Numeric simulation using finite elements

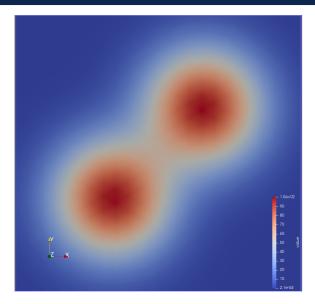
Sparse but not scarce

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Original implementation: dense matrix



Assignment: Sparse but not scarce

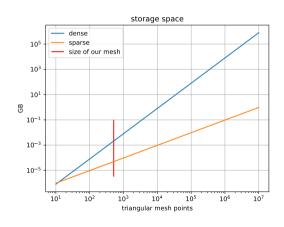
- Convert PDE solver matrix to sparse format and compare the performance with your dense matrix implementation.
- Use library implementation and compare it with a self-implemented CSR format.

Why Sparse?

Storage space



- 1. N = number of mesh points
- 2. $\approx 6 \cdot N$ -nonzero elements in matrix
- 3. storage for dense matrix ($\propto N^2$): 2.11 MB
- 4. storage for sparse matrix ($\propto N$): 0.05 MB



Different Sparse Formats

- sparse manual
 - values = $\begin{bmatrix} 5.3, & 1.5, & 4.2, & 3.1, & 2, & 2.2, & 1.9 \end{bmatrix}$
 - pos = [1, 4, 5, 7, 9, 18, 20]
- sparse COO (coordinate list)
 - values = $\begin{bmatrix} 5.3, & 1.5, & 4.2, & 3.1, & 2, & 2.2, & 1.9 \end{bmatrix}$
 - $\operatorname{col.ind} = \begin{bmatrix} 1, & 4, & 0, & 2, & 4, & 3, & 0 \end{bmatrix}$
 - $row_{ind} = [0, 0, 1, 1, 1, 3, 4]$
- sparse CSR (compressed row storage)
 - values = $\begin{bmatrix} 5.3, & 1.5, & 4.2, & 3.1, & 2, & 2.2, & 1.9 \end{bmatrix}$
 - $col_ind = [1, 4, 0, 2, 4, 3, 0]$
 - $\bullet \ \operatorname{row_ptr} = \begin{bmatrix} 0, & 2, & 5, & 5, & 6, & 7 \end{bmatrix}$

```
\begin{pmatrix}
0 & 5.3 & 0 & 0 & 1.5 \\
4.2 & 0 & 3.1 & 0 & 2 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 2.2 & 0 \\
1.9 & 0 & 0 & 0 & 0
\end{pmatrix}
```

Matrix assembly

class sparse_mat:

preliminaries:

```
vector<int> col_ind;
vector<int> row_ind;
vector<double> values;
```

filling:

```
if (Bij != 0) {
    Bij /= H;
    row_ind.push_back(i);
    col_ind.push_back(j);
    values.push_back(Bij);
```

constructing the sparse_mat object:

```
// construct B
sparse_mat B;
B = sparse_mat(points.size(), col_ind, row_ind, values);
return B;
```

Matrix assembly: Conversion COO to CSR

COO format:

```
row_ind = [0, 0, 1, 1, 1, 3, 4]

for (int i = 0; i < row_ind.size(); i++) {
    row_ptr[row_ind[i] + 1]++;
}</pre>
```

how many elements in each row:

```
\operatorname{row\_step} = \begin{bmatrix} 0, & 2, & 3, & 0, & 1, & 1 \end{bmatrix}
```

```
for (int i = 0; i < dim; i++) {
    row_ptr[i + 1] += row_ptr[i];
}</pre>
```

CSR format:

```
\operatorname{row\_ptr} = \begin{bmatrix} 0, & 2, & 5, & 6, & 7 \end{bmatrix}
```

```
\left(\begin{array}{cccccc}
0 & 5.3 & 0 & 0 & 1.5 \\
4.2 & 0 & 3.1 & 0 & 2 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 2.2 & 0 \\
1.9 & 0 & 0 & 0 & 0
\end{array}\right)
```

