Improving The Memory Performance of Loops And Arrays

Optimizing And Tuning Scientific Codes

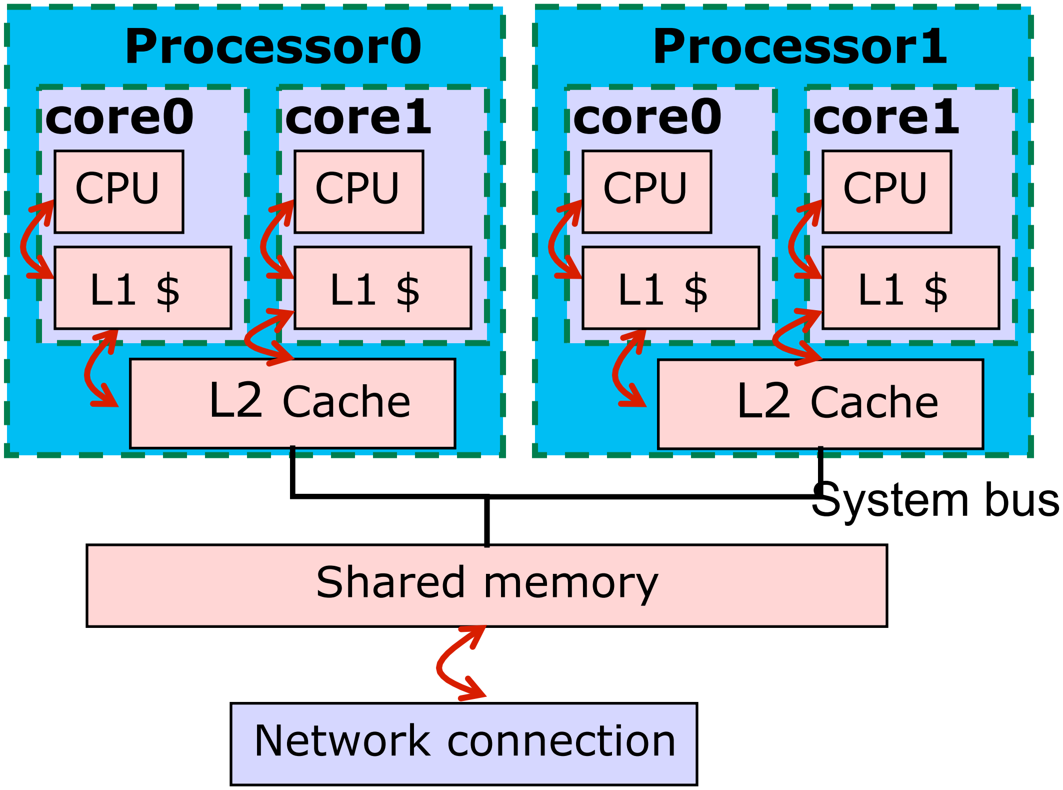
Scientific Computing

- Use high-end computers to solve scientific problems
  - Computation and/or data intensive simulations
- Use loops to operate on multi-dimensional arrays
  - Structured data (regular computation):
    - Locations/offsets of data known before runtime
    - E.g., subscripting arrays via linear combinations of loop index variables
    - Represented by dense matrix and stencil computations
  - Unstructured data (irregular computation):
    - Structure of data unknown until runtime
    - E.g., subscripting arrays via indirect arrays
    - Represented by sparse matrices, trees, and graphs
- Here, we focus on regular scientific computations

Optimizing For Multicore

- Efficient utilization of
  - Single CPU
    - Cache hierarchy
      - Data affinity and locality
    - SIMD Vectorization
  - Concurrent CPU
    - Multi-threading in OpenMP, Pthread, …
    - Shared memory

    Synchronization



Source-level Optimizations

- Automatically applied by compilers to program source
  - Goal: efficient utilization of machine resources
- Reordering of computation and data structures
  - Loop optimizations: reordering of loop evaluation
    - Loop interchange, fusion, blocking, parallelization, unrolling, and unroll&jam
  - Data optimizations: re-organization of data layout
    - Array blocking, scalar replacement
- Reduction of computation cost
  - Prefetching, strength reduction

