




nimCSO: A Nim package for Compositional Space Optimization

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Summary

nimCSO is a high-performance tool implementing several methods for selecting components (data dimensions) in compositional datasets, which optimize the data availability and density for applications such as machine learning. Making said choice is a combinatorically hard problem for complex compositions existing in highly dimensional spaces due to the interdependency of components being present. Such spaces are encountered, for instance, in materials science, where datasets on Compositionally Complex Materials (CCMs) often span 20-45 chemical elements, 5-10 processing types, and several temperature regimes, for up to 60 total data dimensions.

At its core, nimCSO leverages the metaprogramming ability of the Nim language ([Rumpf, 2023](#)) to optimize itself at the compile time, both in terms of speed and memory handling, to the specific problem statement and dataset at hand based on a human-readable configuration file. As demonstrated in [Methods and Performance](#) section, nimCSO reaches the physical limits of the hardware (L1 cache latency) and can outperform an efficient native Python implementation over 400 times in terms of speed and 50 times in terms of memory usage (*not* counting interpreter), while also outperforming NumPy implementation 35 and 17 times, respectively, when checking a candidate solution.

nimCSO is designed to be both (1) a user-ready tool, implementing two efficient brute force approaches (for handling up to 25 dimensions), a custom search algorithm (for up to 40 dimensions), and a genetic algorithm (for any dimensionality), and (2) a scaffold for building even more elaborate methods in the future, including heuristics going beyond data availability. All configuration is done with a simple human-readable YAML config file and plain text data files, making it easy to modify the search method and its parameters with no knowledge of programming and only basic command line skills.

Statement of Need

nimCSO is an interdisciplinary tool applicable to any field where data is composed of a large number of independent components and their interaction is of interest in a modeling effort, ranging from market economics, through medicine where drug interactions can have a significant impact on the treatment, to materials science, where the composition and processing history are critical to resulting properties. The latter has been the root motivation for the development of nimCSO within the [ULTERA Project](#) ([ultera.org](#)) carried under the [US DOE ARPA-E ULTIMATE](#) program which aims to develop a new generation of ultra-high temperature materials for aerospace applications, through generative machine learning models ([Debnath et al., 2021](#)) driving thermodynamic modeling and experimentation ([Li et al., 2024](#)).

One of the most promising materials for such applications are the aforementioned CCMs and their metal-focused subset of Refractory High Entropy Alloys (RHEAs) (Senkov et al., 2018), which have rapidly grown since first proposed by (Cantor et al., 2004) and (Yeh et al., 2004). Contrary to most of the traditional alloys, they contain many chemical elements (typically 4-9) in similar proportions in the hope of thermodynamically stabilizing the material by increasing its configurational entropy ($\Delta S_{conf} = \sum_i^N x_i \ln x_i$ for ideal mixing of N elements with fractions x_i), which encourages sampling from a large palette of chemical elements. At the time of writing, the ULTERA Database is the largest collection of HEA data, containing over 6,300 points manually extracted from almost 550 publications. It covers 37 chemical elements resulting in extremely large compositional spaces (Krajewski et al., 2024); thus, it becomes critical to answer questions like “Which combination of 15 elements will result in the largest dataset?” which has $\binom{37}{15}$ or 10 billion possible solutions.

Another significant example of intended use is to perform similar optimizations over large (many millions) datasets of quantum mechanics calculations spanning 93 chemical elements and accessible through OPTIMADE API (Evans et al., 2024).

56 Methods and Performance

57 Overview

As shown in Figure 1, nimCS0 can be used as a user-tool based on human-readable configuration and a data file containing data “elements” which can be any strings representing problem-specific names of, e.g., market stocks, drug names, or chemical formulas. A single command is then used to recompile (`nim c -f`) and run (`-r`) problem (`-d:configPath=config.yaml`) with nimCS0 (`src/nimcso`) using one of several methods. Advanced users can also quickly customize the provided methods with brief scripts using the nimCS0 as a data-centric library.

