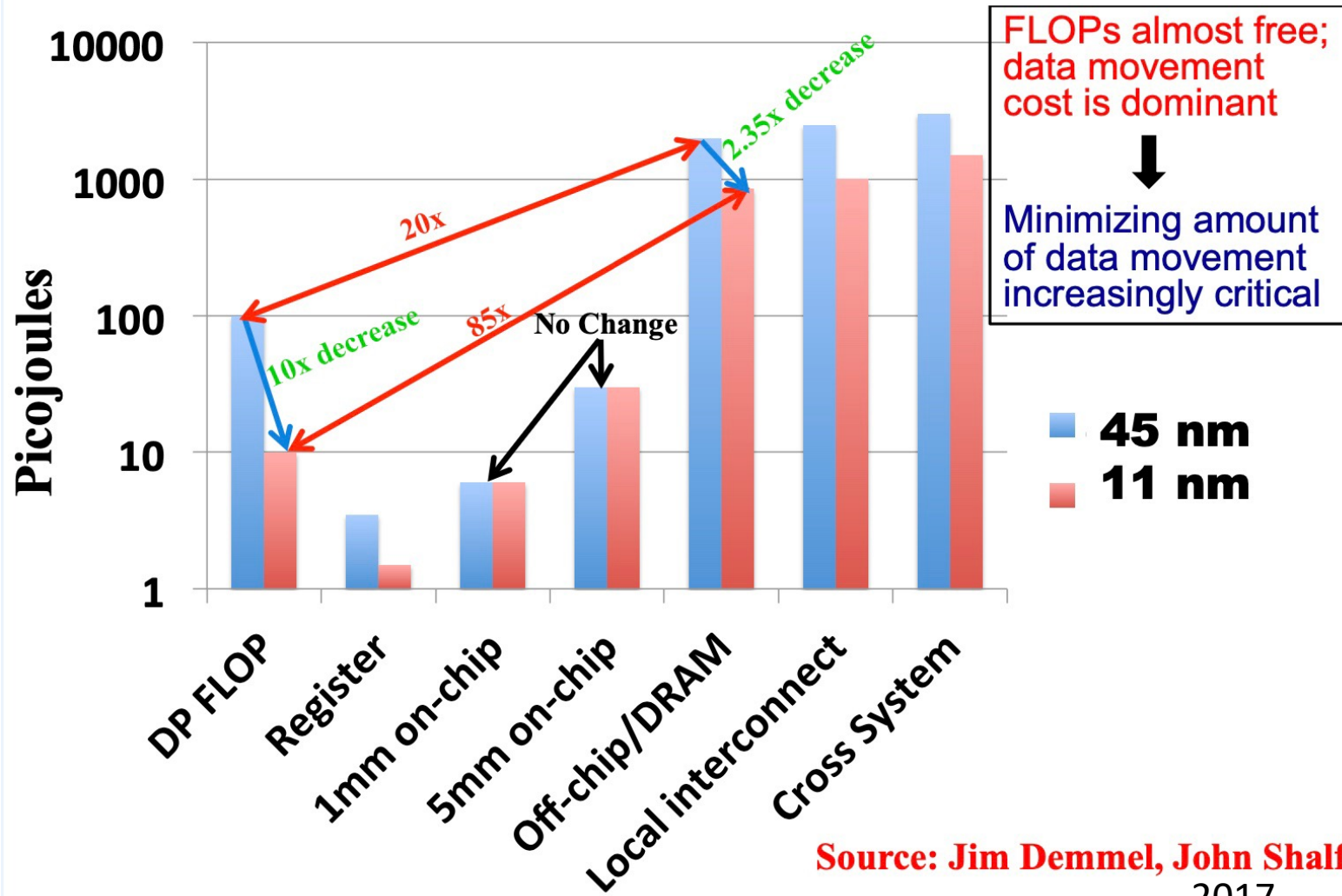


# The I/O Requirements of Various Numerical Linear Algebra Kernels

Julien Langou

Wednesday June 26<sup>th</sup> 2024

# Data Movement Cost: Energy Trends



**Source: Jim Demmel, John Shalf**  
2017



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H. T. Kung

## I/O complexity: The red-blue pebble game

Authors Hong Jia-Wei, HT Kung

Publication date 1981/5/11

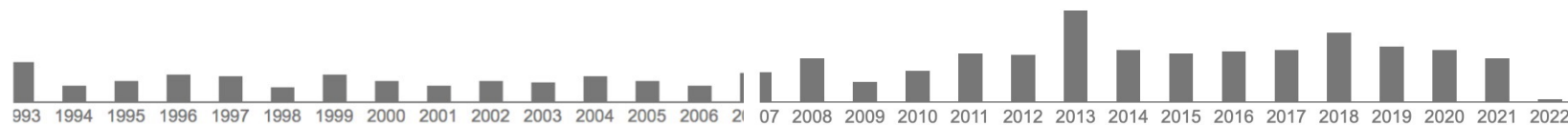
Conference Proceedings of the thirteenth annual ACM symposium on Theory of computing

Pages 326-333

Publisher ACM

Description Abstract In this paper, the red-blue pebble game is proposed to model the input-output complexity of algorithms. Using the pebble game formulation, a number of lower bound results for the I/O requirement are proven. For example, it is shown that to perform the  $n$ -point FFT or the ordinary  $n \times n$  matrix multiplication algorithm with  $O(S)$  memory, at least  $\Omega(n \log n / \log S)$  or  $\Omega(n^{3/4} / S)$ , respectively, time is needed for the I/O. Similar results are obtained for algorithms for several other problems. All of the lower ...

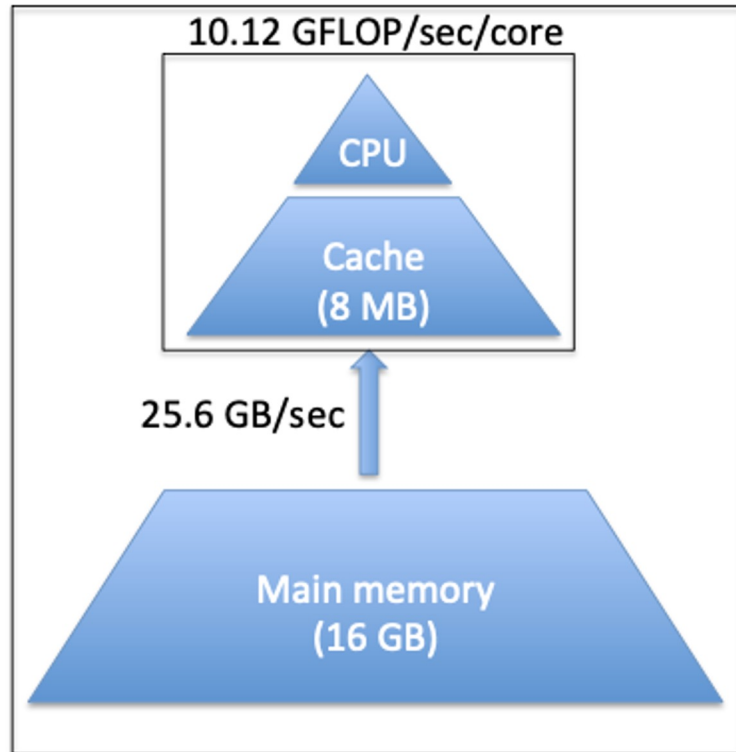
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H Jia-Wei, HT Kung - Proceedings of the thirteenth annual ACM symposium ..., 1981  
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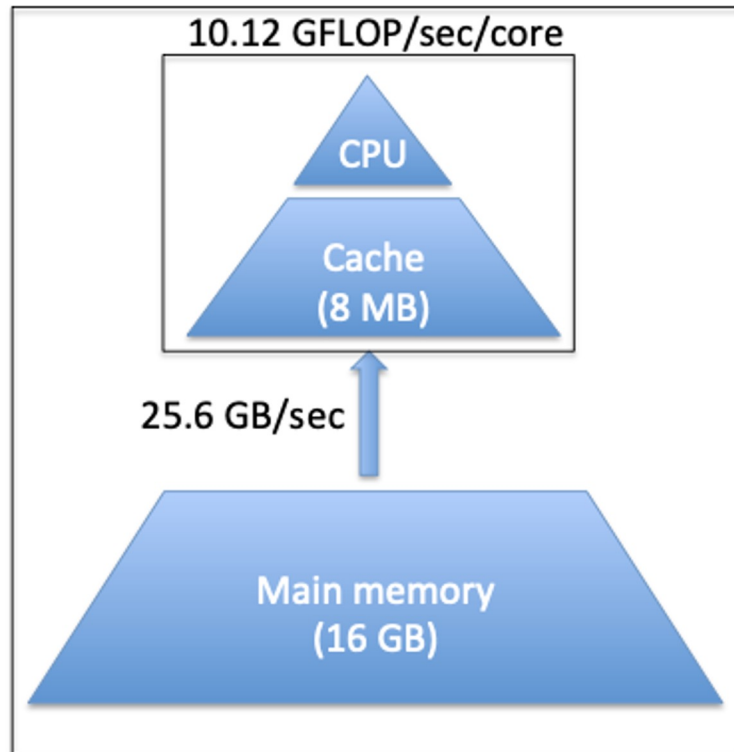
# I/O lower bound for computer programs

Intel Xeon Processor E5520 (Nehalem)



# I/O lower bound for computer programs

Intel Xeon Processor E5520 (Nehalem)



For MM

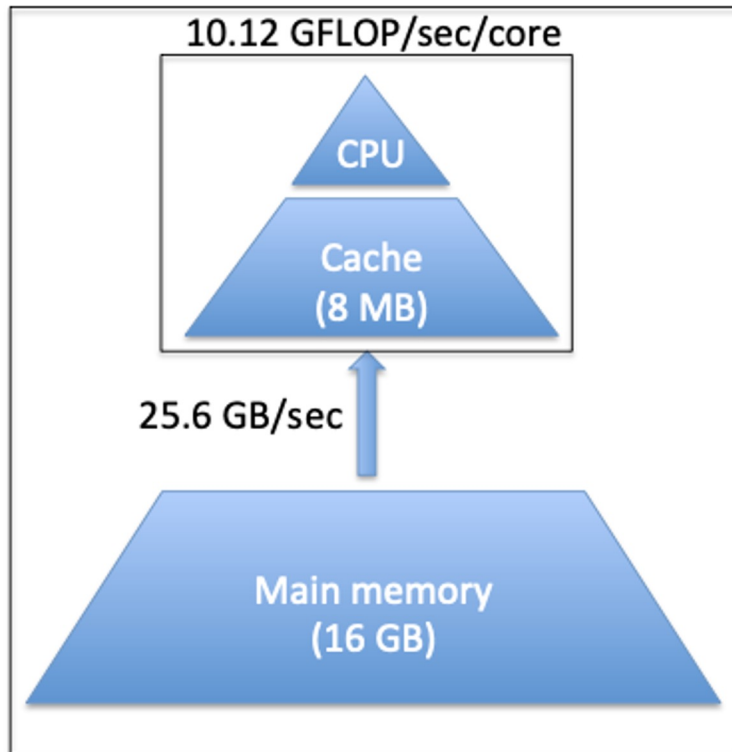
The number of words transferred between slow and fast memory is at least

$$2 \left( \frac{n^3}{\sqrt{M}} \right) - 2M.$$

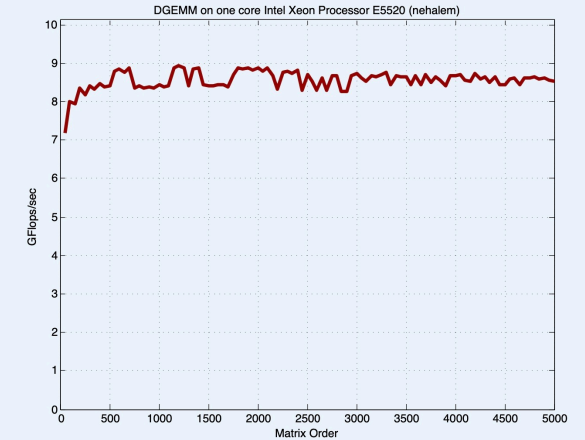
where  $n$  is matrix size and  $M$  is size of cache.

# I/O lower bound for computer programs

Intel Xeon Processor E5520 (Nehalem)



One core Intel Xeon Processor E5520 (nehalem)  
 $\beta^{-1} = 580 \cdot 10^6$  words/sec  $\gamma^{-1} = 10.12 \cdot 10^9$  flops/sec  $M = 10^6$  words



For MM

The number of words transferred between slow and fast memory is at least

$$2 \left( \frac{n^3}{\sqrt{M}} \right) - 2M.$$

where  $n$  is matrix size and  $M$  is size of cache.

## gemm

```
for (i = 0; i < m; i++)  
  for (j = 0; j < n; j++)  
    for (k = 0; k < p; k++)  
      C[i][j] += A[i][k] * B[k][j];
```

## gemm

```
for (i = 0; i < m; i++)  
  for (j = 0; j < n; j++)  
    for (k = 0; k < p; k++)  
      C[i][j] += A[i][k] * B[k][j];
```

## syrk

```
for (i = 0; i < n; i++)  
  for (k = 0; k < m; k++)  
    for (j = 0; j <= i; j++)  
      C[i][j] += A[i][k] * A[j][k];
```



## gemm

```
for (i = 0; i < m; i++)
  for (j = 0; j < n; j++)
    for (k = 0; k < p; k++)
      C[i][j] += A[i][k] * B[k][j];
```

## syrk

```
for (i = 0; i < n; i++)
  for (k = 0; k < m; k++)
    for (j = 0; j <= i; j++)
      C[i][j] += A[i][k] * A[j][k];
```

## lu

```
for (i = 0; i < n; i++) {
  for (j = 0; j < i; j++) {
    for (k = 0; k < j; k++) {
      A[i][j] -= A[i][k] * A[k][j];
    }
    A[i][j] /= A[j][j];
  }
  for (j = i; j < n; j++) {
    for (k = 0; k < i; k++) {
      A[i][j] -= A[i][k] * A[k][j];
    }
  }
}
```

## cholesky

```
for (i = 0; i < n; i++) {
  for (j = 0; j < i; j++) {
    for (k = 0; k < j; k++) {
      A[i][j] -= A[i][k] * A[j][k];
    }
    A[i][j] /= A[j][j];
  }
  for (k = 0; k < i; k++) {
    A[i][i] -= A[i][k] * A[i][k];
  }
  A[i][i] = sqrt(A[i][i]);
}
```

## gemm

```
for (i = 0; i < m; i++)  
  for (j = 0; j < n; j++)  
    for (k = 0; k < p; k++)  
      C[i][j] += A[i][k] * B[k][j];
```

## syrk

```
for (i = 0; i < n; i++)  
  for (k = 0; k < m; k++)  
    for (j = 0; j <= i; j++)  
      C[i][j] += A[i][k] * A[j][k];
```

## lu

```
for (i = 0; i < n; i++) {  
  for (j = 0; j < i; j++) {  
    for (k = 0; k < j; k++) {  
      A[i][j] -= A[i][k] * A[k][j];  
    }  
    A[i][j] /= A[j][j];  
  }  
  for (j = i; j < n; j++) {  
    for (k = 0; k < i; k++) {  
      A[i][j] -= A[i][k] * A[k][j];  
    }  
  }  
}
```

## apply\_givens\_rot\_sequence

```
for (p = 0; p < k; p++) {  
  for (j = 0; j < n - 1; j++) {  
    for (i = 0; i < m; i++) {  
      temp = C[j][p] * A[i][j] + S[j][p] * A[i][j + 1];  
      A[i][j + 1] = -S[j][p] * A[i][j] + C[j][p] * A[i][j + 1];  
      A[i][j] = temp;  
    }  
  }  
}
```

## cholesky

```
for (i = 0; i < n; i++) {  
  for (j = 0; j < i; j++) {  
    for (k = 0; k < j; k++) {  
      A[i][j] -= A[i][k] * A[j][k];  
    }  
    A[i][j] /= A[j][j];  
  }  
  for (k = 0; k < i; k++) {  
    A[i][i] -= A[i][k] * A[i][k];  
  }  
  A[i][i] = sqrt(A[i][i]);  
}
```

## cgs – Classical Gram-Schmidt

```
for (j = 0; j < N; j++) {
  for (i = 0; i < j; i++) {
    R[i][j] = 0.0e+00;
    for (k = 0; k < M; k++)
      R[i][j] += A[k][i] * A[k][j];
  }
  for (i = 0; i < j; i++)
    for (k = 0; k < M; k++)
      A[k][j] -= A[k][i] * R[i][j];
  R[j][j] = 0.0e+00;
  for (k = 0; k < M; k++)
    R[j][j] += A[k][j] * A[k][j];
  R[j][j] = sqrt(R[j][j]);
  for (k = 0; k < M; k++)
    A[k][j] /= R[j][j];
}
```

## a2v – geqr2 – Householder QR factorization

```
for(k = 0; k < N; k++){
  norma2 = 0.e+00;
  for(i = k+1; i < M; i++){
    norma2 += A[i][k] * A[i][k];
  }
  norma = sqrt( A[k][k] * A[k][k] + norma2 );
  A[k][k] = ( A[k][k] > 0 ) ? ( A[k][k] + norma ) : ( A[k][k] - norma );

  tau[k] = 2.0 / ( 1.0 + norma2 / ( A[k][k] * A[k][k] ) );

  for(i = k+1; i < M; i++){
    A[i][k] /= A[k][k];
  }
  A[k][k] = ( A[k][k] > 0 ) ? ( - norma ) : ( norma );

  for(j = k+1; j < N; j++){
    tau[j] = A[k][j];
    for(i = k+1; i < M; i++){
      tau[j] += A[i][k] * A[i][j];
    }
    tau[j] = tau[k] * tau[j];
    A[k][j] = A[k][j] - tau[j];
    for(i = k+1; i < M; i++){
      A[i][j] = A[i][j] - A[i][k] * tau[j];
    }
  }
}
```

## mgs – Modified Gram-Schmidt

```
for (j = 0; j < N; j++) {
  for (i = 0; i < j; i++) {
    R[i][j] = 0.0e+00;
    for (k = 0; k < M; k++)
      R[i][j] += A[k][i] * A[k][j];
    for (k = 0; k < M; k++)
      A[k][j] -= A[k][i] * R[i][j];
  }
  R[j][j] = 0.0e+00;
  for (k = 0; k < M; k++)
    R[j][j] += A[k][j] * A[k][j];
  R[j][j] = sqrt(R[j][j]);
  for (k = 0; k < M; k++)
    A[k][j] /= R[j][j];
}
```

## v2q – orqr2 – Construction of Q from Householder

```
for(k = N-1; k > -1; k--){
  for(j = k+1; j < N; j++){
    tau[j] = 0.e+00;
    for(i = k+1; i < M; i++){
      tau[j] += A[i][k] * A[i][j];
    }
  }
  for(j = k+1; j < N; j++){
    tau[j] *= tau[k];
  }
  A[k][k] = 1.0e+00 - tau[k];
  for(j = k+1; j < N; j++){
    A[k][j] = -tau[j];
  }
  for(j = k+1; j < N; j++){
    for(i = k+1; i < M; i++){
      A[i][j] -= A[i][k] * tau[j];
    }
  }
  for(i = k+1; i < M; i++){
    A[i][k] = - A[i][k] * tau[k];
  }
}
```

## gebd2 – reduction to bidiagonalization

```

for(k = 0; k < N; k++){
  norma2 = 0.e+00;
  for(i = k+1; i < M; i++){
    norma2 += A[i][k] * A[i][k];
  }
  norma = sqrt( A[k][k] * A[k][k] + norma2 );
  A[k][k] = ( A[k][k] > 0 ) ? ( A[k][k] + norma ) : ( A[k][k] - norma );
  tauq[k] = 2.0 / ( 1.0 + norma2 / ( A[k][k] * A[k][k] ) );
  for(i = k+1; i < M; i++){
    A[i][k] /= A[k][k];
  }
  A[k][k] = ( A[k][k] > 0 ) ? ( - norma ) : ( norma );
  for(j = k+1; j < N; j++){
    ttmp = A[k][j];
    for(i = k+1; i < M; i++){
      ttmp += A[i][k] * A[i][j];
    }
    ttmp = tauq[k] * ttmp;
    A[k][j] = A[k][j] - ttmp;
    for(i = k+1; i < M; i++){
      A[i][j] = A[i][j] - A[i][k] * ttmp;
    }
  }
  norma2 = 0.e+00;
  for(j = k+2; j < N; j++){
    norma2 += A[k][j] * A[k][j];
  }
  norma = sqrt( A[k][k+1] * A[k][k+1] + norma2 );
  A[k][k+1] = ( A[k][k+1] > 0 ) ? ( A[k][k+1] + norma ) : ( A[k][k+1] - norma );
  taup[k] = 2.0 / ( 1.0 + norma2 / ( A[k][k+1] * A[k][k+1] ) );
  for(j = k+2; j < N; j++){
    A[k][j] /= A[k][k+1];
  }
  A[k][k+1] = ( A[k][k+1] > 0 ) ? ( - norma ) : ( norma );
  for(i = k+1; i < M; i++){
    ttmp = A[i][k+1];
    for(j = k+2; j < N; j++){
      ttmp += A[i][j] * A[k][j];
    }
    ttmp = ttmp * taup[k];
    A[i][k+1] = A[i][k+1] - ttmp;
    for(j = k+2; j < N; j++){
      A[i][j] = A[i][j] - ttmp * A[k][j];
    }
  }
}
}

```

## gehd2 – reduction to Hessenberg form

```

for ( j = 0; j < n-2; j++ ) {
  norma2 = 0.0;
  for ( i = j+2; i < n; i++ ) {
    norma2 += A[i][j] * A[i][j];
  }
  norma = sqrt ( A[j+1][j] * A[j+1][j] + norma2 );
  A[j+1][j] = ( A[j+1][j] > 0 ) ? ( A[j+1][j] + norma ) : ( A[j+1][j] - norma );
  tau = 2.0 / ( 1.0 + norma2 / ( A[j+1][j] * A[j+1][j] ) );
  for ( i = j+2; i < n; i++ ) {
    A[i][j] /= A[j+1][j];
  }
  A[j+1][j] = ( A[j+1][j] > 0 ) ? ( - norma ) : ( norma );
  for ( i = j+1; i < n; i++ ) {
    tmp[i] = A[j+1][i];
    for ( k = j+2; k < n; k++ ) {
      tmp[i] += A[k][j] * A[k][i];
    }
  }
  for ( i = j+1; i < n; i++ ) {
    tmp[i] *= tau;
  }
  for ( i = j+1; i < n; i++ ) {
    A[j+1][i] -= tmp[i];
  }
  for ( i = j+2; i < n; i++ ) {
    for ( k = j+1; k < n; k++ ) {
      A[i][k] -= A[i][j] * tmp[k];
    }
  }
  for ( i = 0; i < n; i++ ) {
    tmp[i] = A[i][j+1];
    for ( k = j+2; k < n; k++ ) {
      tmp[i] += A[i][k] * A[k][j];
    }
  }
  for ( i = 0; i < n; i++ ) {
    tmp[i] *= tau;
  }
  for ( i = 0; i < n; i++ ) {
    A[i][j+1] -= tmp[i];
  }
  for ( i = 0; i < n; i++ ) {
    for ( k = j+2; k < n; k++ ) {
      A[i][k] -= tmp[i] * A[k][j];
    }
  }
}
}

```

## sytd2 – reduction to symmetric tridiagonal form

```

for(i = 0; i < n-2; i++){
  norma2 = 0.0e+00 ;
  for ( k = i+2; k < n ; k++ ) {
    norma2 += A[k][i] * A[k][i];
  }
  norma = sqrt( A[i+1][i] * A[i+1][i] + norma2 );
  A[i+1][i] = ( A[i+1][i] > 0 ) ? (A[i+1][i] + norma) : (A[i+1][i] - norma) ;
  tau_i = 2.0e+00 / ( 1.0e+00 + norma2 / ( A[i+1][i] * A[i+1][i] ) );

  for (k = i+2; k < n ; k++) {
    A[k][i] /= A[i+1][i] ;
  }
  A[i+1][i] = ( A[i+1][i] > 0.0e+00 ) ? ( - norma ) : ( norma ) ;
  for(k = i+1; k < n; k++){
    tau[k-1] = A[k][i+1];
    for(j = i+2; j <= k; j++){
      tau[k-1] += A[k][j] * A[j][i];
    }
    for(j = k+1; j < n; j++){
      tau[k-1] += A[j][k] * A[j][i];
    }
    tau[k-1] *= tau_i;
  }
  alpha = tau[i];
  for(k = i+2; k < n; k++){
    alpha += tau[k-1] * A[k][i];
  }
  alpha = -0.5e+00 * tau_i * alpha;
  tau[i] += alpha ;
  for(k = i+2; k < n; k++){
    tau[k-1] += alpha * A[k][i];
  }
  A[i+1][i+1] -= 2.0e+00 * tau[i] ;
  for(j = i+2; j < n; j++){
    A[j][i+1] -= tau[j-1] ;
    A[j][i+1] -= tau[i] * A[j][i];
    for(k = i+2; k <= j; k++){
      A[j][k] -= tau[j-1] * A[k][i];
      A[j][k] -= tau[k-1] * A[j][i];
    }
  }
  tau[i] = tau_i;
}

```

## gghd2 – reduction to triangular Hessenberg form

```

for ( j = 0; j < _PB_N-2; j++ ) {
  for ( i = _PB_N-2; i > j; i-- ) {
    nrm = SQRT_FUN ( A[i][j] * A[i][j] + A[i+1][j] * A[i+1][j] );
    c = A[i][j] / nrm;
    s = A[i+1][j] / nrm;
    A[i][j] = nrm;
    A[i+1][j] = SCALAR_VAL(0.0);
    for ( k = j+1; k < _PB_N; k++ ) {
      tmp = c * A[i][k] + s * A[i+1][k];
      A[i+1][k] = - s * A[i][k] + c * A[i+1][k];
      A[i][k] = tmp;
    }
    for ( k = i; k < _PB_N; k++ ) {
      tmp = c * B[i][k] + s * B[i+1][k];
      B[i+1][k] = - s * B[i][k] + c * B[i+1][k];
      B[i][k] = tmp;
    }
    for ( k = 0; k < _PB_N; k++ ) {
      tmp = c * Q[i][k] + s * Q[i+1][k];
      Q[i+1][k] = - s * Q[i][k] + c * Q[i+1][k];
      Q[i][k] = tmp;
    }
    nrm = SQRT_FUN ( B[i+1][i+1] * B[i+1][i+1] + B[i+1][i] * B[i+1][i] );
    c = B[i+1][i+1] / nrm;
    s = B[i+1][i] / nrm;
    B[i+1][i+1] = nrm;
    B[i+1][i] = SCALAR_VAL(0.0);
    for ( k = 0; k <= i; k++ ) {
      tmp = c * B[k][i] - s * B[k][i+1];
      B[k][i+1] = s * B[k][i] + c * B[k][i+1];
      B[k][i] = tmp;
    }
    for ( k = 0; k < _PB_N; k++ ) {
      tmp = c * A[k][i] - s * A[k][i+1];
      A[k][i+1] = s * A[k][i] + c * A[k][i+1];
      A[k][i] = tmp;
    }
    for ( k = i-j; k < _PB_N; k++ ) {
      tmp = c * Z[k][i] - s * Z[k][i+1];
      Z[k][i+1] = s * Z[k][i] + c * Z[k][i+1];
      Z[k][i] = tmp;
    }
  }
}
}

```

```

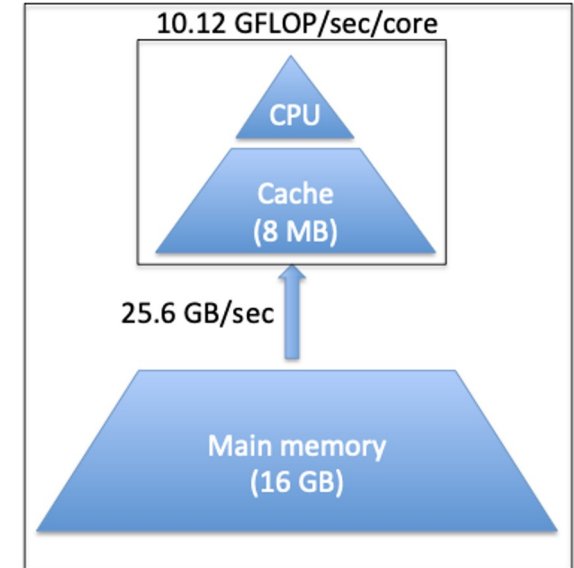
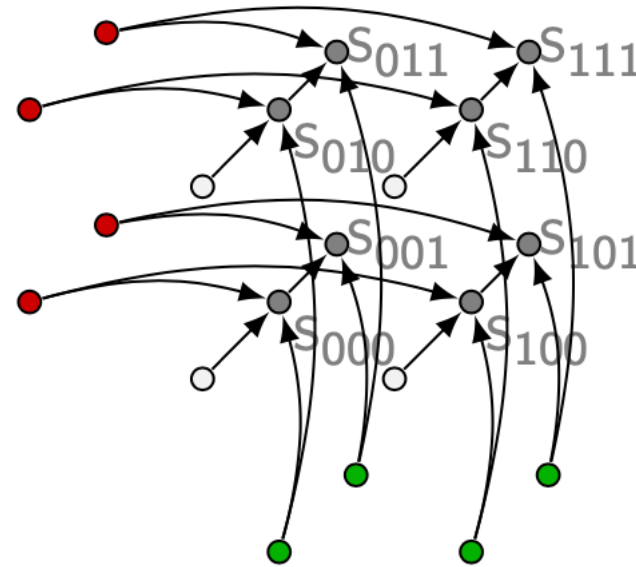
for (i = 0; i < m; i++)
  for (j = 0; j < n; j++)
    for (k = 0; k < p; k++)
      C[i][j] += A[i][k] * B[k][j];

```

```

C[0][0] += A[0][0] * B[0][0]; // S000
C[0][0] += A[0][1] * B[1][0]; // S001
C[0][0] += A[0][2] * B[2][0]; // S002
C[0][0] += A[0][3] * B[3][0]; // S003
...
C[0][1] += A[0][0] * B[0][1]; // S010
C[0][1] += A[0][1] * B[1][1]; // S011
C[0][1] += A[0][2] * B[2][1]; // S012
C[0][1] += A[0][3] * B[3][1]; // S013

```



A. Olivry, J. Langou, L-N Pouchet, P. Sadayappan, and F. Rastello. **Automated derivation of parametric data movement lower bounds for affine programs.** In the Proceedings of PLDI 2020: Proceedings of the 41st ACM SIGPLAN Conference on Programming Language Design and Implementation, page 808–822, June 2020. ( [link](#) )

**input** is an affine code

```
for (i = 0; i < _PB_N; i++) {
  for (j = 0; j < i; j++) {
    for (k = 0; k < j; k++) {
      A[i][j] -= A[i][k] * A[j][k];
    }
    A[i][j] /= A[j][j];
  }
  for (k = 0; k < i; k++) {
    A[i][i] -= A[i][k] * A[i][k];
  }
  A[i][i] = SqrtFun(A[i][i]);
}
```

**cholesky code**

A. Olivry, J. Langou, L-N Pouchet, P. Sadayappan, and F. Rastello. **Automated derivation of parametric data movement lower bounds for affine programs**. In the Proceedings of PLDI 2020: Proceedings of the 41st ACM SIGPLAN Conference on Programming Language Design and Implementation, page 808–822, June 2020. ( [link](#) )

**input** is an affine code with parameter **N** and parameter **S** for cache size

```
for (i = 0; i < _PB_N; i++) {
  for (j = 0; j < i; j++) {
    for (k = 0; k < j; k++) {
      A[i][j] -= A[i][k] * A[j][k];
    }
    A[i][j] /= A[j][j];
  }
  for (k = 0; k < i; k++) {
    A[i][i] -= A[i][k] * A[i][k];
  }
  A[i][i] = SqrtFun(A[i][i]);
}
```

**cholesky code**

Unit is for **N** for, **S** for and IO lower bound is “number”.



