizo podatkov za upravljanje velikih podatkov, HPC in strojno učenje). Najnovejša programska oprema iz DAPHNE repozitorija `daphne` na računu GitHub `daphne-eu`, z uporabo zadnje veje `main` iz julija 2024 (548ea01), je prevedena in nameščena na superračunalniku EuroHPC Vega v Mariboru, Sloveniji. Namestitev je nato pognana z uporabo Slurma za izvedbo niza zagonov ROA z različnimi razredi nastavitev, ob povečevanju števila optimiziranih parametrov na sto tisoč. Nazadnje so poročani in analizirani še novo dobljeni računski rezultati iz zagonov ROA.

Abstract — This paper presents the Very Large Scale Global Optimization (VLSGO) in context of Randomised Optimization Algorithms (ROA) in DAPHNE (Integrated Data Analysis Pipelines for Large-Scale Data Management, HPC, and Machine Learning). The latest software from DAPHNE repository `daphne` at the GitHub account `daphne-eu`, using the last July 2024 commit to the `main` branch (548ea01), is compiled and deployed on EuroHPC Vega supercomputer in Maribor, Slovenia. The compilation is then deployed using Slurm to execute a set of ROA runs with different configuration classes for VLSGO, increasing the optimized parameter sizes. Finally, the newly obtained computational results from ROA runs are reported and analysed.

1 Introduction

This paper presents the Very Large Scale Global Optimization (VLSGO) in context of Randomised Optimization Algorithms (ROA) in DAPHNE (Integrated Data Analysis Pipelines for Large-Scale Data Management, HPC, and Machine Learning) [1–4]. VLSGO as characterized in this paper is with ten thousand floating-point encoded parameters dimension sizes and above, where ROA with large population sizes are applied as well (here, in size of a thousand). When benchmarking ROAs, they also need to be run multiple times, with independent and different random number seeds, because ROAs can be statistically evaluated only with aggregated statistics from these independent runs [5], to further use this in Machine Learning [6].

Some results were already presented at [7, 8] and are now extended to VLSGO and more recent DAPHNE software. Progress on High-Performance Computing (HPC), with DAPHNE, and Computational Intelligence (CI, as defined through IEEE CIS [9]) in Slovenia has also previously been reported in e.g. [10–12], and with EuroHPC Vega the use of HPC with latest CI and DAPHNE has become more accessible. Therefore, this paper benchmarks the latest progress in ROA and DAPHNE with Vega, where latest July 2024 compilation, deployment, and results from DAPHNE is performed, where a ROA algorithm is executed on VLSGO.

In the next section, the related work is described, then the methods are described in Section 3. Section 4 provides the results and Section 5 the conclusion.

2 Related Work

ROA in DAPHNE has already been identified as an opportunity to scale structures like matrices in [10] and an implementation was also deployed on EuroHPC Vega [7], implemented in DaphneDSL [13]. Additionally to be a partner in the DAPHNE project, the decision to choose a HPC DSL is substantiated further especially after considering that University of Maribor is part of SLING (Slovenian National Supercomputing Network), the coordination body of various HPCs in Slovenia, including the first EuroHPC supercomputer [14], the Vega with 240 A100 GPUs and 122 thousand CPU (Central Processing Unit) cores [15]. More about how to deploy ROA in DAPHNE on EuroHPC was already presented in [7] and more about DAPHNE in Maribor is in [4, 7, 10, 12, 15–17].

The DaphneDSL syntax [13] is inspired by C/Java-like languages and the DSL is a case-sensitive language inspired by ML systems as well as languages and libraries

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for numerical computation like Julia, Python NumPy, R, and Apache SystemDS DML [18], but also with compiler hints for data/operator placement (i. e. local/distributed, CPU/GPU/FPGA, computational storage, still in experimental state and not guaranteed by the compiler) [13].

2.1 Population-based Randomised Optimization Algorithms

Population-based ROAs are surveyed in works like [19–26], with several CI applications like [24,27–30]. A sample ROA consists of e.g. an evolutionary loop [31], within which are evolved new population D-dimensional population vectors $\mathbf{x}_i$, $\forall i \in \{1, 2, ..., NP\}$. During each generation step number $g \in \{1, 2, ..., G\}$, on the population, computational operators are performed like mutation, crossover, and selection, until a termination criterion is satisfied, like a fixed number of maximum fitness evaluations (*MAX_FES*). ROA has also been winning competitions at GECCO [32] and applied in context of HPC in works like [33], where a large number of fitness evaluations was executed. Also, parallelization of benchmarking using HPC, from text summarization in natural language processing, glider piloting in deep-sea missions, and search algorithms in computational intelligence has been presented in [12] and then reflected for generative AI in [11]. As indicated further for [34], “Traditionally, single objective benchmark problems are also the first test for new evolutionary and swarm algorithms,” therefore in this paper a challenging single-objective optimisation function HappyCat [35] is applied to test a ROA on VLSGO, where the fitness evaluation of a numerical input vector $\mathbf{x}$ is computed by the function $f = \left(\left(\sum\left(x^2\right) - 10\right)^2\right)^{0.125} + \left(\sum\left(x^2\right)/2 + \sum\left(x\right)\right)/10 + 0.5$.