Reordering Optimizations

- A reordering transformation
  - Changes the ordering of code or data, without adding or deleting any operations.
  - Goal: better utilization of machine resources
- Computation reordering
  - Does not eliminate dependences. Unsafe optimizations may change the relative source and sink of a dependence
- Data reordering
  - It does not change the data, but can change where the data is located
- A computation reordering optimization is safe if it preserves the relative direction of each dependence
- A data reordering optimization is safe if all accesses to each original data item are correctly redirected to the new location

Optimizing Memory Accesses

- Optimizations
  - Reuse data already in cache (locality)
    - Reduce memory bandwidth requirement
  - Prefetch data ahead of time
    - Reduce memory latency requirement
- Two types of cache reuse
  - Temporal reuse
    - After bringing a value into cache, use the same value multiple times
  - Spatial reuse
    - After bringing a value into cache, use its neighboring values in the same cache line
- Cache reuse is limited by
  - cache size, cache line size, cache associativity, replacement policy

```
DO I = 1, M
   DO J = 1, N
      A(I) = A(I) + B(J)
   ENDDO
ENDDO
```

```
DO I = 1, M
   DO J = 1, N
      A(I, J)=A(I,J)+B(I,J)
   ENDDO
ENDDO
```

Optimizing Memory Performance

- Computation optimizations: reordering of instructions
  - Improve temporal and spatial cache reuse
    - **Loop interchange/permutation**
    - **Loop blocking (strip-mining + interchange)**
  - Improve register reuse
    - **Loop unrolling and unroll&jam**
- Data optimizations: rearrange layout of data
  - Static layout transformation
    - A single layout for each variable
  - Dynamic layout transformation
    - Different layout based on variable use
    - **Array blocking and scalar replacement**

Loop Interchange

- A reordering transformation that
  - Changes the nesting order of loops
- Example

```
 DO I = 1, N
   DO J = 1, M
S      A(I,J+1) = A(I,J) + B
    ENDDO
 ENDD
```

- Direction vector: (=, <)

  - After loop interchange

```
 DO J = 1, M
   DO I = 1, N
S      A(I,J+1) = A(I,J) + B
   ENDDO
 ENDDO
```

- Direction vector: (<, =)

  - Leads to

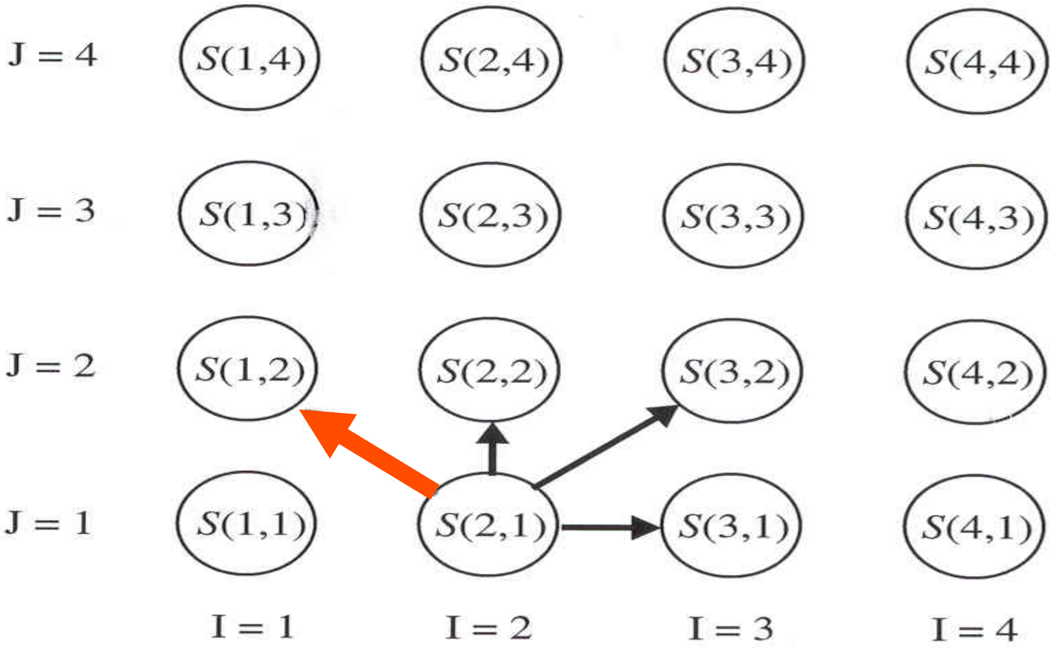
```
DO J = 1, M
S   A(1:N,J+1) = A(1:N,J) + B
ENDDO
```

