Matrix Exponential Optimization

Advanced Systems Lab

Team 28

ETH

Eidgenössische Technische Hochschule Zürich

Swiss Federal Institute of Technology Zurich

Algorithm

- **Goal**
  - Algorithm 5.1 proposes a new way to approximate e^A, where *A* is a square matrix.
- **Motivation**
  - Previous implementation had poor precision with big matrices (overscaling)
- **Extensive use of matrix multiplication**
  - Wipes out cache
  - *Blas* allowed for MMM
  - Main focus in optimization code fragments between MMM

Infrastructure

- **Validation**
  - Existing implementation: *scipy expm* in scipy.linalg module (Python)
  - The C++ infrastructure interacts with a Python script to get the a valid computation
- **Timing**
  - Processor used: i5-6400, Skylake microarchitecture @2700 Mhz
  - Cycles computed using *TSC* counter

Cost analysis

- **Cost measure**
  - Total number of FLOPS
  - All floating-point operations have the same weight
  - Code instructed to count FLOPS through macros

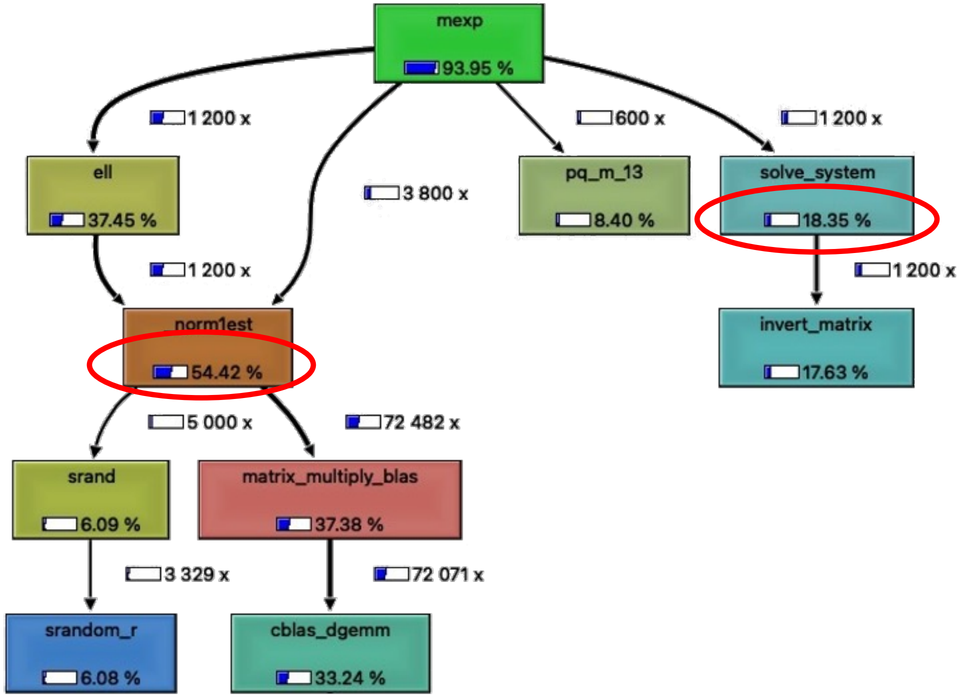
```
#ifdef FLOPS
#define FLOPS_RESET
#define FLOPS_ADD(x)
#define FLOPS_ADD_N(x)
#define FLOPS_ADD_N2(x)
#define FLOPS_ADD_N3(x)
#define FLOPS_PRINT
#endif
```

Straightforward C Implementation

- **Codebase**
  - **mexp_basic_.c**: performs the Matrix Exponential (Memexp), utilizing functions from utils_.c and queries *normest* from norms_.c to get an estimation of the norm from a matrix
  - **utils_.c** and **utils_.h**: utility functions needed in mexp_basic_.c, promoting modularity
  - **norms_.c**: houses *normest* for norm estimation, used by mexp_basic_.c for matrix calculations
- **BLAS is used to perform MMMs**
- **Matrices are represented as array in row-major order**

Callgrind analysis

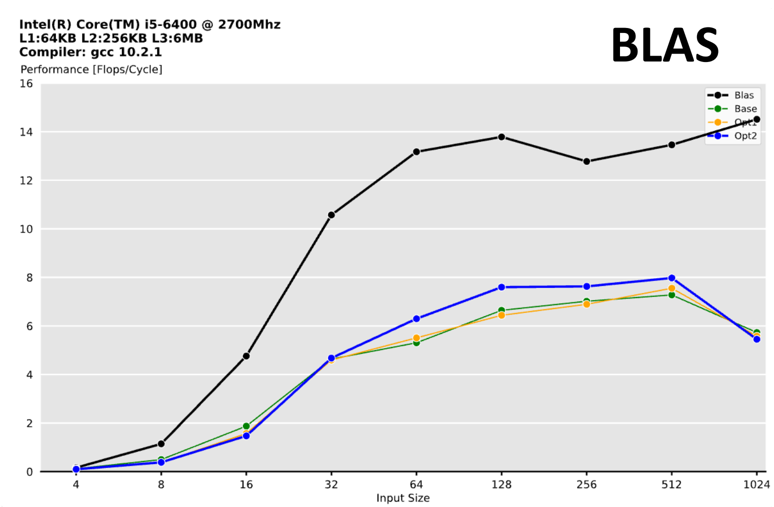
- **Bottlenecks**
  - solve-system
  - normest

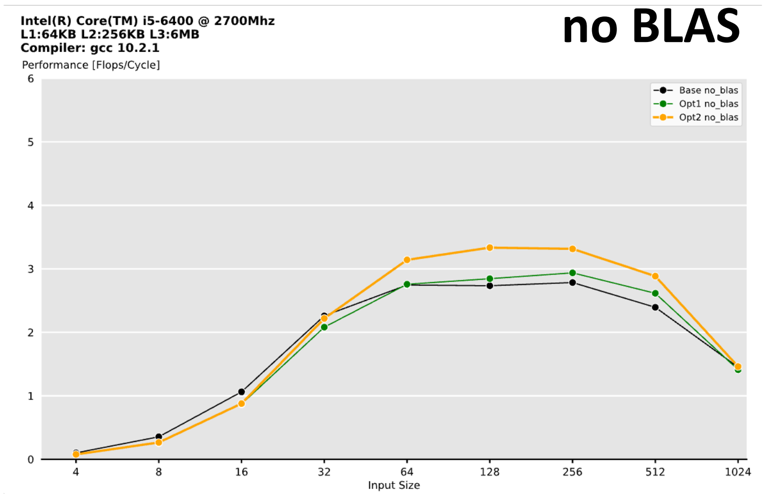


Basic optimizations

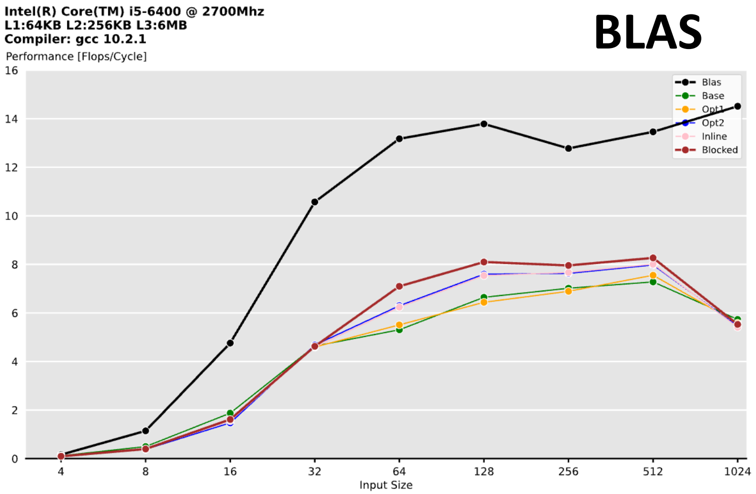
- **OPT-1 and OPT-2 modifications involved the following scalar optimizations:**
  - Ensure the constant use of arrays
  - Save precomputed data and reused after
  - Removed calls to abs(), ceil() or divisions
  - ILP improvements, unrolling and scalar replacement
  - Function inlining

