Transforming Imperfectly Nested Loops

Classes of loop transformations:

- Iteration re-numbering: (eg) loop interchange

  Example

```
DO 10 J = 1,100                  DO 10 I = 1,100
  DO 10 I = 1,100         vs      DO 10 J = 1,100
    Y(I) = Y(I)+A(I,J)*X(J)         Y(I) = Y(I) + A(I,J)*X(J)
10  Z(I) = ....                  10 Z(I) = ....
```

  All statements in body affected identically.

- Statement re-ordering: (eg) loop distribution/jamming

  Example

```
DO 10 I = 1,100                  DO 10 I = 1,100
     Y(I) = ....                   10 Y(I) = ...
 10  Z(I) = ...Y(I)...   vs.     DO 20 J = 1,100
                                   20 Z(I) = ...Y(I)..
```

  Statement re-ordering can be static or dynamic

- Statement transformation:

Example: scalar expansion

```
DO 10 I = 1,100                        DO 10 I = 1,100
  T = f(I)                vs             T[I] = f(I)
10 X(I,J) = T*T                        10 X(I,J) = T[I]*T[I]
```

Statements themselves are altered.

Iteration renumbering transformations

We have already studied linear loop transformations.

Index set splitting: $N \rightarrow N1 + N2$

```
DO 10 I = 1, N               DO 10 I = 1, N1
10   S                       10   S
                       vs
                             DO 20 I = N1+1, N
                             10   S
```

Special case: loop peeling - only the first/last/both first and last iterations are done separately from main loop.

Legality: always legal

Typical use: Eliminate a 'problem iteration'

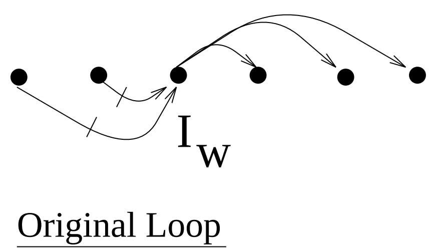
```
DO 10 I = 1, N
10 X(aI + b) = X(c) + ....   vs
```

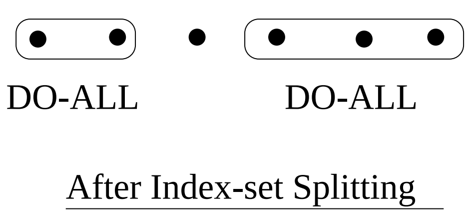
Weak SIV subscript: dependence equation is $aI_w + b = c$

$$\Rightarrow I_w = (c - b)/a$$

Split index set of loop into 3 parts:

- DO-ALL loop that does all iterations before I_w
- Iteration I_w by itself
- DO-ALL loop that does all iterations after I_w

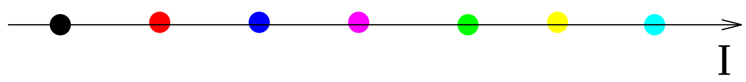




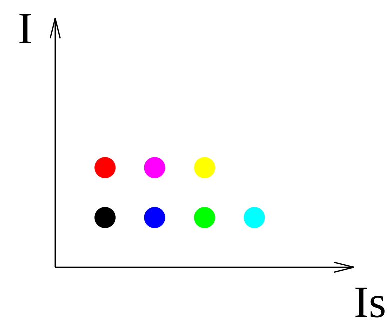
Note: distance/direction are not adequate abstractions

Strip-mining: $N = N1 * N2$

```
DO 10 I = 1, N                 DO 10 Is = 1, N, s
10 Y(I) = X(I)+1   =>            DO 10 I = Is, min(Is + s - 1, N)
                                 10  Y(I) = X(I) + 1
```



Original Loop



Stripmined Loop: strip size = 2

Inner loop does ‘s’ iterations at a time.

Important transformation for vector machines:

‘s’ = vector register length

Strip-mining is always legal.