A. Olivry, J. Langou, L-N Pouchet, P. Sadayappan, and F. Rastello. **Automated derivation of parametric data movement lower bounds for affine programs**. In the Proceedings of PLDI 2020: Proceedings of the 41st ACM SIGPLAN Conference on Programming Language Design and Implementation, page 808–822, June 2020. ( [link](#) )

**Output #1** is an IO lower bound

cholesky	$\max\left(\frac{1}{2}N(N+1), \frac{1}{6} \frac{1}{\sqrt{S}}(N-1)(N-2)(N-3) + \frac{1}{2\sqrt{2}} \frac{1}{S}(N-1)(N-2) - (N-2)(N-7) - 4\sqrt{2}S\right)$	$\frac{1}{6} \frac{1}{\sqrt{S}} N^3$
----------	---	--------------------------------------

**input** is an affine code with parameter **N** and parameter **S** for cache size

```

for (i = 0; i < _PB_N; i++) {
  for (j = 0; j < i; j++) {
    for (k = 0; k < j; k++) {
      A[i][j] -= A[i][k] * A[j][k];
    }
    A[i][j] /= A[j][j];
  }
  for (k = 0; k < i; k++) {
    A[i][i] -= A[i][k] * A[i][k];
  }
  A[i][i] = SqrtFun(A[i][i]);
}

```

**cholesky code**

**IO lower bound** with parameter **N** and parameter **S** for cache size      asymptotic IO lower bound

Unit is for **N** for, **S** for and **IO lower bound** is “number”.

# A. Olivry, J. Langou, L-N Pouchet, P. Sadayappan, and F. Rastello. Automated derivation of parametric data movement lower bounds for affine programs. In the Proceedings of PLDI 2020: Proceedings of the 41st ACM SIGPLAN Conference on Programming Language Design and Implementation, page 808–822, June 2020. ( [link](#) )

## Output #1 is an IO lower bound

cholesky	$\max\left(\frac{1}{2}N(N+1), \frac{1}{6}\frac{1}{\sqrt{S}}(N-1)(N-2)(N-3) + \frac{1}{2\sqrt{2}}\frac{1}{S}(N-1)(N-2) - (N-2)(N-7) - 4\sqrt{2}S\right)$	$\frac{1}{6}\frac{1}{\sqrt{S}}N^3$
----------	---	------------------------------------

input is an affine code

```

for (i = 0; i < _PB_N; i++) {
  for (j = 0; j < i; j++) {
    for (k = 0; k < j; k++) {
      A[i][j] -= A[i][k] * A[j][k];
    }
    A[i][j] /= A[j][j];
  }
  for (k = 0; k < i; k++) {
    A[i][i] -= A[i][k] * A[i][k];
  }
  A[i][i] = SQRT_FUN(A[i][i]);
}

```

## cholesky code

Cholesky

**G Full example: Cholesky decomposition**

IOLB uses two proof techniques, namely the  $K$ -partition and the wavefront based proofs that are respectively described in Sec. 5 and Sec. 6. In this section, we demonstrate the complete process on a concrete example: the cholesky kernel. In this example, the  $K$ -partition method is the method of choice. (So we do not use the wavefront method). The pseudo-code and associated DFG for cholesky are reported in Fig. 8.

The DFG contains three statement vertices  $\{S_1, S_2, S_3\}$  (the vertex corresponding to input array  $A$  and the corresponding dependences are omitted as they do not play a role in the lower bound derivation). The main loop of Alg. 1 iterates on those statements and computes some lower bound complexities for each of them. We here consider statement  $S_1$  for which the  $K$ -partition reasoning is the one that leads to the largest lower bound of the three.

Out of the six paths, procedure `genpaths` will select three "interesting paths" for statement  $S_1$ . These are the three paths pointing to  $S_1$ , namely:

- $P_1 = (e_1)$  is a chain path
- $P_2 = (e_2)$  is a broadcast path
- $P_3 = (e_3)$  is a broadcast path

The "S-centric" sub-CDAG is obtained by intersecting the domain of  $S$  with the corresponding individual domains of the paths of interests  $\mathcal{P} = \{P_1, P_2, P_3\}$  which are:

$\text{Dom}(P_1) = \{S_1[k,i,j] : 1 \leq k < N \wedge k+1 \leq i < N \wedge k+1 \leq j \leq i\}$   
 $\text{Dom}(P_2) = \{S_1[k,i,j] : 0 \leq k < N \wedge k+1 \leq i < N \wedge k+1 \leq j \leq i\}$   
 $\text{Dom}(P_3) = \{S_1[k,i,j] : 0 \leq k < N \wedge k+1 \leq i < N \wedge k+1 \leq j \leq i\}$

Leading to an intersection domain:

$D_2 = \text{Dom}(P_2) \cap \text{Dom}(P_3) \cap \text{Dom}(P_1)$   
 $= \{S_1[k,i,j] : 1 \leq k < N \wedge k+1 \leq i < N \wedge k+1 \leq j \leq i\}$

For those paths, the corresponding projections and kernels are:

$\phi_1(k,i,j) = \text{proj}_{(1,0,0)}(k,i,j) = (0,i,i)$  kernel  $k_1 = \text{Ker}(\phi_1) = ((1,0,0))$   
 $\phi_2(k,i,j) = (k,j)$  kernel  $k_2 = \text{Ker}(\phi_2) = ((0,1,0))$   
 $\phi_3(k,i,j) = (k,i)$  kernel  $k_3 = \text{Ker}(\phi_3) = ((0,0,1))$

The explicit embedding  $\rho$  of the parametrized CDAG into  $E$  is trivial in this case. (See Section D.1.)

In order to apply Theorem B.1 to  $E$  with  $\phi_1, \phi_2$  and  $\phi_3$ , we need to find constant  $s_1, s_2$  and  $s_3$  such that Equation (3) is true. Since the projection kernels,  $\text{Ker}(\phi_i)$ , are linearly independent, in this case, there is no need to compute the generated lattice of subgroups. Simply testing on each kernel individually for Equation (3) is sufficient (see proof in [11], Sec. 6.3). This leads to the following conditions on  $s_1, s_2$  and  $s_3$ :

$$\begin{cases} 0 \leq s_1, s_2, s_3 \leq 1 \\ 1 \leq s_1 + s_2 \\ 1 \leq s_1 + s_3 \\ 1 \leq s_1 + s_2 \end{cases} \quad (8)$$

We can apply Theorem B.1 to  $E$  with  $\phi_1, \phi_2$  and  $\phi_3$  for any  $s_1, s_2$  and  $s_3$  satisfying Equation (8) to get Equation (4). This gives that

$$|E| \leq |\phi_1(E)|^{s_1} \cdot |\phi_2(E)|^{s_2} \cdot |\phi_3(E)|^{s_3}. \quad (9)$$

Each of the  $|\phi_i(E)|$  is bounded by  $K$ , where  $K = (S+T)$ , where  $S$  is the cache size, and  $T$  is the length of a segment. (See Section D.1 and Equation (1):

$$|\phi_i(E)| \leq K, i=1,2,3. \quad (10)$$

Therefore, denoting  $\sigma = s_1 + s_2 + s_3$ , we can bound  $|E|$  with

$$|E| \leq K^\sigma \quad (11)$$

We note that we have introduced 4 parameters:  $T, s_1, s_2, s_3$ . We will choose  $s_1, s_2, s_3$  when we minimize the upper bound  $E$  for all possible values of  $s_1, s_2, s_3$ . We will choose  $T$  when we maximize the lower bound in  $I/O$  for all possible values of  $T$ . For now, we leave these variables as parameters in the reasoning.

Equation (11) is a valid upper bound on the cardinality on any  $K$ -bounded set  $E$  in the parametrized CDAG. This upper bound enables us to finish the reasoning to find a lower bound on  $I/O$  using the  $K$ -partitioning method.

However, we are able to obtain a tighter (higher)  $I/O$  lower bound if we can find more constraining inequalities on  $|\phi_i(E)|$  than Equation (10). In order to do so, we use the "sum-the-projections" trick. (See Section D.1.1.)

In order to use the "sum-the-projections" trick, we need to check the independence of the projections, so we first intersect the inverse domains of the different paths which are:

$R_{P_1}^{-1}(D) = \{S_1[k,i,j] : 0 \leq k < N-1 \wedge k+1 \leq i < N-1 \wedge k+1 \leq j\}$   
 $R_{P_2}^{-1}(D) = \{S_1[k,i,j] : 1 \leq k < N \wedge k+1 \leq j < N\}$   
 $R_{P_3}^{-1}(D) = \{S_1[k,i,j] : 1 \leq k < N \wedge k+1 \leq i < N\}$

Thus getting:

$R_{P_1}^{-1}(D) \cap R_{P_2}^{-1}(D) = \emptyset \Rightarrow P_1$  is independent from  $P_2$   
 $R_{P_1}^{-1}(D) \cap R_{P_3}^{-1}(D) = \emptyset \Rightarrow P_1$  is independent from  $P_3$   
 $R_{P_2}^{-1}(D) \cap R_{P_3}^{-1}(D) \neq \emptyset \Rightarrow P_2$  interferes with  $P_3$

We can thus write, for every  $K$ -bounded-set ( $K = (S+T)$ )  $E$  in the parametrized CDAG:

$$\begin{cases} |\phi_1(E)| + |\phi_2(E)| \leq K \\ |\phi_2(E)| + |\phi_3(E)| \leq K \end{cases}$$

And summing the two:

$$|\phi_1(E)| + \frac{1}{2}|\phi_2(E)| + \frac{1}{2}|\phi_3(E)| \leq K. \quad (12)$$

Since Equation (12) is more constraining on  $|\phi_1(E)|$  than Equation (10), it enables us to obtain a tighter (higher)  $I/O$  lower bound.

In the framework of Lemma D.2, we call  $(\beta_1, \beta_2, \beta_3) = (1, 1/2, 1/2)$ , so that Equation (12) reads

$$\beta_1|\phi_1(E)| + \beta_2|\phi_2(E)| + \beta_3|\phi_3(E)| \leq K.$$

We now use Lemma D.2 to bound  $|E|$  as follows:

**(a) Source code**

```

for (k = 0; k < n; k++) {
  A[k][k] = sqrt(A[k][k]); // S1
  for (i = k+1; i < n; i++)
    A[i][k] /= A[k][k]; // S2
  for (i = k+1; i < n; i++)
    for (j = k+1; j <= i; j++)
      A[i][j] -= A[i][k] * A[j][k]; // S3
}

```

**(b) DFG (input nodes are omitted)**

**Figure 8. Cholesky decomposition**

$R_{e_1} = \{S_1[k-1,i,j] \rightarrow S_1[k,i,j] : 1 \leq k < N \wedge k+1 \leq i < N \wedge k+1 \leq j \leq i\}$   
 $R_{e_2} = \{S_1[k,j] \rightarrow S_1[k,i,j] : 0 \leq k < N \wedge k+1 \leq i < N \wedge k+1 \leq j \leq i\}$   
 $R_{e_3} = \{S_1[k,i] \rightarrow S_1[k,i,j] : 0 \leq k < N \wedge k+1 \leq i < N \wedge k+1 \leq j \leq i\}$   
 $R_{e_4} = \{S_1[k-1,i,k] \rightarrow S_2[k,i,j] : 1 \leq k < N \wedge k+1 \leq i < N\}$   
 $R_{e_5} = \{S_1[k] \rightarrow S_2[k,i] : 0 \leq k < N \wedge k+1 \leq i < N\}$   
 $R_{e_6} = \{S_1[k-1,k,k] \rightarrow S_3[k,i] : 1 \leq k < N \wedge k+1 \leq i < N\}$

So (omitting lower-order terms)  $|V \setminus \text{Sources}(V)| = \frac{N^3}{6}$  and  $|\text{Sources}(V)| = N^2$ . Taking for  $U$  our upper bound on  $|E|$  provides the following inequality for which the objective is to set a value for  $T$  that maximizes its right hand side:

$$Q \geq T \times \left[ \frac{N^3/6}{2 \cdot (K/3)^{3/2}} \right] - N^2 \approx \frac{T}{(S+T)^{3/2}} \times \frac{N^3/6}{2 \cdot (1/3)^{3/2}}.$$

Setting  $T = 2S$  (so  $K = S+T = 3S$ ) leads to the following lower bound

$$Q \geq (2S) \times \frac{N^3/6}{2S^{3/2}} = \frac{N^3}{6\sqrt{S}}.$$

Lower order terms have been omitted at a few places in this reasoning so this bound is asymptotic. The full expression for the lower bound found by IOLB is given in Table 1.

Output #2 is a proof

We consider a segmentation of the execution every  $T$  IOs. For each segment, we have at most  $K = S + T$  “input” data to perform the statements in the segment.

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the maximum number of statements in a segment

We consider a segmentation of the execution every  $T$  IOs. For each segment, we have at most  $K = S + T$  input data to perform the statements in the segment.

$$2 \cdot (K/3)^{3/2}$$

  
the maximum number of statements in a segment

We consider a segmentation of the execution every  $T$  IOs. For each segment, we have at most  $K = S + T$  input data to perform the statements in the segment.

the total number of statements in the execution

the IO of a segment

$$Q \geq T \times \left\lceil \frac{N^3/6}{2 \cdot (K/3)^{3/2}} \right\rceil$$

the maximum number of statements in a segment

is greater than or equal to

the IO of any schedule

The minimum number of segments in a schedule

We consider a segmentation of the execution every  $T$  IOs. For each segment, we have at most  $K = S + T$  input data to perform the statements in the segment.

$$2 \cdot (K/3)^{3/2}$$

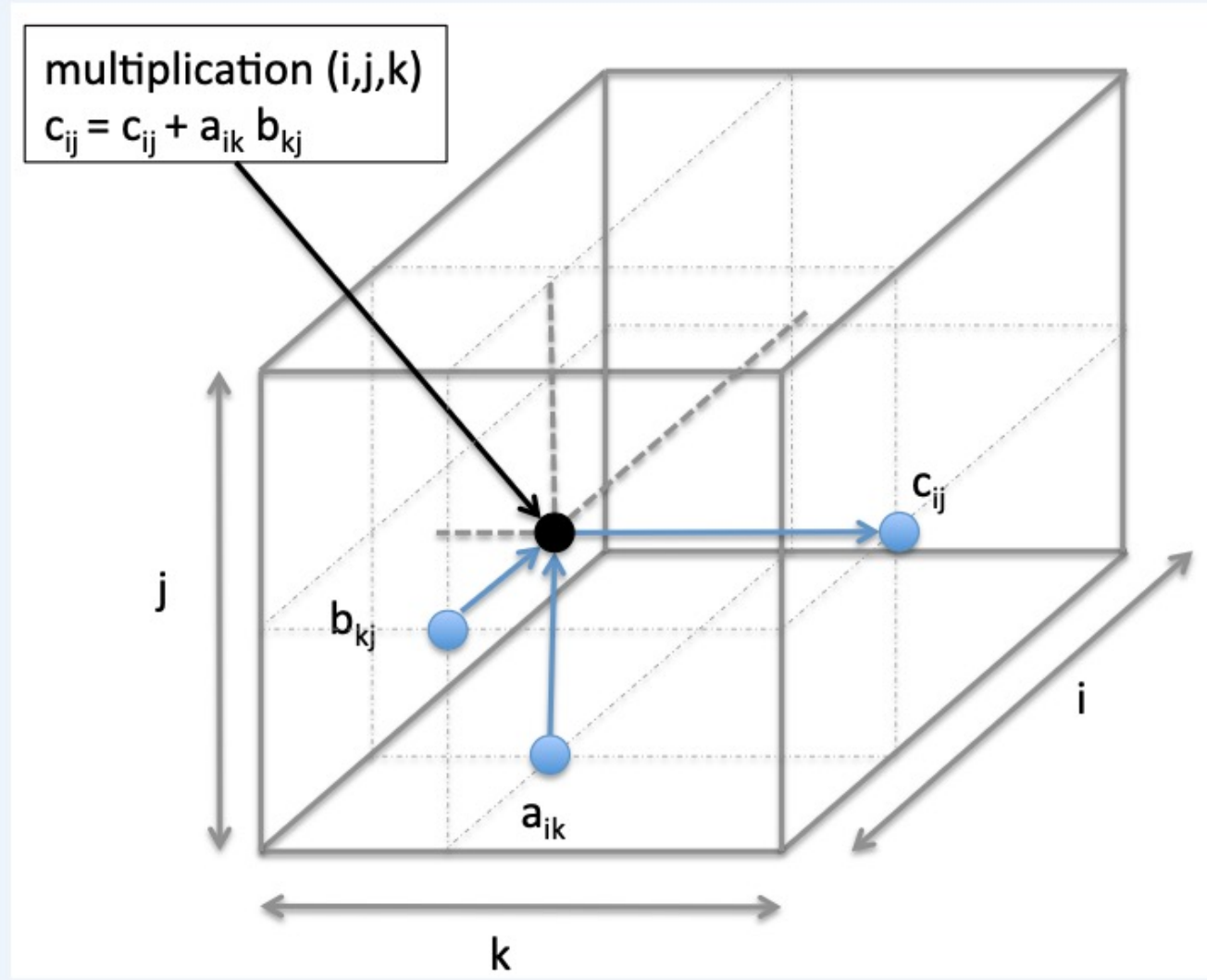
  
the maximum number of statements in a segment

# What do we want to compute?

We want to compute the  $n^3$

$$c_{ijk} = a_{ik} b_{kj}.$$

The computation of  $c_{ijk}$  requires  $a_{ik}$  and  $b_{kj}$  to be in cache.

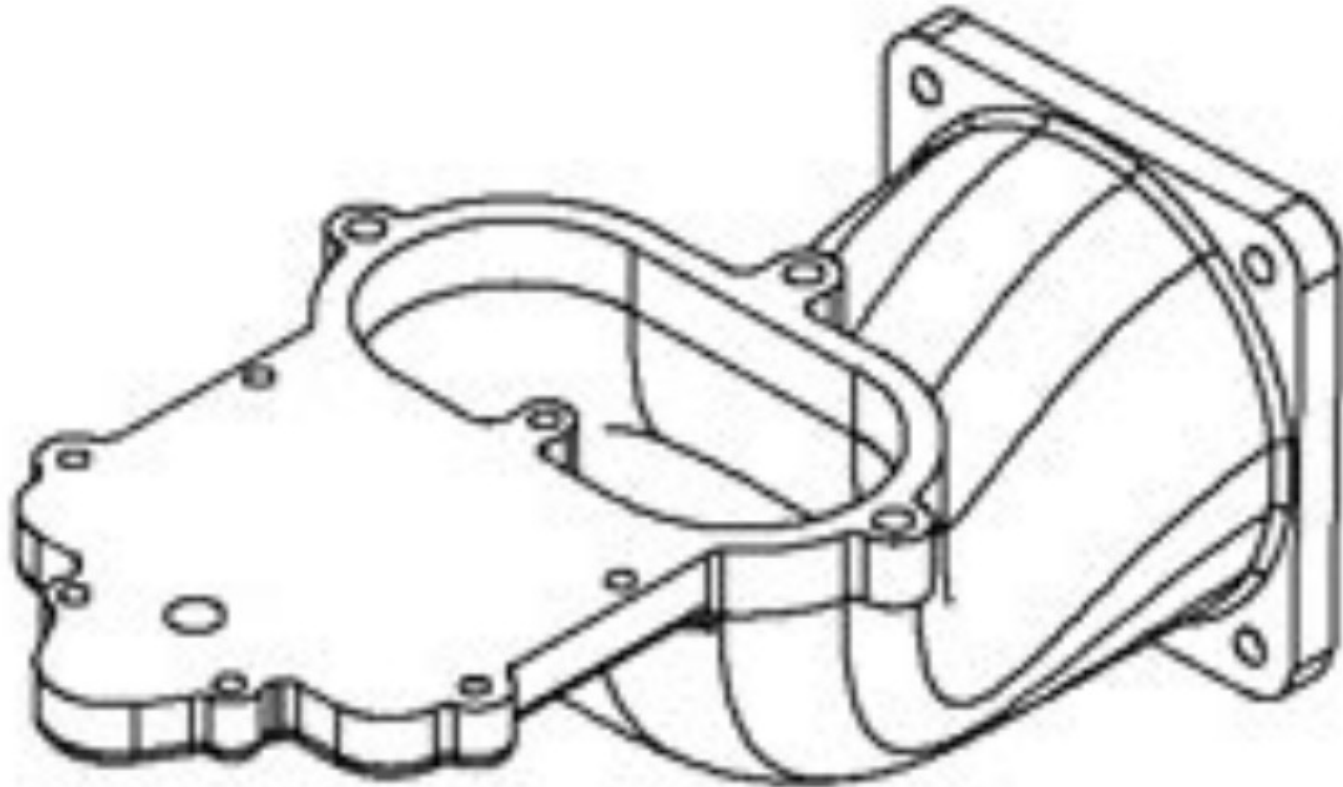




## Lemma (Loomis-Whitney Inequality)

Let  $V \in Z[3]$  be a finite set, and let  $V_x$ ,  $V_y$ , and  $V_z$  be orthogonal projections of  $V$  onto the coordinate planes. The cardinality of  $V$ ,  $|V|$ , satisfies

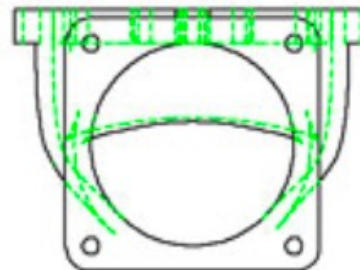
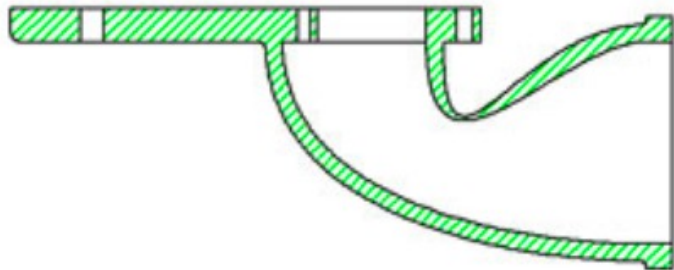
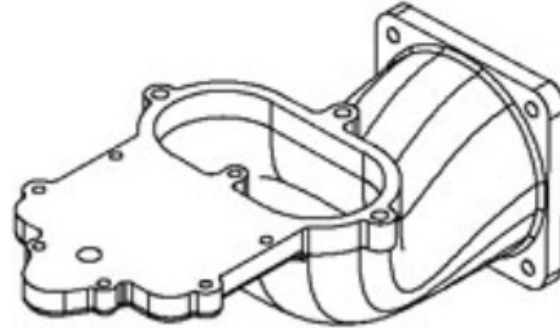
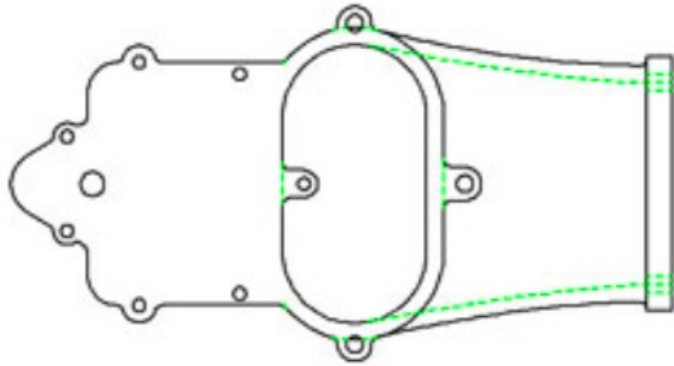
$$|V| \leq \sqrt{|V_x| \cdot |V_y| \cdot |V_z|}.$$



## Lemma (Loomis-Whitney Inequality)

Let  $V \in Z[3]$  be a finite set, and let  $V_x$ ,  $V_y$ , and  $V_z$  be orthogonal projections of  $V$  onto the coordinate planes. The cardinality of  $V$ ,  $|V|$ , satisfies

$$|V| \leq \sqrt{|V_x| \cdot |V_y| \cdot |V_z|}.$$



We consider a segmentation of the execution every  $T$  IOs. For each segment, we have at most  $K = S + T$  input data to perform the statements in the segment.