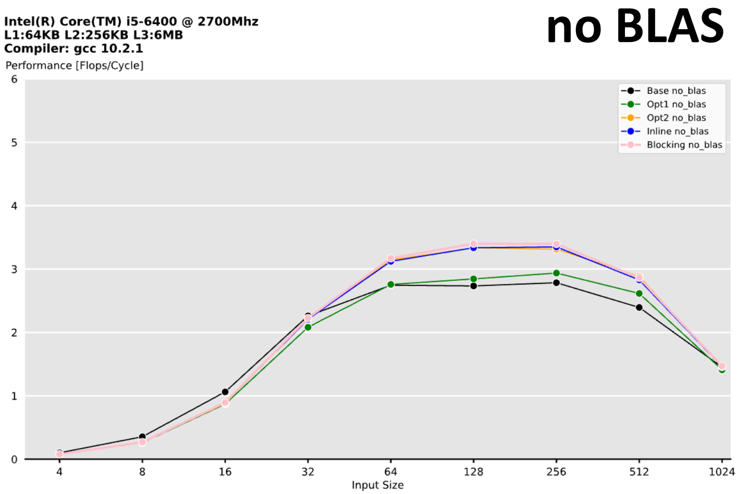
Basic optimizations



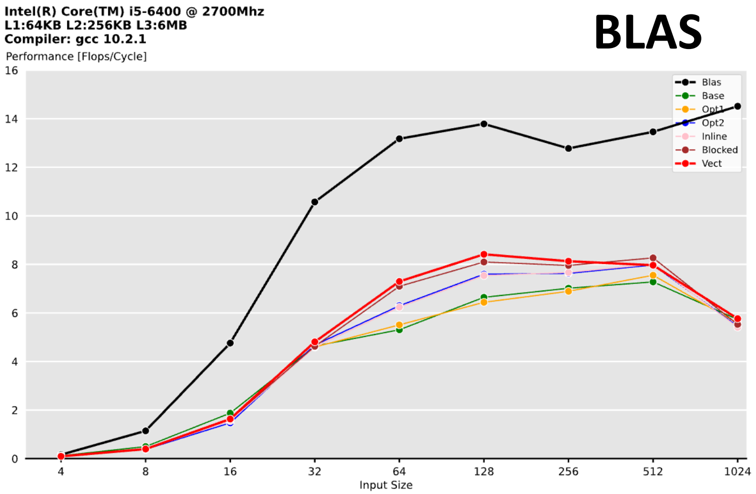


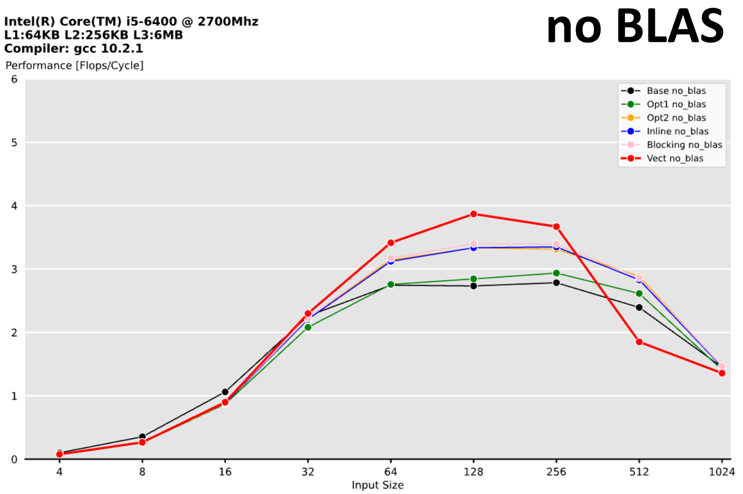
Blocking Plot



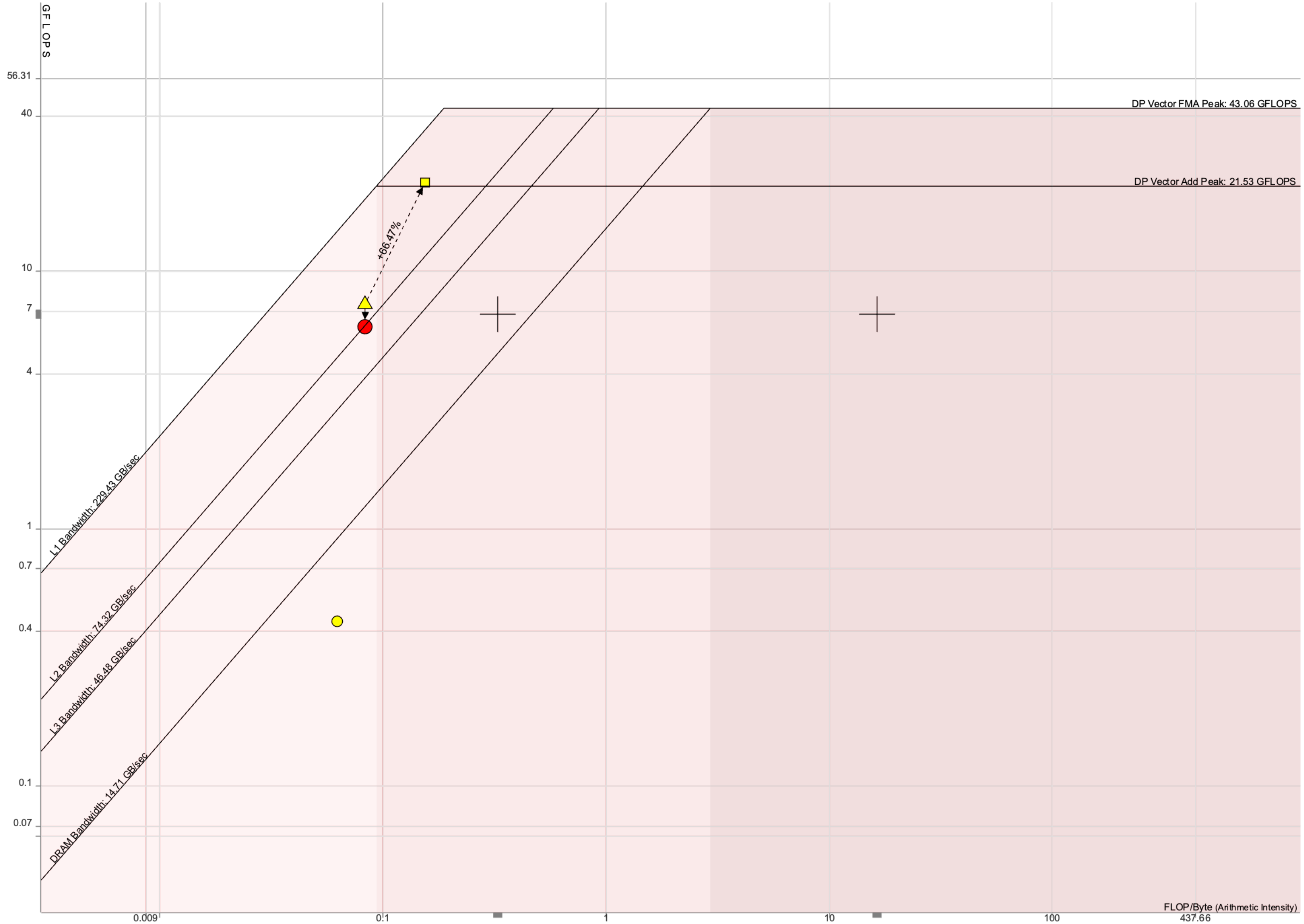


Vectorization Plot





Roofline plot *inverse (Base, BB and BV)*



Gaussian Elimination

- **The straightforward implementation used Gaussian Elimination to solve the system QX=P, where all matrices are NxN.**
- **Limitation**
  - No possible blocking in Gaussian Elimination
  - LU decomposition is the matrix form of Gaussian Elimination
- **In LU decomposition computations can be reused by backward and forward substitution applied to every column of P.**