To get clean bounds for inner loop, do last ‘N mod s’ iterations separately: index-set splitting

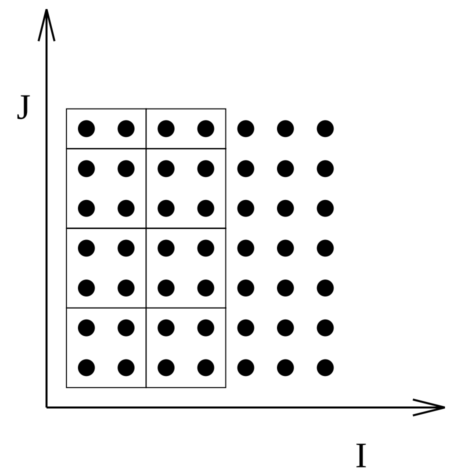
```
DO 10 Is = 1, N, s
  DO 10 I = Is, min(Is + s - 1, N)
  10  Y(I) = X(I) + 1


   =>


DO 10 Is = 1, s*(N div s)
 DO 10 I = Is, Is + s - 1
 10 Y(I) = X(I) + 1

DO 20 I = (N div s)*s + 1 to N
   20 Y(I) = X(I) + 1
```

Tiling: multi-dimensional strip-mining $N1XN2 = t1 * t2 * N3 * N4$




```
DO  I = ...                DO Ti = ...
  DO J = ...         =>      DO Tj = ...
    S                           DO I = ...
                                  DO J = ...
                                   S
```

Old names for tiling: stripmine and interchange, loop quantization

Statement Sinking: useful for converting some imperfectly-nested loops into perfectly-nested ones

```
do k = 1, N
  A(k,k) = sqrt (A(k,k))
  do i = k+1, N
    A(i,k) = A(i,k) / A(k,k) <---- sink into inner loop
    do j = k+1, i
      A(i,j) -= A(i,k) * A(j,k)
```

```
=>
```

```
do k = 1, N
  A(k,k) = sqrt (A(k,k))
  do i = k+1, N
    do j = k, i
      if (j==k) A(i,k) = A(i,k) / A(k,k)
      if (j!=k) A(i,j) -= A(i,k) * A(j,k)
```

Basic idea of statement sinking:

1. Execute a pre/post-iteration of loop in which only sunk statement is executed.
2. Requires insertion of guards for all statements in new loop.

Singly-nested loop (SNL): imperfectly-nested loop in which each loop has only one other loop nested immediately within it.

Locality enhancement of SNL's in MIPSPro compiler:

- convert to perfectly-nested loop by statement sinking,
- locality-enhance perfectly-nested loop, and
- convert back to imperfectly-nested loop in code generation.

Statement Reordering Transformations

loop jamming/fusion <=> loop distribution/fission

Example

```
DO 10 I = 1,100                     DO 10 I = 1,100
     Y(I) = ....                      10 Y(I) = ...
 10  Z(I) = ...Y(I)...    vs.       DO 20 J = 1,100
                                      20 Z(I) = ...Y(I)..
```

Utility of distribution: Can produce parallel loops as below

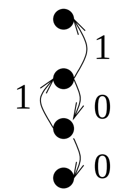
```
DO 10 I = 1, 100                   DOALL 10 I = 1,100
    Y(I) = ....             vs.    10 Y(I) = ....
10  Z(I) = Y(I-1)....              DOALL 20 I' = 1,100
                                   20 Z(I') = Y(I'-1) .....
```

Loop fusion: promote reuse, eliminate array temporaries

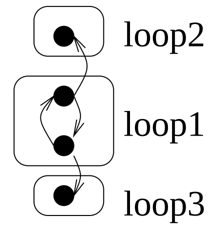
Legality of loop fission: build the statement dependence graph

```
DO I = 1,N
  A(I) = A(I) + B(I-1)
  B(I)  = C(I-1)*X + 1
  C(I)  = 1/B(I)
  D(I)  = sqrt(C(I))
```

Program



Statement Dependence Graph



Acyclic Condensate

```
DO I = 1,N
 B(I) = C(I-1)*X  +1
 C(I) = 1/B(I)
DO I = 1,N
 A(I) = A(I)+B(I-1)
DO I = 1,N
 D(I) = sqrt(C(I))
```

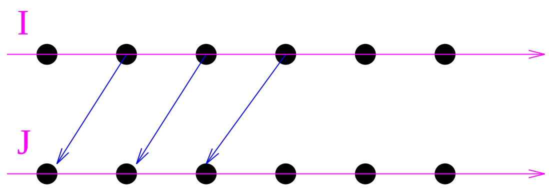
New Code

- Build the statement dependence graph:
  - nodes: assignment statements/if-then-else's
  - edges: dependences between statements (distance/direction is irrelevant)
- Find the acyclic condensate of statement dependence graph
- Each node in acyclic condensate can become one loop nest
- Order of new loop nests: any topological sort of condensate
- Nested loop fission: do in inside-out order, treating inner loop nests as black boxes

Legality of loop fusion:

```
DO   I = 1,N
  X(I) = .....

DO J = 1,N
  Y(J) = X(J+1) ....
```



illegal

```
DO  I = 1,N
  X(I) = ....
  Y(I) = X(I+1) ....
```

Usually, we do not compute dependences across different loop nests.