Safety of Loop Interchange

- Not all loop interchanges are safe

```
DO J = 1, M
  DO I = 1, N
    A(I,J+1) = A(I+1,J) + B
  ENDDO
ENDDO
```

Direction vector: (<, >)



Dependence Direction Matrix

- ***Direction matrix*** of a loop nest contains
  - A row for each dependence direction vector between statements contained in the nest.

```
DO I = 1, N
   DO J = 1, M
      DO K = 1, L
         A(I+1,J+1,K) = A(I,J,K) + A(I,J+1,K+1)
      ENDDO
   ENDDO
ENDDO
```

  - The direction matrix for the loop nest is: $\begin{pmatrix} < & < & = \\ < & = & > \end{pmatrix}$
- A loop permutation is legal if and only if
  - the direction matrix, after the same permutation is applied to its columns, has no dependence with ">" as the leftmost non-"=" direction

Optimization Profitability

- Which loop should be innermost or outermost ?
  - Reduce the number of interfering data accesses between reuse of the same (or neighboring) data
- Approach: attach a cost function when each loop is placed innermost
  - Assuming cache line size is L

```
DO I = 1, N
  DO J = 1, N
     DO K = 1, N
        C(I, J) = C(I, J) + A(I, K) * B(K, J)
     ENDDO
  ENDDO
ENDDO
```

  - Innermost K loop = N*N*N*(1+1/L)+N*N
  - Innermost J loop = 2*N*N*N+N*N
  - Innermost I loop = 2*N*N*N/L+N*N
- Reorder loop from innermost in the order of increasing cost
  - Limited by safety of loop interchange

Loop Blocking

- Goal: separate computation into blocks, where cache can hold the entire data used by each block
- Example

```
DO J = 1, M
   DO I = 1, N
      D(I) = D(I) + B(I,J)
   ENDDO
ENDDO
```

- Assuming N is large, 2*N*M/C cache misses (memory accesses)

- After blocking (**strip-mine-and-interchange)**

```
DO jj = 1, M, T
   DO I = 1, N
      DO J = jj, MIN(jj+T-1, M)
         D(I) = D(I) + B(I, J)
      ENDDO
   ENDDO
ENDDO
```

  - Assuming T is small, (**M/T)*(N/C) + M*N/C** misses

Alternative Ways of Blocking

```
DO jj = 1, M, T
   DO I = 1, N
      DO J = jj, MIN(jj+T-1, M)
         D(I) = D(I) + B(I, J)
      ENDDO
   ENDDO
ENDDO
```

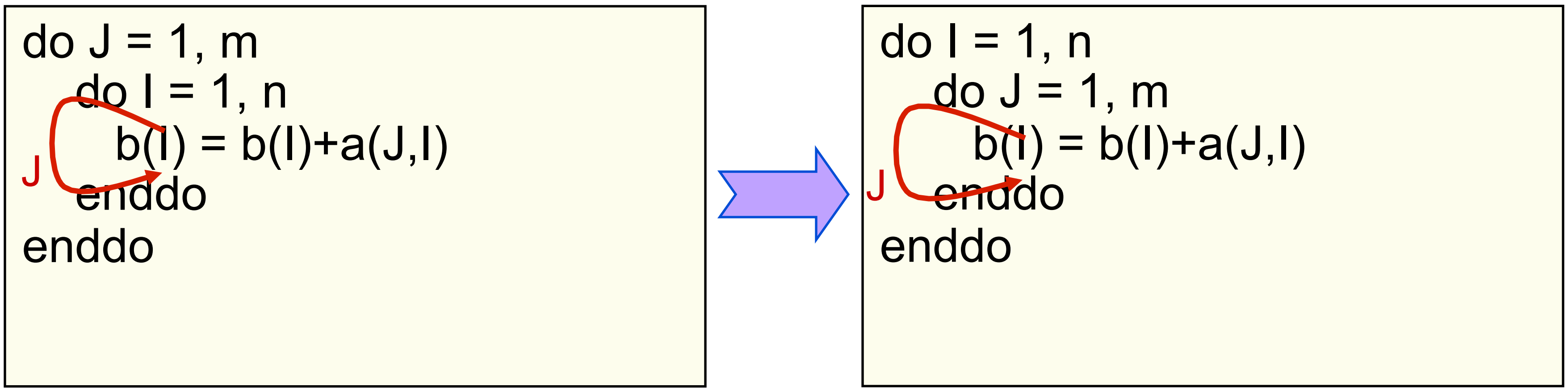
```
DO ii = 1, N, T
   DO J = 1, M
      DO I = ii, MIN(ii+T-1, N)
         D(I) = D(I) + B(I, J)
      ENDDO
   ENDDO
ENDDO
```

```
DO jj = 1, M, Tj
   DO ii = 1, N, Ti
      DO J = jj, MIN(jj+Tj-1,M)
         DO I = ii, MIN(ii+Ti-1, N)
              D(I) = D(I) + B(I, J)
         ENDDO
      ENDDO
   ENDDO
ENDDO
```