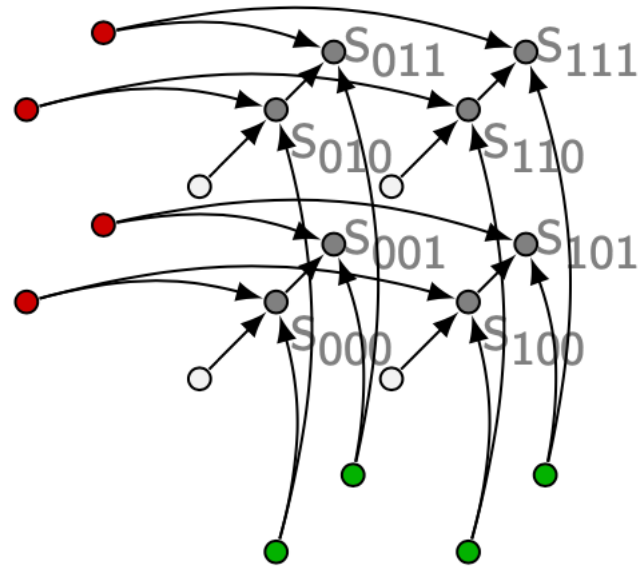
We will use a generalization: the Brascamp-Lieb inequality.

```
for (i = 0; i < m; i++)  
  for (j = 0; j < n; j++)  
    for (k = 0; k < p; k++)  
      C[i][j] += A[i][k] * B[k][j];
```

```
C[0][0] += A[0][0] * B[0][0]; // S000  
C[0][0] += A[0][1] * B[1][0]; // S001  
C[0][0] += A[0][2] * B[2][0]; // S002  
C[0][0] += A[0][3] * B[3][0]; // S003
```

...

```
C[0][1] += A[0][0] * B[0][1]; // S010  
C[0][1] += A[0][1] * B[1][1]; // S011  
C[0][1] += A[0][2] * B[2][1]; // S012  
C[0][1] += A[0][3] * B[3][1]; // S013
```



```

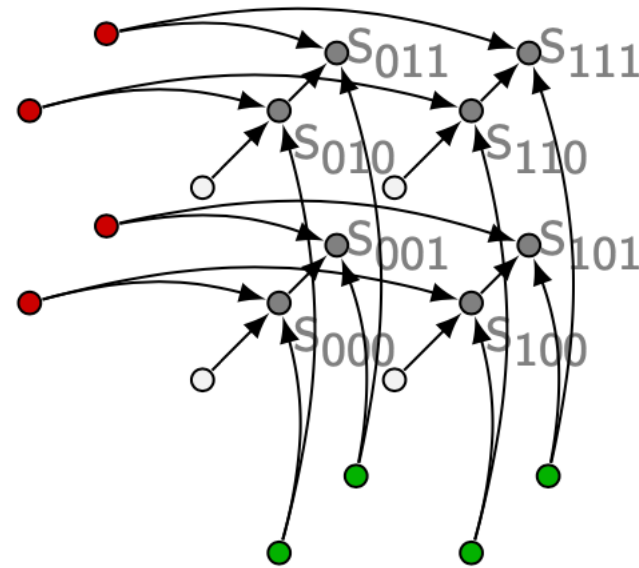
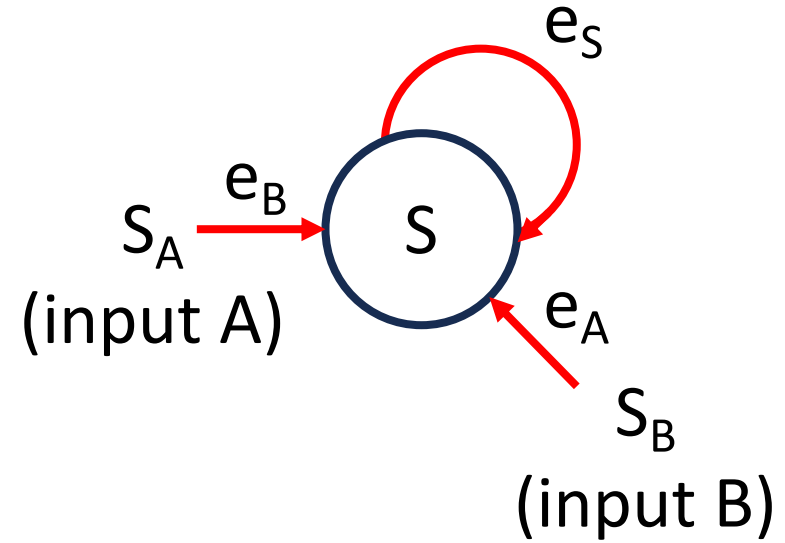
for (i = 0; i < m; i++)
  for (j = 0; j < n; j++)
    for (k = 0; k < p; k++)
      C[i][j] += A[i][k] * B[k][j];

```

```

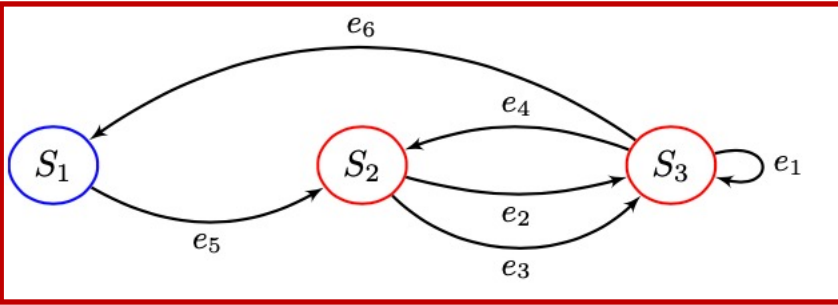
C[0][0] += A[0][0] * B[0][0]; // S000
C[0][0] += A[0][1] * B[1][0]; // S001
C[0][0] += A[0][2] * B[2][0]; // S002
C[0][0] += A[0][3] * B[3][0]; // S003
...
C[0][1] += A[0][0] * B[0][1]; // S010
C[0][1] += A[0][1] * B[1][1]; // S011
C[0][1] += A[0][2] * B[2][1]; // S012
C[0][1] += A[0][3] * B[3][1]; // S013

```



```
for(k = 0; k < n; k++) {  
    A[k][k] = sqrt(A[k][k]);           //S1  
    for(i = k+1; i < n; i++)  
        A[i][k] /= A[k][k];           // S2  
    for(i = k+1; i < n; i++)  
        for(j = k+1; j <= i; j++)  
            A[i][j] -= A[i][k] * A[j][k]; // S3  
}
```

```
for(k = 0; k < n; k++) {  
    A[k][k] = sqrt(A[k][k]);           // S1  
    for(i = k+1; i < n; i++)  
        A[i][k] /= A[k][k];           // S2  
    for(i = k+1; i < n; i++)  
        for(j = k+1; j <= i; j++)  
            A[i][j] -= A[i][k] * A[j][k]; // S3  
}
```

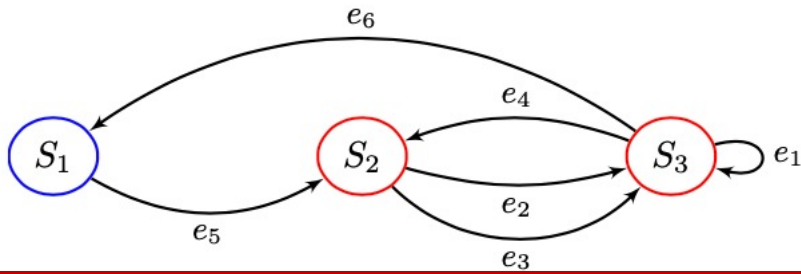


Cholesky

```

for(k = 0; k < n; k++) {
    A[k][k] = sqrt(A[k][k]);           // S1
    for(i = k+1; i < n; i++)
        A[i][k] /= A[k][k];          // S2
    for(i = k+1; i < n; i++)
        for(j = k+1; j <= i; j++)
            A[i][j] -= A[i][k] * A[j][k]; // S3
}

```



$$R_{e_1} = \{S_3[k-1, i, j] \rightarrow S_3[k, i, j] : 1 \leq k < N \wedge k+1 \leq i < N \wedge k+1 \leq j \leq i\}$$

$$R_{e_2} = \{S_2[k, j] \rightarrow S_3[k, i, j] : 0 \leq k < N \wedge k+1 \leq i < N \wedge k+1 \leq j \leq i\}$$

$$R_{e_3} = \{S_2[k, i] \rightarrow S_3[k, i, j] : 0 \leq k < N \wedge k+1 \leq i < N \wedge k+1 \leq j \leq i\}$$

$$R_{e_4} = \{S_3[k-1, i, k] \rightarrow S_2[k, i] : 1 \leq k < N \wedge k+1 \leq i < N\}$$

$$R_{e_5} = \{S_1[k] \rightarrow S_2[k, i] : 0 \leq k < N \wedge k+1 \leq i < N\}$$

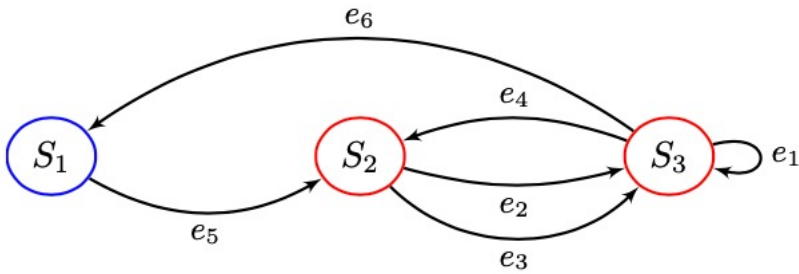
$$R_{e_6} = \{S_1[k-1, k, k] \rightarrow S_1[k] : 1 \leq k < N \wedge k+1 \leq i < N\}$$

```

for(k = 0; k < n; k++) {
    A[k][k] = sqrt(A[k][k]);           // S1
    for(i = k+1; i < n; i++)
        A[i][k] /= A[k][k];         // S2
    for(i = k+1; i < n; i++)
        for(j = k+1; j <= i; j++)
            A[i][j] -= A[i][k] * A[j][k]; // S3
}

```

$$\begin{aligned}
 \text{Dom}(P_1) &= \{S_3[k, i, j] : 1 \leq k < N \wedge k+1 \leq i < N \wedge k+1 \leq j \leq i\} \\
 \text{Dom}(P_2) &= \{S_3[k, i, j] : 0 \leq k < N \wedge k+1 \leq i < N \wedge k+1 \leq j \leq i\} \\
 \text{Dom}(P_3) &= \{S_3[k, i, j] : 0 \leq k < N \wedge k+1 \leq i < N \wedge k+1 \leq j \leq i\} \\
 D_S &:= \text{Dom}(P_1) \cap \text{Dom}(P_2) \cap \text{Dom}(P_3) \\
 &= \{S_3[k, i, j] : 1 \leq k < N \wedge k+1 \leq i < N \wedge k+1 \leq j \leq i\}
 \end{aligned}$$



$$\begin{aligned}
 R_{e_1} &= \{S_3[k-1, i, j] \rightarrow S_3[k, i, j] : 1 \leq k < N \wedge k+1 \leq i < N \wedge k+1 \leq j \leq i\} \\
 R_{e_2} &= \{S_2[k, j] \rightarrow S_3[k, i, j] : 0 \leq k < N \wedge k+1 \leq i < N \wedge k+1 \leq j \leq i\} \\
 R_{e_3} &= \{S_2[k, i] \rightarrow S_3[k, i, j] : 0 \leq k < N \wedge k+1 \leq i < N \wedge k+1 \leq j \leq i\} \\
 R_{e_4} &= \{S_3[k-1, i, k] \rightarrow S_2[k, i] : 1 \leq k < N \wedge k+1 \leq i < N\} \\
 R_{e_5} &= \{S_1[k] \rightarrow S_2[k, i] : 0 \leq k < N \wedge k+1 \leq i < N\} \\
 R_{e_6} &= \{S_1[k-1, k, k] \rightarrow S_1[k] : 1 \leq k < N \wedge k+1 \leq i < N\}
 \end{aligned}$$

$P_1 = (e_1)$	is a chain path
$P_2 = (e_2)$	is a broadcast path
$P_3 = (e_3)$	is a broadcast path

Cholesky



```

for(k = 0; k < n; k++) {
    A[k][k] = sqrt(A[k][k]);           // S1
    for(i = k+1; i < n; i++)
        A[i][k] /= A[k][k];          // S2
    for(i = k+1; i < n; i++)
        for(j = k+1; j <= i; j++)
            A[i][j] -= A[i][k] * A[j][k]; // S3
}

```

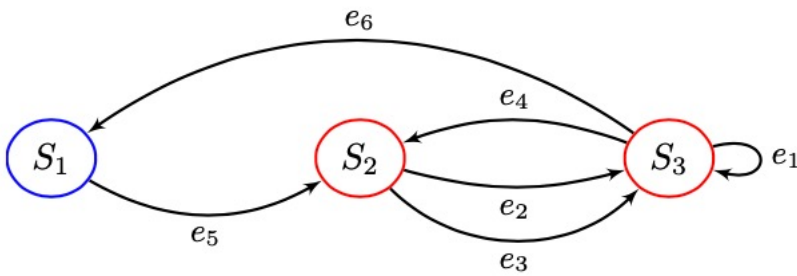
$$\text{Dom}(P_1) = \{S_3[k, i, j] : 1 \leq k < N \wedge k+1 \leq i < N \wedge k+1 \leq j \leq i\}$$

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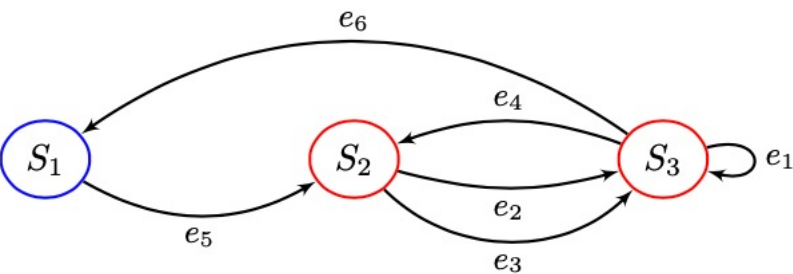
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Cholesky

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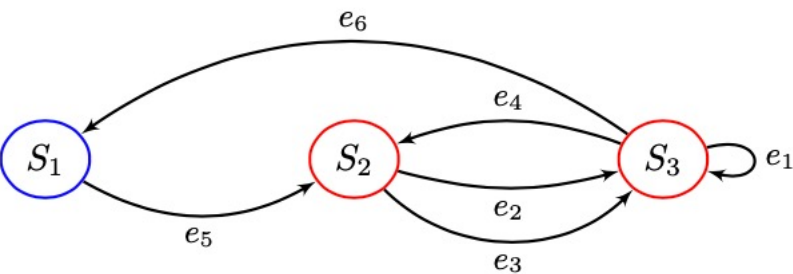
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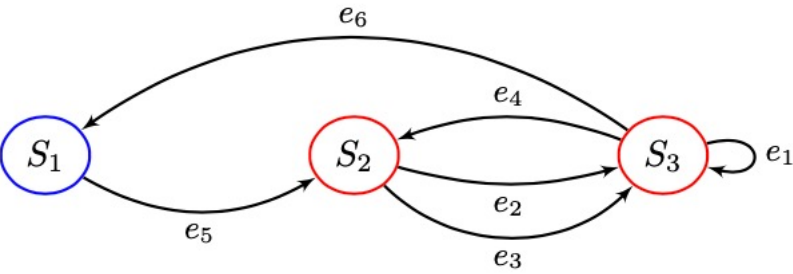
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Cholesky

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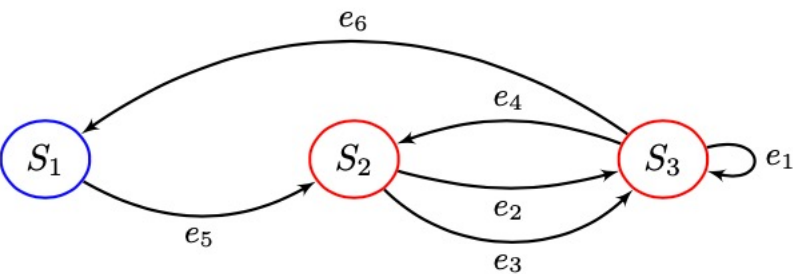
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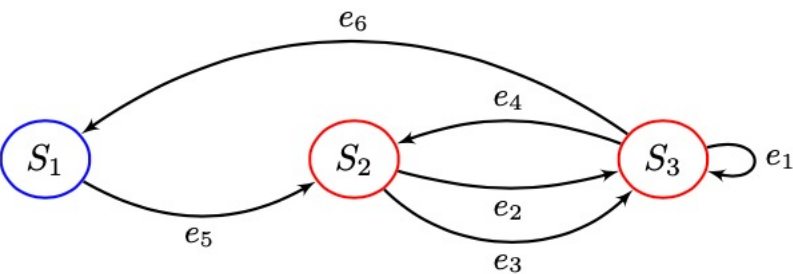
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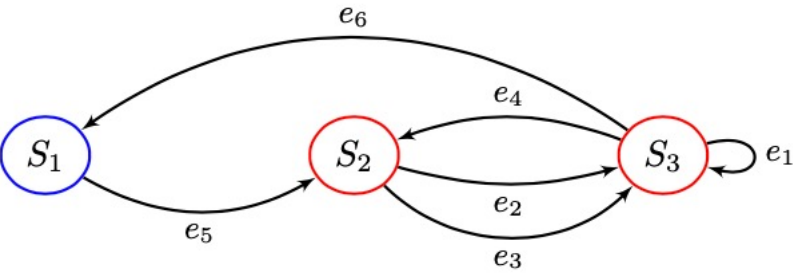
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 |\phi_i(E)| &\leq K, \quad i = 1, 2, 3 \\
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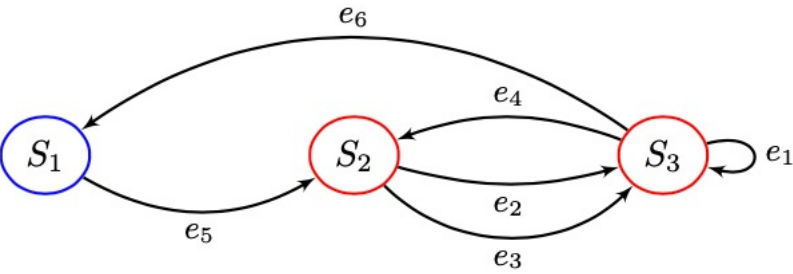
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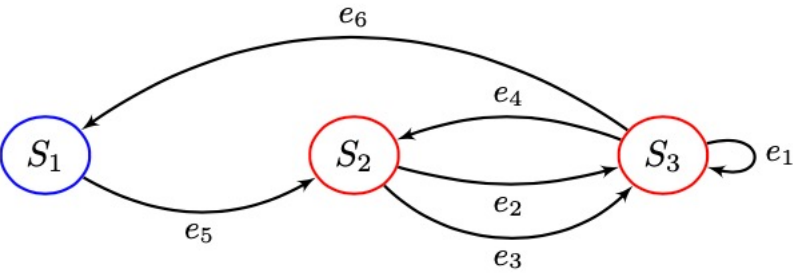
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```

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We consider a segmentation of the execution every  $T$  IOs. For each segment, we have at most  $K = S + T$  input data to perform the statements in the segment.

the total number of statements in the execution

the IO of a segment

$$Q \geq T \times \left\lfloor \frac{N^3/6}{2 \cdot (K/3)^{3/2}} \right\rfloor$$

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is greater than or equal to

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The minimum number of  $K$ -partition in a schedule

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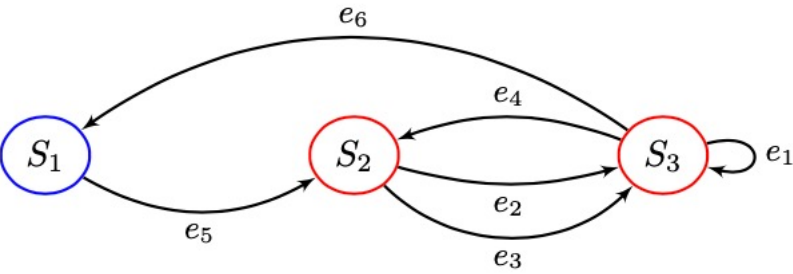
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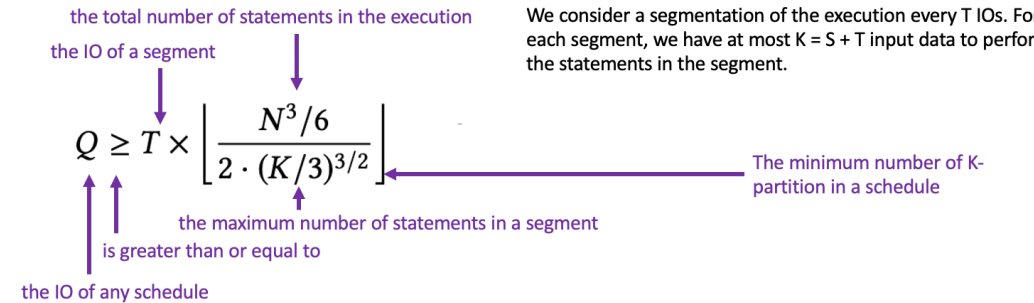
Then:

$$\begin{aligned}
 0 &\leq s_1, s_2, s_3 \leq 1 \\
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$|\phi_1|$



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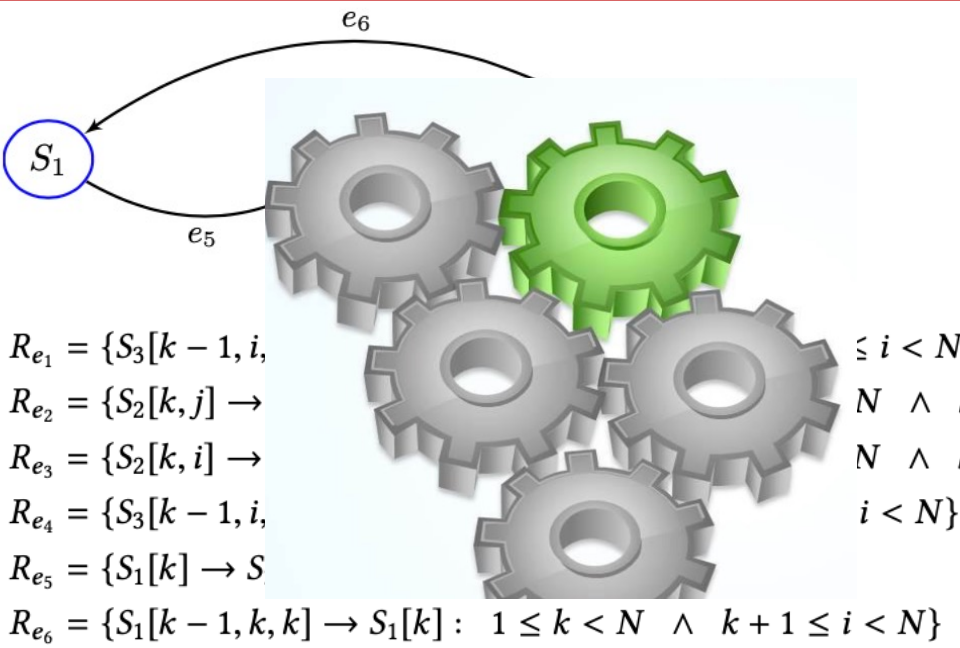
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**IOLB: I/O Lower Bound**  
<https://iocomplexity.corse.inria.fr/iolb>

Cholesky

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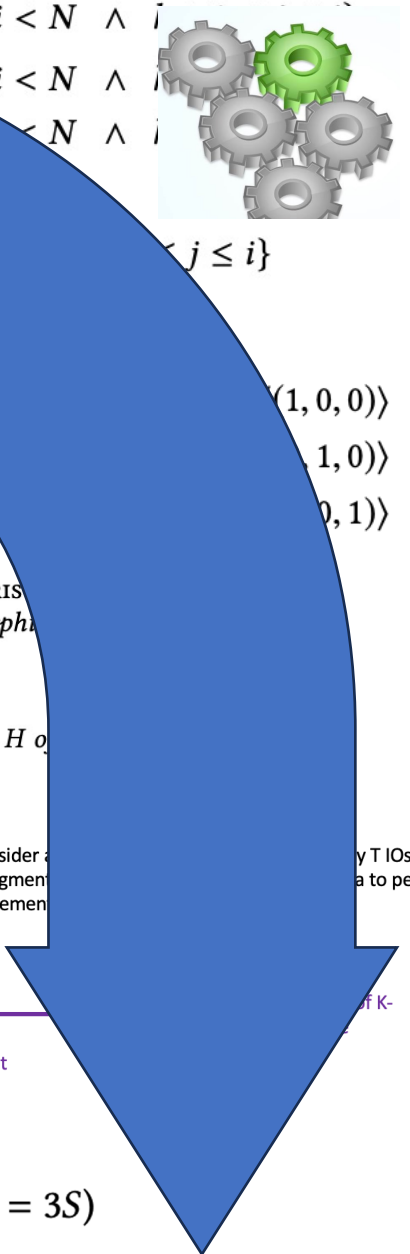
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## IOLB: I/O Lower Bound

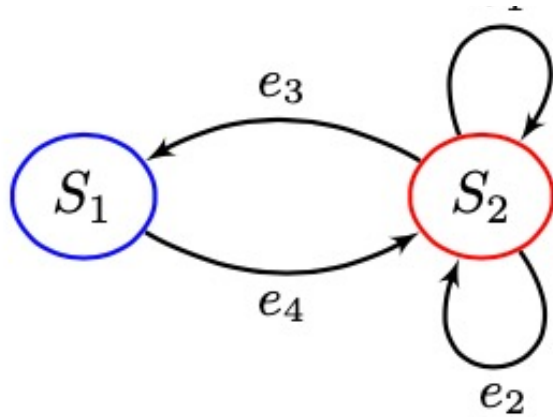
<https://iocomplexity.corse.inria.fr/iolb>

- PET: parse the C code (PET = Polyhedral Extraction Tool )
- DFG (in house) Data Flow Graph
- Piplib: for the ILP (PIP = Parametric Integer Programming )
- GINAC: manipulate symbolic expressions
- Lib ISL: (Integer Set Library) Barvinok: computes cardinalities of  $\mathbb{Z}$  polyhedron. Main tool for polyhedral compiling.

```

for(k = 0; k < n; k++) {
  for(i = k+1; i < n; i++)
    A[i][k] /= A[k][k];           // S1
  for(i = k+1; i < n; i++)
    for(j = k+1; j < n; j++)
      A[i][j] += A[i][k] * A[k][j]; // S2
}

```



$$Q \geq (2S) \frac{N^3/3}{S^{3/2}} = \frac{2N^3}{3\sqrt{S}}$$

Operational intensity of LU is at most  $\sqrt{S}$

# LU

similar algorithm as Béreux's Cholesky (SIMAX 2008)

```
lu
for (i = 0; i < n; i++) {
  for (j = 0; j < i; j++) {
    for (k = 0; k < j; k++) {
      A[i][j] -= A[i][k] * A[k][j];
    }
    A[i][j] /= A[j][j];
  }
  for (j = i; j < n; j++) {
    for (k = 0; k < i; k++) {
      A[i][j] -= A[i][k] * A[k][j];
    }
  }
}
```

Reorder  
statements to  
add blocking in  
the update



explicit cache  
directives



```
for( j = 0; j < n; j+=nb ){
  jb = (( nb < n-j ) ? ( nb ) : ( n-j ));
  for( k= j+jb; k < n; k+=nb ){
    kb = (( nb < n-k ) ? ( nb ) : ( n-k ));
    read A[ k:k+kb, j:j+jb ]
    for( kk= 0; kk < j; kk++){
      read A[ k:k+kb, kk ]
      read A[ kk, j:j+jb ]
      for( ii= k; ii < k+kb; ii++ )
        for( jj= j; jj < j+jb; jj++ )
          A[ ii ][ jj ] -= A[ ii ][ kk ] * A[ kk ][ jj ];
    }
    erase A[ k:k+kb, kk ]
    erase A[ kk, j:j+jb ]
  }
  write A[ k:k+kb, j:j+jb ]
}
for( k= j+jb; k < n; k+=nb ){
  kb = (( nb < n-k ) ? ( nb ) : ( n-k ));
  read A[ j:j+jb, k:k+kb ]
  for( kk= 0; kk < j; kk++){
    read A[ j:j+jb, kk ]
    read A[ kk, k:k+kb ]
    for( ii= j; ii < j+jb; ii++ )
      for( jj= k; jj < k+kb; jj++ )
        A[ ii ][ jj ] -= A[ ii ][ kk ] * A[ kk ][ jj ];
    erase A[ j:j+jb, kk ]
    erase A[ kk, k:k+kb ]
  }
  write A[ j:j+jb, k:k+kb ]
}
read A[ 1:jb, 1:jb ]
for( kk= 0; kk < j; kk++){
  read A[ 1:jb, kk ]
  read A[ kk, 1:jb ]
  for( ii= j; ii < j+jb; ii++ )
    for( jj= j; jj < j+jb; jj++ )
      A[ ii ][ jj ] -= A[ ii ][ kk ] * A[ kk ][ jj ];
  erase A[ 1:jb, kk ]
  erase A[ kk, 1:jb ]
}
for( jj= j; jj < j+jb; jj++){
  for(ii= j; ii < jj; ii++)
    for(kk= j; kk < ii; kk++)
      A[ ii ][ jj ] -= A[ ii ][ kk ] * A[ kk ][ jj ];
  for(ii= jj; ii < j+jb; ii++)
    for(kk= j; kk < jj; kk++)
      A[ ii ][ jj ] -= A[ ii ][ kk ] * A[ kk ][ jj ];
  for( ii = jj+1; ii < j+jb; ii++ )
    A[ ii ][ jj ] /= A[ jj ][ jj ];
}
for(ii= j+jb; ii < n; ii++){
  // read A[ ii, 1:jb ]
  for( jj= j; jj < j+jb; jj++){
    for(kk= j; kk < jj; kk++){
      A[ ii ][ jj ] -= A[ ii ][ kk ] * A[ kk ][ jj ];
    }
    A[ ii ][ jj ] /= A[ jj ][ jj ];
  }
  // write A[ ii, 1:jb ]
}
for(jj= j+jb; jj < n; jj++){
  // read A[ 1:jb, jj ]
  for( ii= j; ii < j+jb; ii++){
    for(kk= j; kk < ii; kk++){
      A[ ii ][ jj ] -= A[ ii ][ kk ] * A[ kk ][ jj ];
    }
  }
  // write A[ 1:jb, jj ]
}
write A[ 1:jb, 1:jb ]
}
```

Operational intensity of LU is at least  $\sqrt{S}$





kernel	# input data	#ops	ratio	$OI_{up}$	$OI_{manual}$	ratio
2mm	$N_i N_k + N_k N_j$ $+ N_j N_l + N_i N_l$	$N_i N_j N_k$ $+ N_i N_j N_l$	-	$\sqrt{S}$	$\sqrt{S}$	1 ✓
3mm	$N_i N_k + N_k N_j$ $+ N_j N_m + N_m N_l$	$N_i N_j N_k + N_j N_l N_m$ $+ N_i N_j N_l$	-	$\sqrt{S}$	$\sqrt{S}$	1 ✓
cholesky	$\frac{1}{2} N^2$	$\frac{1}{3} N^3$	$\frac{2}{3} N$	$2\sqrt{S}$	$\sqrt{S}$	2
correlation	$MN$	$M^2 N$	$M$	$2\sqrt{S}$	$\sqrt{S}$	2
covariance	$MN$	$M^2 N$	$M$	$2\sqrt{S}$	$\sqrt{S}$	2
doitgen	$N_p N_q N_r$	$2N_q n_r N_p^2$	$2N_p$	$\sqrt{S}$	$\sqrt{S}$	1 ✓
fdtd-2d	$3N_x N_y$	$11N_x N_y T$	$\frac{11}{3} T$	$22\sqrt{2}\sqrt{S}$	$\frac{11}{24}\sqrt{3}\sqrt{S}$	$\frac{48\sqrt{2}}{\sqrt{3}}$
floyd-warshall	$N^2$	$2N^3$	$2N$	$2\sqrt{S}$	$\sqrt{S}$	2
gemm	$N_i N_j + N_j N_k + N_i N_k$	$2N_i N_j N_k$	-	$\sqrt{S}$	$\sqrt{S}$	1 ✓
heat-3d	$N^3$	$30N^3 T$	$30T$	$\frac{160}{3}\sqrt[3]{S}$	$\frac{5}{2}\sqrt[3]{S}$	$\frac{64}{3\sqrt[3]{3}}$
jacobi-1d	$N$	$6NT$	$6T$	$24S$	$\frac{3}{2}S$	16
jacobi-2d	$N^2$	$10N^2 T$	$10T$	$15\sqrt{3}\sqrt{S}$	$\frac{5}{4}\sqrt{S}$	$12\sqrt{3}$
lu	$N^2$	$\frac{2}{3} N^3$	$\frac{2}{3} N$	$\sqrt{S}$	$\sqrt{S}$	1 ✓
ludcmp	$N^2$	$\frac{2}{3} N^3$	$\frac{2}{3} N$	$\sqrt{S}$	$\sqrt{S}$	1 ✓
seidel-2d	$N^2$	$9N^2 T$	$9T$	$\frac{27\sqrt{3}}{2}\sqrt{S}$	$\frac{9}{4}\sqrt{S}$	$6\sqrt{3}$
symm	$\frac{1}{2} M^2 + 2MN$	$2M^2 N$	-	$\sqrt{S}$	$\sqrt{S}$	1 ✓
syr2k	$\frac{1}{2} N^2 + 2MN$	$2MN^2$	-	$2\sqrt{S}$	$\sqrt{S}$	2
syrk	$\frac{1}{2} N^2 + MN$	$MN^2$	-	$2\sqrt{S}$	$\sqrt{S}$	2
trmm	$\frac{1}{2} M^2 + MN$	$M^2 N$	-	$\sqrt{S}$	$\sqrt{S}$	1 ✓
atax	$MN$	$4MN$	4	4	4	1 ✓
bicg	$MN$	$4MN$	4	4	4	1 ✓
deriche	$HW$	$32HW$	32	32	$\frac{16}{3}$	6
gemver	$N^2$	$10N^2$	10	10	5	2
gesummv	$2N^2$	$4N^2$	2	2	2	1 ✓
mvt	$N^2$	$4N^2$	4	4	4	1 ✓
trisolv	$\frac{1}{2} N^2$	$N^2$	2	2	2	1 ✓
adi	$N^2$	$30N^2 T$	$30T$	30	5	6
durbin	$N$	$2N^2$	$2N$	4	$\frac{2}{3}$	6
gramschmidt	$MN$	$2MN^2$	$2N$	$2\sqrt{S}$	1	$2\sqrt{S}$
nussinov	$\frac{1}{2} N^2$	$\frac{1}{3} N^3$	$\frac{2}{3} N$	$2\sqrt{S}$	1	$2\sqrt{S}$

polybench test suite

A. Olivry, J. Langou, L-N Pouchet, P. Sadayappan, and F. Rastello. **Automated derivation of parametric data movement lower bounds for affine programs.** In the Proceedings of PLDI 2020: Proceedings of the 41st ACM SIGPLAN Conference on Programming Language Design and Implementation, page 808–822, June 2020. ( [link](#) )

