High-Performance Computing

COMP 40370

Alexey Lastovetsky

(B2.06, alexey.lastovetsky@ucd.ie)

Array Libraries

Array Libraries

- Function extensions of C and Fortran 77 with array or vector libraries
 - The libraries are supposed to be optimised for each particular computer
 - Regular compilers can be used => no need in dedicated optimising compilers
- One of the most well-known and well-designed array libraries is the Basic Linear Algebra Subprograms (BLAS)
 - Provides basic array operations for numerical linear algebra
 - Available for most modern VP and SP computers

BLAS

- All BLAS routines are divided into 3 main categories:
 - Level 1 BLAS addresses scalar and vector operations
 - Level 2 BLAS addresses matrix-vector operations
 - Level 3 BLAS addresses matrix-matrix operations
- Routines of Level 1 do
 - vector reduction operations
 - vector rotation operations
 - element-wise and combined vector operations
 - data movement with vectors

Level 1 BLAS

- A vector reduction operation
 - The addition of the scaled dot product of two real vectors X and Y into a scaled scalar I'

$$r \leftarrow \beta r + \alpha x^T y = \beta r + \alpha \sum_{i=0}^{n-1} x_i y_i$$

The C interface of the routine implementing the operation is

```
void BLAS_ddot(
   enum blas_conj_type conj, int n, double alpha,
   const double *x, int incx, double beta,
   const double *y, int incy, double *r);
```

- Other routines doing reduction operations
 - Compute different vector norms of vector x
 - Compute the sum of the entries of vector x
 - Find the smallest or biggest component of vector x
 - Compute the sum of squares of the entries of vector x
- Routines doing rotation operations
 - Generate Givens plane rotation
 - Generate Jacobi rotation
 - Generate Householder transformation

- An element-wise vector operation
 - The scaled addition of two real vectors x and y

$$w \leftarrow \alpha x + \beta y$$

The C interface of the routine implementing the operation is

```
void BLAS_dwaxpby(
    int n, double alpha, const double *x, int incx,
    double beta, const double *y, int incy,
    double *w, int incw );
```

 Function BLAS_cwaxpby does the same operation but on complex vectors

- Other routines doing element-wise operations
 - Scale the entries of a vector x by the real scalar 1/a
 - Scale a vector x by a and a vector y by b, add these two vectors to one another and store the result in the vector y
 - Combine a scaled vector accumulation and a dot product
 - Apply a plane rotation to vectors x and y

- An example of data movement with vectors
 - The interchange of real vectors X and Y
- The C interface of the routine implementing the operation is

 Function BLAS_cswap does the same operation but on complex vectors

- Other routines doing data movement with vectors
 - Copy vector x into vector y
 - Sort the entries of real vector x in increasing or decreasing order and overwrite this vector x with the sorted vector as well as compute the corresponding permutation vector p
 - Scale the entries of a vector x by the real scalar 1/a
 - Permute the entries of vector x according to permutation vector p

Level 2 BLAS

- Routines of Level 2
 - Compute different matrix vector products
 - Do addition of scaled matrix vector products
 - Compute multiple matrix vector products
 - Solve triangular equations
 - Perform rank one and rank two updates
 - Some operations use symmetric or triangular matrices

- To store matrices, the following schemes are used
 - Conventional column-based and row-based storage
 - Packed storage for symmetric or triangular matrices
 - Band storage for band matrices
- Conventional storage
 - An nxn matrix A is stored in a one-dimensional array a
 - a_{ij} => a[i+j*s] (C, column-wise storage)
 - $a_{ij} \Rightarrow a[j+i*s]$ (C, row-wise storage)
 - If s=n, rows (columns) will be contiguous in memory
 - If s>n, there will be a gap of (s-n) memory elements between two successive rows (columns)
 - Only significant elements of symmetric/triangular matrices need be set