The Blocking Transformation

- The transformation takes a group of loops L0,…,Lk
  - Strip-mine each loop Li into two loops Li’ and Li’’
  - Move all strip counting loops L0’,L1’,…,Lk’ to the outside
  - Leave all strip traversing loops L0’’,L1’’,…,L,’’ inside
- Safety of blocking
  - Strip-mining is always legal
  - Loop interchange is not always legal
  - All participating loops must be safe to be moved outside
    - Each loop has only “=“ or “<“ in all dependence vectors
- Profitability of Blocking: can enable cache reuse by an outer loop that
  - Carries small-threshold dependences (including input dep)
  - With loop index (in small stride) enumerating the contiguous dimension of an array and in no other dimension

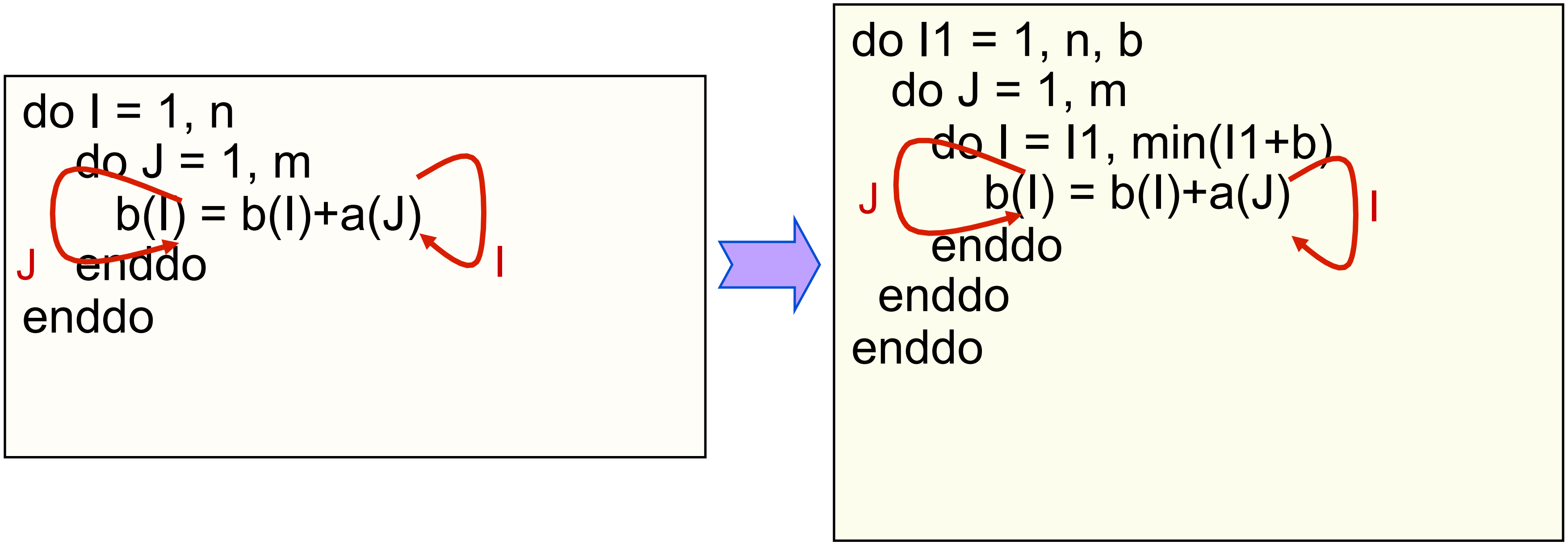
Loop Interchange For Locality



```
do J = 1, m
   do I = 1, n
      b(I) = b(I)+a(J,I)
   enddo
enddo
```

```
do I = 1, n
   do J = 1, m
      b(I) = b(I)+a(J,I)
   enddo
enddo
```