Comparison

- **Gaussian Elimination optimizations**
  - Basic optimizations
    - *Inline swap_rows and avoid repeated calculations*
    - *Strength reduction*
  - Vectorization
- **LU decomposition optimizations**
  - Basic optimizations
    - *Loop reordering provided a major improvement (x10)*
  - Blocking
  - Vectorization

Loop ordering

- **Improved spatial and temporal locality**

```
// Forward substitution
for (int i = 0; i < n; i++){
    for (int j = 0; j < n; j++){
        for (int k = 0; k < j; k++){
            P[j*n + i] -= P[k*n + i] * Q[j*n + k];
        }
    }
}

// Backward substitution
for (int i = 0; i < n; i++){
    for (int j = n - 1; j >= 0; j--){
        double temp = P[j*n + i];
        for (int k = j + 1; k < n; k++){
            temp -= P[k*n + i] * Q[j*n + k];
        }
        P[j*n + i] = temp / Q[j*n + j];
    }
}
```

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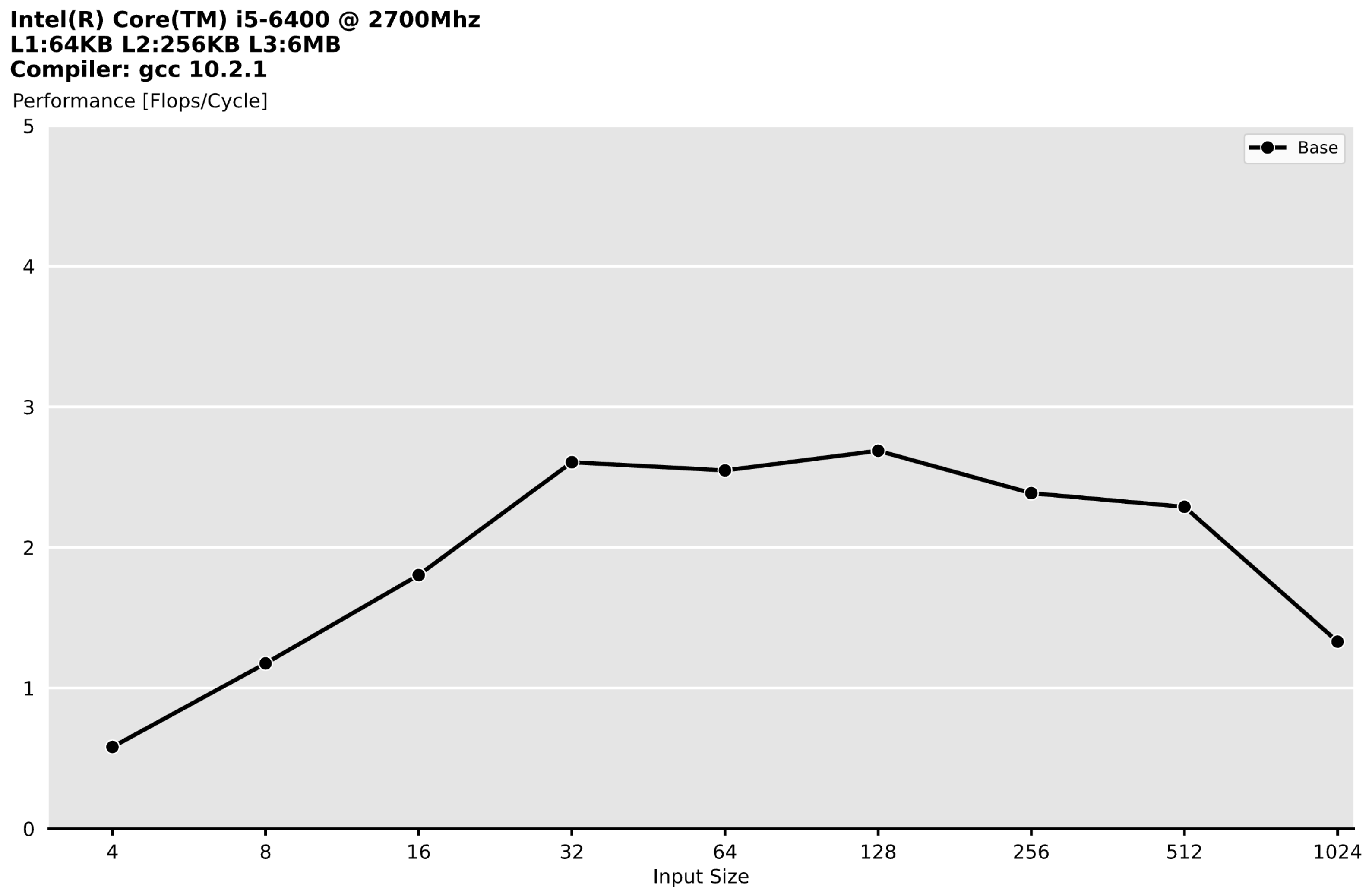
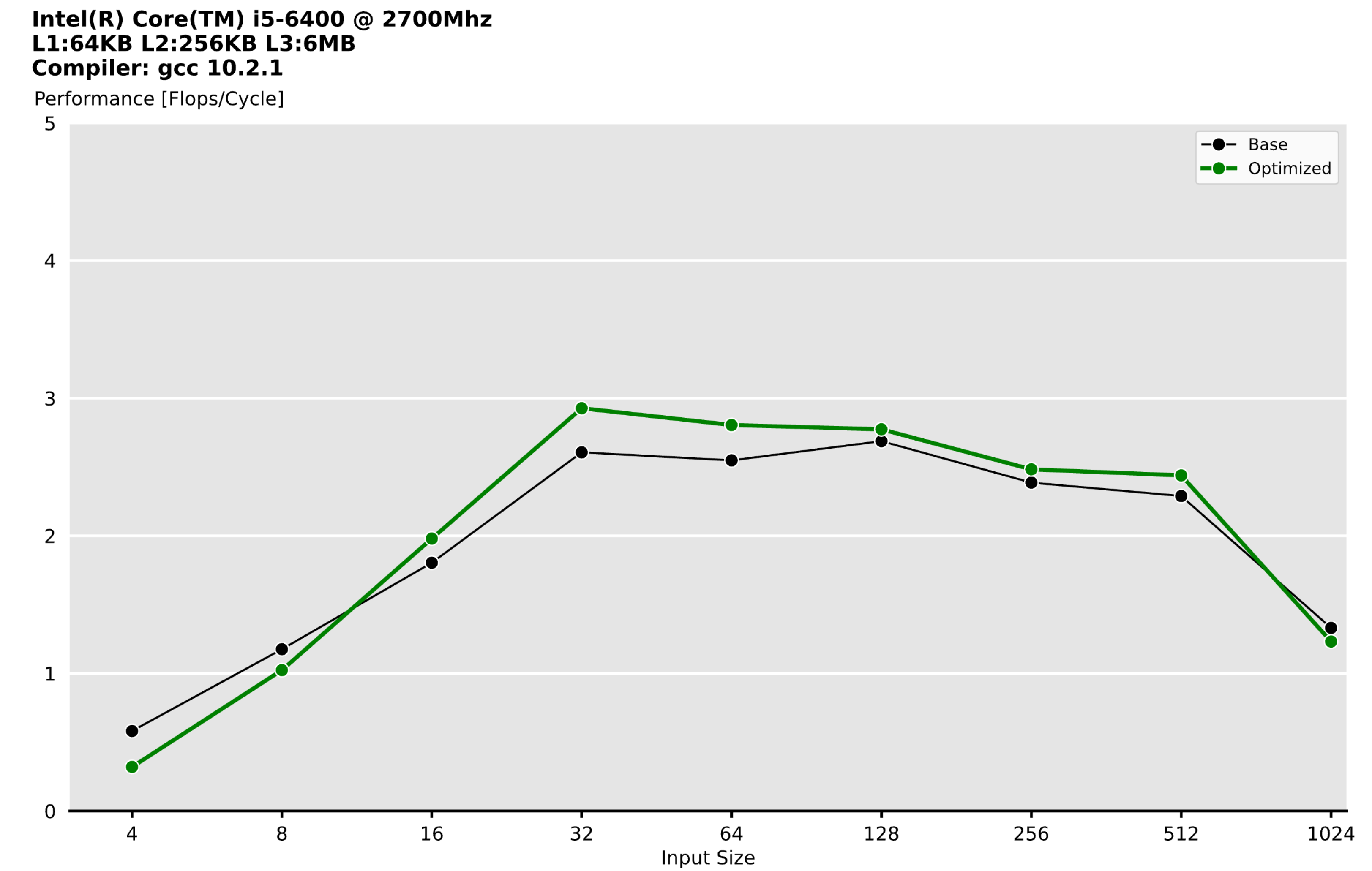
        }
    }
}

