

Evolutionary Mechanics

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Abstract

We developed an application that is able to develop mechanical structures using an evolutionary algorithm. This approach can be scaled efficiently across many different nodes. It is able to evolve 1000 generations of 112 organisms of a 80×80 structure on 256 cores on bridges in 36.05 minutes.

1 Introduction

With increasing computing power available, a new approach is becoming more relevant in engineering: Evolutionary algorithms. Instead of developing a mechanical structure for a problem, an engineer just specifies the forces it has to withstand and lets the computer come up with a solution. The hope is that the computer will come up with a better solution the engineer did not think of. The computer uses a try-and-error approach by making random alterations and only keeping the best mechanical structure. “Best” means, that it uses the least material possible while still withstanding the force. Figure 4 shows the outcome of such a process.

2 Method

Our project is divided in two sections and corresponding layers of parallelism. The first one is solving the mechanical equations to check if a mechanical structure can withstand a force. Figure 1 shows the result of such a simulation. The shape of a figure is approximated through squares consisting of two triangles. A detailed introduction on how to use the finite element method can be found at [1]. We used OpenMP for this part.

The second stage is the evolutionary algorithm. The best 10% survive in each round. The structures mutate and are simulated again. We used MPI for this part.

2.1 Speeding up the equation solver

The reason for using OpenMP is the tight coupling between the data in the sparse matrix multiplication. `gprof` revealed that the equation solver spends most of its time in the sparse matrix multiplication, however the whole equation solver class works parallelized. Algorithm 1 shows the approach.

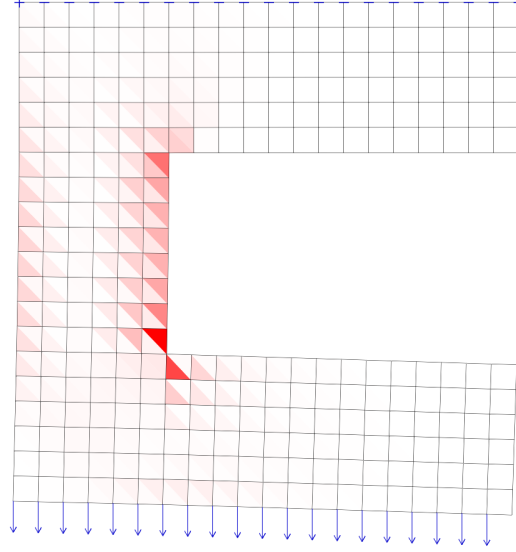


Figure 1: Result of a mechanical simulation and the evolutionary algorithm.

- **Threads are spawned at the highest level** of the `PerformanceEvaluator` class. Subsequent calls to the equation setup, equation solver or linear algebra operations will not spawn new threads. They require the threads to be set up already, and process only their chunk using the `omp for` directive. All for loops are executed in chunks to **prevent false sharing**.
- The **equation setup** process adds the local element stiffness matrix into the global equation system. Depending on the mechanical structure, the position of different planes appears rather random. Therefore, a lock is needed to prevent a race condition. Because the matrix is sparse and each thread works on its own plane, that typically are not directly connected, it is improbable that two threads operate on the same equation row at the same time. A global lock would introduce an unnecessary penalty, therefore each row uses its own **local lock**.

- **All linear algebra operations of the equation solver work in parallel**, we can divide these in two types:

For addition, scalar multiplication, matrix multiplication or assigning a constant value, each thread processes its **own chunk of rows**. These operations do not require an implicit or explicit barrier. If for example, a scalar multiplication follows a vector addition, it is fine if the first thread begins with the scalar multiplication before the second thread has finished the vector addition, since each of them operates on its own set of rows.

However, in the conjugate gradient method there are also operations like the scalar product or the norm of the vector. These operations require a **reduction** and have an implicit barrier.

- In the beginning, a unique index has to be assigned to each Plane and corner. This is