3 Methods: VLSGO with ROA in DAPHNE

The latest software from DAPHNE repository `daphne` at the GitHub account `daphne-eu` using the last July 2024 commit to the `main` branch `548ea01` as seen in Figure 2, is compiled as seen in Figure 3 taking several hours to compile and deployed on EuroHPC Vega supercomputer in Maribor, Slovenia. This compilation is also possible much faster due to CMake, parallel in minutes, if adding more compute resources, while recompilations during development of reprogrammed code parts are down to seconds and well supported in open or closed source code editors like Vim and Qt Creator, or Visual Studio Code. The DaphneDSL code snippet to evaluate a fitness function f is provided in Figure 1: the arithmetics is listed in line 2, while the function definition and input type parameter x is defined as `matrix<f64>`, a 64-bit floating-point matrix, processed with the DaphneDSL kernel operations (see [7] for their list in f on CPU).

The compilation is deployed using Slurm and large maximum stack size, to execute a set of ROA runs with different configuration classes for VLSGO (line 1: scaled from scale level $S = 1$ to $S = 10$), increasing the optimized parameter sizes (line 3: dimensions per ten thousand) and the allowed runtime according to this increase (line 8: 288 minutes per scaling level S, which is 28880 minutes for $D = 100.000$, i.e. two days for the largest configurations expecting to run the longest) as seen in Figure 4. If rerun with same parameters, algorithm results are reproducible and provide same output numbers.

4 Results

The optimisation results from the ROA runs (fitness convergence through generations) as explained in the above deployment preparation, are presented in Figure 5 as a set of convergence graphs, in configurations with dimensions $D = 1000$ and population sizes NP from 10.000 to 100.000 in increases of 10.000 as the scaled parameter classes (S from 1 to 10), capped up to the allocated time limit for each run.

Considering that the allocated time limit might stop an execution of a task, the plots in Figure 5 ran with this timing stopping condition up to their allocated time, all jobs started, and produced useful output results. The plots are drawn after all tasks have executed the allocated runs. As the runs with dimension ten thousand were running the longest, to cap the runtimes on the `cpu` partition, the multiplier of 288 minutes per scale S was used as shown in Figure 4 on line 8. All jobs have successfully reached target generations of 300 for the VLSGO tasks, except 4 cancelled earlier by Slurm due to timeout on node cn0514 (jobs 31746064 on $S = 5$, $RNi = 6$ at $G = 298$; 31746065 on $S = 3$, $RNi = 6$ and $RNi = 1$ both at $G = 289$) and cn0570 (31746113, $G = 269$).

For each of the runs plotted, it is observed that the fitness function optimised by the ROA is successfully improving, hence, the ROA CI is performing its main functionality of optimisation.

Further, using Universal Machine Learning Analysis Utility (Umlaut) from GitHub `https://github.com/daphne-eu/umlaut`, the resource usage is tracked during execution. As an example, for configuration $D = 10.000$, $NP = 1000$, the total runtime over these independent runs is seen in Figure 6. Furthermore, Figures 7 and 10 provide usage of memory and CPU resources, respectively. The memory usage plot peeks at approximately 105.87 MB for these runs, by initially rising to roughly 89 MB and then staying almost all of the time at that usage, slightly varying because of iterative allocations. As memory was seen increasing during the run, in meanwhile after experiments have already been done in August using lates July code updates and by the time of revision of this paper in September, also for loops [17], the implementation of allocations has been upgraded in the language implementation with newest

```
1 def eval_f(x: matrix<f64>) -> matrix<f64> {
2     return ( (sum(x * x, 0) - 10) ^ 2 ) ^ 0.125 + ( sum(x * x, 0) / 2 + sum(x) ) / 10 + 0.5;
3 }
```

Figure 1: Fitness function f evaluation snippet in DaphneDSL.

```
git clone https://github.com/daphne-eu/daphne.git
```

Figure 2: Cloning the DAPHNE main repository from daphne-eu repository of daphne-eu at GitHub, from July 26, 2024.

```
[DAPHNE]..Successfully built Daphne://daphne (took 4h 37min 624ms 452us 620ns)........................[31.07.24 15:22:43]
```