Automated I/O Lower Bound Analysis

PLDI'20, June 15 - 20, 2020, London, United Kingdom

kernel	Complete Lower Bound Formulae for PolyBENCH obtained with the current version of IOLB	asymptotic simplified formula
2mm	$\max(N_i N_j + N_j N_k + N_i N_k + N_j N_i + 2, \left(\frac{2}{\sqrt{S}} N_i N_j (N_k - 1) + 2N_i + 2N_j + N_k - 4\sqrt{2S}\right) + \left(\frac{2}{\sqrt{S}} N_i N_j (N_j - 1) + 2N_i + 2N_j + N_j - 4\sqrt{2S}\right) - 2N_i N_j - 2)$	$\frac{2}{\sqrt{S}} N_i N_j N_k + \frac{2}{\sqrt{S}} N_i N_j N_j$
3mm	$\max(N_i N_k + N_j N_k + N_j N_m + N_i N_m, \left(\frac{2}{\sqrt{S}} N_i N_j (N_k - 1) + 2N_i + 2N_j + N_k - 4\sqrt{2S}\right) + \left(\frac{2}{\sqrt{S}} N_i N_j (N_j - 1) + 2N_i + 2N_j + N_j - 4\sqrt{2S}\right) + \left(\frac{2}{\sqrt{S}} N_j N_i (N_m - 1) + 2N_j + 2N_i + N_m - 4\sqrt{2S}\right) - 2N_j N_i - 2N_j N_j - N_i N_i - 6)$	$\frac{2}{\sqrt{S}} N_i N_j N_k + \frac{2}{\sqrt{S}} N_i N_j N_j + \frac{2}{\sqrt{S}} N_j N_i N_m$
adi	$4N^2 + \max(0, (N^2 - 4N - S + 5)(T - 2))$	$N^2 T$
atax	$MN + N + \max(0, \frac{1}{3} \frac{1}{3} ((2M - 1 - 8S)(2N - 1 - 8S) - 1) - 10S + 2)$	$MN$
bicg	$MN + M + N + \max(0, \frac{1}{3} \frac{1}{3} ((2M - 1 - 8S)(2N - 1 - 8S) - 1) - 10S + 2)$	$MN$
cholesky	$\max(\frac{1}{2} N(N+1), \frac{1}{6} \frac{1}{\sqrt{S}} (N-1)(N-2)(N-3) + \frac{1}{2\sqrt{2}} \frac{1}{3} (N-1)(N-2) - (N-2)(N-7) - 4\sqrt{2S})$	$\frac{1}{6} \frac{1}{\sqrt{S}} N^3$
correlation	$\max(MN + 2, \frac{1}{2} \frac{1}{\sqrt{S}} M(M-1)(N-1 + \frac{\sqrt{2}}{2} \frac{1}{\sqrt{S}}) - \frac{1}{2} (M-3)(M+2N-2) + 4S\sqrt{2})$	$\frac{1}{2} \frac{1}{\sqrt{S}} M^2 N$
covariance	$\max(MN + 2, \frac{1}{2} \frac{1}{\sqrt{S}} M(M-1)(N-1 + \frac{\sqrt{2}}{2} \frac{1}{\sqrt{S}}) - \frac{1}{2} (M-3)(M+2N-2) + 4S\sqrt{2})$	$\frac{1}{2} \frac{1}{\sqrt{S}} M^2 N$
deriche	$HW + 1$	$HW$
doitgen	$\max(N_p^2 + N_p N_q N_r, \frac{2}{\sqrt{S}} N_q N_r N_p (N_p - 1 + \frac{1}{\sqrt{2}} \frac{1}{\sqrt{S}}) - N_q N_r (N_p - 1) + 2N_p - 8\sqrt{2S} - 1)$	$2 \frac{1}{\sqrt{S}} N_q N_r N_p^2$
durbin	$2N + \max(0, \frac{1}{2} (N-3)(N-2-2S))$	$\frac{1}{2} N^2$
fdtd-2d	$\max(3N_x N_y - N_y + T - 1, \frac{2}{\sqrt{2}} \frac{1}{\sqrt{S}} (N_x - 2)(N_y - 2)(T - 1) + 2(N_x + 2)(N_y + 2) - T(N_x + N_y - 6) - N_y - S - 23)$	$\frac{2}{\sqrt{2}} \frac{1}{\sqrt{S}} N_x N_y T$
floyd-warshall	$\max(N^2, \frac{1}{\sqrt{S}} (N-1)^2 - (6N-19)(N-2) - 8\sqrt{2S})$	$\frac{1}{\sqrt{S}} N^3$
gemm	$\max(N_i N_j + N_j N_k + N_i N_k + 2, \frac{2}{\sqrt{S}} N_i N_j (N_k - 1) + 2N_i + 2N_j + N_k - 4\sqrt{2S})$	$2 \frac{1}{\sqrt{S}} N_i N_j N_k$
gemver	$N^2 + 8N + 2 + \max(0, \frac{1}{3} \frac{1}{3} (3N - 2)(N - 8S) - 3S + 1)$	$N^2$
gesummv	$2N^2 + N + 2 + \max(0, \frac{1}{3} \frac{1}{3} (N - 1)(N - 8S) - 2S)$	$2N^2$
gramschmidt	$\max(MN, \frac{1}{\sqrt{S}} MN(N-3) - M(N-5 - \frac{2}{\sqrt{S}}) - \frac{1}{2} (N-1)(N-6) - 4\sqrt{2S} - 3)$	$\frac{1}{\sqrt{S}} MN^2$
heat-3d	$\max((N-10)(N+2)^2, \frac{9\sqrt{3}}{16} \frac{1}{\sqrt{S}} (T-1)(N-3)^3 - 3(T-7)(N-3)(N-4) + 42N - T - \frac{9\sqrt{3}}{4\sqrt{4}} S - 111)$	$\frac{9\sqrt{3}}{16} \frac{1}{\sqrt{S}} N^3 T$
jacobi-1d	$\max(2 + n, \frac{1}{3} \frac{1}{3} (T-1)(N-3) - T - S + 7)$	$\frac{1}{3} \frac{1}{3} NT$
jacobi-2d	$\max((N-2)(N+6), \frac{2}{3\sqrt{2}} \frac{1}{\sqrt{S}} (N-3)^2 (T-1) - \frac{4\sqrt{2}}{3\sqrt{2}} S - (T-7)(2N-7) + 14)$	$\frac{2}{3\sqrt{2}} \frac{1}{\sqrt{S}} N^2 T$
lu	$\max(N^2, \frac{2}{3} \frac{1}{\sqrt{S}} (N-2)(N^2 - 4N + 6) - 2(N^2 - 10N + 18) - 8\sqrt{2S})$	$\frac{2}{3} \frac{1}{\sqrt{S}} N^3$
ludcmp	$\max(N^2 + N, \frac{1}{3} \frac{1}{3} (2N-3)(N-1)(N-2)\sqrt{2} \frac{1}{\sqrt{S}} (N-1)(N-2) - (2N^2 - 15N + 19) - 16\sqrt{2S})$	$\frac{2}{3} \frac{1}{\sqrt{S}} N^3$
mvt	$N^2 + 4N + \max(0, \frac{1}{3} \frac{1}{3} N(N-1) - 2S - 4N + 4)$	$N^2$
nussinov	$\frac{1}{2} N^2 + \frac{5}{2} N - 1 + \max(0, \frac{1}{6} \frac{1}{\sqrt{S}} (N-3)(N-4)(N-5) + \frac{1}{3} \sqrt{2}(3N^2 - 19N + 6) - (N^2 - 13N + 22) - 8\sqrt{2S})$	$\frac{1}{6} \frac{1}{\sqrt{S}} N^3$
seidel-2d	$\max(N^2, \frac{2}{3\sqrt{2}} \frac{1}{\sqrt{S}} (N-3)^2 (T-1) - (2N-7)(T-5) - \frac{4\sqrt{2}}{3\sqrt{2}} S + 12)$	$\frac{2}{3\sqrt{2}} \frac{1}{\sqrt{S}} N^2 T$
symm	$\max(\frac{1}{2} M(M+1) + 2MN + 2.2 \frac{1}{\sqrt{S}} (M-1)(M-2)N - \frac{1}{2} ((4N+M)(M-5) + 5(M-2) - 8\sqrt{2S})$	$2 \frac{1}{\sqrt{S}} M^2 N$
syr2k	$\max(2 + 2MN + \frac{1}{2} N(N+1), \frac{1}{\sqrt{S}} (M-1)(N+1)N + M + 4N - 4\sqrt{2S})$	$\frac{1}{\sqrt{S}} MN^2$
syrk	$\max(MN + \frac{1}{2} (N+1)N + 2, \frac{1}{2} \frac{1}{\sqrt{S}} (M-1)(N+1)N - (M-4)(N-1) - 2\sqrt{2S} + 4)$	$\frac{1}{2} \frac{1}{\sqrt{S}} MN^2$
trisolv	$\frac{1}{2} N(N+1) + N + \max(0, \frac{1}{3} \frac{1}{3} (N-1)(N-2) - 2N - S + 5)$	$\frac{1}{2} N^2$
trmm	$\max(\frac{1}{2} M(M-1) + MN + 1, \frac{2}{\sqrt{2}} (M-2 + \frac{3\sqrt{2}}{\sqrt{S}} (M-1)N - (M-4)(N-2) - 8\sqrt{2S} + 5)$	$\frac{1}{\sqrt{2}} M^2 N$

Table 2. Complete Lower Bound Formulae for POLYBENCH obtained with the current version of IOLB

gemm	$\max(N_i N_j + N_j N_k + N_i N_k + 2, \frac{2}{\sqrt{S}} N_i N_j (N_k - 1) + 2N_i + 2N_j + N_k - 4\sqrt{2S})$	$2 \frac{1}{\sqrt{S}} N_i N_j N_k$
------	--	------------------------------------

gemm

```

for (i = 0; i < _PB_NI; i++) {
  for (j = 0; j < _PB_NJ; j++)
    C[i][j] *= beta;
  for (k = 0; k < _PB_NK; k++) {
    for (j = 0; j < _PB_NJ; j++)
      C[i][j] += alpha * A[i][k] * B[k][j];
  }
}

```

Operational intensity of GEMM is at sqrt(S)

A. Olivry, J. Langou, L-N Pouchet, P. Sadayappan, and F. Rastello. **Automated derivation of parametric data movement lower bounds for affine programs.** In the Proceedings of PLDI 2020: Proceedings of the 41st ACM SIGPLAN Conference on Programming Language Design and Implementation, page 808–822, June 2020. ( [link](#) )

Automated I/O Lower Bound Analysis

PLDI'20, June 15 - 20, 2020, London, United Kingdom

kernel	Complete Lower Bound Formulae for POLYBENCH obtained with the current version of IOLB	asymptotic simplified formula
2mm	$\max(N_i N_j + N_j N_k + N_i N_k + N_j N_i + 2, \left(\frac{2}{\sqrt{3}} N_i N_j (N_k - 1) + 2N_i + 2N_j + N_k - 4\sqrt{2S}\right) + \left(\frac{2}{\sqrt{3}} N_i N_j (N_j - 1) + 2N_i + 2N_j + N_j - 4\sqrt{2S}\right) - 2N_i N_j - 2)$	$\frac{2}{\sqrt{3}} N_i N_j N_k + \frac{2}{\sqrt{3}} N_i N_j N_j$
3mm	$\max(N_i N_k + N_j N_k + N_j N_m + N_i N_m, \left(\frac{2}{\sqrt{3}} N_i N_j (N_k - 1) + 2N_i + 2N_j + N_k - 4\sqrt{2S}\right) + \left(\frac{2}{\sqrt{3}} N_i N_j (N_j - 1) + 2N_i + 2N_j + N_j - 4\sqrt{2S}\right) + \left(\frac{2}{\sqrt{3}} N_i N_j (N_m - 1) + 2N_i + 2N_j + N_m - 4\sqrt{2S}\right) - 2N_i N_j - 2N_j N_i - N_i N_j - 6)$	$\frac{2}{\sqrt{3}} N_i N_j N_k + \frac{2}{\sqrt{3}} N_i N_j N_j + \frac{2}{\sqrt{3}} N_i N_j N_m$
adi	$4N^2 + \max(0, (N^2 - 4N - S + 5)(T - 2))$	$N^2 T$
atax	$MN + N + \max(0, \frac{1}{3}((2M - 1 - 8S)(2N - 1 - 8S) - 1) - 10S + 2)$	$MN$
bigc	$MN + M + N + \max(0, \frac{1}{3}((2M - 1 - 8S)(2N - 1 - 8S) - 1) - 10S + 2)$	$MN$
cholesky	$\max\left(\frac{1}{2}N(N+1), \frac{1}{6}\frac{1}{\sqrt{S}}(N-1)(N-2)(N-3) + \frac{1}{2\sqrt{2}}\frac{1}{S}(N-1)(N-2) - (N-2)(N-7) - 4\sqrt{2S}\right)$	$\frac{1}{6}\frac{1}{\sqrt{S}}N^3$
correlation	$\max\left(MN + 2, \frac{1}{\sqrt{3}}M(M-1)(N-1) + \frac{2\sqrt{2}}{3}M - \frac{1}{2}(M-3)(M+2N-2) + 2 - 4S\sqrt{2}\right)$	$\frac{1}{2}\frac{1}{\sqrt{3}}M^2 N$
covariance	$\max\left(MN + 2, \frac{1}{\sqrt{3}}M(M-1)(N-1) + \frac{2\sqrt{2}}{3}M - \frac{1}{2}(M-3)(M+2N-2) + 1 - 4S\sqrt{2}\right)$	$\frac{1}{2}\frac{1}{\sqrt{3}}M^2 N$
deriche	$HW + 1$	$HW$
doitgen	$\max(N_p^2 + N_p N_q N_r - \frac{2}{\sqrt{3}}N_q N_r N_p(N_p - 1) + \frac{1}{\sqrt{3}}N_q - N_q N_r(N_p - 1) + 2N_p - 8\sqrt{2S} - 1)$	$2\frac{2}{\sqrt{3}}N_q N_r N_p^2$
durbin	$2N + \max(0, \frac{1}{2}(N-3)(N-2-2S))$	$\frac{1}{2}N^2$
fdtd-2d	$\max\left(3N_x N_y - N_y + T - 1, \frac{1}{2\sqrt{2}}\frac{1}{\sqrt{S}}(N_x - 2)(N_y - 2)(T - 1) + 2(N_x + 2)(N_y + 2) - T(N_x + N_y - 6) - N_y - S - 23\right)$	$\frac{1}{2\sqrt{2}}\frac{1}{\sqrt{S}}N_x N_y T$
floyd-warshall	$\max(N^2, \frac{1}{\sqrt{3}}(N-1)^3 - (6N-19)(N-2) - 8\sqrt{2S})$	$\frac{1}{\sqrt{3}}N^3$
gemm	$\max\left(N_i N_j + N_j N_k + N_i N_k + 2, \frac{2}{\sqrt{3}}N_i N_j (N_k - 1) + 2N_i + 2N_j + N_k - 4\sqrt{2S}\right)$	$2\frac{2}{\sqrt{3}}N_i N_j N_k$
gemver	$N^2 + 8N + 2 + \max(0, \frac{1}{3}(3N-2)(N-8S) - 3S + 1)$	$N^2$
gesummv	$2N^2 + N + 2 + \max(0, \frac{1}{3}(N-1)(N-8S) - 2S)$	$2N^2$
gramschmidt	$\max\left(MN, \frac{1}{\sqrt{3}}MN(N-3) - M(N-5 - \frac{2}{\sqrt{3}}) - \frac{1}{2}(N-1)(N-6) - 4\sqrt{2S} - 3\right)$	$\frac{1}{\sqrt{3}}MN^2$
heat-3d	$\max\left((N-10)(N+2)^2, \frac{2\sqrt{3}}{16}\frac{1}{\sqrt{S}}(T-1)(N-3)^3 - 3(T-7)(N-3)(N-4) + 42N - T - \frac{2\sqrt{3}}{4\sqrt{2}}S - 111\right)$	$\frac{2\sqrt{3}}{16}\frac{1}{\sqrt{S}}N^3 T$
jacobi-1d	$\max(2 + n, \frac{1}{3}(T-1)(N-3) - T - S + 7)$	$\frac{1}{3}NT$
jacobi-2d	$\max\left((N-2)(N+6), \frac{2}{3\sqrt{3}}\frac{1}{\sqrt{S}}(N-3)^2(T-1) - \frac{4\sqrt{2}}{3\sqrt{3}}S - (T-7)(2N-7) + 14\right)$	$\frac{2}{3\sqrt{3}}\frac{1}{\sqrt{S}}N^2 T$
lu	$\max\left(N^2, \frac{2}{3}\frac{1}{\sqrt{3}}(N-2)(N^2 - 4N + 6) - 2(N^2 - 10N + 18) - 8\sqrt{2S}\right)$	$\frac{2}{3}\frac{1}{\sqrt{3}}N^3$
ludcmp	$\max\left(N^2 + N, \frac{1}{3}\frac{1}{\sqrt{3}}(2N-3)(N-1)(N-2)\sqrt{2}\frac{1}{S}(N-1)(N-2) - (2N^2 - 15N + 19) - 16\sqrt{2S}\right)$	$\frac{2}{3}\frac{1}{\sqrt{3}}N^3$
mvt	$N^2 + 4N + \max(0, \frac{1}{3}N(N-1) - 2S - 4N + 4)$	$N^2$
nussinov	$\frac{1}{2}N^2 + \frac{1}{2}N - 1 + \max(0, \frac{1}{6}\frac{1}{\sqrt{S}}(N-3)(N-4)(N-5) + \frac{1}{3}\sqrt{2}(3N^2 - 19N + 6) - (N^2 - 13N + 22) - 8\sqrt{2S})$	$\frac{1}{6}\frac{1}{\sqrt{S}}N^3$
seidel-2d	$\max\left(N^2, \frac{2}{3\sqrt{3}}\frac{1}{\sqrt{S}}(N-3)^2(T-1) - (2N-7)(T-5) - \frac{4\sqrt{2}}{3\sqrt{3}}S + 12\right)$	$\frac{2}{3\sqrt{3}}\frac{1}{\sqrt{S}}N^2 T$
symm	$\max\left(\frac{1}{2}M(M+1) + 2MN + 2, 2\frac{1}{\sqrt{3}}(M-1)(M-2)N - \frac{1}{2}((4N+M)(M-5)) + 5(M-2) - 8\sqrt{2S}\right)$	$2\frac{1}{\sqrt{3}}M^2 N$
syr2k	$\max\left(2 + 2MN + \frac{1}{2}N(N+1), \frac{1}{\sqrt{3}}(M-1)(N+1)N + M + 4N - 4\sqrt{2S}\right)$	$\frac{1}{\sqrt{3}}MN^2$
syrk	$\max\left(MN + \frac{1}{2}(N+1)N + 2, \frac{1}{\sqrt{3}}(M-1)(N+1)N - (M-4)(N-1) - 2\sqrt{2S} + 4\right)$	$\frac{1}{2}\frac{1}{\sqrt{3}}MN^2$
trisolv	$\frac{1}{2}N(N+1) + N + \max(0, \frac{1}{3}\frac{1}{\sqrt{3}}(N-1)(N-2) - 2N - S + 5)$	$\frac{1}{2}N^2$
trmm	$\max\left(\frac{1}{2}M(M-1) + MN + 1, \frac{1}{\sqrt{3}}(M-2 + \frac{2\sqrt{2}}{3})(M-1)N - (M-4)(N-2) - 8\sqrt{2S} + 5\right)$	$\frac{1}{\sqrt{3}}M^2 N$

cholesky	$\max\left(\frac{1}{2}N(N+1), \frac{1}{6}\frac{1}{\sqrt{S}}(N-1)(N-2)(N-3) + \frac{1}{2\sqrt{2}}\frac{1}{S}(N-1)(N-2) - (N-2)(N-7) - 4\sqrt{2S}\right)$	$\frac{1}{6}\frac{1}{\sqrt{S}}N^3$
----------	---	------------------------------------

cholesky

```

for (i = 0; i < _PB_N; i++) {
  for (j = 0; j < i; j++) {
    for (k = 0; k < j; k++) {
      A[i][j] -= A[i][k] * A[j][k];
    }
    A[i][j] /= A[j][j];
  }
  for (k = 0; k < i; k++) {
    A[i][i] -= A[i][k] * A[i][k];
  }
  A[i][i] = SQRT_FUN(A[i][i]);
}

```

Table 2. Complete Lower Bound Formulae for POLYBENCH obtained with the current version of IOLB

A. Olivry, J. Langou, L-N Pouchet, P. Sadayappan, and F. Rastello. **Automated derivation of parametric data movement lower bounds for affine programs.** In the Proceedings of PLDI 2020: Proceedings of the 41st ACM SIGPLAN Conference on Programming Language Design and Implementation, page 808–822, June 2020. ( [link](#) )

Automated I/O Lower Bound Analysis

PLDI'20, June 15 - 20, 2020, London, United Kingdom

kernel	Complete Lower Bound Formulae for POLYBENCH obtained with the current version of IOLB	asymptotic simplified formula
2mm	$\max(N_i N_j + N_j N_k + N_i N_k + N_j N_i + 2, \left(\frac{2}{\sqrt{3}} N_i N_j (N_k - 1) + 2N_i + 2N_j + N_k - 4\sqrt{2S}\right) + \left(\frac{2}{\sqrt{3}} N_i N_j (N_j - 1) + 2N_i + 2N_j + N_j - 4\sqrt{2S}\right) - 2N_i N_j - 2)$	$\frac{2}{\sqrt{3}} N_i N_j N_k + \frac{2}{\sqrt{3}} N_i N_j N_j$
3mm	$\max(N_i N_k + N_j N_k + N_j N_m + N_i N_m, \left(\frac{2}{\sqrt{3}} N_i N_j (N_k - 1) + 2N_i + 2N_j + N_k - 4\sqrt{2S}\right) + \left(\frac{2}{\sqrt{3}} N_i N_j (N_j - 1) + 2N_i + 2N_j + N_j - 4\sqrt{2S}\right) + \left(\frac{2}{\sqrt{3}} N_i N_j (N_m - 1) + 2N_i + 2N_j + N_m - 4\sqrt{2S}\right) - 2N_i N_j - 2N_j N_i - N_i N_j - 6)$	$\frac{2}{\sqrt{3}} N_i N_j N_k + \frac{2}{\sqrt{3}} N_i N_j N_j + \frac{2}{\sqrt{3}} N_i N_j N_m$
adi	$4N^2 + \max(0, (N^2 - 4N - S + 5)(T - 2))$	$N^2 T$
atax	$MN + N + \max(0, \frac{1}{3}((2M - 1 - 8S)(2N - 1 - 8S) - 1) - 10S + 2)$	$MN$
bigc	$MN + M + N + \max(0, \frac{1}{3}((2M - 1 - 8S)(2N - 1 - 8S) - 1) - 10S + 2)$	$MN$
cholesky	$\max\left(\frac{1}{2}N(N+1), \frac{1}{6}\frac{1}{\sqrt{S}}(N-1)(N-2)(N-3) + \frac{1}{2\sqrt{2}}\frac{1}{S}(N-1)(N-2) - (N-2)(N-7) - 4\sqrt{2S}\right)$	$\frac{1}{6}\frac{1}{\sqrt{S}}N^3$
correlation	$\max\left(MN + 2, \frac{1}{\sqrt{3}}M(M-1)(N-1) + \frac{2\sqrt{2}}{3}\frac{1}{\sqrt{S}} - \frac{1}{2}(M-3)(M+2N-2) + 2 - 4S\sqrt{2}\right)$	$\frac{1}{2}\frac{1}{\sqrt{3}}M^2 N$
covariance	$\max\left(MN + 2, \frac{1}{\sqrt{3}}M(M-1)(N-1) + \frac{2\sqrt{2}}{3}\frac{1}{\sqrt{S}} - \frac{1}{2}(M-3)(M+2N-2) + 1 - 4S\sqrt{2}\right)$	$\frac{1}{2}\frac{1}{\sqrt{3}}M^2 N$
deriche	$HW + 1$	$HW$
doitgen	$\max(N_p^2 + N_p N_q N_r - \frac{2}{\sqrt{3}}N_q N_r N_p(N_p - 1) + \frac{1}{\sqrt{3}}\frac{1}{\sqrt{S}} - N_q N_r(N_p - 1) + 2N_p - 8\sqrt{2S} - 1)$	$2\frac{2}{\sqrt{3}}N_q N_r N_p^2$
durbin	$2N + \max(0, \frac{1}{2}(N-3)(N-2-2S))$	$\frac{1}{2}N^2$
fdtd-2d	$\max\left(3N_x N_y - N_y + T - 1, \frac{1}{2\sqrt{2}}\frac{1}{\sqrt{S}}(N_x - 2)(N_y - 2)(T - 1) + 2(N_x + 2)(N_y + 2) - T(N_x + N_y - 6) - N_y - S - 23\right)$	$\frac{1}{2\sqrt{2}}\frac{1}{\sqrt{S}}N_x N_y T$
floyd-warshall	$\max(N^2, \frac{1}{\sqrt{3}}(N-1)^3 - (6N-19)(N-2) - 8\sqrt{2S})$	$\frac{1}{\sqrt{3}}N^3$
gemm	$\max\left(N_i N_j + N_j N_k + N_i N_k + 2, \frac{2}{\sqrt{3}}N_i N_j (N_k - 1) + 2N_i + 2N_j + N_k - 4\sqrt{2S}\right)$	$2\frac{2}{\sqrt{3}}N_i N_j N_k$
gemver	$N^2 + 8N + 2 + \max(0, \frac{1}{3}(3N-2)(N-8S) - 3S + 1)$	$N^2$
gesummv	$2N^2 + N + 2 + \max(0, \frac{1}{3}(N-1)(N-8S) - 2S)$	$2N^2$
gramschmidt	$\max\left(MN, \frac{1}{\sqrt{3}}MN(N-3) - M(N-5 - \frac{2}{\sqrt{3}}) - \frac{1}{2}(N-1)(N-6) - 4\sqrt{2S} - 3\right)$	$\frac{1}{\sqrt{3}}MN^2$
heat-3d	$\max\left((N-10)(N+2)^2, \frac{2\sqrt{3}}{16}\frac{1}{\sqrt{S}}(T-1)(N-3)^3 - 3(T-7)(N-3)(N-4) + 42N - T - \frac{2\sqrt{3}}{4\sqrt{2}}S - 111\right)$	$\frac{2\sqrt{3}}{16}\frac{1}{\sqrt{S}}N^3 T$
jacobi-1d	$\max(2 + n, \frac{1}{3}(T-1)(N-3) - T - S + 7)$	$\frac{1}{3}NT$
jacobi-2d	$\max\left((N-2)(N+6), \frac{2}{3\sqrt{3}}\frac{1}{\sqrt{S}}(N-3)^2(T-1) - \frac{4\sqrt{2}}{3\sqrt{3}}S - (T-7)(2N-7) + 14\right)$	$\frac{2}{3\sqrt{3}}\frac{1}{\sqrt{S}}N^2 T$
lu	$\max\left(N^2, \frac{2}{3}\frac{1}{\sqrt{3}}(N-2)(N^2 - 4N + 6) - 2(N^2 - 10N + 18) - 8\sqrt{2S}\right)$	$\frac{2}{3}\frac{1}{\sqrt{3}}N^3$
ludcmp	$\max\left(N^2 + N, \frac{1}{3}\frac{1}{\sqrt{3}}(2N-3)(N-1)(N-2)\sqrt{2}\frac{1}{S}(N-1)(N-2) - (2N^2 - 15N + 19) - 16\sqrt{2S}\right)$	$\frac{2}{3}\frac{1}{\sqrt{3}}N^3$
mvt	$N^2 + 4N + \max(0, \frac{1}{3}N(N-1) - 2S - 4N + 4)$	$N^2$
nussinov	$\frac{1}{2}N^2 + \frac{1}{2}N - 1 + \max(0, \frac{1}{6}\frac{1}{\sqrt{S}}(N-3)(N-4)(N-5) + \frac{1}{3}\sqrt{2}(3N^2 - 19N + 6) - (N^2 - 13N + 22) - 8\sqrt{2S})$	$\frac{1}{6}\frac{1}{\sqrt{S}}N^3$
seidel-2d	$\max\left(N^2, \frac{2}{3\sqrt{3}}\frac{1}{\sqrt{S}}(N-3)^2(T-1) - (2N-7)(T-5) - \frac{4\sqrt{2}}{3\sqrt{3}}S + 12\right)$	$\frac{2}{3\sqrt{3}}\frac{1}{\sqrt{S}}N^2 T$
symm	$\max\left(\frac{1}{2}M(M+1) + 2MN + 2, 2\frac{1}{\sqrt{3}}(M-1)(M-2)N - \frac{1}{2}((4N+M)(M-5)) + 5(M-2) - 8\sqrt{2S}\right)$	$2\frac{1}{\sqrt{3}}M^2 N$
syr2k	$\max\left(2 + 2MN + \frac{1}{2}N(N+1), \frac{1}{\sqrt{3}}(M-1)(N+1)N + M + 4N - 4\sqrt{2S}\right)$	$\frac{1}{\sqrt{3}}MN^2$
syrk	$\max\left(MN + \frac{1}{2}(N+1)N + 2, \frac{1}{\sqrt{3}}(M-1)(N+1)N - (M-4)(N-1) - 2\sqrt{2S} + 4\right)$	$\frac{1}{2}\frac{1}{\sqrt{3}}MN^2$
trisolv	$\frac{1}{2}N(N+1) + N + \max(0, \frac{1}{3}\frac{1}{\sqrt{3}}(N-1)(N-2) - 2N - S + 5)$	$\frac{1}{2}N^2$
trmm	$\max\left(\frac{1}{2}M(M-1) + MN + 1, \frac{1}{\sqrt{3}}(M-2 + \frac{2\sqrt{2}}{3})(M-1)N - (M-4)(N-2) - 8\sqrt{2S} + 5\right)$	$\frac{1}{\sqrt{3}}M^2 N$