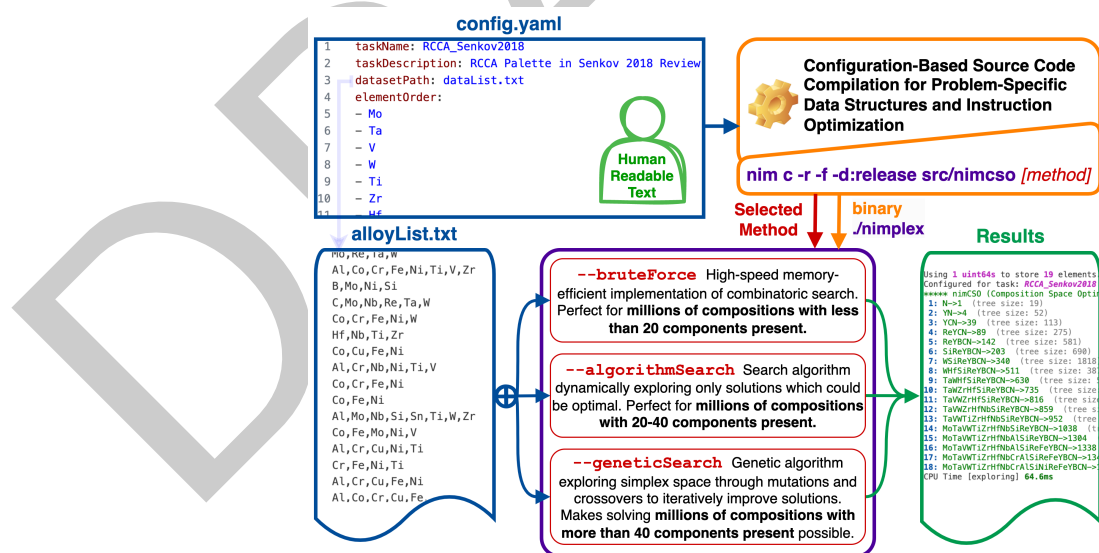


Figure 1: Schematic of core nimCSO data flow with a description of key methods. Metaprogramming is used to compile the software optimized to the human-readable data and configuration files at hand.

Internally, nimCSO is built around storing the data and solutions in one of two ways. The first is as bits inside an integer (`uint64`), which allows for the highest speed and lowest memory consumption possible but is limited to 64 dimensions and does not allow for easy extension to other use cases; thus, as of publication, it is used only in a particular `bruteForceInt` routine. The second one, used in `bruteForce`, `algorithmSearch`, and `geneticSearch`, implements a

69 custom easily extensible `ElSolution` type containing heuristic value and `BitArray` payload,
 70 which is defined at compile time based on the configuration file to minimize necessary overheads.
 71 Both encodings outperform typical native Python and NumPy implementations, as shown in
 72 Table 1.

Table 1: Benchmarks of (1) average time to evaluate how many datapoints would be lost if 5 selected components were removed from a dataset with 2,150 data points spanning 37 components, averaged over 10,000 runs, and (2) the size of the data structure representing the dataset. Values were obtained by running scripts in benchmarks directory on Apple M2 Max CPU.

Tool	Object	Time per Dataset	Time per Entry (Relative)	Database Size (Relative)
Python ^{3.11}	set	327.4 μ s	152.3 ns ($\times 1$)	871.5 kB ($\times 1$)
NumPy ^{1.26}	array	40.1 μ s	18.6 ns ($\times 8.3$)	79.7 kB ($\times 10.9$)
nimCSO ^{0.6}	BitArray	9.2 μ s	4.4 ns ($\times 34.6$)	50.4 kB ($\times 17.3$)
nimCSO ^{0.6}	uint64	0.79 μ s	0.37 ns ($\times 413$)	16.8 kB ($\times 52$)

73 Brute-Force Search

74 The brute force search is a naïve method of evaluating all possibilities; however, its near-zero
 75 overhead can make it the most efficient for small problems. In this implementation, all entries
 76 in the *power set* of N considered elements are represented as a range of integers from 0 to
 77 $2^N - 1$, and used to initialize `uint64`/`BitArrays` on the fly. To minimize the memory footprint
 78 of solutions, the algorithm only keeps track of the best solution for a given number of elements
 79 present in the solution. Current implementations are limited to 64 elements, as it is not
 80 feasible beyond approximately 30 elements; however, the one based on `BitArray` could be
 81 easily extended if needed.