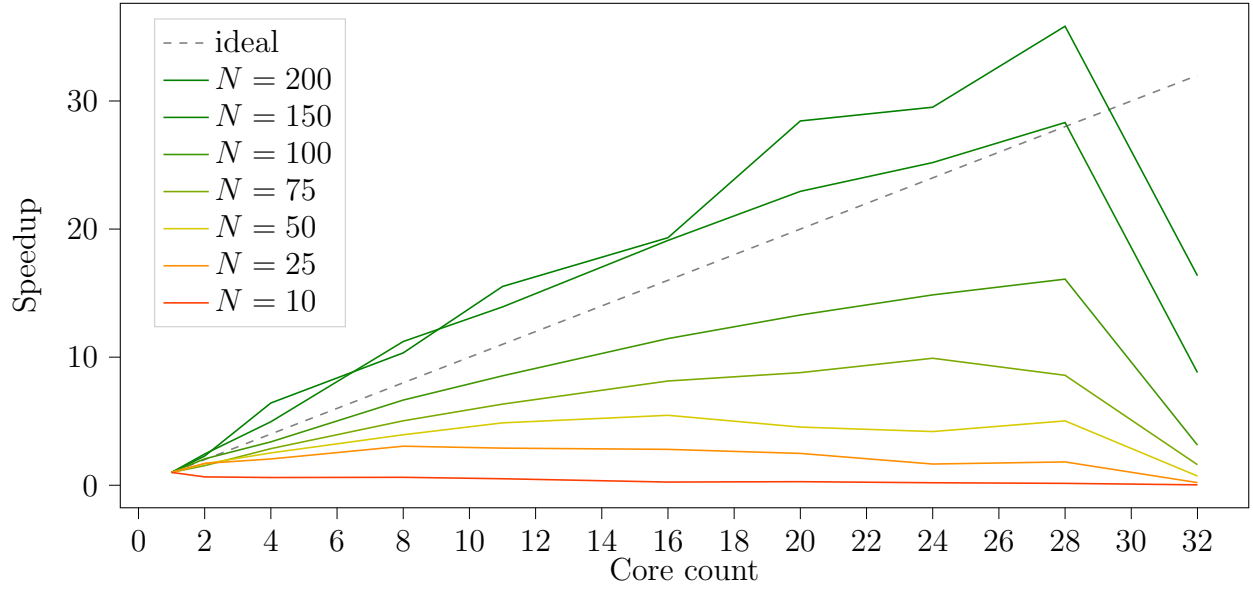


Figure 2: Speedup of the equation solver for different problem sizes N .

	$N = 10$	$N = 25$	$N = 50$	$N = 75$	$N = 100$	$N = 150$	$N = 200$
Equations	230	1325	5150	11475	20300	45450	80600
$C = 1$	3	43	311	1153	3306	19869	97932
$C = 2$	4	25	185	754	1604	8149	42934
$C = 4$	5	21	123	403	976	4008	15251
$C = 8$	5	14	79	229	497	1771	9477
$C = 11$	6	15	64	182	387	1427	6311
$C = 16$	11	15	57	142	289	1040	5067
$C = 20$	10	17	69	131	249	866	3443
$C = 24$	14	26	74	116	222	789	3318
$C = 28$	19	24	62	134	205	702	2733
$C = 32$	91	209	432	718	1055	2257	5986

Table 1: Execution time for the equation solver for different field sizes N and cores C .

Algorithm 1 Simulate

Setup the equation system
Solve the equation system with the conjugate gradient method
Calculate the stress using the Van-Mises-Equation

not parallelizable, as the total number of planes and corners is unknown and does not follow a predictable pattern.

- Using the **conjugate gradient method** reduced the time complexity by $O(N)$ [2].
- Using a **sparse matrix multiplication** reduced the the time complexity by $O(N^2)$ [2].

The time complexity of the sequential equation solver is dominated by the sparse matrix multiplication, having a complexity of

$$O_{seqSolve}(N) = O(N^3) \quad (1)$$

as explained in the progress report [2]. The sparse matrix multiplication has been fully parallelized. The indexing of the equation requires $O(N^2)$. Leaving the overhead for thread creation aside, the runtime complexity is

$$O_{parSolve}(N, C) = O\left(\frac{N^3}{C}\right) + O(N^2) \quad (2)$$

for a sufficiently large N . The efficiency is

$$E = \frac{O_{seqSolve}}{O_{parSolve}C} = O\left(\frac{N^3}{N^3 + C^2}\right) \quad (3)$$

As the efficiency remains only if $N \propto C$, we can asses that the equation solver has weak scalability. However, there is a significant overhead due to creating the threads. The speedup becomes only notable for problem sizes $N > 100$.

The Equation Solver is still a powerful solver. It is able to solve a 200×200 mechanical structure with 80600 equations in 2.732s using 28 cores on bridges. The speedup of the execution time of table 2 are shown in figure 1.

2.2 Speeding up the evolutionary algorithm

Evolutionary algorithms are easily parallelizable by nature. Each organism can be evaluated independently by each node, while the results will be gathered by a single node in charge of sorting them. The best 10% get broadcasted to the other nodes again. This is visualized in algorithm 2.

A MPI Message for an evaluated board consists of

- 1 float for the score
- $R \times C$ bytes, each containing the boolean value of the field.