Packed Storage

- Packed storage
 - The relevant triangle of a symmetric/triangular matrix is packed by columns or rows in a one-dimensional array
 - The upper triangle of an nxn matrix A may be stored in a onedimensional array a
 - $a_{ij}(i \le j) = a[j+i*(2*n-i-1)/2]$ (C, row-wise storage)
- Example.

$$\begin{pmatrix} a_{00} & a_{01} & a_{02} \\ 0 & a_{11} & a_{12} \\ 0 & 0 & a_{22} \end{pmatrix} \implies a_{00} \quad a_{01} \quad a_{02} \quad a_{11} \quad a_{12} \quad a_{22}$$

Band Storage

- Band storage
 - A compact storage scheme for band matrices
- Consider a band storage scheme
 - An mxn band matrix A with I subdiagonals and u superdiagonals may be stored in a 2-dimensional array A with I+u+1 rows and I columns
 - Columns of matrix A are stored in corresponding columns of array A
 - Diagonals of matrix A are stored in rows of array A
 - $a_{ii} \Rightarrow A(u+i-j,j)$ for $max(0,j-u) \le i \le min(m-1,j+l)$
- Example.

$$\begin{pmatrix} a_{00} & a_{01} & 0 & 0 & 0 \\ a_{10} & a_{11} & a_{12} & 0 & 0 \\ a_{20} & a_{21} & a_{22} & a_{23} & 0 \\ 0 & a_{31} & a_{32} & a_{33} & a_{34} \\ 0 & 0 & a_{42} & a_{43} & a_{44} \end{pmatrix} = > \begin{array}{c} * & a_{01} & a_{12} & a_{23} & a_{34} \\ * & a_{00} & a_{11} & a_{22} & a_{33} & a_{44} \\ * & a_{10} & a_{21} & a_{32} & a_{43} & * \\ * & a_{20} & a_{31} & a_{42} & * & * \end{array}$$

- An example of matrix vector multiplication operation
 - The scaled addition of a real n-length vector y, and the product of a general real mxn matrix A and a real n-length vector x

$$y \leftarrow \alpha Ax + \beta y$$

The C interface of the routine implementing this operation is

Parameters

```
order => blas_rowmajor or blas_colmajor
trans => blas_no_trans (do not transpose A)
```

 If matrix A is a general band matrix with I subdiagonals and u superdiagonals, the function

better uses the memory. It assumes that a *band storage* scheme is used to store matrix *A*.

Other routines of Level 2 perform the following operations

$$y \leftarrow \alpha Ax + \beta y$$
 where $A = A^T$
 $x \leftarrow \alpha Ax$ or $x \leftarrow \alpha A^T x$ where A is triangular
 $y \leftarrow \alpha Ax + \beta Bx$
 $x \leftarrow \beta A^T y$, $w \leftarrow \alpha Ax$
 $x \leftarrow A^T y$, $w \leftarrow Az$ where A is triangular

as well as many others

 For any matrix-vector operation with a specific matrix operand (triangular, symmetric, banded, etc.), there is a routine for each storage scheme that can be used to store the operand

Level 3 BLAS

- Routines of Level 3 do
 - O(n²) matrix operations
 - norms, diagonal scaling, scaled accumulation and addition
 - different storage schemes to store matrix operands are supported
 - O(n³) matrix-matrix operations
 - multiplication, solving matrix equations, symmetric rank k and 2k updates
 - Data movement with matrices

- An example of O(n2) matrix operation, which scales two real mxn matrices A and B and stores their sum in a matrix C, is $C \leftarrow \alpha A + \beta B$
- The C interface of the routine implementing this operation under assumption that the matrices A, B and C are of the general form, is

 There are other 15 routines performing this operation for different types and forms of the matrices A, B and C

• An example of $O(n^3)$ matrix-matrix operation involving a real mxn matrix A, a real nxk matrix B, and a real mxk matrix C is

$$C \leftarrow \alpha AB + \beta C$$

 The C routine implementing the operation for matrices A, B and C in the general form is