82 Algorithm-Based Search

83 The algorithm implemented in the `algorithmSearch` routine, targeting high dimensional prob-
 84 lems (20-50), iteratively expands and evaluates candidates from a priority queue (implemented
 85 through an efficient binary heap (Williams, 1964)) while leveraging the fact that *the number*
 86 *of data points lost when removing elements A and B from the dataset has to be at least as*
 87 *large as when removing either A or B alone* to delay exploration of candidates until they can
 88 contribute to the solution. Furthermore, to (1) avoid revisiting the same candidate without
 89 keeping track of visited states and (2) further inhibit the exploration of unlikely candidates,
 90 the algorithm *assumes* that while searching for a given order of solution, elements present in
 91 already expanded solutions will not improve those not yet expanded. This effectively prunes
 92 candidate branches requiring two or more levels of backtracking. In the authors' tests, this
 93 method has generated the same results as `bruteForce`, except for occasional differences in the
 94 last explored solution.

95 Genetic Search

96 Beyond 50 components, the [algorithm-based](#) method will likely run out of memory on most
 97 personal systems. The `geneticSearch` routine resolves this issue through an evolution strategy
 98 to iteratively improve solutions based on custom mutate and crossover procedures. Both
 99 are of uniform type (Goldberg, 1989) with additional constraint of Hamming weight (Knuth,
 100 2009) preservation in order to preserve number of considered elements in parents and offspring.
 101 In mutate this is achieved by using purely random bit swapping, rather than more common
 102 flipping, as demonstrated in the Figure 2.

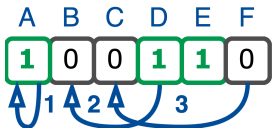


Figure 2: Schematic of mutate procedure where bits are swapping randomly, so that (1) bit can swap itself, (2) bits can swap causing a flip, or (3) bits can swap with no effect.

103 Meanwhile, in crossover, this constraint is satisfied by passing overlapping bits directly, while
104 non-overlapping bits are shuffled and distributed at positions present in one of the parents, as
105 shown in Figure 3.

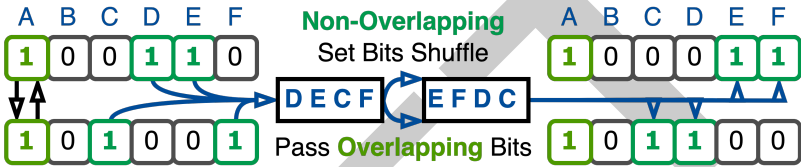


Figure 3: Schematic of uniform crossover procedure preserving Hamming weight implemented in nimCSO.

106 The above are applied iteratively, with best solutions carried to next generation, until the
107 solution converges or the maximum number of iterations is reached. Unlike the other methods,
108 the present method is not limited by the number of components and lets user control both
109 time and memory requirements, either to make big problems feasible or to get a good-enough
110 solution quickly in small problems. However, it comes with no optimality guarantees.

111 **Use Examples**

112 The tool comes with two pre-defined example problems to demonstrate its use. The first one is
113 defined in the default config.yaml file and goes through the complete dataset of 2,150 data
114 points spanning 37 components in dataList.txt based on the ULTERA Dataset (Debnath et
115 al., 2021). It is intended to showcase algorithmSearch/-as and geneticSearch/-gs methods,
116 as brute-forcing would take around one day. The second one is defined in config_rhea.yaml
117 and uses the same dataset but a limited scope of components critical to RHEAs (Senkov et
118 al., 2018) and is intended to showcase bruteForce/-bf and bruteForceInt/-bfi methods.
119 With four simple commands (see Table 2), the user can compare the methods' performance
120 and the solutions' quality.

Table 2: Four example tasks alongside typical CPU time and memory usage on Apple M2 Max.

Task Definition (nim c -r -f -d:release ...)	Time (s)	Memory (MB)
-d:configPath=config.yaml src/nimcso -as	302s	488 MB
-d:configPath=config.yaml src/nimcso -gs	5.8s	3.2 MB
-d:configPath=config_rhea.yaml src/nimcso -as	0.076s	2.2 MB
-d:configPath=config_rhea.yaml src/nimcso -gs	0.429s	2.1 MB
-d:configPath=config_rhea.yaml src/nimcso -bf	4.171s	2.0 MB
-d:configPath=config_rhea.yaml src/nimcso -bfi	0.459s	2.0 MB

121 In case of issues, the help message can be accessed by running the tool with -h flag or by
122 referring to documentation at amkrajewski.github.io/nimCSO.

Contributions

A.M.K. was responsible for conceptualization, methodology, software, testing and validation, writing of manuscript, and visualization; A.D. was responsible for testing software and results in training machine learning models; A.M.B., W.F.R., Z-K.L. were responsible for funding acquisition, review, and editing. Z-K.L. was also supervising the work.

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