Loop Blocking For Locality



```
do I = 1, n
   do J = 1, m
      b(I) = b(I)+a(J)
   enddo
enddo
```

```
do I1 = 1, n, b
  do J = 1, m
    do I = I1, min(I1+b)
       b(I) = b(I)+a(J)
    enddo
  enddo
enddo
```

Optimizing for Register Usage

- Registers are part of the memory hierarchy
  - Compare to cache, compilers have complete control over what data to put in register
  - Can use registers to hold scalar variables
- Goal: use scalars to replace multiple array references
  - Enable reuse of array references in a single loop body
  - Through loop unrolling and unroll&jam

Loop Unrolling

- An enabling transformation to expose opportunities for other optimizations
    - Reduce the number of branches by a factor 4
    - Provide a bigger basic block (loop body) for local optimization
        - Better instruction scheduling and register allocation
    - Always safe if applied correctly. But must be careful when handling loop bounds do not divide unrolling factors

```
do i = 1 to n by 1
  a(i) = a(i) + b(i)
end
```

Original loop

```
do i = 1 to 100 by 4
  a(i) = a(i) + b(i)
  a(i+1) = a(i+1) + b(i+1)
  a(i+2) = a(i+2) + b(i+2)
  a(i+3) = a(i+3) + b(i+3)
end
```

Unrolled by 4, n = 100

Loop Unroll-and-Jam

```
DO I = 1, N*2
    DO J = 1, M
        A(I) = A(I) + B(J)
    ENDDO
ENDDO
```

- Can we put B(J) into a register and reuse the reference?

```
DO I = 1, N*2, 2
    DO J = 1, M
        A(I) = A(I) + B(J)
        A(I+1) = A(I+1) + B(J)
    ENDDO
ENDDO
```

- Unroll outer loop twice and then fuse the copies of the inner loop
- Now can reuse register for B(J)
- But require one more register for A

- Goal: explore register reuse by outer loops
  - Compare to loop blocking
    - Different iterations of outer loop unrolled
  - Often called register blocking
    - May increase register pressure at the innermost loop
- Transformation: two alternative ways to get the combined result
  - Unroll an outer loop, apply multi-level loop fusion to the unrolled loops
  - Strip-mine outer loop, interchange strip loop inside, then unroll strip loop

Safety of Unroll-and-Jam

```
DO I = 1, N*2
   DO J = 1, M
     A(I+1,J-1)=A(I,J)+B(I,J)
   ENDDO
ENDDO
```

- Apply unroll-and-jam

```
DO I = 1, N*2, 2
   DO J = 1, M
      A(I+1,J-1)=A(I,J)+B(I,J)
      A(I+2,J-1)=A(I+1,J)+B(I+1,J)
   ENDDO
ENDDO
```

- **This is wrong!**

- Direction vector: (<,>)
  - This makes loop interchange illegal
- Unroll-and-Jam is similar to blocking
  - It must be safe to interchange the strip traversing outer loop with the inner loop

Array Copying vs. Scalar Replacement

- Array copying: dynamic layout transformation for arrays
  - Copy arrays into local buffers before computation
  - Copy modified local buffers back to array
- Previous work
  - Lam, Rothberg and Wolf, Temam, Granston and Jalby
    - Copy arrays after loop blocking
  - Optimizing irregular applications
    - Data access patterns not known until runtime
    - Dynamic layout transformation --- through libraries
  - Scalar Replacement
    - Equivalent to copying single array element into scalars
    - Carr and Kennedy: applied to inner loops
- Unify scalar replacement and array copying (Yi LCPC' 05)
  - Improve cache and register locality
  - Automaticly insert copy operations to ensure safety
  - Heuristics to reduce buffer size and copy cost

Scalar Replacement

- Convert array references to scalar variables to improve performance of register allocation

```
DO I = 1, N
   DO J = 1, M
        A(I) = A(I) + B(J)
   ENDDO
ENDDO
```