Easy to compute though:

Flow dependence: test for fusion preventing dependence

$$\begin{aligned} Iw &= Jr + 1 \\ Jr &< Iw \\ 1 \leq\ & Iw \leq N \\ 1 \leq\ & Jr \leq N \end{aligned}$$

Loop fusion is legal if
(i) loop bounds are identical
(ii) loops are adjacent
(iii) no fusion-preventing dependence

Statement transformation:

Example: scalar expansion

```
DO 10 I = 1,100                    DO 10 I = 1,100
  T = f(I)            vs             T[I] = f(I)
10 X(I,J) = T*T                    10 X(I,J) = T[I]*T[I]
```

Anti- and output-dependences (*resource dependences*)arise from "storage reuse" in imperative languages (cf. functional languages).

Eliminating resource dependences: eliminate storage reuse.

Standard transformations: scalar/array expansion (shown above)

We got into perfectly-nested loop transformations by studying the effect of interchange and tiling on key kernels like matrix-vector product and matrix-matrix multiplication.

Let us study how imperfectly-nested loop transformations can be applied to other key routines to get a feel for the issues in applying these transformations.

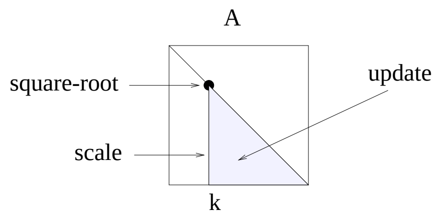
Cholesky factorization from a numerical analyst's viewpoint:

- used to solve a system of linear equations $Ax = b$
- A must be symmetric positive-definite
- compute L such that $L * L^T = A$, overwriting lower-triangular part of A with L
- obtain x be solving two triangular systems

Cholesky factorization from a compiler writer's viewpoint:

- Cholesky factorization has 6 loops like MMM, but loops are imperfectly-nested.
- All 6 permutations of these loops are legal.
- Variations of these 6 basic versions can be generated by transformations like loop distribution.

Column Cholesky: kij, right-looking versions




```
do k = 1, N
  A(k,k) = sqrt (A(k,k))  //square root statement
  do i = k+1, N
    A(i,k) = A(i,k) / A(k,k) //scale statement
  do i = k+1, N
    do j = k+1, i
      A(i,j) -= A(i,k) * A(j,k) //update statement
```

- Three assignment statements are called square root, scale and update statements.
- Compute columns of L column-by-column (indexed by `k`).
- Eagerly update portion of matrix to right of current column.
- Note: most data references and computations in update.

Interchanging i and j loops in `kij` version gives `kji` version.

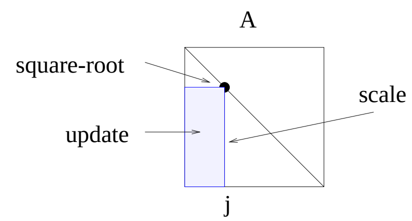
Update is performed row by row.

```
do k = 1, N
  A(k,k) = sqrt (A(k,k))
do i = k+1, N
  A(i,k) = A(i,k) / A(k,k)
do j = k+1, N
  do i = j, N
    A(i,j) -= A(i,k) * A(j,k)
```

Fusion of the two `i` loops in `kij` version produces a SNL.

```
do k = 1, N
  A(k,k) = sqrt (A(k,k))
  do i = k+1, N
    A(i,k) = A(i,k) / A(k,k)
    do j = k+1, i
      A(i,j) -= A(i,k) * A(j,k)
```

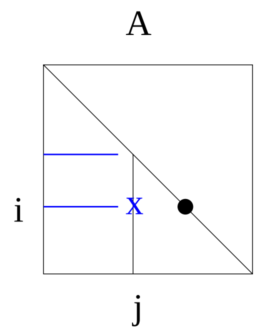
Column Cholesky: jik left-looking versions




```
do j = 1, N
  do i = j, N    //interchange i and k loops for jki version
    do k = 1, j-1
      A(i,j) -= A(i,k) * A(j,k)
  A(j,j) = sqrt (A(j,j))
  do i = j+1, N
    A(i,j) = A(i,j) / A(j,j)
```

- Compute columns of L column-by-column.
- Updates to column are done lazily, not eagerly.
- To compute column `j`, portion of matrix to left of column is used to update current column.