We typically simulate grid sizes of 20, meaning the message has a size of 404 bytes. Since all processes will be initialized with the same field size it has not to be stored in the message. The message size grows with

$$O_{msgSize} = O(N^2) \quad (4)$$

The runtime complexity of the single thread evolutionary algorithm is

Algorithm 2 Evolute on node

```
Initialize all local fields fully set
for all epochs do
  Mutate the fields
  Evaluate the fields
  Gather all fields into the master
  Sort the fields on the master
  Broadcast the best 10% to everyone
  Replace local fields
end for
```

Cores	7	14	28	56	112	224
Cores per Task	1	1	1	1	1	2
Tasks	7	14	28	56	112	112
Nodes	1	1	1	2	4	8
<hr/>						
$N = 10$	33.667	18.519	9,399	5.432	2.950	4.256
$N = 20$	296.997	164.875	91.958	43.114	25.199	29.429
$N = 40$	*2029.938	*1073.118	*631.448	335.852	200.529	164.243
$N = 80$	-	*19588.620	*14045.210	*7105.495	*3729.680	2163.535

Table 2: Execution time in seconds for the evolution for different field sizes N and cores C . The generation size is set fixed to 112 and 1000 epochs are simulated. Values marked with * are extrapolated from a run with less epochs.

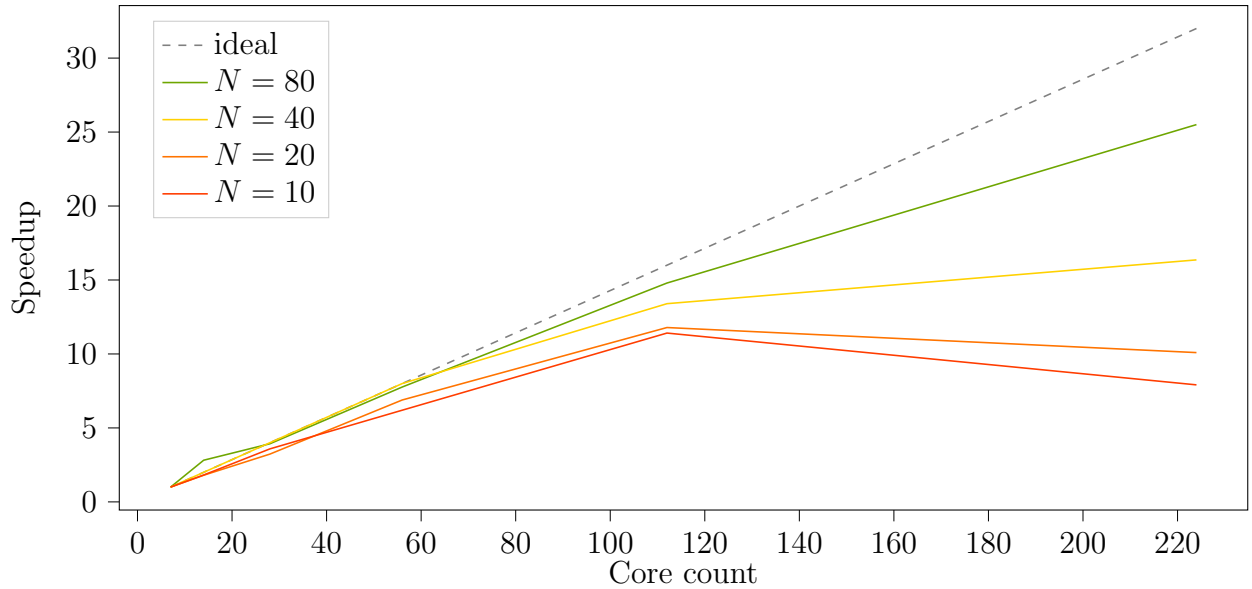


Figure 3: Speedup of the equation solver for different problem sizes N .

$$O_{evolSeq}(N, G, A) = O_{seqSolve} \cdot O(GA) \quad (5)$$

with generations size G and A epochs. The parallel version has

$$O_{evolPar}(N, C, G, A) = O\left(\frac{N^3GA}{C} + N^2GA\right) \quad (6)$$

with $O(\frac{N^3GA}{C})$ being the work for solving the equation system per core and $O(N^2GA)$ being the communication cost for sending $O(G)$ bytes of data over the network each epoch A . The efficiency is

$$E = O\left(\frac{N^3 + N^2}{N^3 + CN^2}\right) \quad (7)$$

so this algorithm has also a weak scalability. Table 2 shows the execution times of the program. They are visualized in figure 3. The algorithm scales well for small core counts $C < 112$, because each generation has 112 organisms. This allows each core to work on its own organism. For $C > 112$, multiple cores process one organism, so the mechanical solver starts to parallelize. This gives a speedup only if the problem size N is sufficient. The result of the finished evolution is shown on figure 4.

2.3 Implementation differences

As requested from the requirements, our submission contains four different implementations of our solution.