- Data movement with matrices includes
 - Copying matrix A or its transpose with storing the result in matrix B

$$B \leftarrow A$$
 or $B \leftarrow A^T$

Transposition of a square matrix A with the result overwriting matrix A

$$A \leftarrow A^T$$

Permutation of the rows or columns of matrix A by a permutation matrix P

$$A \leftarrow PA$$
 or $A \leftarrow AP$

 Different types and forms of matrix operands as well as different storage schemes are supported

Sparse BLAS

- Sparse BLAS
 - Provides routines for unstructured sparse matrices
 - Poorer functionality compared to Dense and Banded BLAS
 - only some basic array operations used in solving large sparse linear equations using iterative techniques
 - matrix multiply, triangular solve, sparse vector update, dot product, gather/scatter
 - Does not specify methods to store a sparse matrix
 - storage format is dependent on the algorithm, the original sparsity pattern, the format in which the data already exists, etc.
 - sparse matrix arguments are a placeholder, or *handle*, which refers to an abstract representation of a matrix, not the actual data components

Sparse BLAS (ctd)

- Several routines provided to create sparse matrices
 - The internal representation is implementation dependent
 - Sparse BLAS applications are independent of the matrix storage scheme, relying on the scheme provided by each implementation
- A typical Sparse BLAS application
 - Creates an internal sparse matrix representation and returns its handle
 - Uses the handle as a parameter in computational Sparse BLAS routines
 - Calls a cleanup routine to free resourses associated with the handle, when the matrix is no longer needed

Example

 Example. Consider a C program using Sparse BLAS performing the matrix-vector operation $y \leftarrow Ax$, where

$$A = \begin{pmatrix} 1.1 & 0 & 0 & 0 \\ 0 & 2.2 & 0 & 2.4 \\ 0 & 0 & 3.3 & 0 \\ 4.1 & 0 & 0 & 4.4 \end{pmatrix} \qquad x = \begin{pmatrix} 1.0 \\ 1.0 \\ 1.0 \\ 1.0 \end{pmatrix}$$

$$x = \begin{pmatrix} 1.0 \\ 1.0 \\ 1.0 \\ 1.0 \end{pmatrix}$$

Example (ctd)

```
#include <blas sparse.h>
int main() {
  const int n = 4, nonzeros = 6;
  double values[] = {1.1, 2.2, 2.4, 3.3, 4.1, 4.4};
  int index_i[] = {0, 1, 1, 2, 3, 3};
  int index_j[] = \{0, 1, 3, 2, 0, 3\};
  double x[] = \{1.0, 1.0, 1.0, 1.0\}, y[] = \{0.0, 0.0, 0.0, 0.0\};
 blas sparse matrix A;
  int k;
 double alpha = 1.0;
 A = BLAS duscr begin(n, n); //Create Sparse BLAS handle
  for(k=0; k < nonzeros; k++) //Insert entries one by one</pre>
   BLAS duscr insert entry(A, values[k], index i[k], index j[k]);
 BLAS uscr end(A); // Complete construction of sparse matrix
 //Compute matrix-vector product y = A*x
 BLAS dusmv(blas no trans, alpha, A, x, 1, y, 1);
 BLAS usds(A); //Release matrix handle
```

Parallel Languages

Parallel Languages

- C and Fortran 77 do not reflect some essential features of VP and SP architectures
 - They cannot play the same role for VPs and SPs
- Optimizing compilers
 - Only for a simple and limited class of applications
- Array libraries
 - Cover a limited class of array operations
 - Other array operations can be only expressed as a combination of the locally-optimized library array operations
 - This excludes global optimization of combined array operations

Parallel Languages (ctd)

- Parallel extensions of C and Fortran 77 allows programmers
 - To explicitly express in a portable form any array operation
 - Compiler does not need to recognize code to parallelize
 - Global optimisation of operations on array is possible
 - We consider a parallel superset of Fortran 77
 - Fortran 90