Row Cholesky versions



for each element in row i

- find inner-product of two blue vectors
- update element x
- scale
- take square-root at end

These compute the matrix L row by row. Here is `ijk`-version of row Cholesky.

```
do i = 1, N
  do j = 1, i
    do k = 1, j-1
       A(i,j) -= A(i,k) * A(j,k)
    if (j < i) A(i,j) = A(i,j)/A(j,j)
    else       A(i,i) = sqrt (A(i,i))
```

Locality enhancement in Cholesky factorization

- Most of data accesses are in update step.
- Ideal situation: distribute loops to isolate update and tile update loops.
- Unfortunately, loop distribution is not legal because it requires delaying all the updates till the end.

```
do k = 1, N
  A(k,k) = sqrt (A(k,k))  //square root statement
  do i = k+1, N
    A(i,k) = A(i,k) / A(k,k) //scale statement
  do i = k+1, N
    do j = k+1, i
      A(i,j) -= A(i,k) * A(j,k) //update statement
```

=> loop distribution (illegal because of dependences)

```
do k = 1, N
  A(k,k) = sqrt (A(k,k))  //square root statement
  do i = k+1, N
    A(i,k) = A(i,k) / A(k,k) //scale statement
do k = 1, N
  do i = k+1, N
    do j = k+1, i
      A(i,j) -= A(i,k) * A(j,k) //update statement
```

After distribution, we could have tiled update statement, and obtained great performance....

```
do k = 1, N
  do i = k+1, N
    do j = k+1, i
      A(i,j) -= A(i,k) * A(j,k) //update statement
```

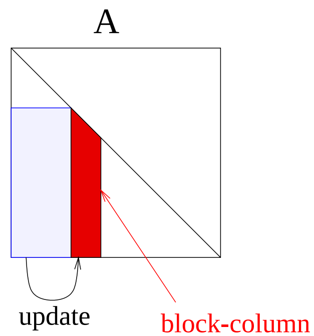
Dependence vectors:

```
(A(i,j) -> A(i,j)):    (+,0,0)
(A(i,j) -> A(i,k)):    (+,0,+)
(A(i,j) -> A(j,k)):    (+,0+,+)
```

Let us study two distinct approaches to locality enhancement of Cholesky factorization:

- transformations to extract MMM computations hidden within Cholesky factorization: improvement of BLAS-3 content
- transformations to permit tiling of imperfectly-nested code

Key idea used in LAPACK library: "partial" distribution



- do processing on block-columns
- do updates to block-columns lazily
- processing of a block-column:
  1. apply all delayed updates to current block-column
  2. perform square root, scale and local update steps on current block column
- Key point: applying delayed updates to current block-column can be performed by calling BLAS-3 matrix-matrix multiplication.

How do we think about this in terms of loop transformations?

Intermediate representation of Cholesky factorization

Perfectly-nested loop that performs Cholesky factorization:

```
do k = 1, N
  do i = k, N
    do j = k, i
      if (i == k && j == k) A(k,k) = sqrt (A(k,k));
      if (i <  k && j == k) A(i,k) = A(i,k) / A(k,k);
      if (i >  k && j >  k) A(i,j) -= A(i,k) * A(j,k);
```

Easy to show that

- loop nest is fully permutable, and
- guards are mutually exclusive, so order of statement is irrelevant.

Generating intermediate form of Cholesky:

Converting kij-Fused version: only requires code sinking.

Converting kji version:

- interchange i and j loops to get kij version,
- apply loop fusion to i loops to get SNL, and
- use code sinking.

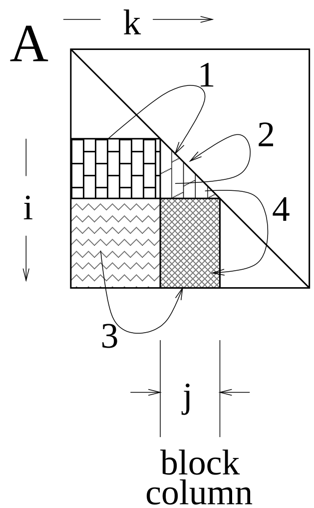
Converting other versions: much more challenging....