Table 2. Complete Lower Bound Formulae for POLYBENCH obtained with the current version of IOLB

cholesky	$\max\left(\frac{1}{2}N(N+1), \frac{1}{6}\frac{1}{\sqrt{S}}(N-1)(N-2)(N-3) + \frac{1}{2\sqrt{2}}\frac{1}{S}(N-1)(N-2) - (N-2)(N-7) - 4\sqrt{2S}\right)$	$\frac{1}{6}\frac{1}{\sqrt{S}}N^3$
----------	---	------------------------------------

Off by a factor of 2 from the lowest known upper bound

```
cholesky
for (i = 0; i < _PB_N; i++) {
  for (j = 0; j < i; j++) {
    for (k = 0; k < j; k++) {
      A[i][j] -= A[i][k] * A[j][k];
    }
    A[i][j] /= A[j][j];
  }
  for (k = 0; k < i; k++) {
    A[i][i] -= A[i][k] * A[i][k];
  }
  A[i][i] = SQRT_FUN(A[i][i]);
}
```

kernel	# input data	#ops	ratio	$OI_{up}$	$OI_{manual}$	ratio
2mm	$N_i N_k + N_k N_j$ $+ N_j N_l + N_i N_l$	$N_i N_j N_k$ $+ N_i N_j N_l$	-	$\sqrt{S}$	$\sqrt{S}$	1 ✓
3mm	$N_i N_k + N_k N_j$ $+ N_j N_m + N_m N_l$	$N_i N_j N_k + N_j N_l N_m$ $+ N_i N_j N_l$	-	$\sqrt{S}$	$\sqrt{S}$	1 ✓
cholesky	$\frac{1}{2} N^2$	$\frac{1}{3} N^3$	$\frac{2}{3} N$	$2\sqrt{S}$	$\sqrt{S}$	2
correlation	$MN$	$M^2 N$	$M$	$2\sqrt{S}$	$\sqrt{S}$	2
covariance	$MN$	$M^2 N$	$M$	$2\sqrt{S}$	$\sqrt{S}$	2
doitgen	$N_p N_q N_r$	$2N_q n_r N_p^2$	$2N_p$	$\sqrt{S}$	$\sqrt{S}$	1 ✓
fdtd-2d	$3N_x N_y$	$11N_x N_y T$	$\frac{11}{3} T$	$22\sqrt{2}\sqrt{S}$	$\frac{11}{24}\sqrt{3}\sqrt{S}$	$\frac{48\sqrt{2}}{\sqrt{3}}$
floyd-warshall	$N^2$	$2N^3$	$2N$	$2\sqrt{S}$	$\sqrt{S}$	2
gemm	$N_i N_j + N_j N_k + N_i N_k$	$2N_i N_j N_k$	-	$\sqrt{S}$	$\sqrt{S}$	1 ✓
heat-3d	$N^3$	$30N^3 T$	$30T$	$\frac{160}{3}\sqrt[3]{S}$	$\frac{5}{2}\sqrt[3]{S}$	$\frac{64}{3\sqrt[3]{3}}$
jacobi-1d	$N$	$6NT$	$6T$	$24S$	$\frac{3}{2}S$	16
jacobi-2d	$N^2$	$10N^2 T$	$10T$	$15\sqrt{3}\sqrt{S}$	$\frac{5}{4}\sqrt{S}$	$12\sqrt{3}$
lu	$N^2$	$\frac{2}{3} N^3$	$\frac{2}{3} N$	$\sqrt{S}$	$\sqrt{S}$	1 ✓
ludcmp	$N^2$	$\frac{2}{3} N^3$	$\frac{2}{3} N$	$\sqrt{S}$	$\sqrt{S}$	1 ✓
seidel-2d	$N^2$	$9N^2 T$	$9T$	$\frac{27\sqrt{3}}{2}\sqrt{S}$	$\frac{9}{4}\sqrt{S}$	$6\sqrt{3}$
symm	$\frac{1}{2} M^2 + 2MN$	$2M^2 N$	-	$\sqrt{S}$	$\sqrt{S}$	1 ✓
syr2k	$\frac{1}{2} N^2 + 2MN$	$2MN^2$	-	$2\sqrt{S}$	$\sqrt{S}$	2
syrk	$\frac{1}{2} N^2 + MN$	$MN^2$	-	$2\sqrt{S}$	$\sqrt{S}$	2
trmm	$\frac{1}{2} M^2 + MN$	$M^2 N$	-	$\sqrt{S}$	$\sqrt{S}$	1 ✓
atax	$MN$	$4MN$	4	4	4	1 ✓
bicg	$MN$	$4MN$	4	4	4	1 ✓
deriche	$HW$	$32HW$	32	32	$\frac{16}{3}$	6
gemver	$N^2$	$10N^2$	10	10	5	2
gesummv	$2N^2$	$4N^2$	2	2	2	1 ✓
mvt	$N^2$	$4N^2$	4	4	4	1 ✓
trisolv	$\frac{1}{2} N^2$	$N^2$	2	2	2	1 ✓
adi	$N^2$	$30N^2 T$	$30T$	30	5	6
durbin	$N$	$2N^2$	$2N$	4	$\frac{2}{3}$	6
gramschmidt	$MN$	$2MN^2$	$2N$	$2\sqrt{S}$	1	$2\sqrt{S}$
nussinov	$\frac{1}{2} N^2$	$\frac{1}{3} N^3$	$\frac{2}{3} N$	$2\sqrt{S}$	1	$2\sqrt{S}$

A. Olivry, J. Langou, L-N Pouchet, P. Sadayappan, and F. Rastello. **Automated derivation of parametric data movement lower bounds for affine programs**. In the Proceedings of PLDI 2020: Proceedings of the 41st ACM SIGPLAN Conference on Programming Language Design and Implementation, page 808–822, June 2020. ( [link](#) )

kernel	# input data	#ops	ratio	$OI_{up}$	$OI_{manual}$	ratio
2mm	$N_i N_k + N_k N_j$ $+ N_j N_l + N_i N_l$	$N_i N_j N_k$ $+ N_i N_j N_l$	-	$\sqrt{S}$	$\sqrt{S}$	1 ✓
3mm	$N_i N_k + N_k N_j$ $+ N_j N_m + N_m N_l$	$N_i N_j N_k + N_j N_l N_m$ $+ N_i N_j N_l$	-	$\sqrt{S}$	$\sqrt{S}$	1 ✓
cholesky	$\frac{1}{2} N^2$	$\frac{1}{3} N^3$	$\frac{2}{3} N$	$2\sqrt{S}$	$\sqrt{S}$	2
correlation	$MN$	$M^2 N$	$M$	$2\sqrt{S}$	$\sqrt{S}$	2
covariance	$MN$	$M^2 N$	$M$	$2\sqrt{S}$	$\sqrt{S}$	2
doitgen	$N_p N_q N_r$	$2N_q n_r N_p^2$	$2N_p$	$\sqrt{S}$	$\sqrt{S}$	1 ✓
fdtd-2d	$3N_x N_y$	$11N_x N_y T$	$\frac{11}{3} T$	$22\sqrt{2}\sqrt{S}$	$\frac{11}{24}\sqrt{3}\sqrt{S}$	$\frac{48\sqrt{2}}{\sqrt{3}}$
floyd-warshall	$N^2$	$2N^3$	$2N$	$2\sqrt{S}$	$\sqrt{S}$	2
gemm	$N_i N_j + N_j N_k + N_i N_k$	$2N_i N_j N_k$	-	$\sqrt{S}$	$\sqrt{S}$	1 ✓
heat-3d	$N^3$	$30N^3 T$	$30T$	$\frac{160}{3}\sqrt[3]{S}$	$\frac{5}{2}\sqrt[3]{S}$	$\frac{64}{3\sqrt[3]{3}}$
jacobi-1d	$N$	$6NT$	$6T$	$24S$	$\frac{3}{2}S$	16
jacobi-2d	$N^2$	$10N^2 T$	$10T$	$15\sqrt{3}\sqrt{S}$	$\frac{5}{4}\sqrt{S}$	$12\sqrt{3}$
lu	$N^2$	$\frac{2}{3} N^3$	$\frac{2}{3} N$	$\sqrt{S}$	$\sqrt{S}$	1 ✓
ludcmp	$N^2$	$\frac{2}{3} N^3$	$\frac{2}{3} N$	$\sqrt{S}$	$\sqrt{S}$	1 ✓
seidel-2d	$N^2$	$9N^2 T$	$9T$	$\frac{27\sqrt{3}}{2}\sqrt{S}$	$\frac{9}{4}\sqrt{S}$	$6\sqrt{3}$
symm	$\frac{1}{2} M^2 + 2MN$	$2M^2 N$	-	$\sqrt{S}$	$\sqrt{S}$	1 ✓
syr2k	$\frac{1}{2} N^2 + 2MN$	$2MN^2$	-	$2\sqrt{S}$	$\sqrt{S}$	2
syrk	$\frac{1}{2} N^2 + MN$	$MN^2$	-	$2\sqrt{S}$	$\sqrt{S}$	2
trmm	$\frac{1}{2} M^2 + MN$	$M^2 N$	-	$\sqrt{S}$	$\sqrt{S}$	1 ✓
atax	$MN$	$4MN$	4	4	4	1 ✓
bicg	$MN$	$4MN$	4	4	4	1 ✓
deriche	$HW$	$32HW$	32	32	$\frac{16}{3}$	6
gemver	$N^2$	$10N^2$	10	10	5	2
gesummv	$2N^2$	$4N^2$	2	2	2	1 ✓
mvt	$N^2$	$4N^2$	4	4	4	1 ✓
trisolv	$\frac{1}{2} N^2$	$N^2$	2	2	2	1 ✓
adi	$N^2$	$30N^2 T$	$30T$	30	5	6
durbin	$N$	$2N^2$	$2N$	4	$\frac{2}{3}$	6
gramschmidt	$MN$	$2MN^2$	$2N$	$2\sqrt{S}$	1	$2\sqrt{S}$
nussinov	$\frac{1}{2} N^2$	$\frac{1}{3} N^3$	$\frac{2}{3} N$	$2\sqrt{S}$	1	$2\sqrt{S}$

(1) Olivier Beaumont, Lionel Eyraud-Dubois, Julien Langou, and Mathieu Verite. [I/O-optimal algorithms for symmetric linear algebra kernels](#). In the 34th ACM Symposium on Parallelism in Algorithms and Architectures (SPAA '22), Philadelphia, PA, USA, July 11–14, 2022. DOI information: [10.1145/3490148.3538587](#).

(2) Olivier Beaumont, Philippe Duchon, Lionel Eyraud-Dubois, Julien Langou, and Mathieu Verite. [Symmetric Block-Cyclic Distribution: Fewer Communications leads to Faster Dense Cholesky Factorization](#).

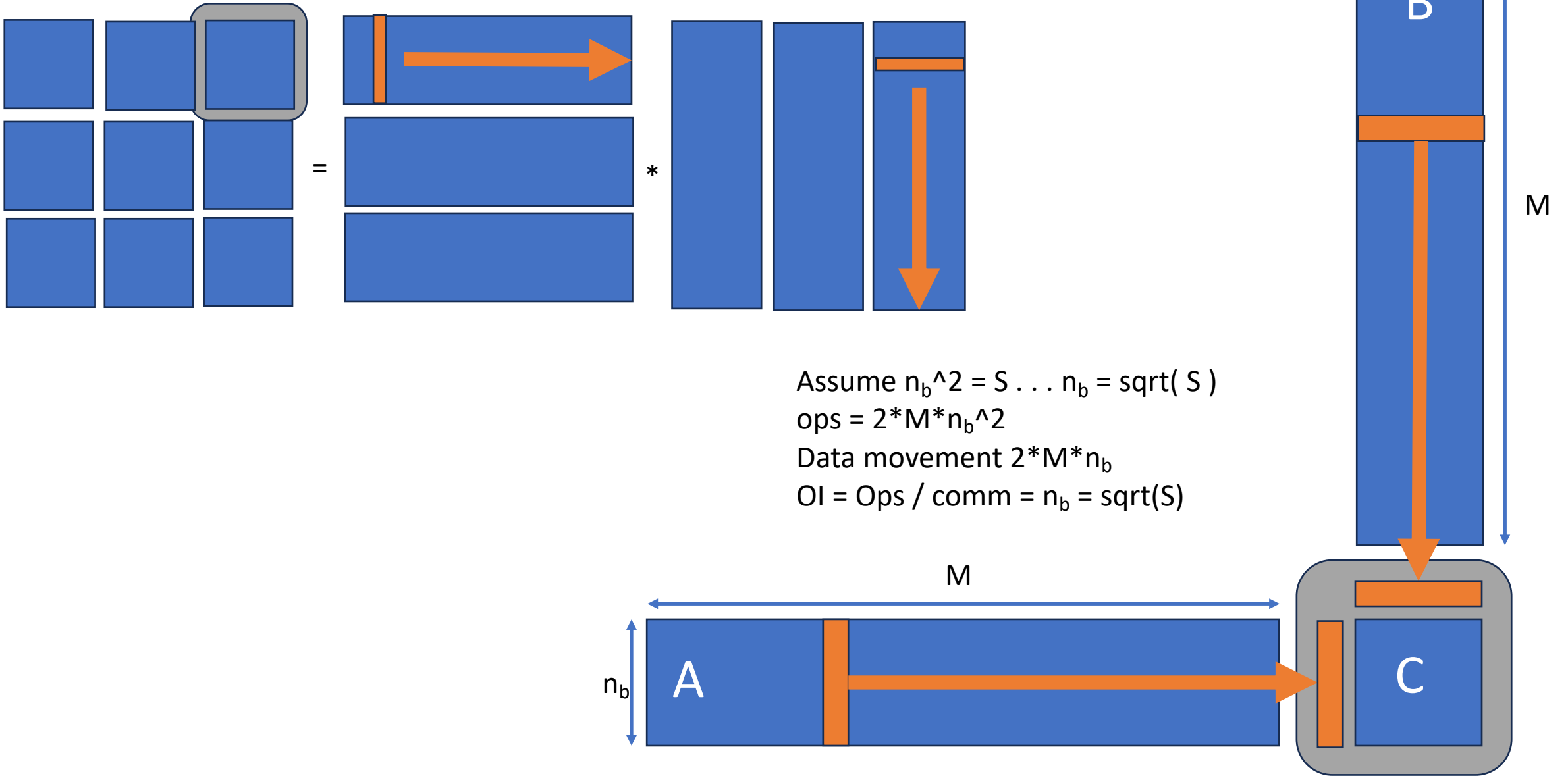
In ACM/IEEE SC 2022 Conference (SC'22), Dallas, TX, USA, November 13-18, 2022. DOI information: [10.1109/SC41404.2022.00034](#). Nominee for Best Paper Award.

(3) Emmanuel Agullo, Alfredo Buttari, Olivier Coulaud, Lionel Eyraud-Dubois, Mathieu Faverge, Alain Franc, Abdou Guermouche, Antoine Jago, Romain Peressoni, and Florent Pruvost. [On the Arithmetic Intensity of Distributed-Memory Dense Matrix Multiplication Involving a Symmetric Input Matrix \(SYMM\)](#). In 2023 IEEE International Parallel and Distributed Processing Symposium (IPDPS'23), St. Petersburg, FL, USA, 15-19 May 2023. DOI information: [10.1109/IPDPS54959.2023.00044](#)

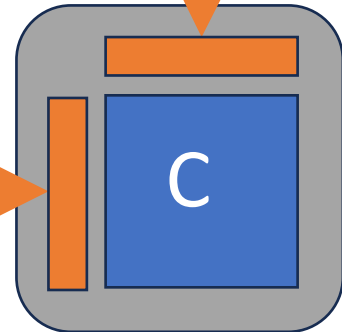
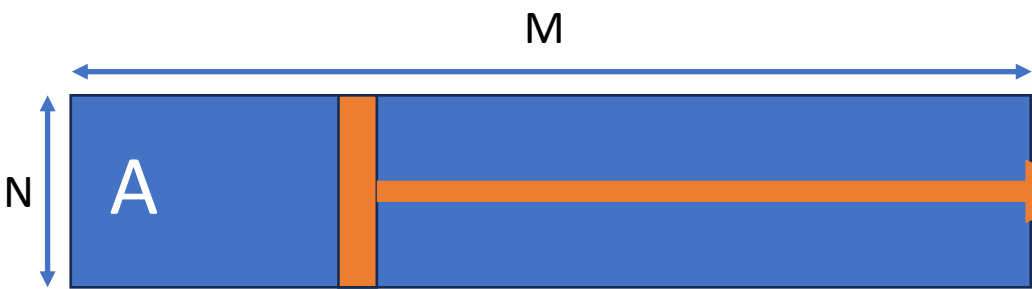
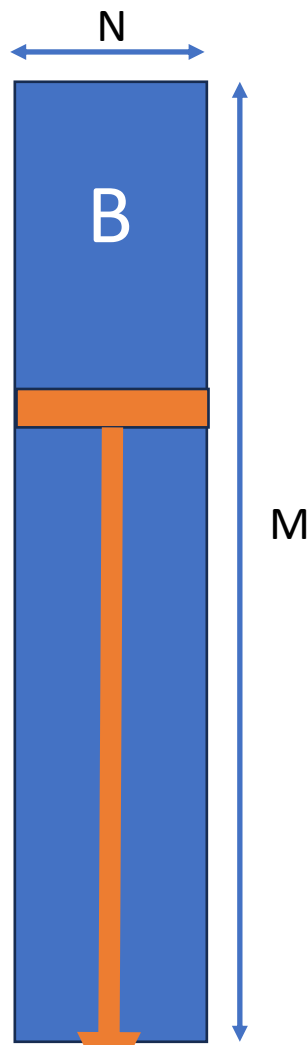
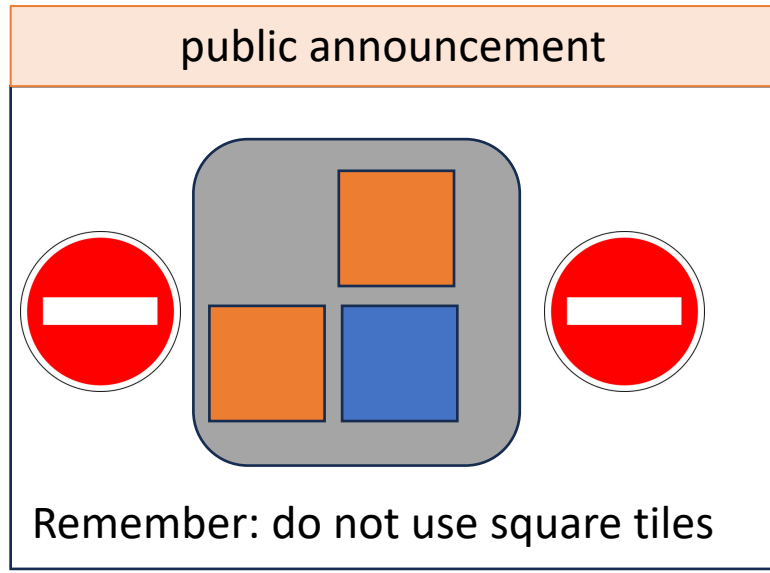
A. Olivry, J. Langou, L-N Pouchet, P. Sadayappan, and F. Rastello. [Automated derivation of parametric data movement lower bounds for affine programs](#). In the Proceedings of PLDI 2020: Proceedings of the 41st ACM SIGPLAN Conference on Programming Language Design and Implementation, page 808–822, June 2020. ( [link](#) )

Operational intensity of LU is at  $\sqrt{2} * \sqrt{S}$

# GEMM



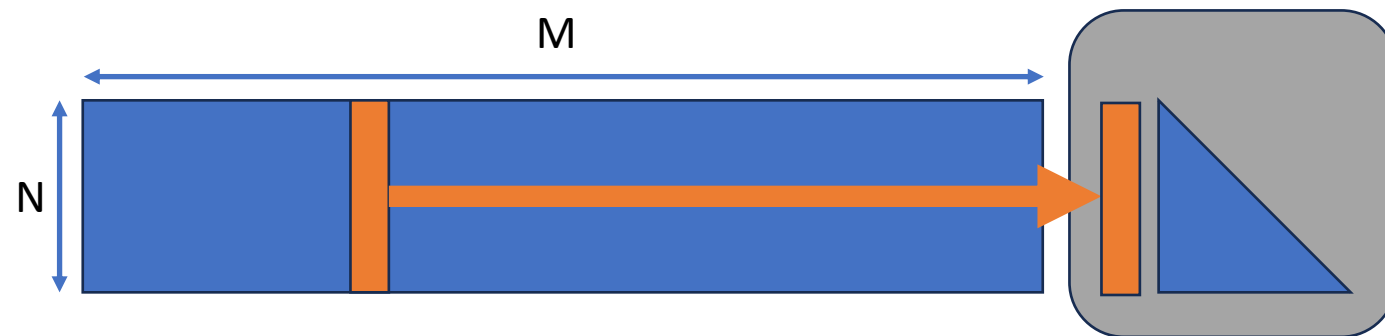
# GEMM





# SYRK

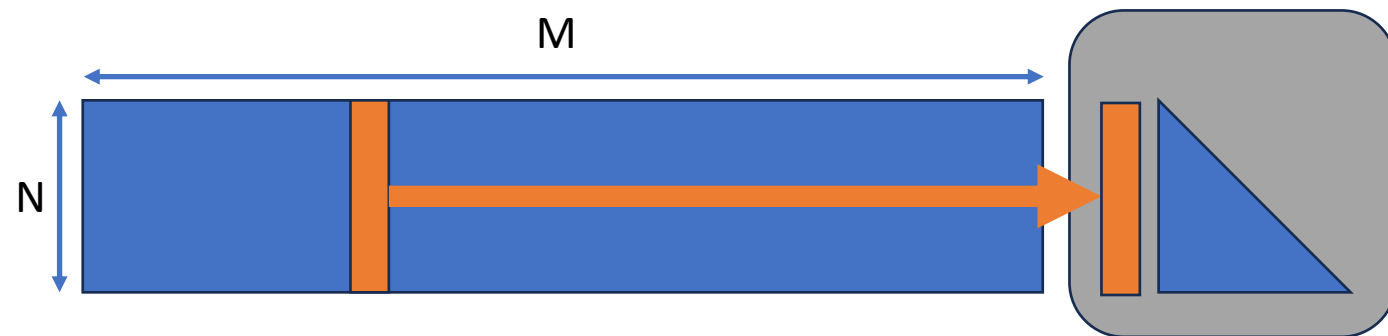
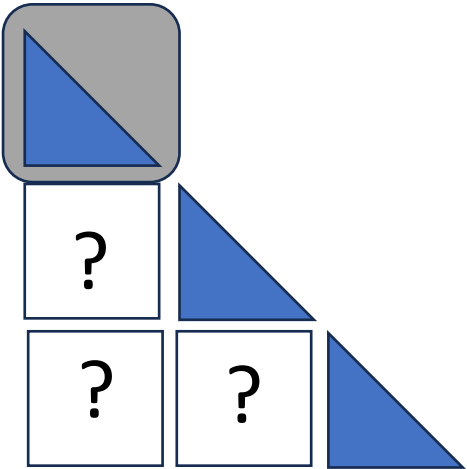
Assume  $(N^2)/2 = S \dots N = \text{sqrt}(S) * \text{sqrt}(2)$   
ops =  $M * N^2$   
Data movement  $M * N$   
OI = Ops / comm =  $N = \text{sqrt}(S) * \text{sqrt}(2)$



Observation:  
SYRK has an OI  $\text{sqrt}(2)$  better  
than MM when a “triangle fit in cache”

# SYRK

Assume  $(N^2)/2 = S \dots N = \text{sqrt}(S) * \text{sqrt}(2)$   
ops =  $M * N^2$   
Data movement  $M * N$   
OI = Ops / comm =  $N = \text{sqrt}(S) * \text{sqrt}(2)$



SYRK has an OI  $\text{sqrt}(2)$  better than MM when a “triangle fit in cache”

- Building an optimal GEMM is easy.
- But how to build an optimal SYRK?

# SYRK

- IOLB says OI is less than  $2 \sqrt{S}$
- Béreux's algorithm has an OI of  $\sqrt{S}$
- This begs the question what is the OI of SYRK?

# SYRK

- IOLB says OI is less than  $2 \sqrt{S}$
- Béreux's algorithm has an OI of  $\sqrt{S}$
- The OI upper bound from IOLB of  $2 \sqrt{S}$  is too optimistic, we can find a lower OI upper bound:  $\sqrt{2} * \sqrt{S}$ .
- And we can improve Béreux's algorithm. Instead of an OI of  $\sqrt{S}$ , we can improve to  $\sqrt{2} * \sqrt{S}$ .

kernel	# input data	#ops	ratio	$OI_{up}$	$OI_{manual}$	ratio
2mm	$N_i N_k + N_k N_j$ $+ N_j N_l + N_i N_l$	$N_i N_j N_k$ $+ N_i N_j N_l$	-	$\sqrt{S}$	$\sqrt{S}$	1 ✓
3mm	$N_i N_k + N_k N_j$ $+ N_j N_m + N_m N_l$	$N_i N_j N_k + N_j N_l N_m$ $+ N_i N_j N_l$	-	$\sqrt{S}$	$\sqrt{S}$	1 ✓
cholesky	$\frac{1}{2} N^2$	$\frac{1}{3} N^3$	$\frac{2}{3} N$	$2\sqrt{S}$	$\sqrt{S}$	2
correlation	$MN$	$M^2 N$	$M$	$2\sqrt{S}$	$\sqrt{S}$	2
covariance	$MN$	$M^2 N$	$M$	$2\sqrt{S}$	$\sqrt{S}$	2
doitgen	$N_p N_q N_r$	$2N_q n_r N_p^2$	$2N_p$	$\sqrt{S}$	$\sqrt{S}$	1 ✓
fdtd-2d	$3N_x N_y$	$11N_x N_y T$	$\frac{11}{3} T$	$22\sqrt{2}\sqrt{S}$	$\frac{11}{24}\sqrt{3}\sqrt{S}$	$\frac{48\sqrt{2}}{\sqrt{3}}$
floyd-warshall	$N^2$	$2N^3$	$2N$	$2\sqrt{S}$	$\sqrt{S}$	2
gemm	$N_i N_j + N_j N_k + N_i N_k$	$2N_i N_j N_k$	-	$\sqrt{S}$	$\sqrt{S}$	1 ✓
heat-3d	$N^3$	$30N^3 T$	$30T$	$\frac{160}{3}\sqrt[3]{S}$	$\frac{5}{2}\sqrt[3]{S}$	$\frac{64}{3\sqrt[3]{3}}$
jacobi-1d	$N$	$6NT$	$6T$	$24S$	$\frac{3}{2}S$	16
jacobi-2d	$N^2$	$10N^2 T$	$10T$	$15\sqrt{3}\sqrt{S}$	$\frac{5}{4}\sqrt{S}$	$12\sqrt{3}$
lu	$N^2$	$\frac{2}{3} N^3$	$\frac{2}{3} N$	$\sqrt{S}$	$\sqrt{S}$	1 ✓
ludcmp	$N^2$	$\frac{2}{3} N^3$	$\frac{2}{3} N$	$\sqrt{S}$	$\sqrt{S}$	1 ✓
seidel-2d	$N^2$	$9N^2 T$	$9T$	$\frac{27\sqrt{3}}{2}\sqrt{S}$	$\frac{9}{4}\sqrt{S}$	$6\sqrt{3}$
symm	$\frac{1}{2} M^2 + 2MN$	$2M^2 N$	-	$\sqrt{S}$	$\sqrt{S}$	1 ✓
syr2k	$\frac{1}{2} N^2 + 2MN$	$2MN^2$	-	$2\sqrt{S}$	$\sqrt{S}$	2
syrk	$\frac{1}{2} N^2 + MN$	$MN^2$	-	$2\sqrt{S}$	$\sqrt{S}$	2
trmm	$\frac{1}{2} M^2 + MN$	$M^2 N$	-	$\sqrt{S}$	$\sqrt{S}$	1 ✓
atax	$MN$	$4MN$	4	4	4	1 ✓
bicg	$MN$	$4MN$	4	4	4	1 ✓
deriche	$HW$	$32HW$	32	32	$\frac{16}{3}$	6
gemver	$N^2$	$10N^2$	10	10	5	2
gesummv	$2N^2$	$4N^2$	2	2	2	1 ✓
mvt	$N^2$	$4N^2$	4	4	4	1 ✓
trisolv	$\frac{1}{2} N^2$	$N^2$	2	2	2	1 ✓
adi	$N^2$	$30N^2 T$	$30T$	30	5	6
durbin	$N$	$2N^2$	$2N$	4	$\frac{2}{3}$	6
gramschmidt	$MN$	$2MN^2$	$2N$	$2\sqrt{S}$	1	$2\sqrt{S}$
nussinov	$\frac{1}{2} N^2$	$\frac{1}{3} N^3$	$\frac{2}{3} N$	$2\sqrt{S}$	1	$2\sqrt{S}$

A. Olivry, J. Langou, L-N Pouchet, P. Sadayappan, and F. Rastello. [Automated derivation of parametric data movement lower bounds for affine programs](#). In the Proceedings of PLDI 2020: Proceedings of the 41st ACM SIGPLAN Conference on Programming Language Design and Implementation, page 808–822, June 2020. ( [link](#) )

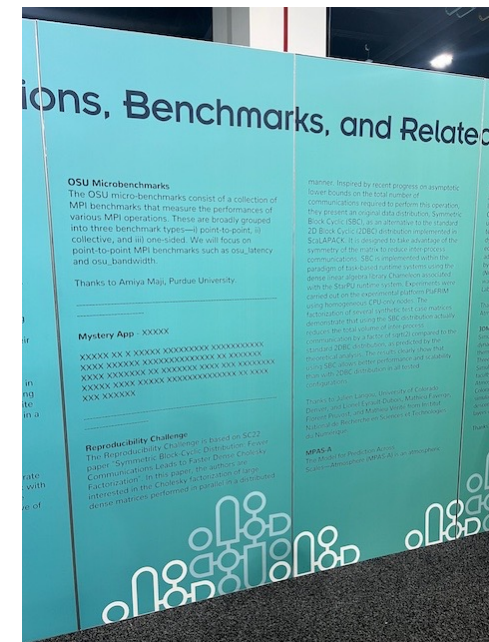
(1) Olivier Beaumont, Lionel Eyraud-Dubois, Julien Langou, and Mathieu Verite. [I/O-optimal algorithms for symmetric linear algebra kernels](#). In the 34th ACM Symposium on Parallelism in Algorithms and Architectures (SPAA '22), Philadelphia, PA, USA, July 11–14, 2022. DOI information: [10.1145/3490148.3538587](#).