Fortran 90

- Fortran 90 is a Fortran standard released in 1991
 - Widely implemented since then
- Two categories of new features
 - Modernization of Fortran according to the state-of-the-art in serial programming languages
 - Support for explicit expression of operations on arrays

- Serial extensions include
 - Free-format source code and some other simple improvements
 - Dynamic memory allocation (automatic arrays, allocatable arrays, and pointers and associated heap storage management)
 - User-defined data types (structures)
 - Generic user-defined procedures (functions and subroutines) and operators

- Serial extensions (ctd)
 - Recursive procedures
 - New control structures to support structured programming
 - A new program unit, MODULE, for encapsulation of data and a related set of procedures

We focus on parallel extensions

- Fortran 90 considers arrays first-class objects
 - Whole-array operations, assignments, and functions
 - Operations and assignments are extended in an obvious way, on an element-by-element basis
 - Intrinsic functions are array-valued for array arguments
 - operate element-wise if given an array as their argument
 - Array expressions may include scalar constants and variables, which are replicated (or expanded) to the required number of elements

Example:

```
REAL, DIMENSION(3,4,5) :: a, b, c, d ... c = a + b d = SQRT(a) c = a + 2.0
```

WHERE Structure

- Sometimes, some elements of arrays in an array-valued expression should be treated specially
 - Division by zero in a = 1./a should be avoided
- WHERE statement

```
WHERE (a /= 0.) a = 1./a
```

WHERE construct

```
WHERE (a /= 0.)
  a = 1./a
ELSEWHERE
  a = HUGE(a)
END WHERE
```

- All the array elements in an array-valued expression or array assignment must be conformable, i.e., they must have the same shape
 - the same number of axes
 - the same number of elements along each axis
- Example.

```
REAL :: a(3,4,5), b(0:2,4,5), c(3,4,-1:3)
```

- Arrays a, b, and c have the same rank of 3, extents of 3,4, and 5, shape of {3,4,5}, size of 60
 - Only differ in the lower and upper dimension bounds

Array Section

- An array section can be used everywhere in array
 assignments and array-valued expressions where a whole
 array is allowed
- An array section may be specified with subscripts of the form of *triplet*: lower:upper:stride
- It designates an ordered set i_1, \dots, i_k such that
 - $i_1 = lower$
 - $i_{j+1} = i_j + stride (j=1,...,k-1)$
 - $|i_k$ upper | < stride

Array Section (ctd)

- Example. **REAL** :: a(50,50)
- What sections are designated by the following expressions? What are the rank and shape for each section?

```
a(i,1:50:1), a(i,1:50)
a(i,:)
a(i,1:50:3)
a(i,50:1:-1)
a(11:40,j)
a(1:10,1:10)
```

Array Section (ctd)

- Vector subscripts may also be used to specify array sections
 - Any expression whose value is a rank 1 integer array may be used as a vector subsript
- Example.

```
REAL :: a(5,5), b(5)

INTEGER :: index(5)

index = (/5,4,3,2,1/)

b = a(index,1)
```

Array Section (ctd)

- Whole arrays and array sections of the same shape can be mixed in expressions and assignments
- Note, that unlike a whole array, an array section may not occupy contiguous storage locations

Array Constants

- Fortran 90 introduces *array constants*, or *array constructors*
 - The simplest form is just a list of elements enclosed in (/ and /)
 - May contain lists of scalars, lists of arrays, and implied-DO loops
- Examples.

```
(/ 0, i=1,50 /)
(/ (3.14*i, i=4,100,3) /)
(/ ( (/ 5,4,3,2,1 /), i=1,5 ) /)
```

Array Constants (ctd)

- The array constructors can only produce 1-dimensional arrays
 - Function RESHAPE can be used to construct arrays of higher rank

```
REAL :: a(500,500)

a = RESHAPE( (/ (0., i=1,250000) /), (/ 500,500 /) )
```