// Backward substitution
for (int i = n - 1; i >= 0; i--) {
    for (int k = n - 1; k > i; k--) {
        for (int j = 0; j < n; j++) {
            P[i*n + j] -= Q[i*n + k] * P[k*n + j];
        }
    }
    for (int j = 0; j < n; j++) {
        P[i*n + j] /= Q[i*n + i];
    }
}
```

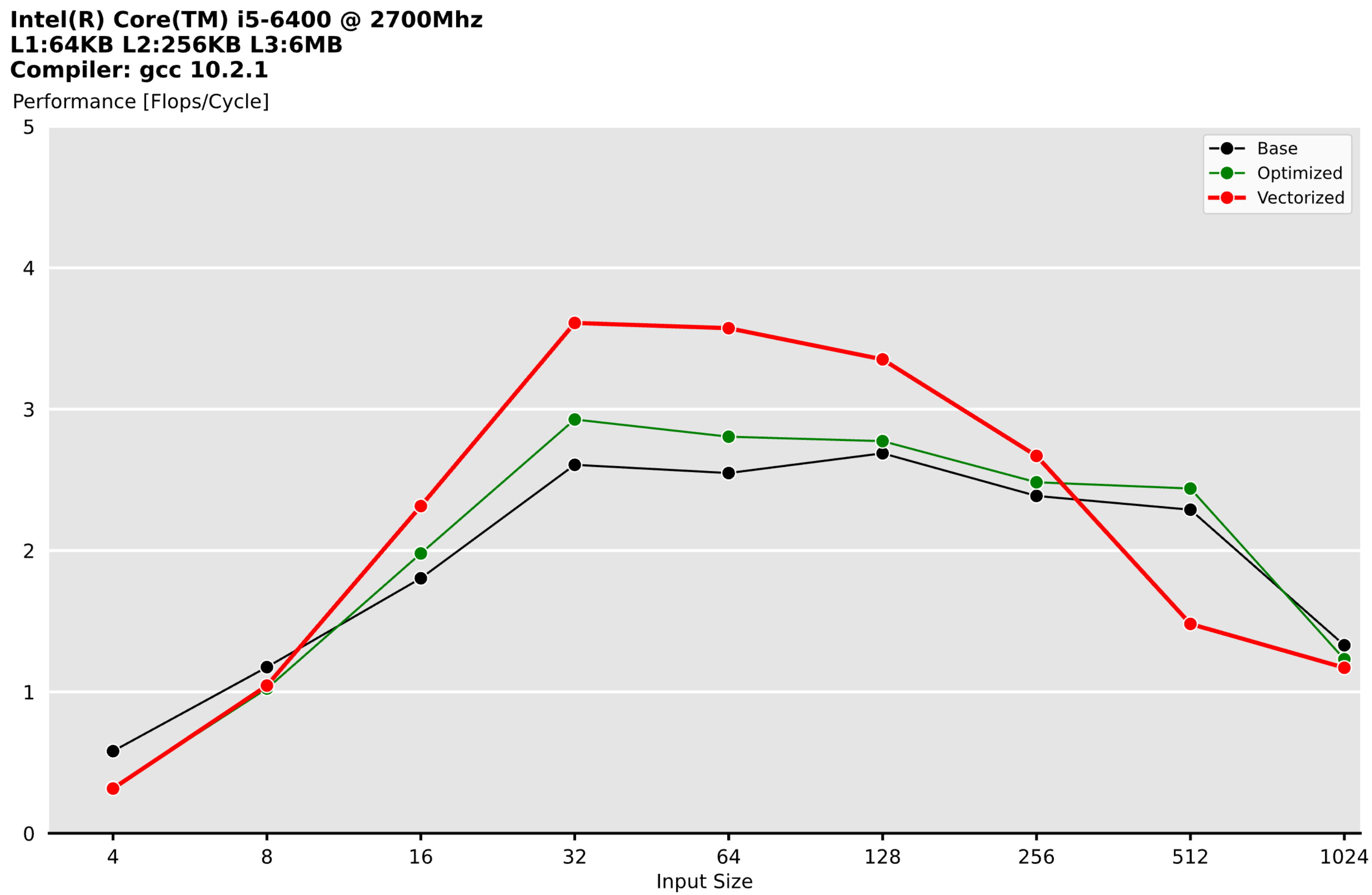
Gaussian Elimination Performance Plot