(2) Olivier Beaumont, Philippe Duchon, Lionel Eyraud-Dubois, Julien Langou, and Mathieu Verite. [Symmetric Block-Cyclic Distribution: Fewer Communications leads to Faster Dense Cholesky Factorization](#).

In ACM/IEEE SC 2022 Conference (SC'22), Dallas, TX, USA, November 13-18, 2022. DOI information: [10.1109/SC41404.2022.00034](#). Nominee for Best Paper Award.

(3) Emmanuel Agullo, Alfredo Buttari, Olivier Coulaud, Lionel Eyraud-Dubois, Mathieu Faverge, Alain Franc, Abdou Guermouche, Antoine Jago, Romain Peressoni, and Florent Pruvost. [On the Arithmetic Intensity of Distributed-Memory Dense Matrix Multiplication Involving a Symmetric Input Matrix \(SYMM\)](#). In 2023 IEEE International Parallel and Distributed Processing Symposium (IPDPS'23), St. Petersburg, FL, USA, 15-19 May 2023. DOI information: [10.1109/IPDPS54959.2023.00044](#)

# SIGHPC Reproducibility Award SCC @ SC'23



Thanks to Mathieu Faverge and Florent Pruvost  
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Olivier Beaumont, Philippe Duchon, Lionel Eyraud-Dubois, Julien Langou, and Mathieu V rit .

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3mm	$N_i N_k + N_k N_j$ $+ N_j N_m + N_m N_l$	$N_i N_j N_k + N_j N_l N_m$ $+ N_i N_j N_l$	-	$\sqrt{S}$	$\sqrt{S}$	1 ✓
cholesky	$\frac{1}{2} N^2$	$\frac{1}{3} N^3$	$\frac{2}{3} N$	$2\sqrt{S}$	$\sqrt{S}$	2
correlation	$MN$	$M^2 N$	$M$	$2\sqrt{S}$	$\sqrt{S}$	2
covariance	$MN$	$M^2 N$	$M$	$2\sqrt{S}$	$\sqrt{S}$	2
doitgen	$N_p N_q N_r$	$2N_q n_r N_p^2$	$2N_p$	$\sqrt{S}$	$\sqrt{S}$	1 ✓
fdtd-2d	$3N_x N_y$	$11N_x N_y T$	$\frac{11}{3} T$	$22\sqrt{2}\sqrt{S}$	$\frac{11}{24}\sqrt{3}\sqrt{S}$	$\frac{48\sqrt{2}}{\sqrt{3}}$
floyd-warshall	$N^2$	$2N^3$	$2N$	$2\sqrt{S}$	$\sqrt{S}$	2
gemm	$N_i N_j + N_j N_k + N_i N_k$	$2N_i N_j N_k$	-	$\sqrt{S}$	$\sqrt{S}$	1 ✓
heat-3d	$N^3$	$30N^3 T$	$30T$	$\frac{160}{3}\sqrt[3]{S}$	$\frac{5}{2}\sqrt[3]{S}$	$\frac{64}{3\sqrt[3]{3}}$
jacobi-1d	$N$	$6NT$	$6T$	$24S$	$\frac{3}{2}S$	16
jacobi-2d	$N^2$	$10N^2 T$	$10T$	$15\sqrt{3}\sqrt{S}$	$\frac{5}{4}\sqrt{S}$	$12\sqrt{3}$
lu	$N^2$	$\frac{2}{3} N^3$	$\frac{2}{3} N$	$\sqrt{S}$	$\sqrt{S}$	1 ✓
ludcmp	$N^2$	$\frac{2}{3} N^3$	$\frac{2}{3} N$	$\sqrt{S}$	$\sqrt{S}$	1 ✓
seidel-2d	$N^2$	$9N^2 T$	$9T$	$\frac{27\sqrt{3}}{2}\sqrt{S}$	$\frac{9}{4}\sqrt{S}$	$6\sqrt{3}$
symm	$\frac{1}{2} M^2 + 2MN$	$2M^2 N$	-	$\sqrt{S}$	$\sqrt{S}$	1 ✓
syr2k	$\frac{1}{2} N^2 + 2MN$	$2MN^2$	-	$2\sqrt{S}$	$\sqrt{S}$	2
syrk	$\frac{1}{2} N^2 + MN$	$MN^2$	-	$2\sqrt{S}$	$\sqrt{S}$	2
trmm	$\frac{1}{2} M^2 + MN$	$M^2 N$	-	$\sqrt{S}$	$\sqrt{S}$	1 ✓
atax	$MN$	$4MN$	4	4	4	1 ✓
bicg	$MN$	$4MN$	4	4	4	1 ✓
deriche	$HW$	$32HW$	32	32	$\frac{16}{3}$	6
gemver	$N^2$	$10N^2$	10	10	5	2
gesummv	$2N^2$	$4N^2$	2	2	2	1 ✓
mvt	$N^2$	$4N^2$	4	4	4	1 ✓
trisolv	$\frac{1}{2} N^2$	$N^2$	2	2	2	1 ✓
adi	$N^2$	$30N^2 T$	$30T$	30	5	6
durbin	$N$	$2N^2$	$2N$	4	$\frac{2}{3}$	6
gramschmidt	$MN$	$2MN^2$	$2N$	$2\sqrt{S}$	1	$2\sqrt{S}$
nussinov	$\frac{1}{2} N^2$	$\frac{1}{3} N^3$	$\frac{2}{3} N$	$2\sqrt{S}$	1	$2\sqrt{S}$

A. Olivry, J. Langou, L-N Pouchet, P. Sadayappan, and F. Rastello. **Automated derivation of parametric data movement lower bounds for affine programs**. In the Proceedings of PLDI 2020: Proceedings of the 41st ACM SIGPLAN Conference on Programming Language Design and Implementation, page 808–822, June 2020. ( [link](#) )



## Classical Gram-Schmidt (CGS)

**Input:**  $a_1, a_2, \dots, a_{n-1}, a_n$

**Output:**  $q_1, q_2, \dots, q_{n-1}, q_n$

**for**  $j=1:n$ ,

$$w = (I - Q_{1:j-1} Q_{1:j-1}^T) a_j$$

$$q_j = w / \|w\|_2$$

**end**

## Modified Gram-Schmidt (MGS)

**Input:**  $a_1, a_2, \dots, a_{n-1}, a_n$

**Output:**  $q_1, q_2, \dots, q_{n-1}, q_n$

**for**  $j=1:n$ ,

$$w = (I - q_{j-1} q_{j-1}^T) \dots (I - q_1 q_1^T) a_j$$

$$q_j = w / \|w\|_2$$

**end**

```
function [ Q, R ] = cgs( A )
```

```
    n = size(A,2);
```

```
    Q = zeros(size(A));
```

```
    R = zeros (n);
```

```
    for j=1:n,
```

```
        Q(:,j) = A(:,j) ;
```

```
        for i=1:j-1,
```

```
            R(i,j) = Q(:,i)' * A(:,j) ;
```

```
            Q(:,j) = Q(:,j) - Q(:,i) * R(i,j);
```

```
        end
```

```
        R(j,j) = norm( Q(:,j) );
```

```
        Q(:,j) = Q(:,j) / R(j,j);
```

```
    end
```

```
end
```

```
function [ Q, R ] = mgs( A )
```

```
    n = size(A,2);
```

```
    Q = zeros(size(A));
```

```
    R = zeros (n);
```

```
    for j=1:n,
```

```
        Q(:,j) = A(:,j) ;
```

```
        for i=1:j-1,
```

```
            R(i,j) = Q(:,i)' * Q(:,j) ;
```

```
            Q(:,j) = Q(:,j) - Q(:,i) * R(i,j);
```

```
        end
```

```
        R(j,j) = norm( Q(:,j) );
```

```
        Q(:,j) = Q(:,j) / R(j,j);
```

```
    end
```

```
end
```

```

#include <math.h>
void qr_cgs_ll (int M, int N, double A[M][N], double R[N][N] )
{
  int i, j, k;
  #pragma scop
  if (M>=N) {
    for (j = 0; j < N; j++) {
      for (i = 0; i < j; i++) {
        R[i][j] = 0.0e+00;
        for (k = 0; k < M; k++)
          R[i][j] += A[k][i] * A[k][j];
      }
      for (i = 0; i < j; i++)
        for (k = 0; k < M; k++)
          A[k][j] -= A[k][i] * R[i][j];
      R[j][j] = 0.0e+00;
      for (k = 0; k < M; k++)
        R[j][j] += A[k][j] * A[k][j];
      R[j][j] = sqrt(R[j][j]);
      for (k = 0; k < M; k++)
        A[k][j] /= R[j][j];
    }
  }
  #pragma endscop
}

```

### CGS

MN input data (+  $N^2 / 2$  for R in output)

2  $MN^2$  operations

IOLB: operational intensity is at most  $2\sqrt{S}$

```

#include <math.h>
void qr_mgs_ll (int M, int N, double A[M][N], double R[N][N] )
{
  int i, j, k;
  #pragma scop
  if (M>=N) {
    for (j = 0; j < N; j++) {
      for (i = 0; i < j; i++) {
        R[i][j] = 0.0e+00;
        for (k = 0; k < M; k++)
          R[i][j] += A[k][i] * A[k][j];
        for (k = 0; k < M; k++)
          A[k][j] -= A[k][i] * R[i][j];
      }
      R[j][j] = 0.0e+00;
      for (k = 0; k < M; k++)
        R[j][j] += A[k][j] * A[k][j];
      R[j][j] = sqrt(R[j][j]);
      for (k = 0; k < M; k++)
        A[k][j] /= R[j][j];
    }
  }
  #pragma endscop
}

```

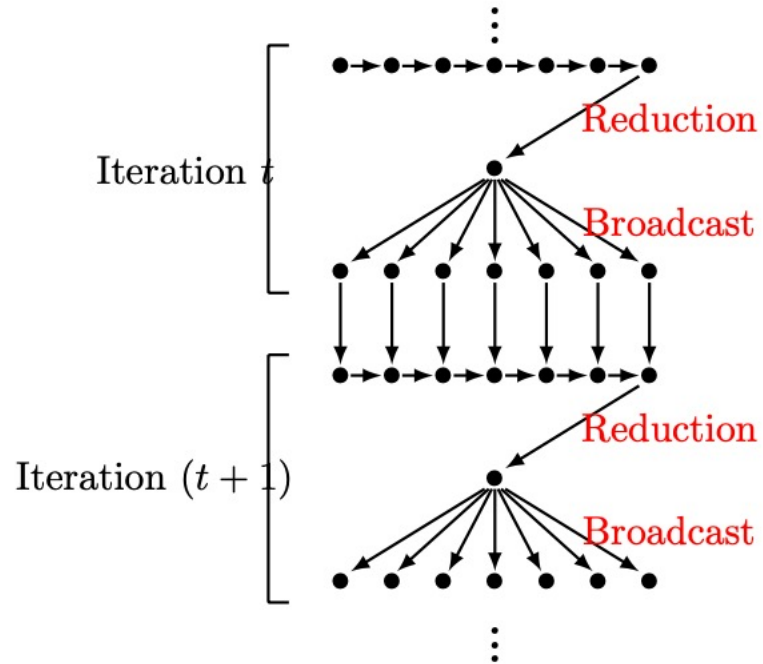
### MGS

MN data (+  $N^2 / 2$  for R in output)

2  $MN^2$  operations

IOLB: operational intensity is at most  $2\sqrt{S}$

# Hourglass pattern



Standard “MM-way” of doing business

$$|E| \leq |\phi_{i,j}(E)|^{\frac{1}{2}} \cdot |\phi_{i,k}(E)|^{\frac{1}{2}} \cdot |\phi_{k,j}(E)|^{\frac{1}{2}} \leq K^{3/2}$$

If Hourglass pattern is detected then

$$|I'| \leq |\phi_i(I')| \times |\phi_j(I')| \times |\phi_k(I')|.$$

$$|I'| \leq M \times \frac{K}{M} \times \frac{K}{M} = \frac{K^2}{M}$$

**Theorem 5** (Lower bounds for MGS). *The communication volume  $Q$  for the MGS algorithm on a  $M \times N$  matrix can be bounded as follows:*

$$\frac{M^2 N(N-1)}{8(S+M)} \leq Q$$

*Furthermore, if  $S \leq M$ , we also have:*

$$\frac{(M-S)N(N-1)}{4} \leq Q$$

Interpretation: (with approximations)

If  $M < N$  then IO is at least  $(1/8) * M^2 N^2 / S$   
 or in another words  $(1/8) * (M/S) * M N^2$

If  $M > N$  then IO is at least  $(1/4) * M N^2$

Interpretation:

Since  $M < \sqrt{S}$ ,  $M^2 N^2 / S$  is a much better lower bound on IO than  $M N^2 / \sqrt{S}$  – (larger is better)

Kernel	Old bound	New bound (hourglass)	
MGS	$\Omega \left( \frac{MN^2}{\sqrt{S}} \right)$	$\Omega \left( \frac{M^2N(N-1)}{S+M} \right)$	
QR HH A2V	$\Omega \left( \frac{MN^2}{\sqrt{S}} \right)$	$\Omega \left( \frac{MN^2(N-M)}{N-M-S} \right)$	GEQR2
QR HH V2Q	$\Omega \left( \frac{MN^2}{\sqrt{S}} \right)$	$\Omega \left( \frac{MN^2(N-M)}{N-M-S} \right)$	ORG2R

Kernel	Old bound [17]	New bound (hourglass)
MGS	$\frac{2M+3MN+MN^2}{\sqrt{S}} + 5M - MN + \frac{7N-N^2}{2} - S - 6$	$\frac{N^2M^2+2M^2-3NM^2}{8(M+S)} + 5M - MN + \frac{7N-N^2}{2} - S - 6$
QR HH A2V	$\frac{3MN^2+6M+7N-N^3-9MN-6}{3\sqrt{S}} + 5M - MN + 5N - S - 13$	$\frac{3MN^2-9MN+7N+6M-6-N^3}{24(1-\frac{S}{N-M})} + 5M - MN + 5N - S - 13$
QR HH V2Q	$\frac{3MN^2-N^3+6M+7N-9MN-6}{3\sqrt{S}} + 2M + 2N + \frac{N-N^2}{2} - S - 4$	$\frac{3MN^2-N^3+6M+7N-9MN-6}{24(1+\frac{S}{M-N})} + 2M + 2N + \frac{N-N^2}{2} - S - 4$

Kernel	Old bound [17]	New bound (hourglass)
MGS	$\Omega \left( \frac{MN^2}{\sqrt{S}} \right)$	$\Omega \left( \frac{M^2N(N-1)}{S+M} \right)$
QR HH A2V	$\Omega \left( \frac{MN^2}{\sqrt{S}} \right)$	$\Omega \left( \frac{MN^2(N-M)}{N-M-S} \right)$
QR HH V2Q	$\Omega \left( \frac{MN^2}{\sqrt{S}} \right)$	$\Omega \left( \frac{MN^2(N-M)}{N-M-S} \right)$
GEBD2	$\Omega \left( \frac{MN^2}{\sqrt{S}} \right)$	$\Omega \left( \frac{MN^2(M-N+1)}{8(S+M-N+1)} \right)$
GEHD2	$\Omega \left( \frac{N^3}{\sqrt{S}} \right)$	$\Omega \left( \frac{N^4}{N+2S} \right)$

Kernel	Old bound [17]	New bound (hourglass)
MGS	$\frac{2M+3MN+MN^2}{\sqrt{S}} + 5M - MN + \frac{7N-N^2}{2} - S - 6$	$\frac{N^2M^2+2M^2-3NM^2}{8(M+S)} + 5M - MN + \frac{7N-N^2}{2} - S - 6$
QR HH A2V	$\frac{3MN^2+6M+7N-N^3-9MN-6}{3\sqrt{S}} + 5M - MN + 5N - S - 13$	$\frac{3MN^2-9MN+7N+6M-6-N^3}{24(1-\frac{S}{N-M})} + 5M - MN + 5N - S - 13$
QR HH V2Q	$\frac{3MN^2-N^3+6M+7N-9MN-6}{3\sqrt{S}} + 2M + 2N + \frac{N-N^2}{2} - S - 4$	$\frac{3MN^2-N^3+6M+7N-9MN-6}{24(1+\frac{S}{M-N})} + 2M + 2N + \frac{N-N^2}{2} - S - 4$
GEBD2	$\frac{3MN^2-N^3-9MN+6M+7N-6}{3\sqrt{S}} + 5N + 5M - MN - S - 13$	$\frac{3MN^2-N^3+3N^2-15MN+4N+18M-12}{24(1+\frac{S}{1+M-N})} + 5N + 7M - MN - S - 18$
GEHD2	$\frac{5N^3-30N^2+55N-30}{3\sqrt{S}} + \frac{69N-9N^2}{2} - 3 * S - 56$	$\frac{N^3-6N^2+11N-6}{12(1+\frac{S}{N-M-1})} - N^2 + 12N - S - 19$

[./iolb-affine-indocker.sh examples/lin-alg/gehd2\\_splitted.c](#)

$$\begin{aligned} & -1+n^2+\max(0,-107+5/24*(S-(2+m-n)^{-1}*S^2)^{-1}*S*n^3-11/12*((1+m-n)^{-1}*S^2-S)^{-1}*S*n-8*m*S^{(-1/2)}*n^2-5/4*(S-(2+m-n)^{-1}*S^2)^{-1}*S*n^2-23*S^{(-1/2)}-27*m*S^{(-1/2)}-1/12*((1+m-n)^{-1}*S^2-S)^{-1}*S*n^3+55/24*(S-(2+m-n)^{-1}*S^2)^{-1}*S*n-2*m^2-5/4*(S-(2+m-n)^{-1}*S^2)^{-1}*S+1/2*((1+m-n)^{-1}*S^2-S)^{-1}*S*n^2+31*m*S^{(-1/2)}*n-9*m+235/6*S^{(-1/2)}*n+7*m^2*S^{(-1/2)}*n-13*m^2*S^{(-1/2)}+5*m*n-25/2*n^2-41/2*S^{(-1/2)}*n^2-10*S+145/2*n+1/2*((1+m-n)^{-1}*S^2-S)^{-1}*S+10/3*S^{(-1/2)}*n^3-2*m^3*S^{(-1/2)}) \end{aligned}$$



**Theorem 5** (Lower bounds for MGS). *The communication volume  $Q$  for the MGS algorithm on a  $M \times N$  matrix can be bounded as follows:*

$$\frac{M^2 N(N-1)}{8(S+M)} \leq Q$$

*Furthermore, if  $S \leq M$ , we also have:*

$$\frac{(M-S)N(N-1)}{4} \leq Q$$

Interpretation:

If  $M < N$  then IO is at least  $(1/8) * M^2 N^2 / S$  or  $(1/8) * (M/S) M N^2$

Interpretation:

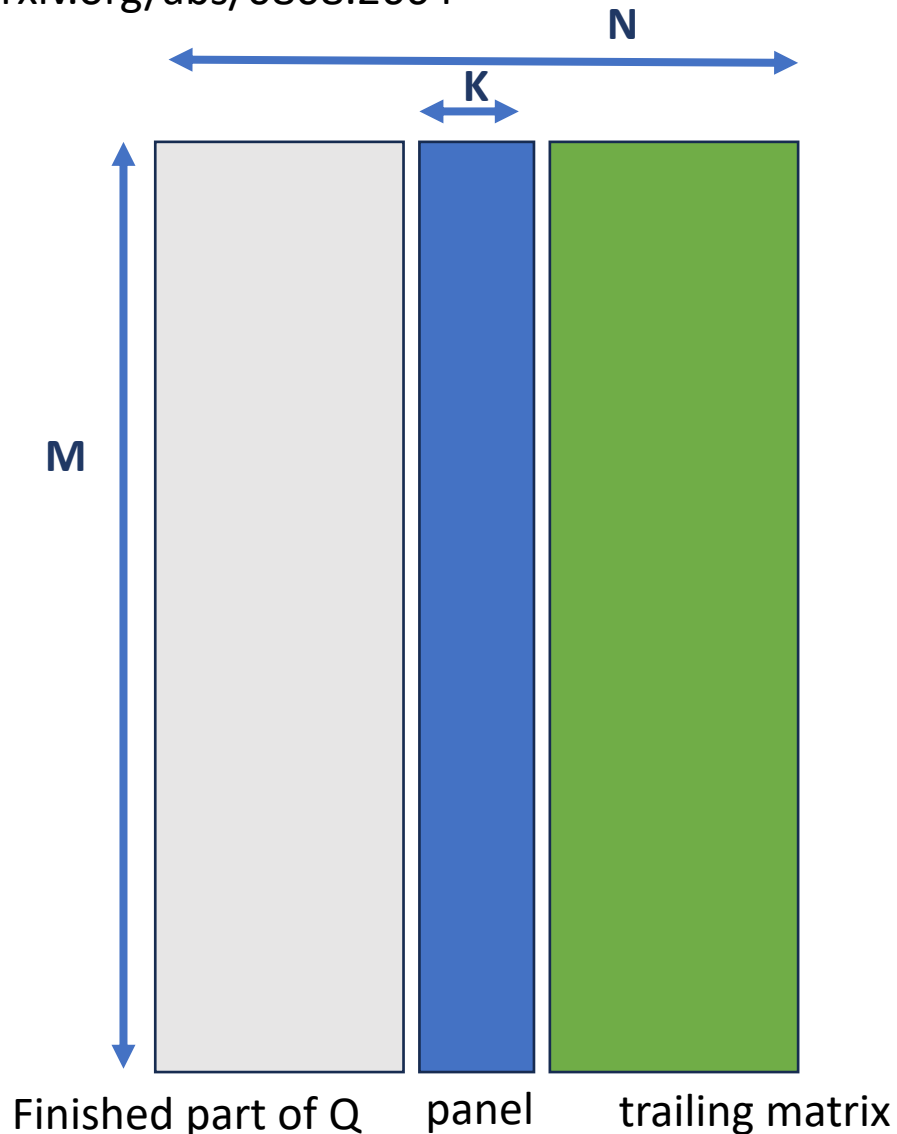
If  $M > N$  then IO is at least  $(1/4) * M N^2$

Much better lower bound on IO than  $M N^2 / \sqrt{S}$

# Communication-optimal parallel and sequential QR and LU factorizations

Demmel, Grigori, Hoemmen and Langou, 2008

<https://arxiv.org/abs/0808.2664>



We need at least a few columns to fit in cache!

Take  $K$  such that

$$M * K + M < S$$

panel fits in cache and stays in cache

At start of step, panel+trailing are updated and ready to go

Load panel

Do MGS on panel (panel factorization)

Update trailing matrix by loading one column at a time

Analysis:

$K$  is about  $M / S$

Load about (less than)  $N$  columns of size  $M$  every  $N / K$  steps

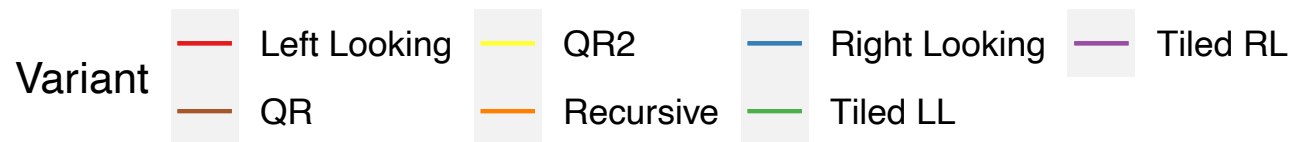
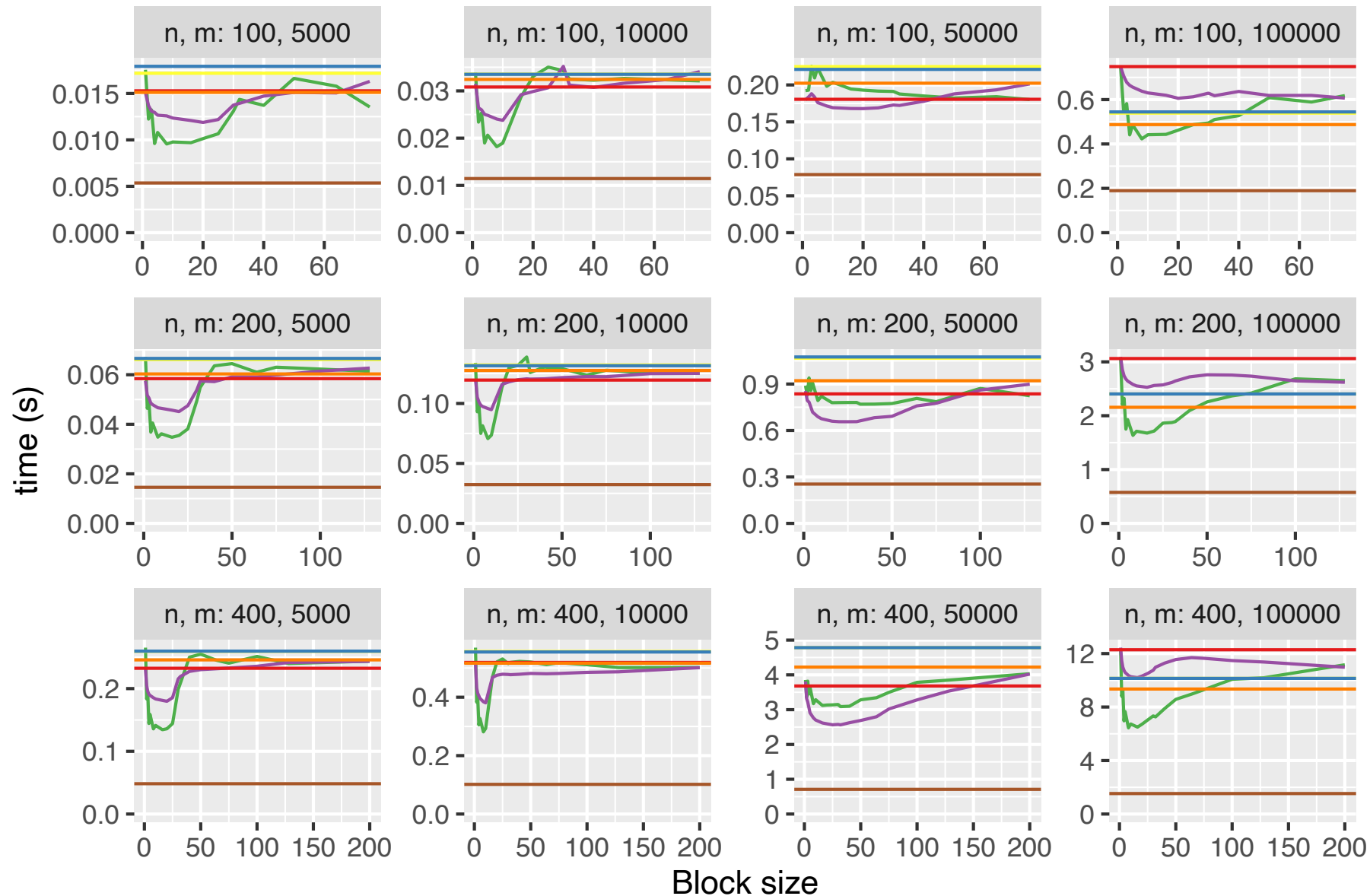
So IO is about  $M^2 N^2 / S$

Which is a factor of  $S/M$  better than  $M N^2$

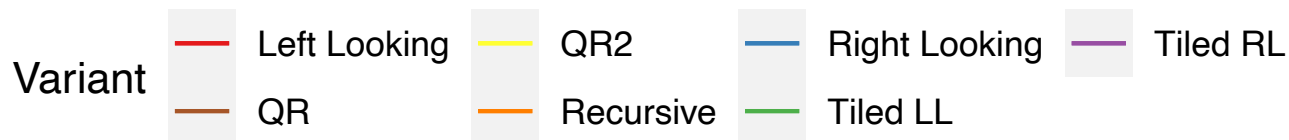
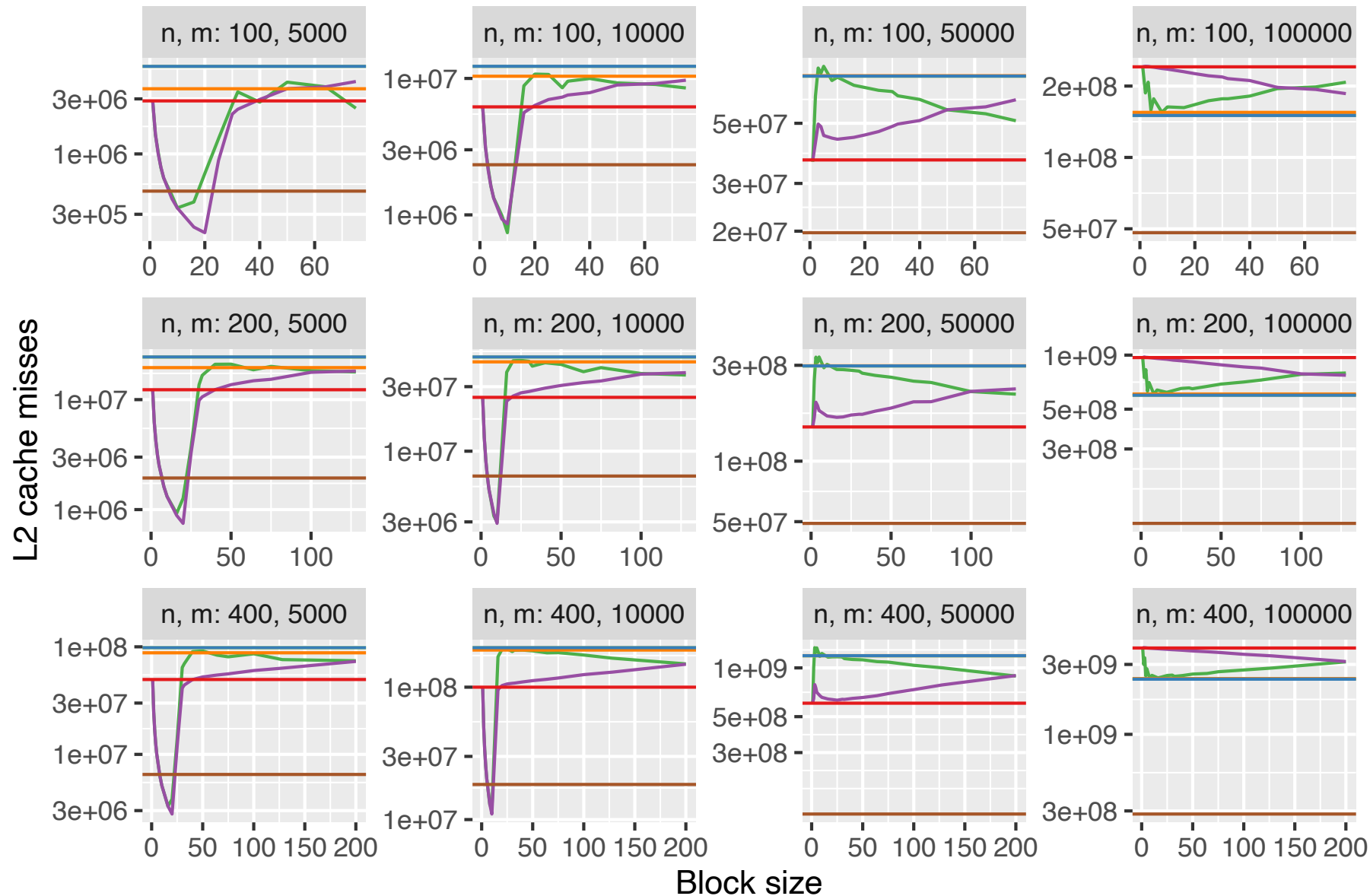
So a factor of  $K$  better than  $M N^2$

This is right looking, you can do a left looking variant too.