Assumed-Shape and Automatic Arrays

Consider the user-defined procedure operating on arrays

```
SUBROUTINE swap(a,b)
REAL, DIMENSION(:,:) :: a, b
REAL, DIMENSION(SIZE(a,1), SIZE(a,2)) :: temp
temp = a
a = b
b = temp
END SUBROUTINE swap
```

Assumed-Shape and Automatic Arrays (ctd)

- Formal array arguments a and b are of assumed shape
 - Only the type and rank are specified
 - The actual shape is taken from that of the actual array arguments
- The local array temp is an example of the automatic array
 - Its size is set at runtime
 - It stops existing as soon as control leaves the procedure

Intrinsic Array Functions

- Intrinsic array functions include
 - Extension of such intrinsic functions as SQRT, SIN, etc. to array arguments
 - Specific array intrinsic functions
- Specific array intrinsic functions do the following
 - Compute the scalar product of two vectors (DOT_PRODUCT) and the matrix product of two matrices (MATMUL)

Specific Intrinsic Array Functions

- Perform diverse reduction operations on an array
 - logical multiplication (ALL) and addition (ANY)
 - counting the number of true elements in the array
 - arithmetical multiplication (PRODUCT) and addition (SUM) of its elements
 - finding the smallest (MINVAL) or the largest (MAXVAL) element

Specific Intrinsic Array Functions (ctd)

- Return diverse attributes of an array
 - its shape (SHAPE)
 - the lower dimension bounds of the array (LBOUND)
 - the upper dimension bounds (UBOUND)
 - the number of elements (SIZE)
 - the allocation status of the array (ALLOCATED)

Specific Intrinsic Array Functions (ctd)

- Construct arrays by means of
 - merging two arrays under mask (MERGE)
 - packing an array into a vector (PACK)
 - replication of an array by adding a dimension (SPREAD)
 - unpacking a vector (a rank 1 array) into an array under mask (UNPACK)

Specific Intrinsic Array Functions (ctd)

- Reshape arrays (RESHAPE)
- Move array elements performing
 - the circular shift (CSHIFT)
 - the end-off shift (EOSHIFT)
 - the transpose of a rank 2 array (TRANSPOSE)
- Locate the first maximum (MAXLOC) or minimum (MINLOC) element in an array

Memory Hierarchy

- Parallel programming systems for VPs and SPs take into account their modern memory structure
 - Optimal memory management is often more efficient than optimal usage of IEUs
 - Approaches to optimal memory management appear surprisingly similar to optimisation of parallel facilities
- Simple two-level memory model
 - Small and fast register memory
 - Large and relatively slow main memory

Memory Hierarchy (ctd)

- A simple modern memory hierarchy
 - Register memory
 - Cache memory
 - Main memory
 - Disk memory
- Cache memory
 - A buffer memory between main memory and registers
 - Holds copies of some data from the main memory

Memory Hierarchy (ctd)

- Execution of instruction reading a data item from the main memory into a register
 - Check if a copy of the data item is already in the cache
 - If so, the data item will be actually transferred into the register from the cache
 - If not, the data item will be transferred into the register from the main memory, and a copy of the item will appear in the cache

Cache

- Cache
 - Partitioned into cache lines
 - Cache line is a minimum unit of data transfer between the cache and the main memory
 - Scalars may be transferred only as a part of a cache line
 - Much smaller than the main memory
 - The same cache line may reflect different data blocks from the main memory

Cache (ctd)

- Types of cache memory
 - Direct mapped
 - each block of the main memory has only one place it can appear in the cache
 - Fully associative
 - a block can be placed anywhere in the cache
 - Set associative
 - a block can be placed in a restricted set of places
 - a set is a group of two or more cache lines
 - n-way associative cache

Cache (ctd)

- Cache miss is the situation when a data item being referenced is not in the cache
- Minimization of cache misses is able to significantly accelerate execution of the program
- Programs intensively using basic operations on arrays are obviously suitable for that type of optimization