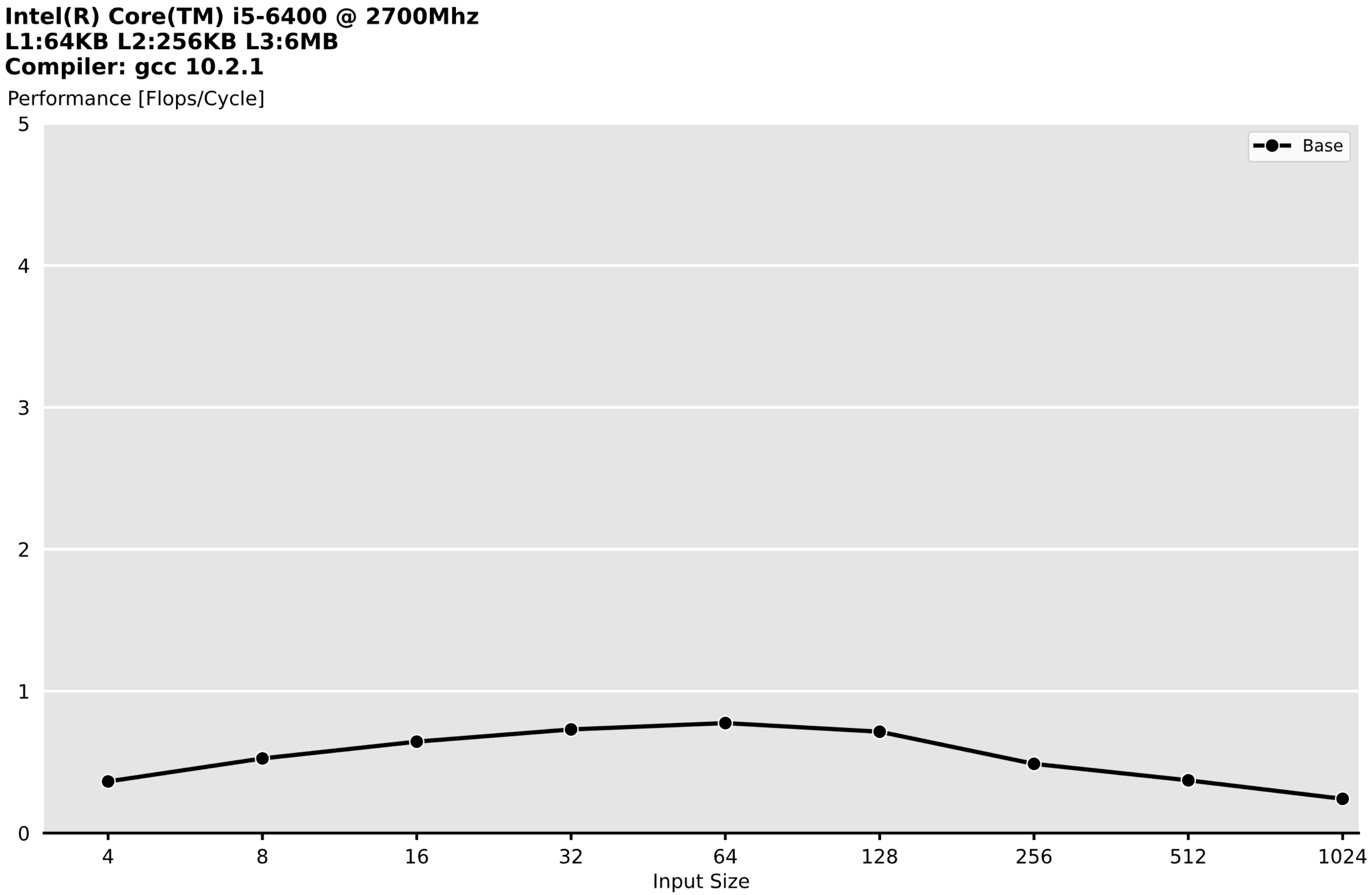
Gaussian Elimination Performance Plot



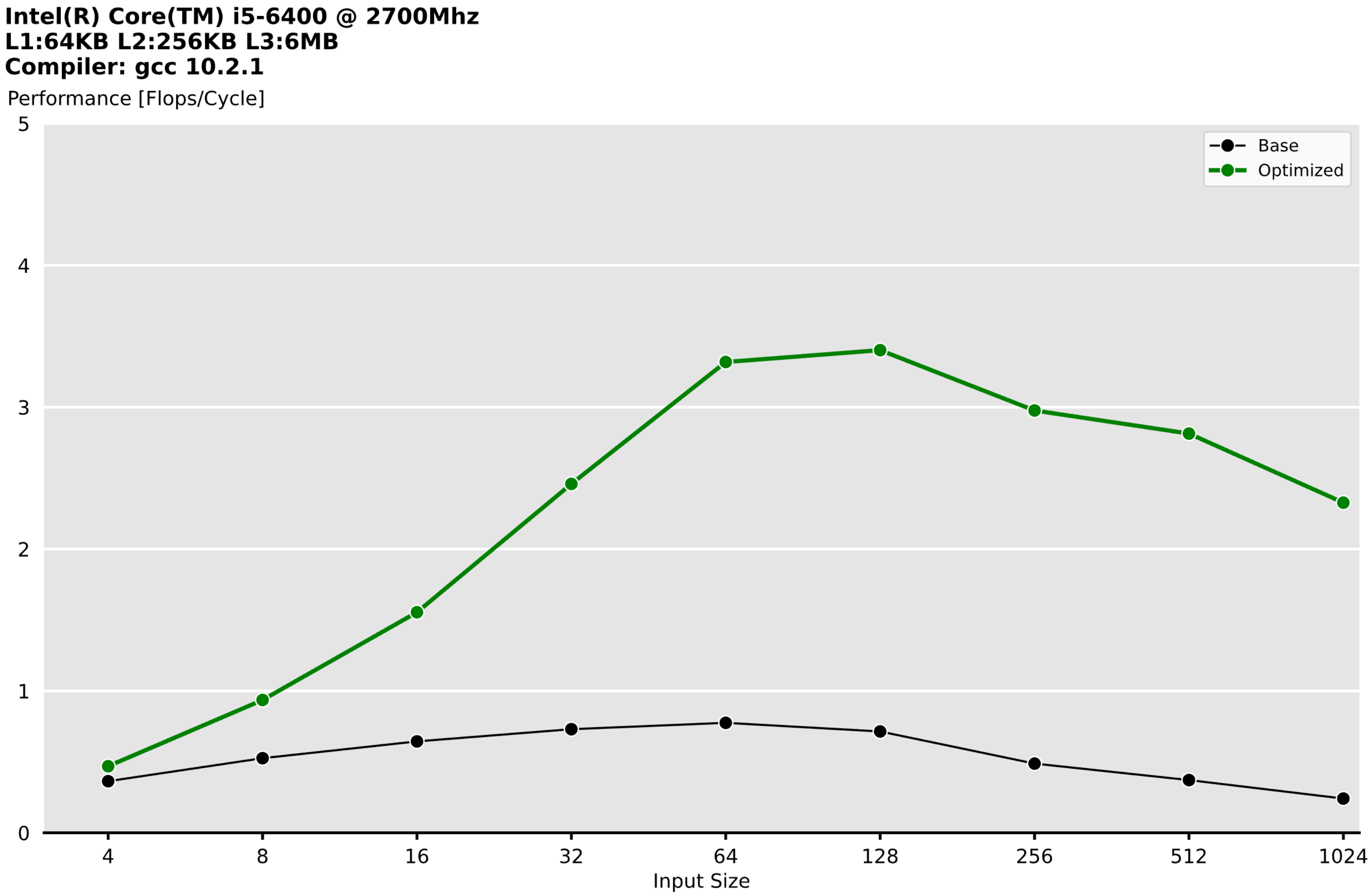
Gaussian Elimination Performance Plot



LU Decomposition Performance Plot



LU Decomposition Performance Plot



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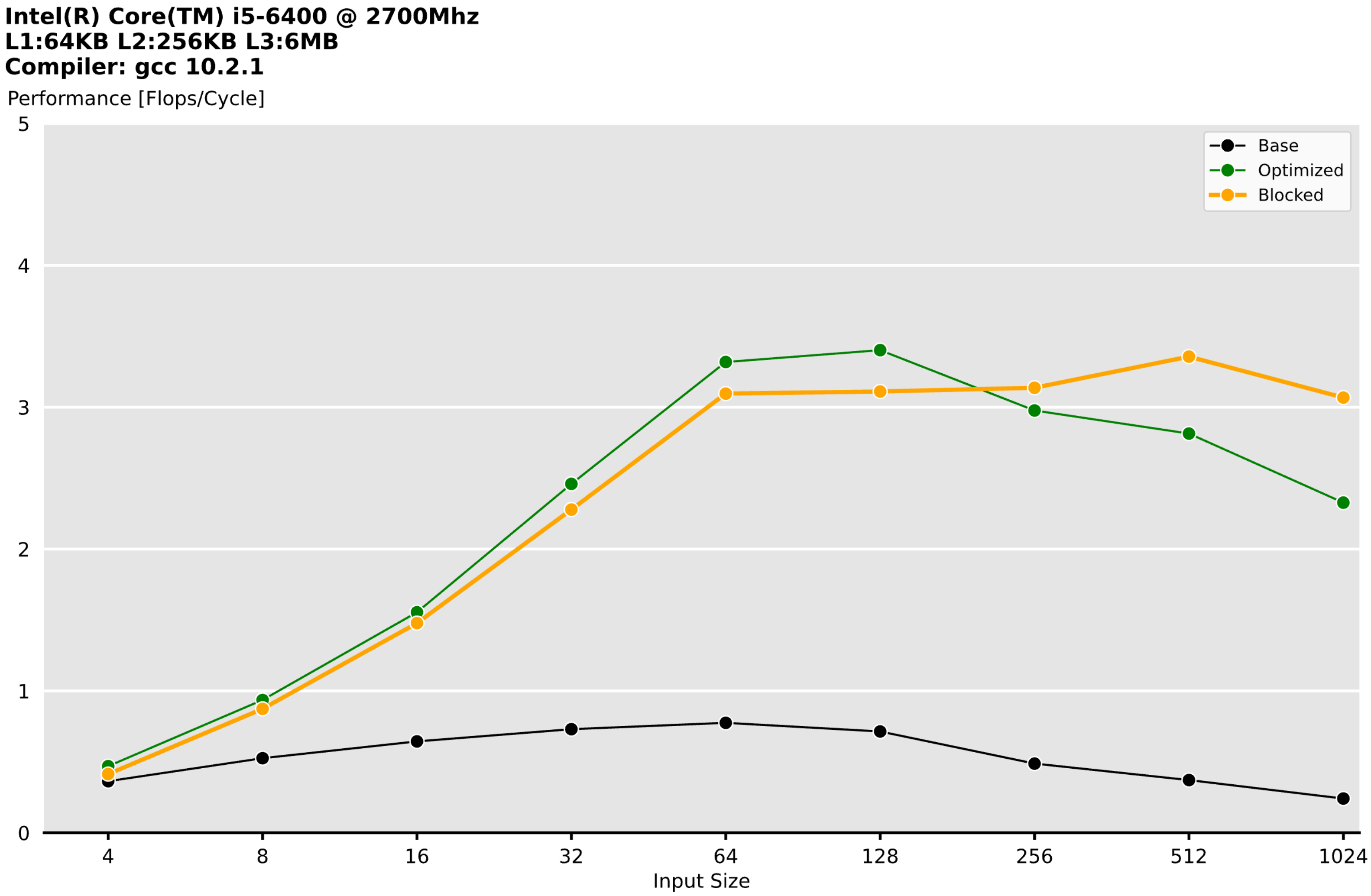

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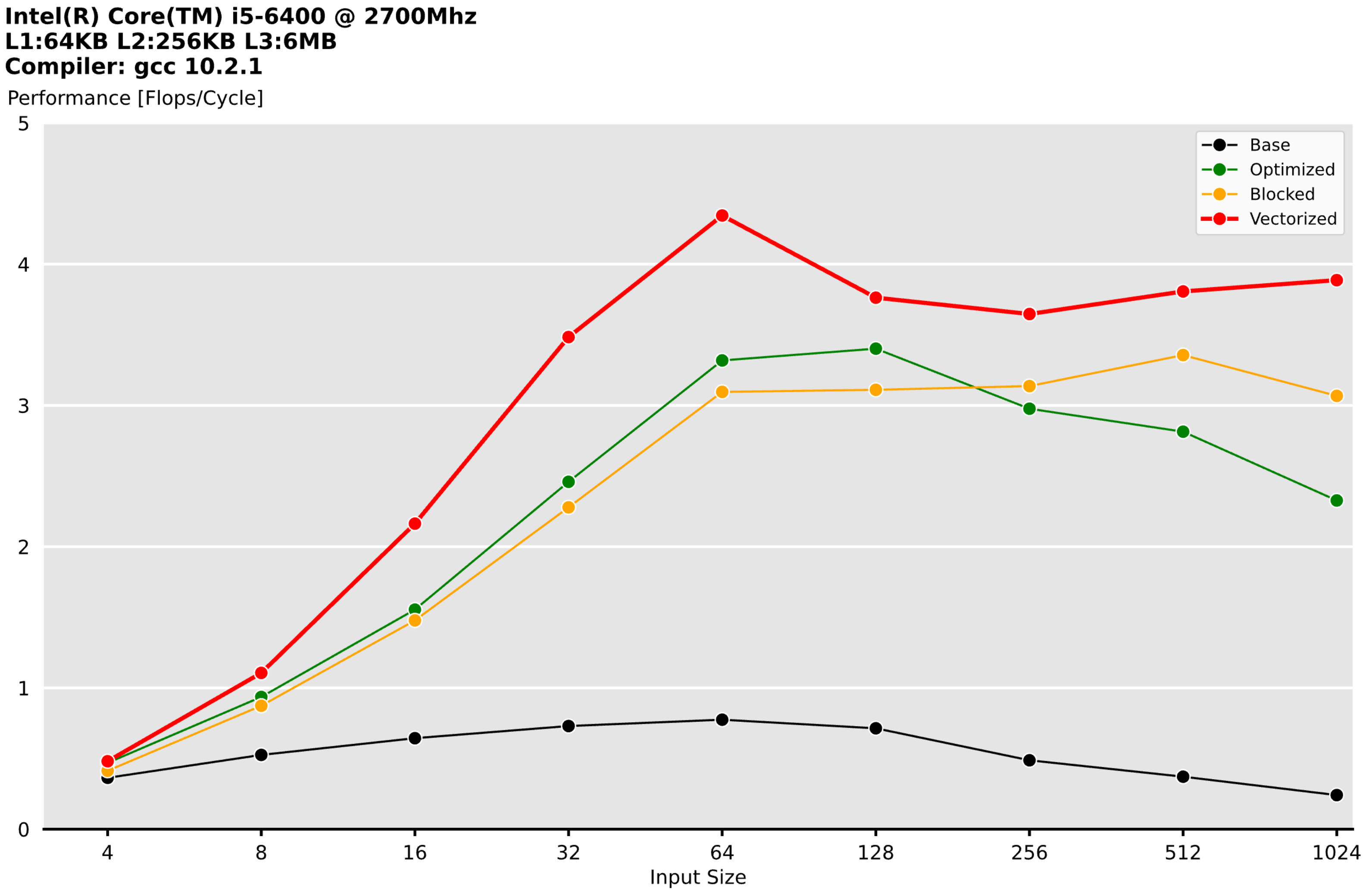