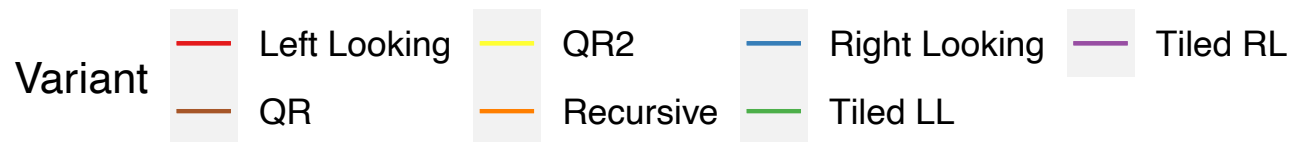
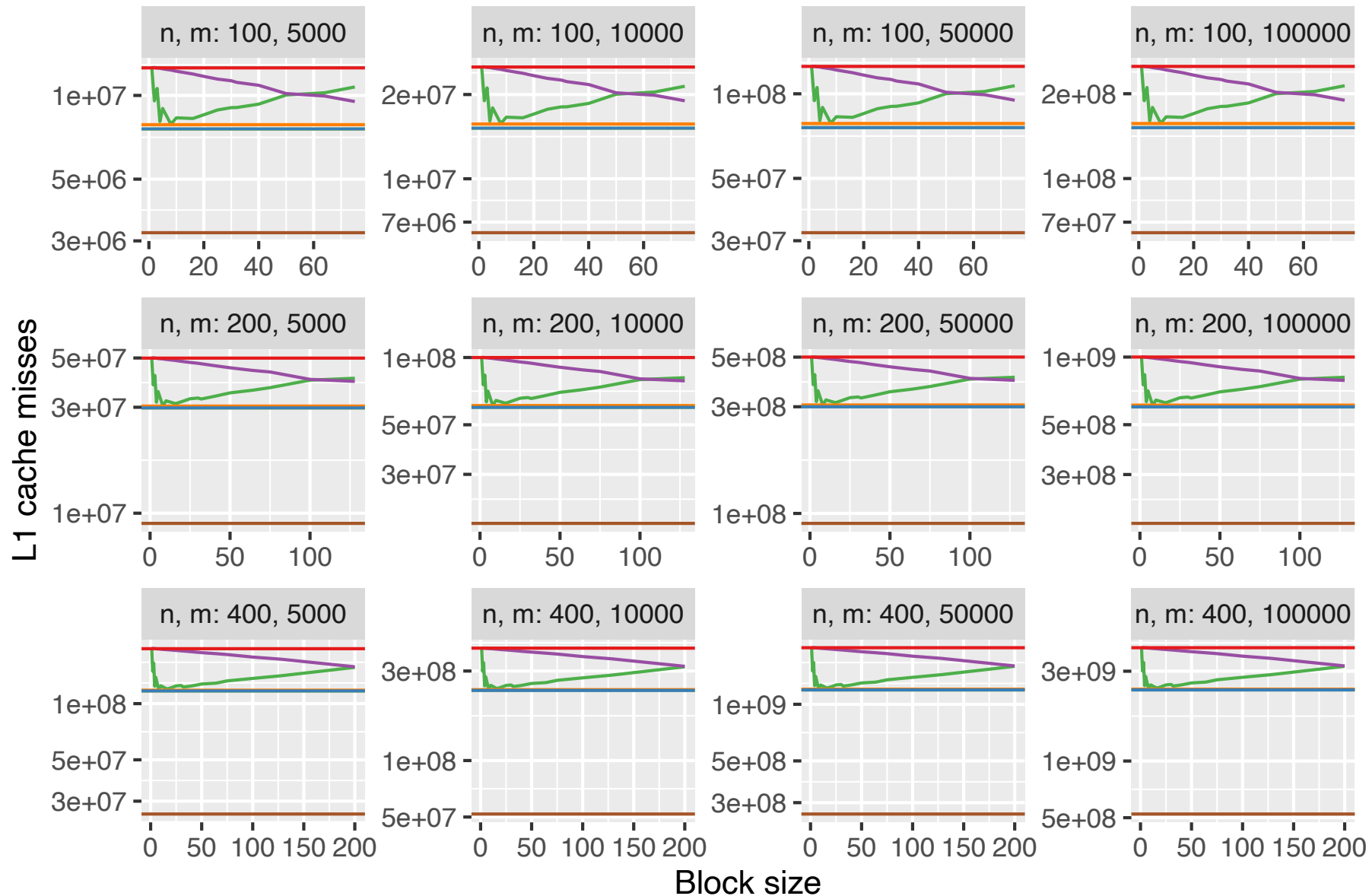
A2V (geqr2)  
bora@plafrim  
Intel CascadeLake



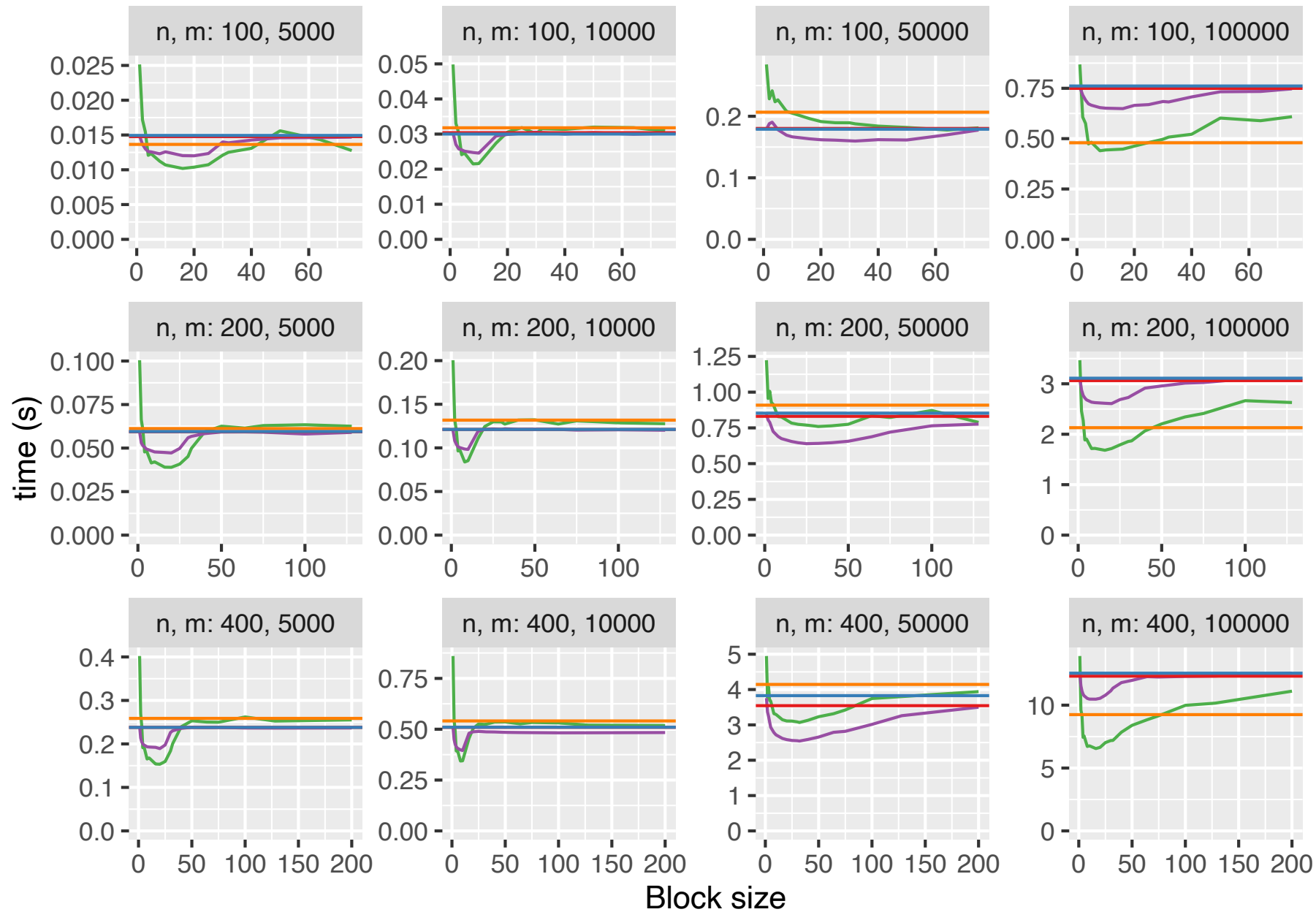
A2V (geqr2)  
 bora@plafrim  
 Intel CascadeLake



A2V (geqr2)  
 bora@plafrim  
 Intel CascadeLake

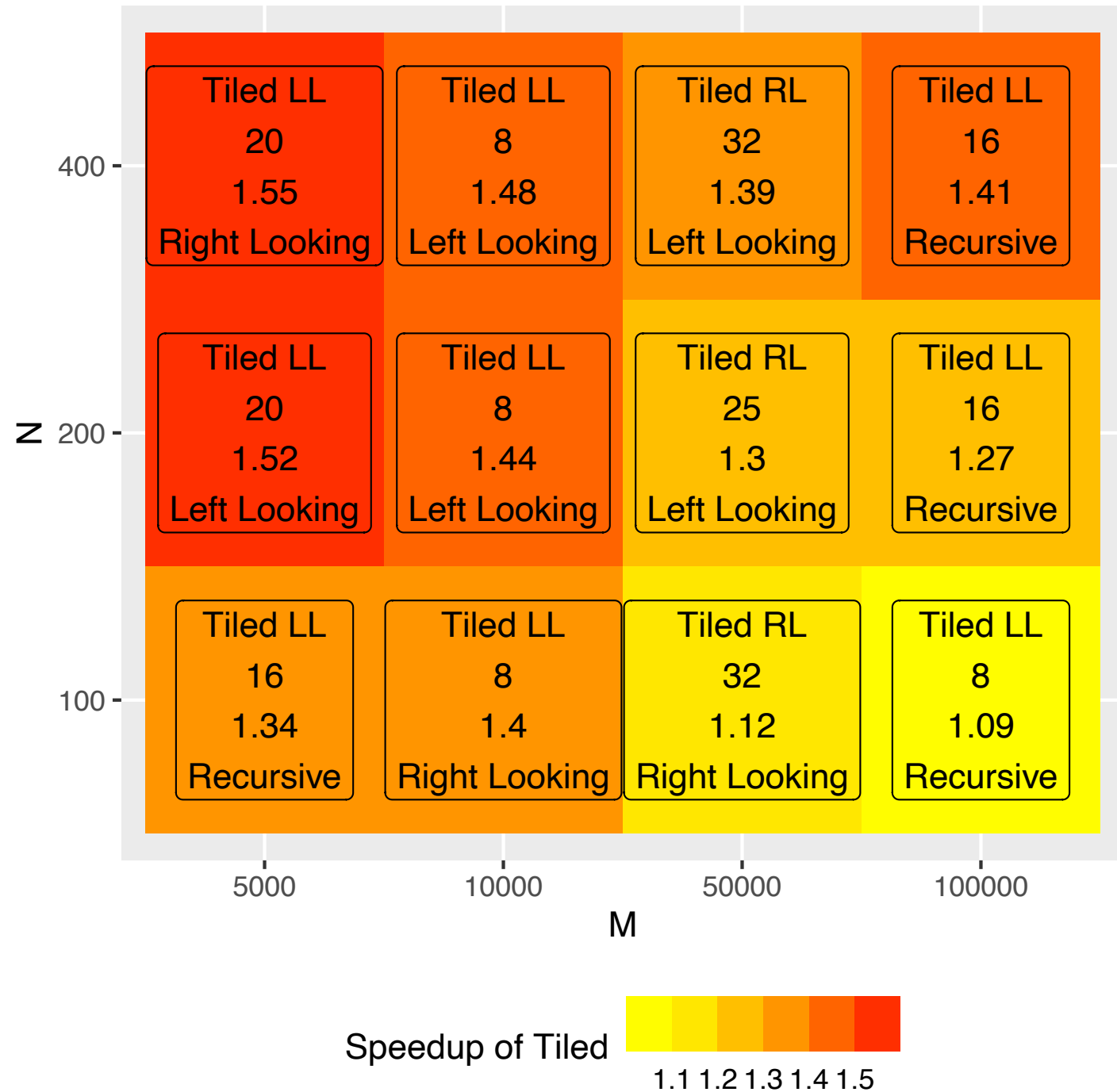


MGS  
bora@plafrim  
Intel CascadeLake

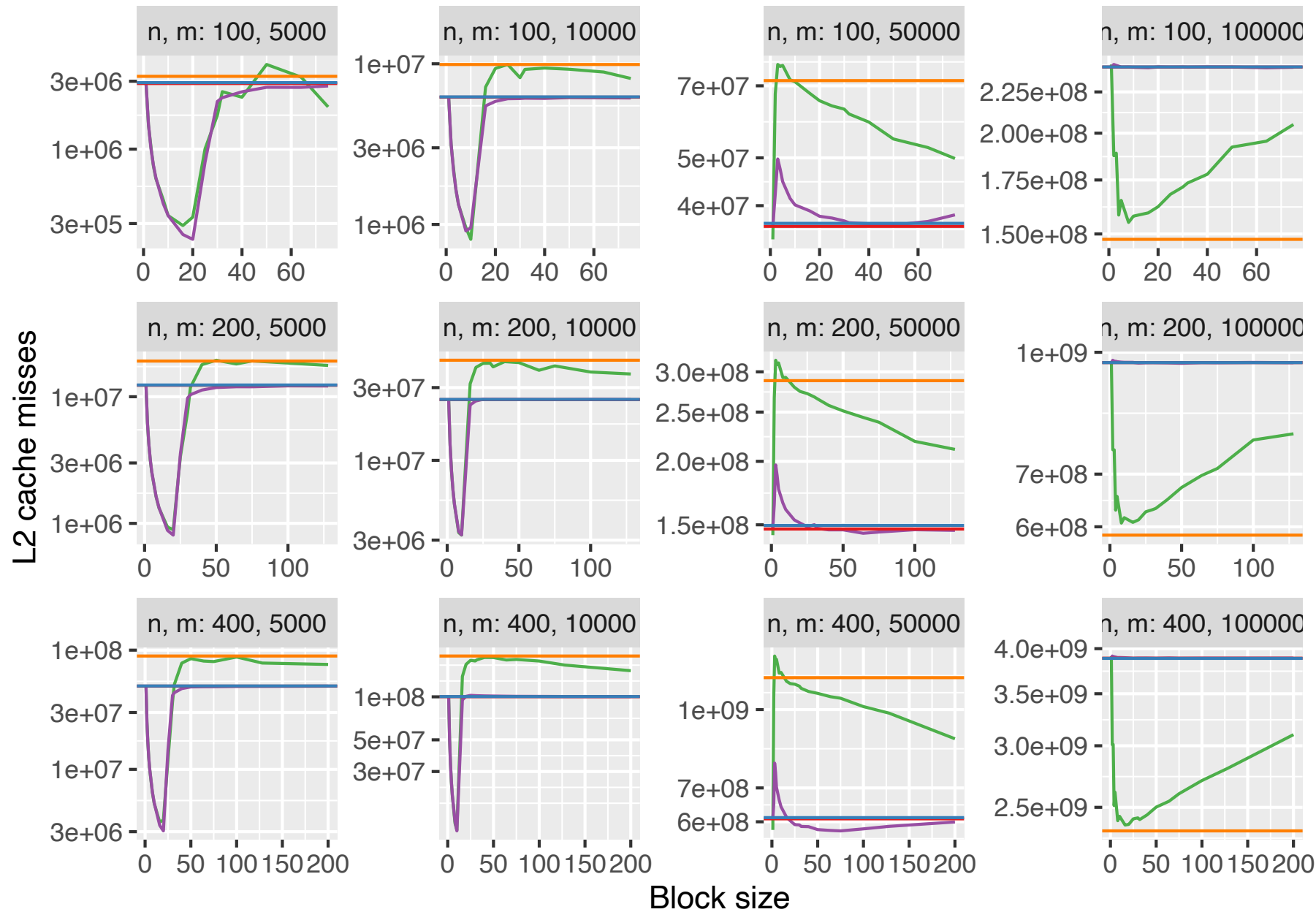


Variant — Left Looking — Recursive — Right Looking — Tiled LL — Tiled RL

MGS  
bora@plafrim  
Intel CascadeLake



MGS  
bora@plafrim  
Intel CascadeLake



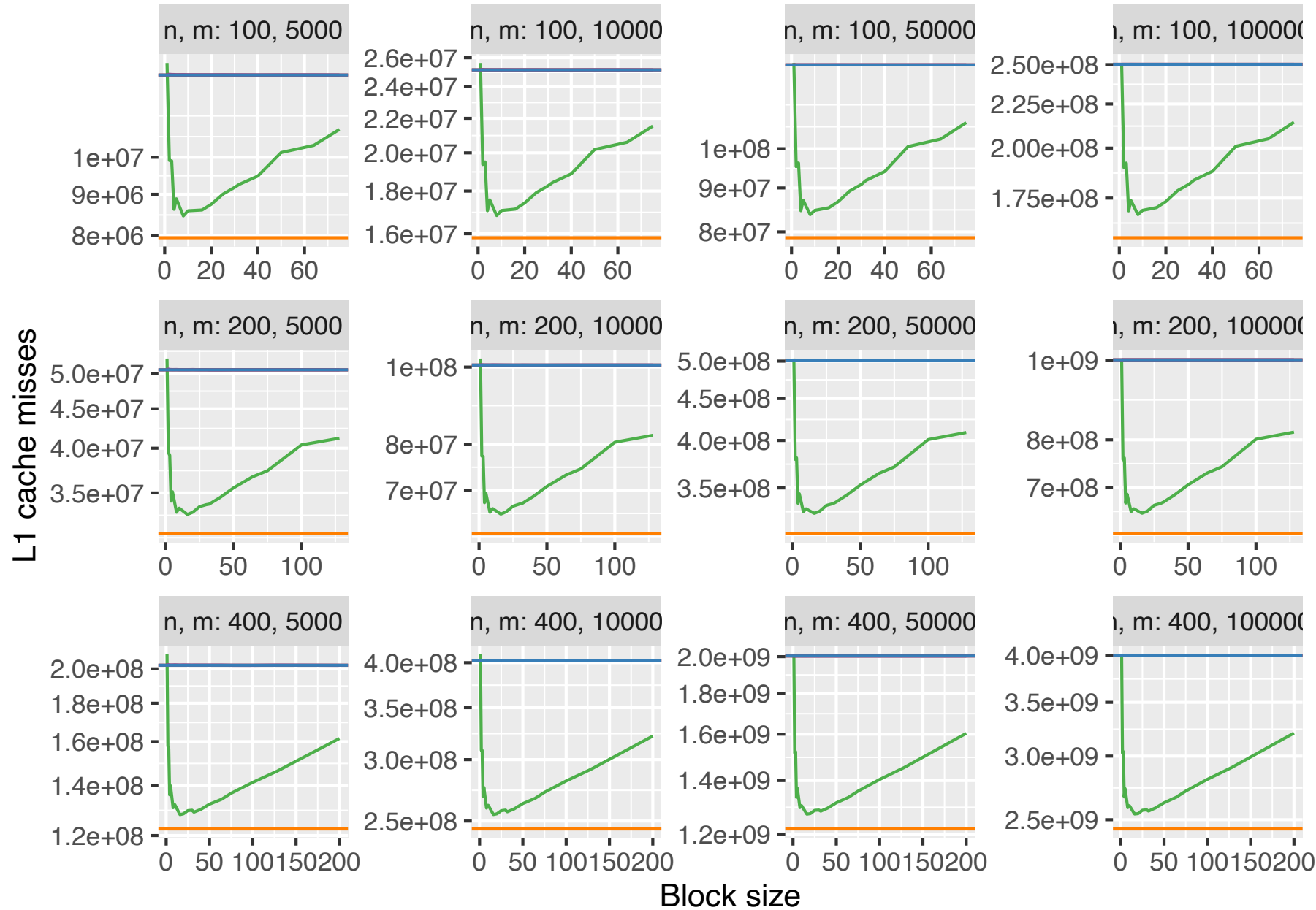
Variant — Left Looking — Recursive — Right Looking — Tiled LL — Tiled RL



# MGS

bora@plafrim

Intel CascadeLake



Variant — Left Looking — Recursive — Right Looking — Tiled LL — Tiled RL

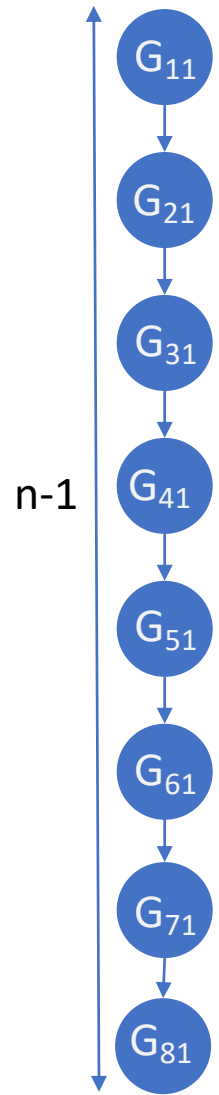
# Current work: chains of Givens rotations with Thijs Steel

```
for (p = 0; p < k; p++) {  
    for (j = 0; j < n - 1; j++) {  
        for (i = 0; i < m; i++) {  
            temp = C[j][p] * A[i][j] + S[j][p] * A[i][j + 1];  
            A[i][j + 1] = -S[j][p] * A[i][j] + C[j][p] * A[i][j + 1];  
            A[i][j] = temp;  
        }  
    }  
}
```