Figure 3: Output feedback after compiling the latest codes on EuroHPC Vega using a single Slurm task.

```
for S in {1..10}; do
 for NP in 1000; do
  D=${S}0000
  echo D=$D NP=$NP
  for RNi in {1..10}; do
   echo -n .
   { time srun --mpi=none \
    --time $((288*$S)) --mem=${S}G \
    ../daphneeu.sif \
    ./run-daphne.sh roa.d \
    D=$D NP=$NP RNi=$RNi \
    > results-D-$D-NP-$NP-RNi-$RNi-out.txt &
   } 2> time-D-$D-NP-$NP-RNi-$RNi-out.txt
  done #RNi
 done #NP
done #D

wait
```

Figure 4: Deploying ROA on EuroHPC Vega with Slurm, scaling the optimized dimension sizes.

software release (version 0.3) and additional regular updates.

A plotting of run times over scaling level S for D is seen in Figures 8 and 9, where runtime dash-dotted linear fit of data points is seen increasing with S. For $RNi = 1$ (the first run) of $D = 10.000$ (smallest S) and $RNi = 4$ (typical, median run) of $D = 100.000$ (largest S), plots for CPU load are drawn in Figure 10. CPU load is baselined at 100% (one thread) and the jitters with higer loads are attributed to multi-threaded executions of DAPHNE kernels with Basic Linear Algebra Subprograms (BLAS). Deviations in running time among independent runs were observed and could be studied further.

5 Conclusion

This paper presented a pipeline benchmarking with latest July 2024 deployment of DAPHNE (Integrated Data Analysis Pipelines for Large-Scale Data Management, HPC, and Machine Learning) on EuroHPC Vega, running ROA CI tasks with Slurm on VLSGO (Very Large Scale Global Optimization). An example ROA benchmarking pipeline scenario using HappyCat function was benchmarked and VLSGO scaling results were discussed, together with resource usage as obtained through Umlaut. All runs have successfully been running, optimizing fitness, and their provided resource usage reported.

Future work still includes further deployment (e.g. to additional hardware and improved scheduling of workload in distributed multi-node Slurm tasks), comparisons of benchmarking results [11, 12], integrated benchmarking, benchmarking using updated versions of DAPHNE software, and extending the ROA scenario and library as well as research in other use cases, especially from CI and remote sensing, including underwater missions like ocean glider path planning and text summarization.

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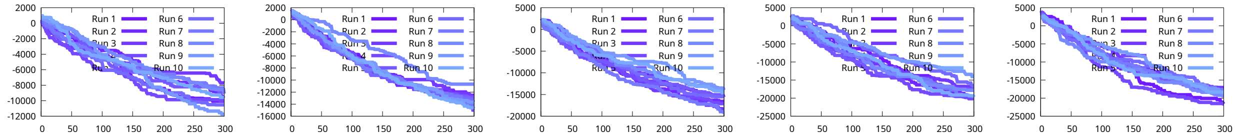
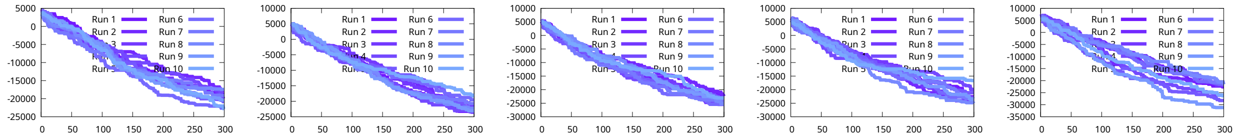


(a) $D = 10.000, NP = 1000$ (b) $D = 20.000, NP = 1000$ (c) $D = 30.000, NP = 1000$ (d) $D = 40.000, NP = 1000$ (e) $D = 50.000, NP = 1000$



(f) $D = 60.000, NP = 1000$ (g) $D = 70.000, NP = 1000$ (h) $D = 80.000, NP = 1000$ (i) $D = 90.000, NP = 1000$ (j) $D = 100.000, NP = 1000$

Figure 5: Convergent optimisation runs (fitness on vertical axis, number of executed generations on horizontal axis) using DAPHNE ROA on function HappyCat, for different independent seeds, with D from $D = 10.000$ (case (a)) upto $D = 100.000$ in case (j).