- The basic sequential implementation is the unoptimized version of the program.
- The best optimized sequential implementation differs from the previous version by the introduction of the SparseMatrix class. This class is able to perform sparse matrix - vector multiplications.
- The basic parallel implementation introduces the usage of OpenMP, which revealed to be a turning point in improving the time taken by solving the equation systems.
- The best optimized parallel implementation adds the usage of MPI for the evolutionary implementation. We decided to distribute the seeking of the best organism through different nodes. The nodes will collaborate in this research finding the best solution in the amount of iterations given. This takes out solution on a new level, forming a distributed, collaborative and parallelized solution.

3 Summary and learning outcomes

All of us learned a lot during the project. We have never experimented with finite element simulation, conjugate gradient method or evolutionary algorithms before. The project provided several challenges for us, for example using locks, combining OpenMP with MPI or separating `omp parallel` from `omp for`. We improved our development technique a lot by using test-driven development, no-push-to-master and code reviews.

References

- [1] G. P. Nikishkov. *Introduction to the finite element method*. 2004.
- [2] Tobias Jacob, Raffaele Galliera, and Ali Muddasar. Progress report. 2020.

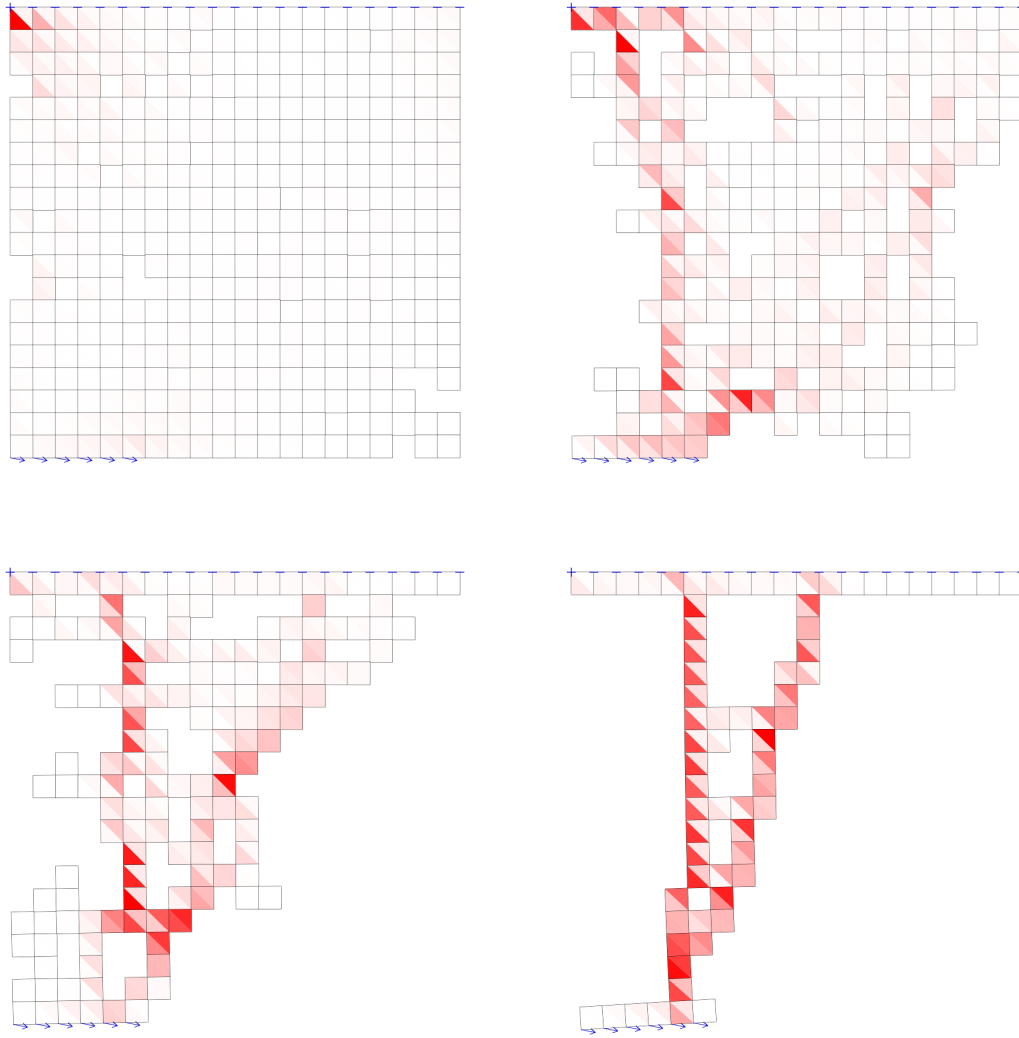


Figure 4: Result of a evolution, using 20×20 grid, 100 organisms per epoch, 1000 epochs and a alterations decay of 0.995. Note, how the structure gets wider on the top to deal with the increased bending stress.