Matrix-Vector multiplication: Sparse - manual

- sparse manual
 - values = $\begin{bmatrix} 5.3, & 1.5, & 4.2, & 3.1, & 2, & 2.2, & 1.9 \end{bmatrix}$ pos = $\begin{bmatrix} 1, & 4, & 5, & 7, & 9, & 18, & 20 \end{bmatrix}$
- matrix-vector multiplication

```
for (int k = 0; k < count; k++) {
   const int i = _pos[k] / dim;
   const int j = pos[k] % dim;
  res[i] += val[k] * u[j];
```

```
\left(\begin{array}{cccccc}
0 & 5.3 & 0 & 0 & 1.5 \\
4.2 & 0 & 3.1 & 0 & 2 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 2.2 & 0 \\
1.9 & 0 & 0 & 0 & 0
\end{array}\right)
```

Matrix-Vector multiplication: Sparse - CSR

- sparse CSR (compressed row storage)
 - values = $\begin{bmatrix} 5.3, & 1.5, & 4.2, & 3.1, & 2, & 2.2, & 1.9 \end{bmatrix}$ col_ind = $\begin{bmatrix} 1, & 4, & 0, & 2, & 4, & 3, & 0 \end{bmatrix}$ row_ptr = $\begin{bmatrix} 0, & 2, & 5, & 5, & 6, & 7 \end{bmatrix}$
- matrix-vector multiplication

```
for (int j= row ptr[i]; j< row ptr[i+1]; j++) {</pre>
    res[i]+= val[j]*u[ col ind[j]];
```

```
\begin{pmatrix}
0 & 5.3 & 0 & 0 & 1.5 \\
4.2 & 0 & 3.1 & 0 & 2 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 2.2 & 0 \\
1.9 & 0 & 0 & 0 & 0
\end{pmatrix}
```

Solution: Sparse but not scarce

- two self-implemented classes for sparse matrices: non-CSR and CSR format.
- Eigen library
 - added to repository as a git submodule
 - SparseMatrix class
 - SparseMatrix::makeCompressed() conversion to CSR format
 - forward Euler simplified using matrix multiplication notation:

Eigen::SparseMatrix B * Eigen::VectorXd u

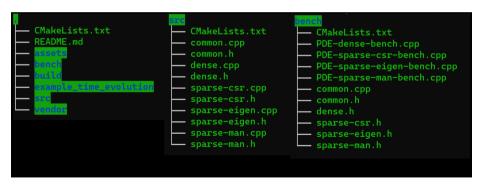
Google Benchmark

- github.com/google/benchmark
- a library to benchmark code snippets (functions)
- added to repository as a git submodule

```
#include <benchmark/benchmark.h>
static void BM_SomeFunction(benchmark::State& state) {
    // Perform setup here
    for (auto _ : state) {
        // This code gets timed
        SomeFunction();
    }
}
// Register the function as a benchmark
BENCHMARK(BM_SomeFunction);
// Run the benchmark
BENCHMARK_MAIN();
```

Code organization

- Cmake build 8 targets, common + unique code
- 4 versions of PDE solver
- corresponding benchmarks, testing functions unique to each implementation