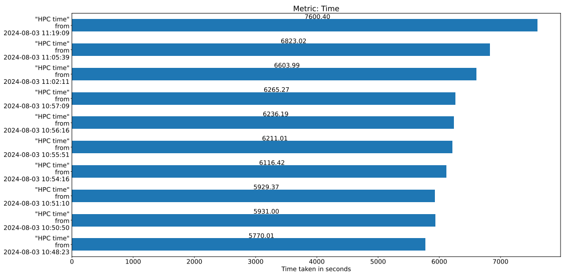


Figure 6: Time duration for DAPHNE ROA on function HappyCat, $D = 10.000$, $NP = 1000$, over 10 RNi configurations, measured through an Umlaut pipeline.

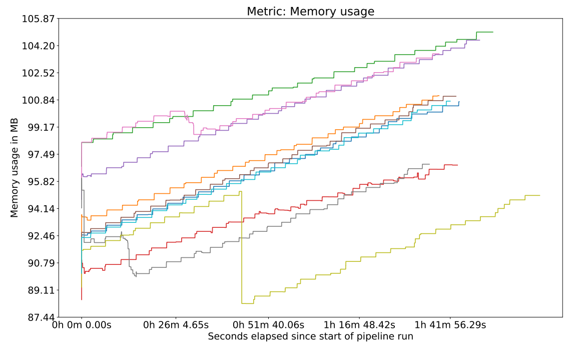


Figure 7: Memory usage profiles during the run execution of DAPHNE ROA on function HappyCat, $D = 10.000$, $NP = 1000$, and 10 RNi configuration values.

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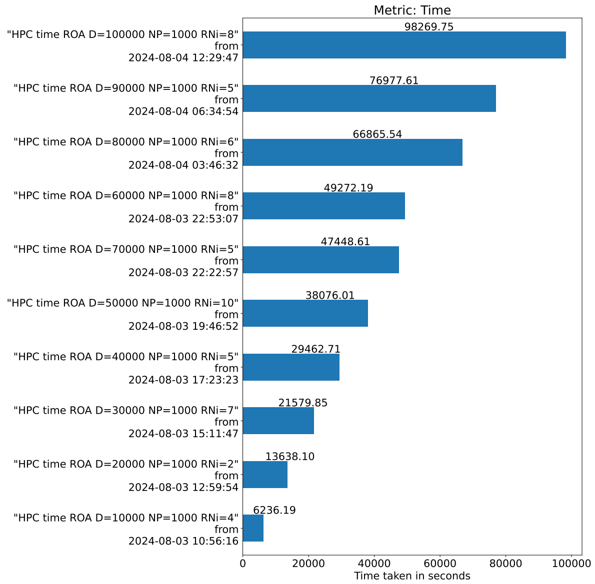


Figure 8: Runtime reported for DAPHNE ROA on function HappyCat, $NP = 1000$, for some selected runs with different D. As D increases, the runtimes are also increasing.

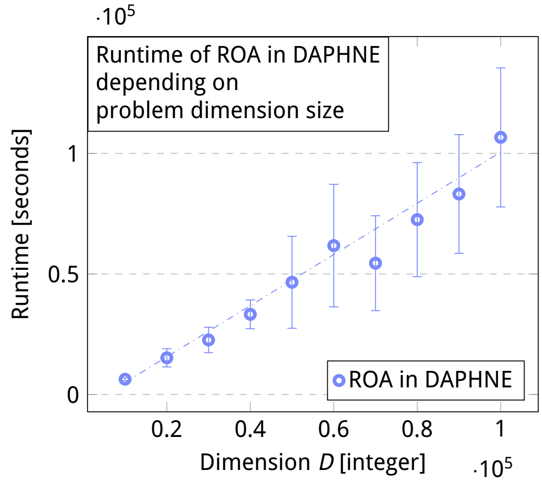
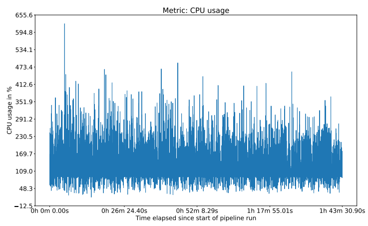
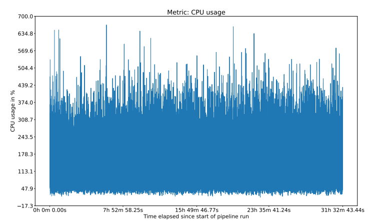


Figure 9: Runtime reported for DAPHNE ROA on function HappyCat, depending on problem dimension size (D), $NP = 1000$, drawn as average and standard deviations.



(a) $D = 10.000, RNi = 1$



(b) $D = 100.000, RNi = 5$

Figure 10: CPU load during run execution using DAPHNE ROA on function HappyCat $NP = 1000$, for case a) $D = 10.000$, $RNi = 1$ and $D = 100.000$, $RNi = 5$.

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