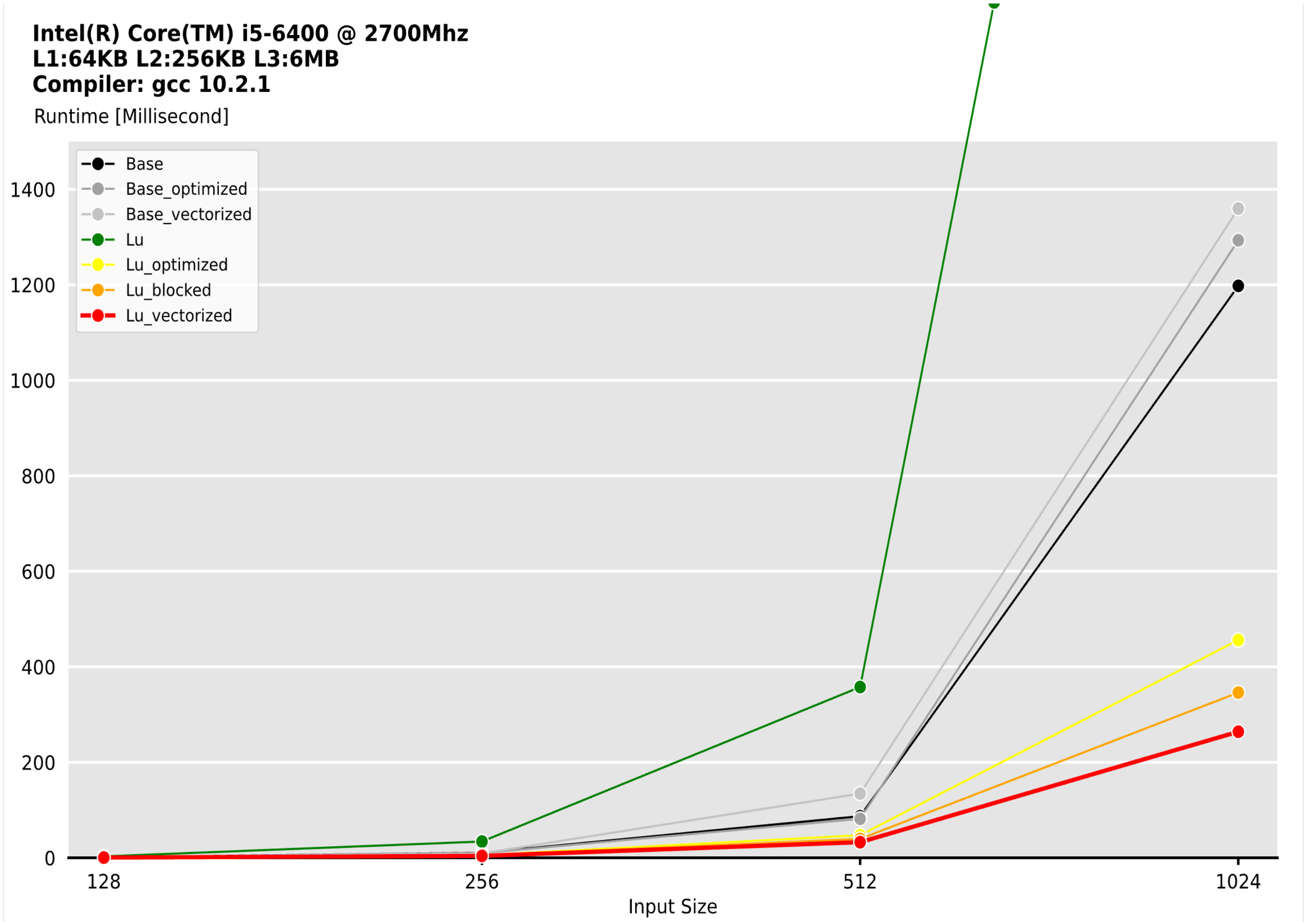
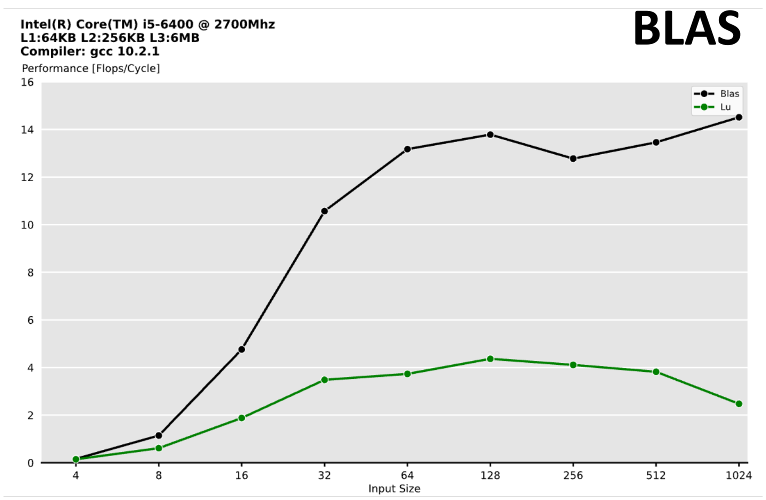


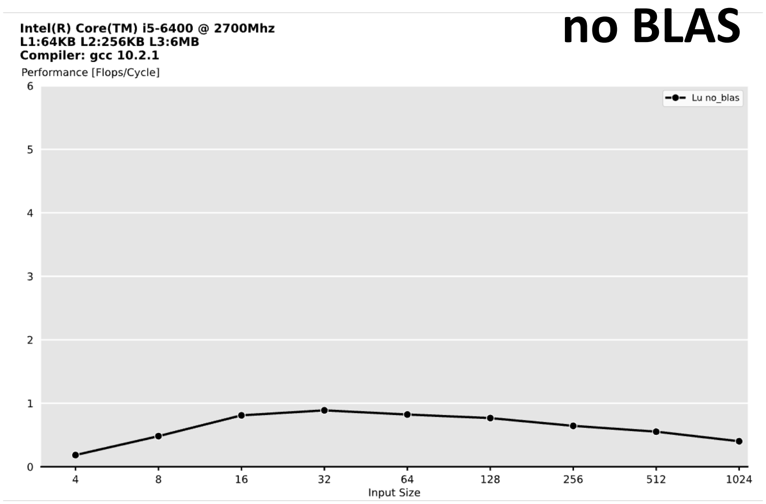
Runtime LU vs GE



Mexp-LU - Base

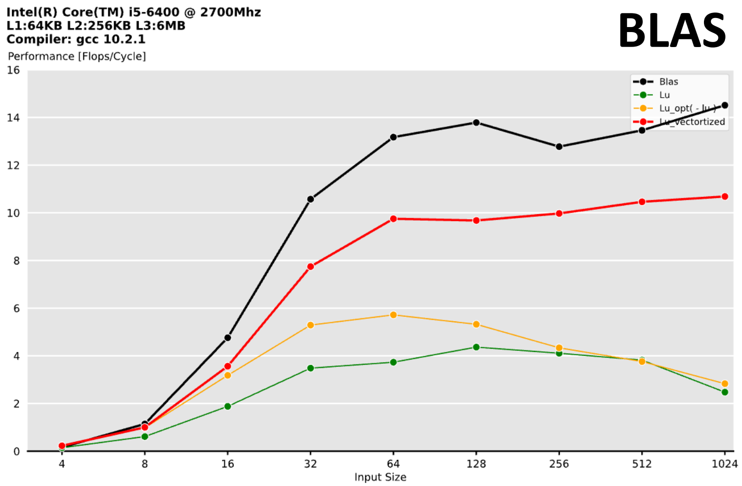


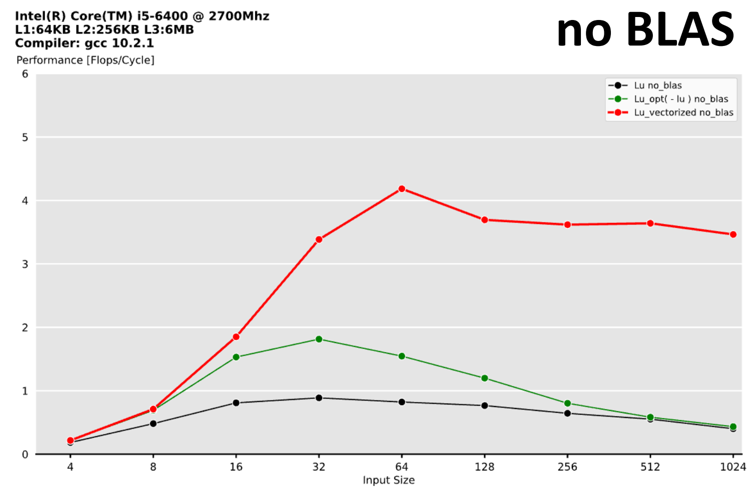
BLAS
Intel(R) Core(TM) i5-6400 @ 2700Mhz
L1:64KB L2:256KB L3:6MB
Compiler: gcc 10.2.1
Performance [Flops/Cycle]