$n$



### A Francis step



work on columns 1 and 2

work on columns 2 and 3

work on columns 3 and 4

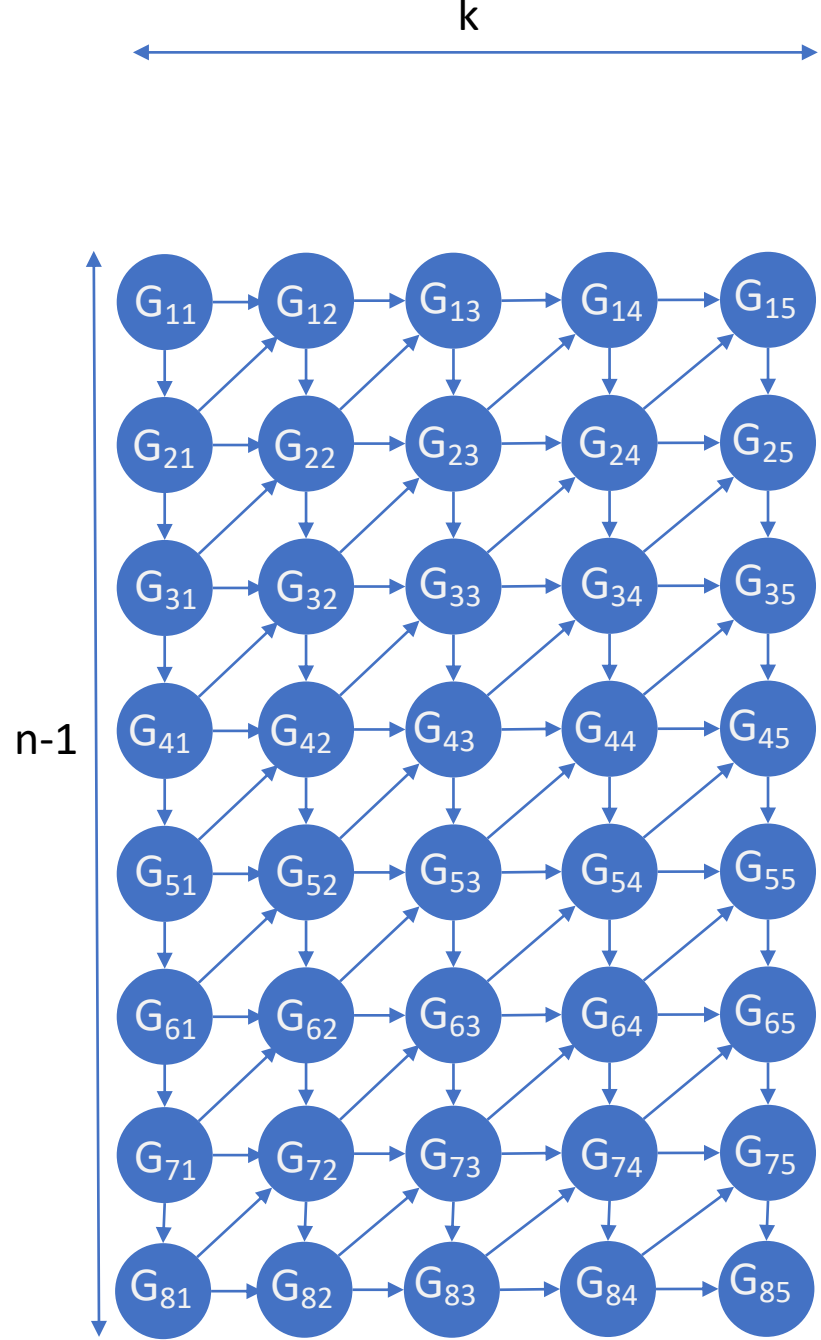
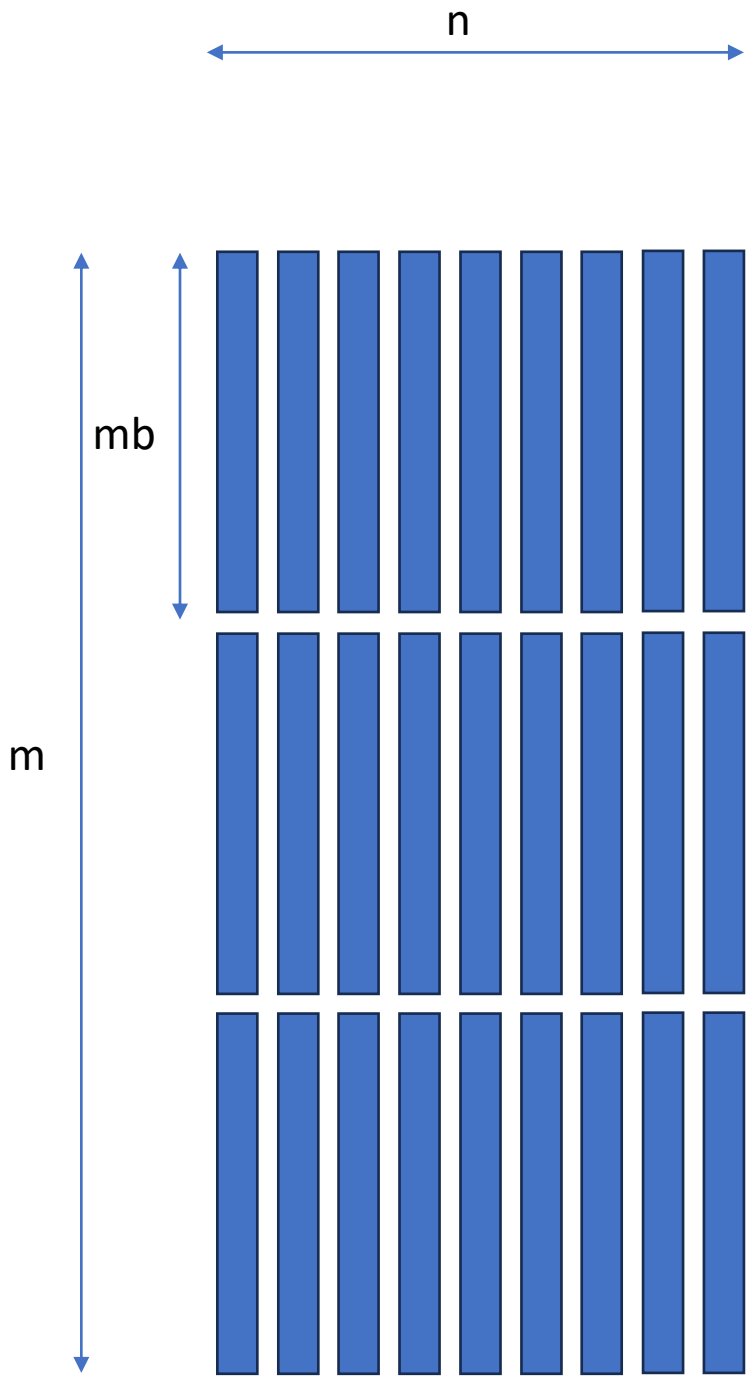
work on columns 4 and 5

work on columns 5 and 6

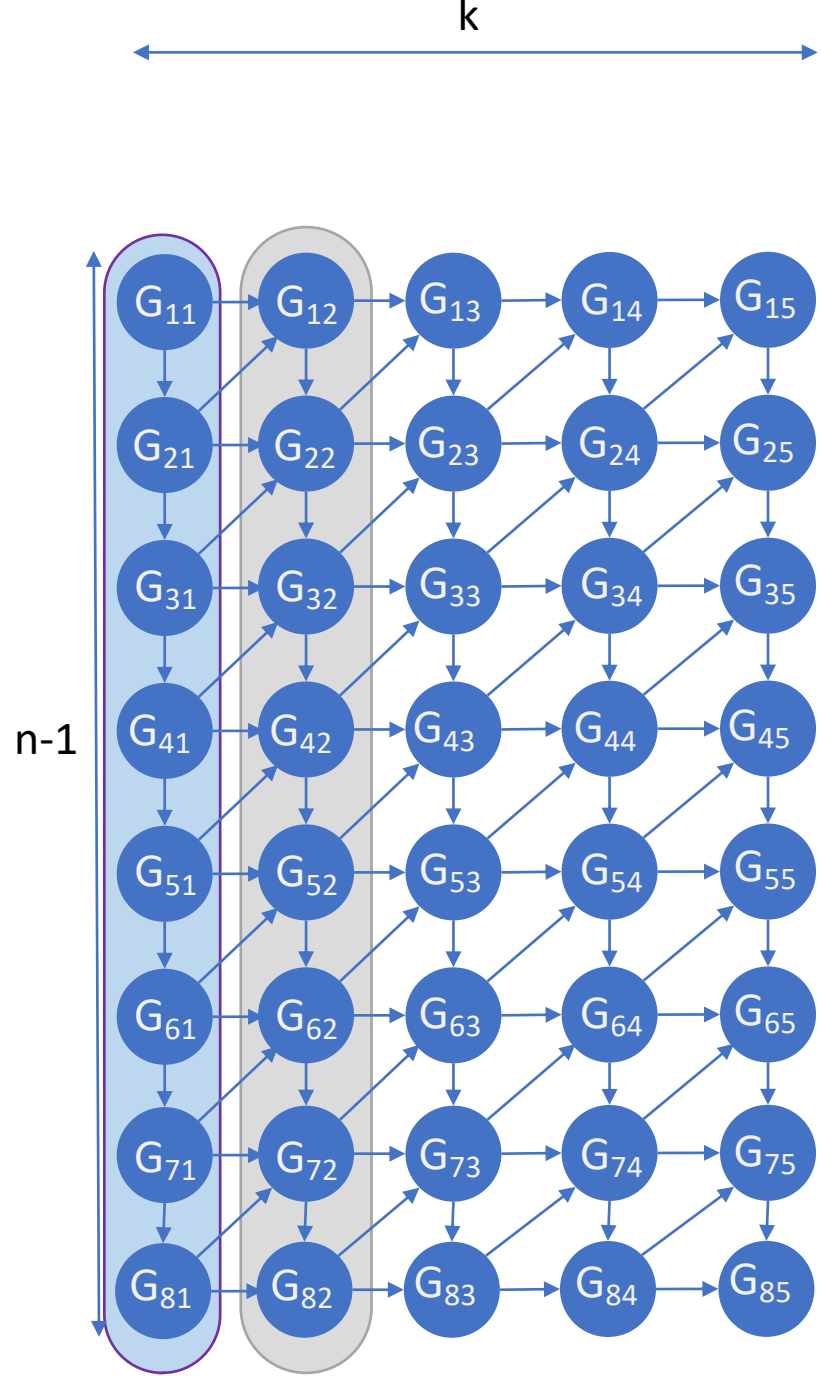
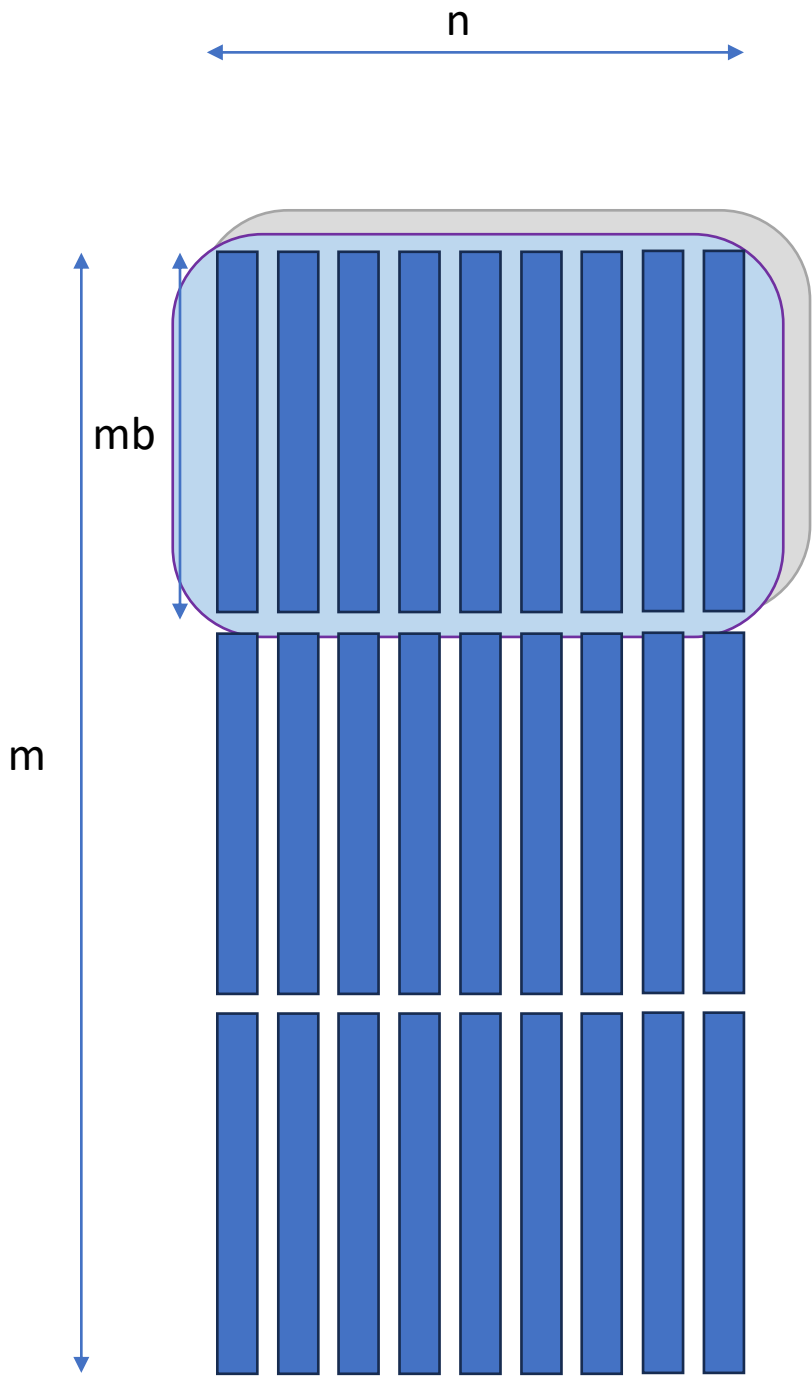
work on columns 6 and 7

work on columns 7 and 8

work on columns 8 and 9



- A waves of five Francis steps
- work on columns 1 and 2
  - work on columns 2 and 3
  - work on columns 3 and 4
  - work on columns 4 and 5
  - work on columns 5 and 6
  - work on columns 6 and 7
  - work on columns 7 and 8
  - work on columns 8 and 9



work on columns 1 and 2

work on columns 2 and 3

work on columns 3 and 4

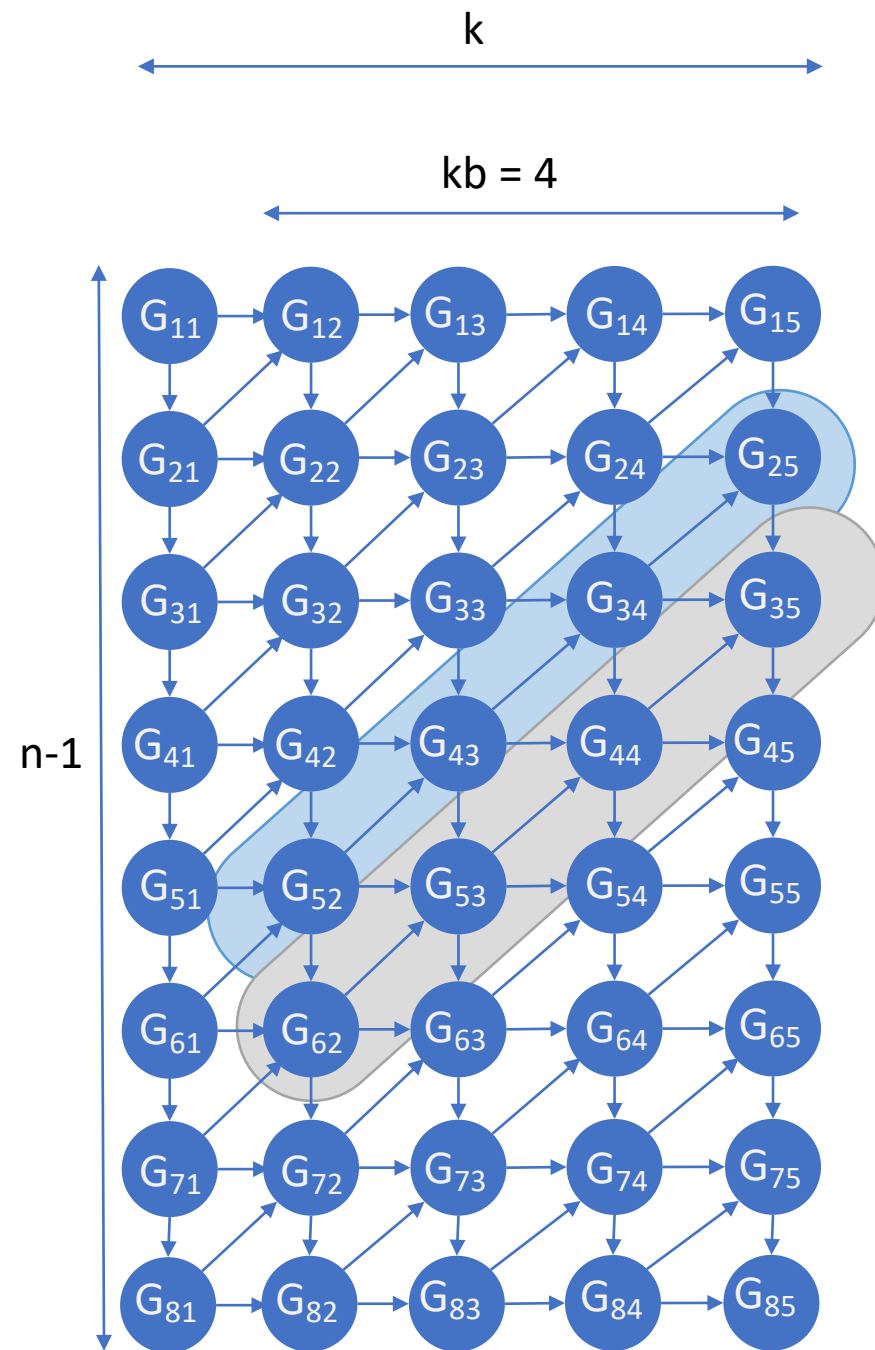
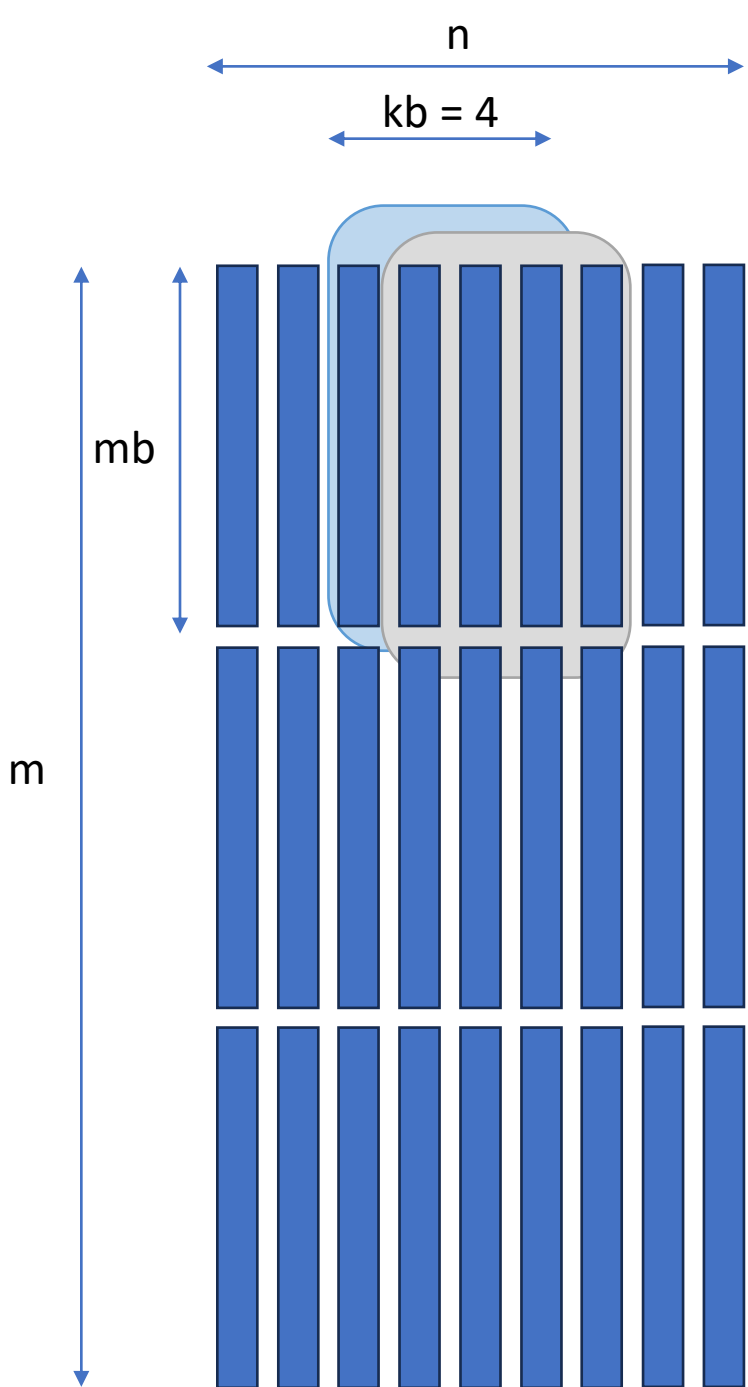
work on columns 4 and 5

work on columns 5 and 6

work on columns 6 and 7

work on columns 7 and 8

work on columns 8 and 9



work on columns 1 and 2

work on columns 2 and 3

work on columns 3 and 4

work on columns 4 and 5

work on columns 5 and 6

work on columns 6 and 7

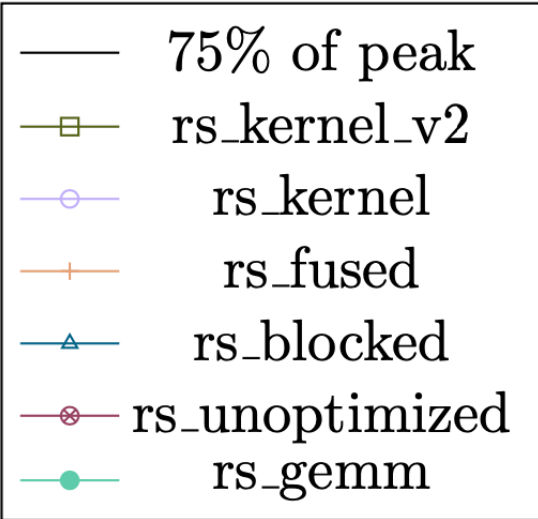
work on columns 7 and 8

work on columns 8 and 9

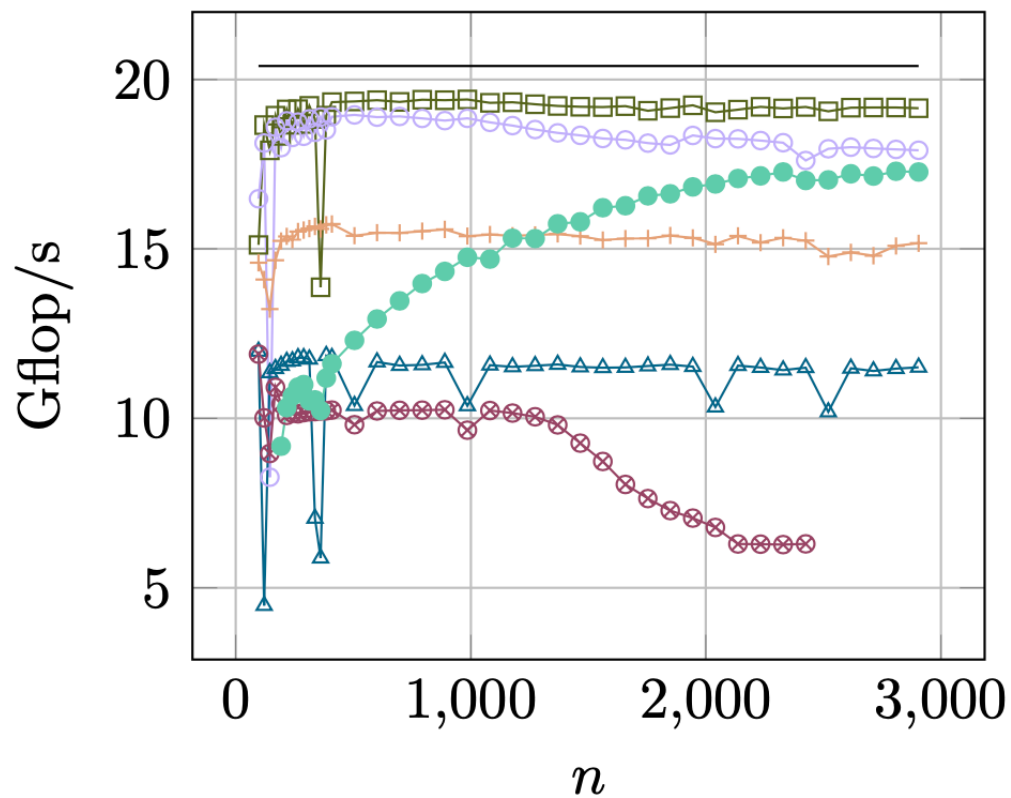
# Analysis

- Going fast.
- We need to apply  $mnk$  Givens rotations.
- We assume that  $k_b * m_b \leq M$
- We move on piece of column of size  $m_b$ , write back one piece of size  $m_b$ , and load  $2k_b$  rotations
- And we will do  $k_b * m_b$  rotations in a segment
- Forgetting start and end clean up code, we need to do  $mnk / m_b / k_b$  segments
- And so the volume of communication of the algorithm is  $( mnk / m_b / k_b ) * ( 2m_b + 2k_b )$
- For  $k_b = \text{sqrt}(M)$  and  $m_b = \text{sqrt}(M)$  we get  $4 mnk / \text{sqrt}( M )$
- Since the total number of operations of our code is  $6mnk$ , this means that the operational intensity for the wavefront algorithm is  **$(3/2) \text{sqrt}\{S\}$**
- IOLB returns  **$6 \text{sqrt}\{S\}$**  as an upper bound for the operational intensity
- So we are a factor of 4 off.

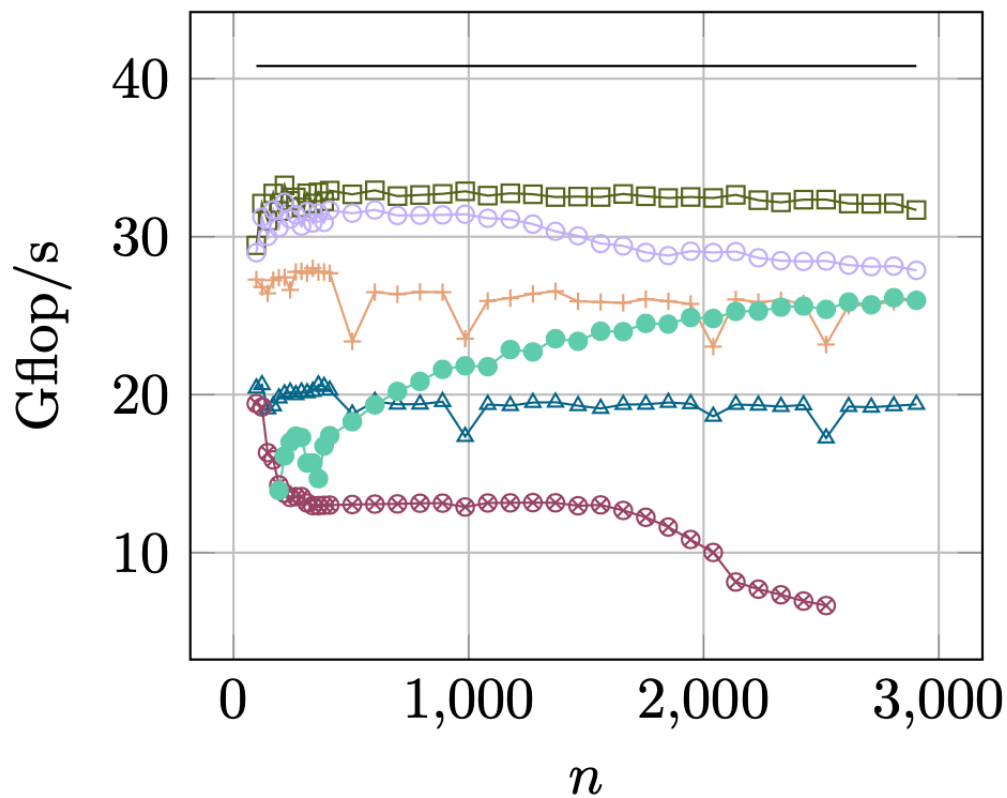
apply\_givens( )  
 $k = 180$ , varying  $n$  and  $m = n$



“fused” is a 2x2 kernel  
 “kernel” is a 16x2 kernel  
 “kernel\_v2” uses packed format for A



(a) Xeon V2 flop rate



(b) Xeon V3 flop rate



### a2v – geqr2 – Householder QR factorization

```

for(k = 0; k < N; k++){
  norma2 = 0.e+00;
  for(i = k+1; i < M; i++){
    norma2 += A[i][k] * A[i][k];
  }
  norma =
  A[k][k]
  tau[k] =
  2. for(k = N-1; k > -1; k--){
    for(j = k+1; j < N; j++){

```

### sytd2 – reduction to symmetric tridiagonal form

```

for(i = 0; i < n-2; i++){
  norma2 = 0.0e+00;
  for ( k = i+2; k < n ; k++ ) {
    norma2 += A[k][i] * A[k][i];
  }
  norma = sqrt( A[
  A[i+1][i] = ( A[

```

### v2q – orqr2 – Construction of Q from Householder

### syrk

```

for ( i = 0; i < n; i++)
  for ( k = 0; k < m; k++)
    for ( j = 0; j <= i; j++)
      C[i][j] += A[i][k] * A[j][k];

```

### gemm

```

for ( i = 0; i < m; i++)
  for ( j = 0; j < n; j++)
    for ( k = 0; k < p; k++)
      C[i][j] += A[i][k] * B[k][j];

```

### geb2 – reduction to bidiagonalization

```

( 1.0e+00 + norma2 / ( A[i+1][i] * A[i+1][i] ) );
for(k = 0; k < N; k++){
  norma2 = 0.e+00;
  for(i = k+1; i < M; i++){
    norma2 += A[i][k] * A[i][k];
  }
  norma = sqrt( A[k][k] * A[k][k] + norma2 );
  A[k][k] = ( A[k][k] > 0 ) ? ( A[k][k] + norma ) : ( A[k][k] -
  tauq[k] = 2.0 / ( 1.0 + norma2 / ( A[k][k] * A[k][k] ) );
  for(i = k+1; i < M; i++){
    A[i][k]

```

### cgs – Classical Gram-Schmidt

```

for ( j = 0; j < N; j++ ) {
  for ( i = 0; i < j; i++ ) {
    R[i][j] = 0.0e+00;
    for ( k = 0; k <

```

### gehd2 – reduction to Hessenk

```

for ( j = 0; j < n-2; j++ ) {
  for ( j = 0; j < n-2; j++ ) {
    tmp = A[
    norma2 = 0.0;
    j+2; i < n; i++ ) {
      += A[i][j] * A[i][j] ;
    }
    rrt ( A[j+1][j] * A[j+1][j] + norma2 )
    = ( A[j+1][j] > 0 ) ? ( A[j+1][j] + no
    / ( 1.0 + norma2 / ( A[j+1][j] * A[j+1]
    j+2; i < n; i++ ) {
      /= A[j+1][j] ;
    }
    = ( A[j+1][j] > 0 ) ? ( - norma ) : (
    +1; i < n; i++ ) {
      = A[j+1][i] ;
      = j+2; k < n; k++ ) {
        tmp[i] += A[k][j] * A[k][i];
      }
    }

```

### mgs – Modified Gram-Schmidt

```

for ( j = 0; j < N; j++ ) {
  for ( i = 0; i < j; i++ ) {
    R[i][j] = 0.0e+00;
    for ( k = 0; k < M; k++ )
      R[i][j] += A[k][i] * A[k][j];
    for ( k = 0; k < M; k++ )
      A[k][j] -= A[k][i] * R[i][j];
  }
  R[j][j] = 0.0e+00;
  for ( k = 0; k < M; k++ )
    R[j][j] += A[k][j] * A[k][j];
  R[j][j] = sqrt(R[j][j]);
  for ( k = 0; k < M; k++ )
    A[k][j] /= R[j][j];
}

```

### apply\_givens\_rot\_sequence

```

for ( p = 0; p < k; p++ ) {
  for ( j = 0; j < n - 1; j++ ) {
    for ( i = 0; i < m; i++ ) {
      temp = C[j][p] * A[i][j] + S[j][p] * A[i][j + 1];
      A[i][j + 1] = -S[j][p] * A[i][j] + C[j][p] * A[i][j + 1];
      A[i][j] = temp;
    }
  }
}

```

### cholesky

```

for ( i = 0; i < n; i++ ) {
  for ( j = 0; j < i; j++ ) {
    for ( k = 0; k < j; k++ ) {
      A[i][j] -= A[i][k] * A[j][k];
    }
    A[i][j] /= A[j][j];
  }
  for ( k = 0; k < i; k++ ) {
    A[i][i] -= A[i][k] * A[i][k];

```

### lu

```

for ( i = 0; i < n; i++ ) {
  for ( j = 0; j < i; j++ ) {
    for ( k = 0; k < j; k++ )
      A[i][j] -= A[i][k] *

```

# The I/O Requirements of Various Numerical Linear Algebra Kernels

Julien Langou

Tuesday June 26<sup>th</sup> 2024