- **A(I) can be left in a register throughout the inner loop**

```
DO I = 1, N
   T = A(I)
   DO J = 1, M
        T = T + B(J)
   ENDDO
   A(I) = T
ENDDO
```

- **All loads and stores to A in the inner loop have been eliminated**
- **High chance of T being allocated to a register by register allocation**

Unroll-and-Jam + Scalar Repl

```
DO I = 1, N*2, 2
   DO J = 1, M
        A(I) = A(I) + B(J)
        A(I+1) = A(I+1) + B(J)
   ENDDO
ENDDO
```

```
DO I = 1, N*2, 2
   s0 = A(I)
   s1 = A(I+1)
   DO J = 1, M
        t = B(J)
        s0 = s0 + t
        s1 = s1 + t
   ENDDO
   A(I) = s0
   A(I+1) = s1
ENDDO
```

- Reduce the number of memory loads by half

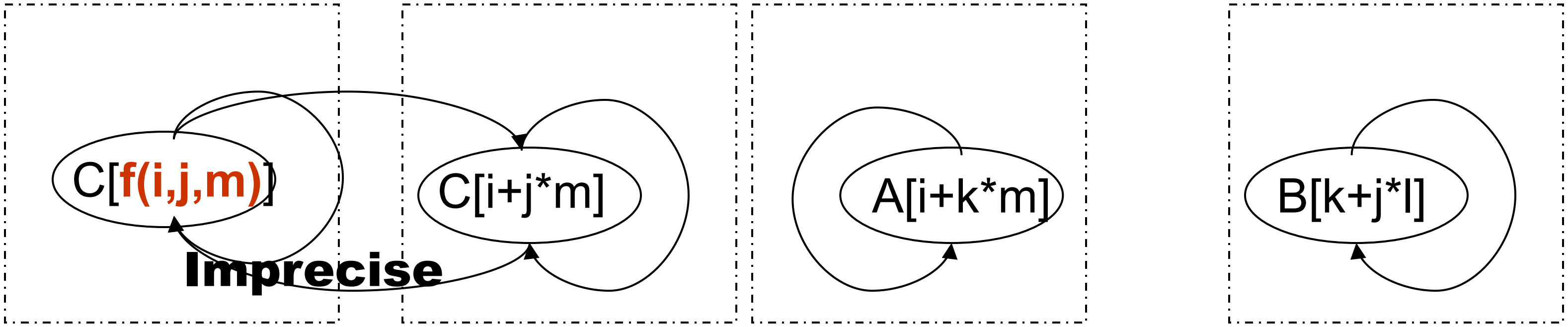
Array Copy: Matrix Multiplication

```
A_buf[0:m*l] = A[0:m,0:l];
for (j=0; j<n; ++j)  {
  C_buf[0:m] = C[0:m, j*m];
  for (k=0; k<l; ++k) {
    B_buf = B[k+j*l];
    for (i=0; i<m; ++i)
       C_buf[i] = C_buf[i] + alpha * A_buf[i+k*m]*B_buf;
  }
  C[0:m,j*m]=C_buf[0:m];
}
```

- Layout of data depends on ordering of their accesses
  - Often applied in sync with blocking

Array Copy: Imprecise Dependences

```
for (j=0; j<n; ++j)
  for (k=0; k<l; ++k)
   for (i=0; i<m; ++i) {
    C[f(i,j,m)]= C[i+j*m] + alpha * A[i+k*m]*B[k+j*l];
```



- Array references connected by imprecise deps
  - Cannot precisely determine a mapping between subscripts
  - Sometimes may refer to the same location, sometimes not
  - Not safe to copy into a single buffer
    - Never attempt to copy them

Profitabilities

- When should we apply scalar replacement?
  - Profitable unless register pressure too high
  - No overhead
- When should we apply array copy?
  - When regular cache conflict misses occur
  - When prefetching of array elements is need
    - 10-40% improvement observed
  - Overhead is 0.5-8% when not beneficial
- How should the different optimizations be combined (composed)?
  - How should each optimization be customized to maximize their collective effectiveness?

Summary

- Common loop optimizations for improving memory performance
  - Transformation, safety and profitability
    - Loop interchange
    - Loop blocking
    - Loop unrolling
    - Loop unroll&jam
    - Scalar replacement
    - Array copying
  - Programmable composition and customization of the optimizations