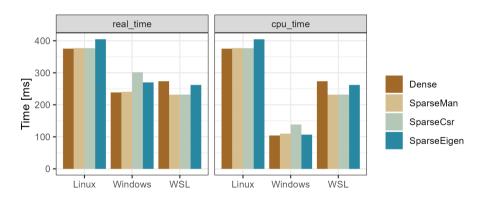


Benchmark example output

```
Run on (4 X 2995 MHz CPU s)
CPU Caches:
  L1 Data 48 KiB (x4)
  L1 Instruction 32 KiB (x4)
  L2 Unified 1280 KiB (x4)
  L3 Unified 12288 KiB (x1)
Benchmark
                                                        Time
                                                                         CPU
                                                                               Iterations
assembleMatrixSparseEigenBench1/iterations:30
                                                     308 ms
                                                                     149 ms
timeEvolutionSparseEigenBench2/iterations:30
                                                     36.7 ms
                                                                     17.2 ms
                                                                                       30
                                                   0.360 s
                                                                    0.180 s
odeSparseEigenBench3/1/iterations:2
                                                                    0.211 s
                                                   0.373 \, s
odeSparseEigenBench3/2/iterations:2
                                                   0.372 s
                                                                    0.195 s
odeSparseEigenBench3/3/iterations:2
                                                   0.363 s
                                                                    0.211 s
odeSparseEigenBench3/4/iterations:2
                                                   0.347 s
                                                                    0.234 s
odeSparseEigenBench3/5/iterations:2
                                                                    0.195 s
                                                   0.335 s
odeSparseEigenBench3/6/iterations:2
                                                   0.382 s
                                                                    0.141 s
odeSparseEigenBench3/7/iterations:2
                                                   0.331 s
                                                                    0.164 5
odeSparseEigenBench3/8/iterations:2
                                                   0.341 s
                                                                    0.172 s
odeSparseEigenBench3/9/iterations:2
                                                   0.353 s
                                                                    0.133 \, s
```

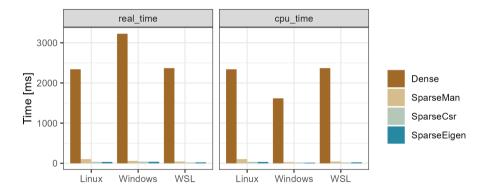
Benchmark assembly matrix B

- 30 iterations
- Linux (Martin's machine), Windows and WSL (Charlotte's machine)



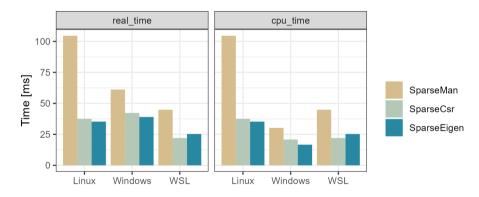
Benchmark time evolution

• 30 iterations



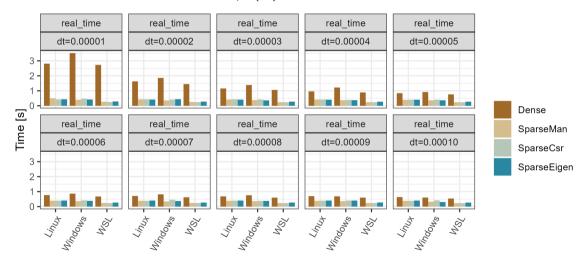
Benchmark time evolution

• 30 iterations



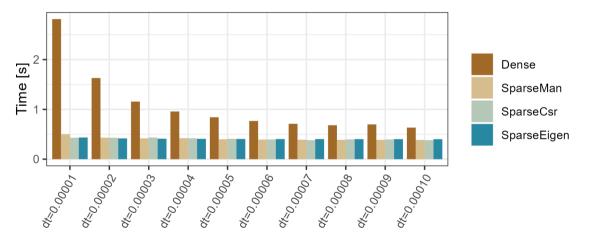
Benchmark matrix assembly + time evolution

• 2 iterations, for different timesteps (dt)



Benchmark matrix assembly + time evolution

- 2 iterations, for different timesteps (dt)
- Linux, real time



Conclusions

- Sparse formats preferred over dense format:
 - Memory issues for large mesh sizes
 - Time needed for matrix assembly similar (dependence on machine and OS used?)
 - Significant 100-fold time-speed up using sparse format for time evolution
- Tradeoff own sparse format vs CSR-format:
 - Extra time needed for converting COO to CSR
 - Speed up at time evolution
- Tradeoff library vs own implementation:
 - Time spent on learning the library (once) vs on correctly implementing the sparse format
 - With Eigen code simplification using matrix product expressions

Questions?