Loop Tiling

- The main specific optimization minimizing the number of cache misses is loop tiling
- Consider the loop nest

```
for(i=0; i<m; i++)  /* loop 1 */
  for(j=0; j<n; j++) /* loop 2 */
    if(i==0)
    b[j]=a[i][j];
    else
    b[j]+=a[i][j];</pre>
```

b[j] are repeatedly used by successive iterations of loop 1

Loop Tiling (ctd)

- If n is large enough, the data items may be flushed from the cache by the moment of their repeated use
- To minimize the flushing of repeatedly used data items,
 the number of iterations of loop 2 may be decreased
- To keep the total number of iterations of this loop nest unchanged, an additional controlling loop is introduced

Loop Tiling (ctd)

The transformed loop nest is:

```
for(k=0; k<n; k+=T) //additional controlling loop 0
    for(i=0; i<m; i++) // loop 1
        for(j=k; j<min(k+T,n); j++) // loop 2
        if(i==0)
            b[j]=a[i][j];
        else
            b[j]+=a[i][j];</pre>
```

- This transformation is called tiling
- T is the tile size

Loop Tiling (ctd)

In general, the loop tiling is applied to loop nests of the

 The goal is to minimize the number of cache misses for reference e[i2]...[in], which is repeatedly used by successive iterations of loop 1

Loop Tiling and Optimising Compilers

- The recognition of the loop nests, which can be tiled is the most difficult problem to be solved by optimising C and Fortran 77 compilers
 - Based on the analysis of data dependencies in loop nests
- Theorem. The loop tiling is legally applicable (to the above loop nest) iff the loops from loop 2 to loop n are fully interchangeable
 - To prove the interchangability an analysis of data dependence between different iterations of the loop nest is needed

Loop Tiling and Array Libraries

- Level 3 BLAS is specified to support block algorithms of matrix-matrix operations
- Partitioning matrices into blocks and performing the computation on the blocks maximizes the reuse of data held in the upper levels of memory hierarchy

Loop Tiling and Parallel Languages

- Compilers for parallel languages do not need to recognize loops suitable for tiling
- They can translate explicit operations on arrays into loop nests with the best possible temporal locality

Virtual memory

- Instructions address virtual memory rather than the real physical memory
- The virtual memory is partitioned into pages of a fixed size
 - Each page is stored on a disk until it is needed
 - When the page is needed, it copied to main memory, with the virtual addresses mapping into real addresses
 - This copying is known as paging or swapping

Virtual memory (ctd)

- Programs processing large enough arrays do not fit into main memory
 - The swapping takes place each time when required data are not in the main memory
 - The swapping is a very expensive operation
 - Minimization of the number of swappings can significantly accelerate the programs
- The problem is similar to minimization of cache misses and can be, therefore, approached similarly

Vector and Superscalar Processors: Summary

- VPs and SPs provide instruction-level parallelism, which is best exploited by applications with intensive operations on arrays
- Such applications can be written in a serial programming language and complied by dedicated optimizing compilers performing some specific loop optimizations
 - Modular, portable, and reliable programming are supported
 - Efficiency and portable efficiency are also supported but only for a limited class of programs

Vector and Superscalar Processors: Summary (ctd)

- Array libraries allow the programmers to avoid the use of dedicated compilers
 - The programmers express operations on arrays directly using calls to carefully implemented subroutines
 - Modular, portable, and reliable programming are supported
 - Limited efficiency and portable efficiency
 - Excludes global optimization of combined array operations

Vector and Superscalar Processors: Summary (ctd)

- Parallel languages combine advantages of the first and second approaches
 - Operations on arrays can be explicitly expressed
 - No need in sophisticated algorithms to recognize parallelizable loops
 - Global optimisation of combined array operations is possible
 - They support general-purpose programming (unlike existing array libraries)