Convenient to express loop bounds of fully permutable perfectly nested loop in the following form:

```
do {i,j,k} in 1 <= k <= j <= i <= N

  if (i == k && j == k) A(k,k) = sqrt (A(k,k));
  if (i >  k && j == k) A(i,k) = A(i,k) / A(k,k);
  if (i >  k && j  > k) A(i,j) -= A(i,k) * A(j,k);
```

LAPACK-style blocking of intermediate form



Computation 1: MMM
Computation 2: unblocked Cholesky
Computation 3: MMM
Computation 4: Triangular solve

Two levels of blocking:

1. convert to block-column computations to expose BLAS-3 computations
2. use handwritten codes to execute the BLAS-3 kernels

(1) Stripmine the j loop into blocks of size B:

```
do js = 0, N/B -1  //js enumerates block columns
  do j = B*js +1, B*js+B
    do {i,k} in 1 <= k <= j <= i <= N

     if (i == k && j == k) A(k,k) = sqrt (A(k,k));
     if (i >  k && j == k) A(i,k) = A(i,k) / A(k,k);
     if (i >  k && j  > k) A(i,j) -= A(i,k) * A(j,k);
```

(2) Interchange the j loop into the innermost position:

```
do js = 0, N/B -1
  do i = B*js +1, N
    do k = 1, min(i,B*js+B)
      do j = max(B*js +1,k), min(i,B*js+B)
         if (i == k && j == k) A(k,k) = sqrt (A(k,k));
         if (i >  k && j == k) A(i,k) = A(i,k) / A(k,k);
         if (i >  k && j  > k) A(i,j) -= A(i,k) * A(j,k);
```

(3) Index-set split i loop into B*js +1:B*js +B and B*js +B+1:N.

(4) Index-set split k loop into 1:B*js and B*js +1:min(i,B*js+B).

```
do js = 0, N/B -1

   //Computation 1: an MMM
   do i= B*js +1, B*js +B
      do k = 1,B*js
         do j = B*js +1,i
              A(i,j) -= A(i,k) * A(j,k);

    //Computation 2: a small Cholesky factorization
   do i = B*js +1,B*js +B
      do k = B*js+1,i
         do j = k,i
              if (i == k && j == k) A(k,k) = sqrt (A(k,k));
              if (i >  k && j == k) A(i,k) = A(i,k) / A(k,k);
              if (i >  k && j  > k) A(i,j) -= A(i,k) * A(j,k);
```

```
//Computation 3: an MMM
do i = B*js+ B+1,N
   do k = 1,B*js
      do j = B*js+1,B*js+B
          A(i,j) -= A(i,k) * A(j,k);

//Computation 4: a triangular solve
do i = B*js+ B+1,N
   do k = B*js+1,B*js+B
      do j = k,B*js+B
         if (j == k) A(i,k) = A(i,k) / A(k,k);
         if (j  > k) A(i,j) -= A(i,k) * A(j,k);
```

Observations on code:

- Computations 1 and 3 are MMM. Call BLAS-3 kernel to execute them.
- Computation 4 is a block triangular-solve. Call BLAS-3 kernel to execute it.
- Only unblocked computations are in the small Cholesky factorization.

Critique of this development from compiler perspective:

- How does a compiler where BLAS-3 computations are hiding in complex codes?
- How do we recognize BLAS-3 operations when we expose them?
- How does a compiler synthesize such a complex sequence of transformations?

Compiler approach:

Tile the fully-permutable intermediate form of Cholesky:

```
do {is,js,ks}   0 <= ks <= js <= is <= N/B -1

  do {i,j,k}    B*is < i <= B*is + B
                B*js < j <= B*js + B
                B*ks < k <= B*ks + B

    if (i == k && j == k) A(k,k) = sqrt (A(k,k));
    if (i >  k && j == k) A(i,k) = A(i,k) / A(k,k);
    if (i >  k && j  > k) A(i,j) -= A(i,k) * A(j,k);
```

- Loop nest is,js,ks is fully permutable, as is i,j,k loop nest.
- Choose k,j,i order to get good spatial locality.

Strategy for locality-enhancement of imperfectly-nested loops:

1. Convert an imperfectly-nested loop into a perfectly-nested intermediate form with guards by code sinking/fusion/etc.
2. Transform intermediate form as before to enhance locality.
3. Convert resulting perfectly-nested loop with guards back into imperfectly-nested loop by index-set splitting/peeling.

How do we make all this work smoothly?