Blas
Lu
Input Size



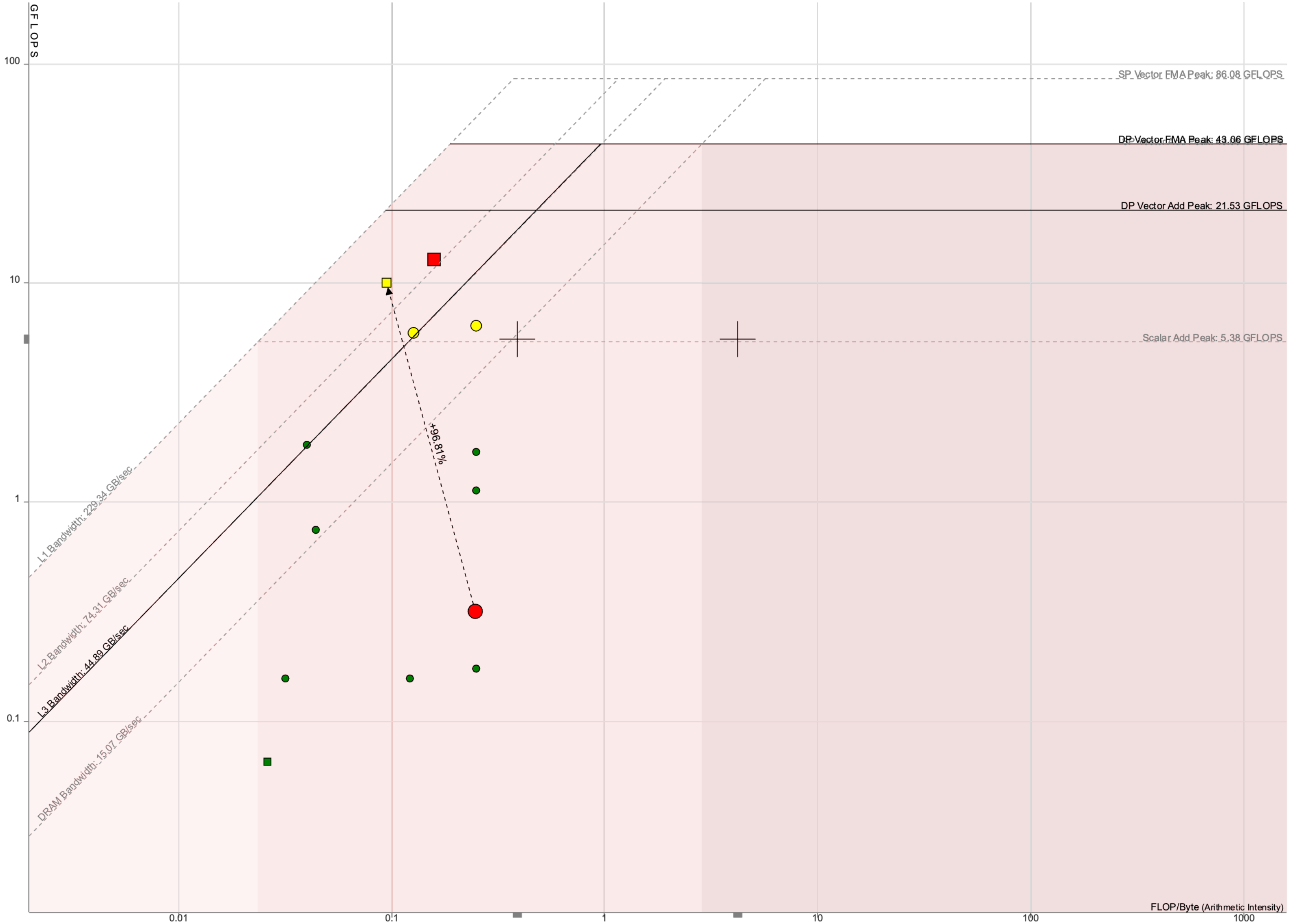
no BLAS
Intel(R) Core(TM) i5-6400 @ 2700Mhz
L1:64KB L2:256KB L3:6MB
Compiler: gcc 10.2.1
Performance [Flops/Cycle]
Lu no_blas
Input Size

Mexp-LU - Vectorised

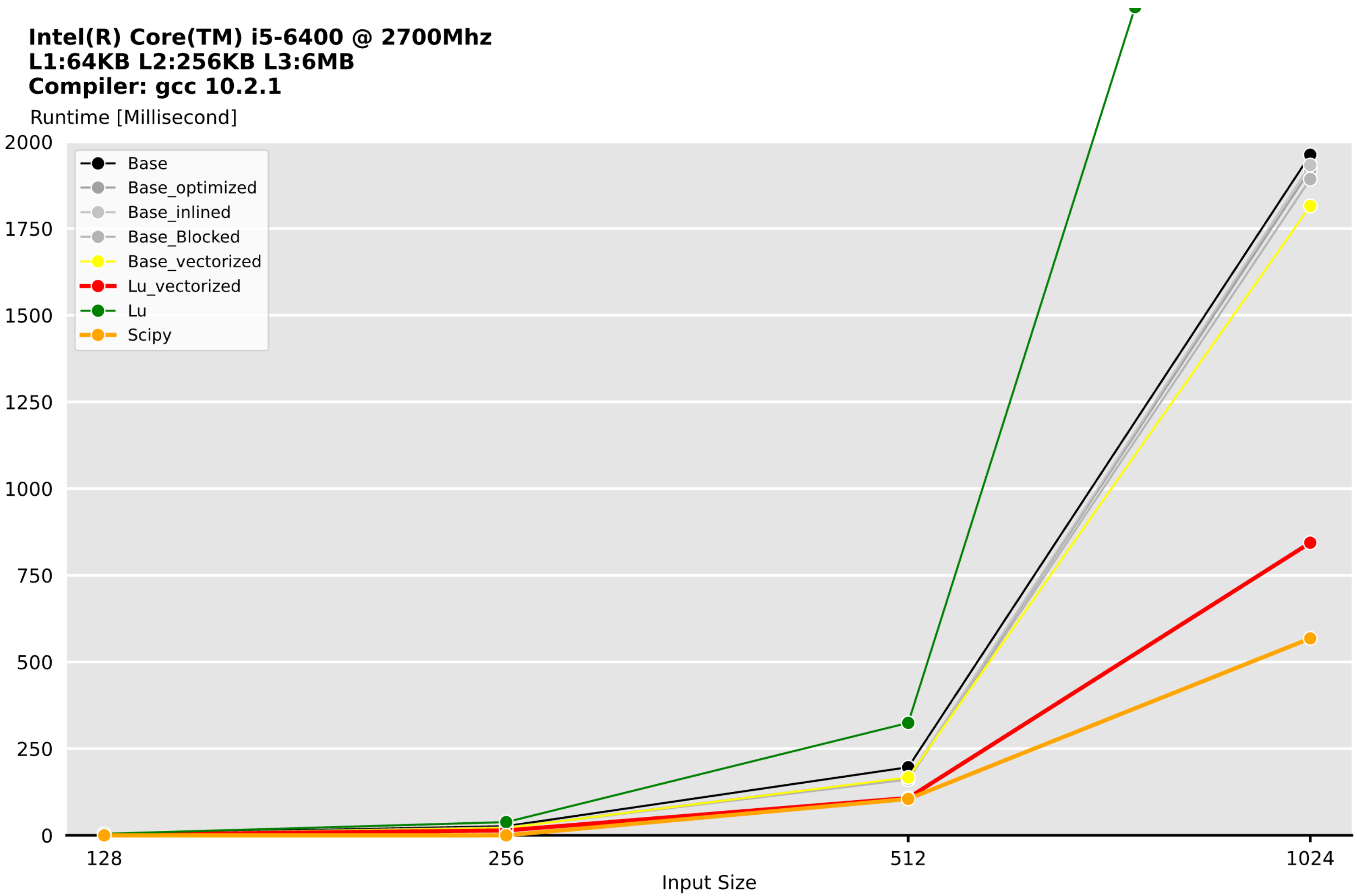




Roofline plot LU



Benchmark runtime comparison



Callgrind analysis

- **Bottlenecks**
  - solve-system
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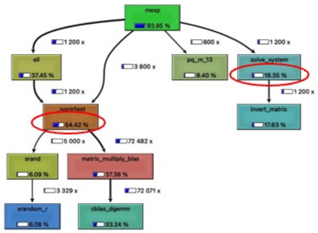

Loop ordering

- **Improved spatial and temporal locality**

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        }
    }
    for (int j = 0; j < n; j++) {
        P[i*n + j] /= Q[i*n + i];
    }
}
```
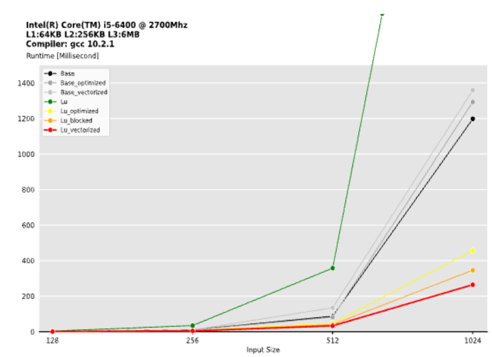

Q & A

Runtime LU vs GE



Roofline plot LU