

Crash Course: FORTRAN 77+

- FORTRAN 77+ is used in these notes to refer to the dialect of FORTRAN 77 used by LAPACK and ScaLAPACK developers.
 - Straight FORTRAN 77 is quite arcane and most compilers have implemented a set of extensions.
- FORTRAN has been the language of choice for scientific and engineering for a long time, partly because it:
 - Has an extensive compiler support for multi-dimensional arrays
 - Has restrictions in the language to allow aggressive compiler optimizations
 - Has language support (in FORTRAN 90 and onwards) for dynamic memory management, derived types, object orientation, operator overloading, generic interfaces, array expressions, distributed arrays (co-arrays), etc

Fixed Source Format

- FORTRAN 77+ has a strict source format known as the "fixed source format" (removed in later standards)
- Columns are used for different things:
 - 1: Comment column
 - 2-5: Label columns
 - 6: Continuation column
 - 7-72: Statement columns



Set your editor to expand

tabs to spaces.

Use 3 as tabstop (two tabs takes

you to colunm 7)

IF-THEN-ELSE

- IF-statement:
 - IF (<logical expression>) <statement>
- IF-construct:
 - IF(<logical expression>) THEN

<block>

[ELSE IF (<logical expression>) THEN <block>]

ELSE

<block>]

END IF

GO TO, CONTINUE and Labels

- Labels
 - Integers from 1 to 9999
 - Placed in columns 2 to 5
 - Used as targets for GO TO statements and in DO loops
- GO TO-statement:
 - GO TO <label>
 - Transfers control to statement labeled with <label>
- CONTINUE-statement:
 - CONTINUE
 - A do-nothing statement often used as target statement and DO loop end statement.

<pre>DO • DO-construct: - Do <label> <var> = <low>, <high>[, <step>] <block> <label> continue • Example:</label></block></step></high></low></var></label></pre>	PROC • In FORTRAN you do not ha MAIN, instead you have the - program [name] <declarations> <statements> END [PROGRAM name]</statements></declarations>	SRAM ve a special function called PROGRAM construct:
SUBROUTINEs and FUNCTIONs	Arithmetic	Operators
 SUBROUTINEs (think of C functions returning void) <u>CALL mysub(<arglist>)</arglist></u> 	FORTRAN	C/Java
FUNCTIONs (think of C functions returning non-void)	+	+
- <ivai> = mytunc(<arglist>)</arglist></ivai>	-	-
Declaring a SUBROUTINE:	*	*
<pre><dummy argument="" declarations="" type=""> END [SUBROUTINE name]</dummy></pre>	/	/
Declaring a FUNCTION:	**	N/A
<pre><dummy argument="" declarations="" type=""> END [FUNCTION name]</dummy></pre>	N/A	+=
- Example:	N/A	++
INTEGER a, b MAX = a IF(b.GT. a) MAX = b END		

Logical Operators

FORTRAN	C/Java
.GT.	>
.LT.	<
.LE.	<=
.GE.	>=
.EQ.	==
.EQV. (logical)	
.NE.	! =
.NEQV. (logical)	(exclusive or)
.AND.	&&
.OR.	
.NOT.	I

Arrays (Matrices and Vectors)

- Declaring a vector of 50 INTEGERs
 - INTEGER vec(50)
- Declaring a 25x47 matrix of 50 INTEGERs
 - INTEGER mtx(25, 47)
- Indexing starts from 1 (unless explicitly stated in the declaration)
- Indexing top left element in matrix:
 - mtx(1, 1)
- Indexing bottom right index in matrix:
 - mtx(25, 47)

Data Types

- INTEGER
 - Signed 32-bit (usually) integer
- LOGICAL
 - .TRUE. Or .FALSE.
- **CHARACTER**(<length>) Or **CHARACTER** (just one character)
 - 'string' or "string"
- REAL
 - Single precision IEEE (usually) floating point f = 5E+0
- DOUBLE PRECISION
 - Double precision IEEE (usually) floating point d = 5D+0
- COMPLEX
 - Single precision IEEE (usually) complex number c = (r, i)
- COMPLEX*16
 - Double precision IEEE (usually) complex number c = (r, i)

Automatic Arrays

- Size of array is either known at compile time or determined by dummy arguments and the array is not a dummy argument itself.
- Storage will be allocated (think of it as being allocated on the stack) at runtime and deallocated automatically when variable falls out of scope.
 - Example:
 - SUBROUTINE auto(N) INTEGER A(N) END

Assumed Shape Array Assumed Size Arrays The shape (extent of all dimensions) need not be known Extent of last dimension in FORTRAN arrays need not at compile time. be known at compile time (or at runtime for that matter) to generate indexing code (first dimension in the case of • An array where the extent of one or more dimension is C). determined by dummy arguments is referred to as an assumed shape array. • An array declared with unknown last dimension extent is referred to as an assumed size array. - Useful for passing arrays as arguments to subroutines. - REAL A(LDA, *) - Example: Indexing code: SUBROUTINE mysub(A, LDA, M, N) $A(i, j) \rightarrow A + (i-1) + (j-1)*LDA$ INTEGER LDA, M, N REAL A(LDA, N) END Comments Continuation (long statements) Comment lines are created by putting (almost) any • Long statements (going beyond column 72) can be broken into several lines by placing (almost) any character (usually * or c) in the first column: character (usually numbers, $s, \varepsilon, +$) in the continuation - Example: column (column 6) • C This is a comment This is also a comment - Example: A = 1 c This is not a comment A(1, 2) = longvariablename +• \$ anotherlongvariable

 FORTRAN 77+/C "Interoperability" Calling FORTRAN 77+ from C: These are usual type relationships: LOGICAL (?) INTEGER	 Other things to know about FORTRAN FORTRAN is case insensitive FORTRAN passes everything by reference FORTRAN 77 has no type checking of arguments FORTRAN 77 has no support for recursive subroutines or functions
 Storage Formats used by the Libraries General matrices: Column Major Symmetric and triangular matrices Column Major Column Packed Band matrices Diagonal Storage Tridiagonal matrices Diagonal Storage 	Full Storage Format Matrix Indices Memory Placement 11 12 13 14 15 16 17 18 19 0 9 18 27 36 45 54 63 72 21 22 23 24 25 26 27 28 29 1 10 19 28 37 46 55 64 73 31 32 33 34 35 36 37 38 39 2 11 20 29 38 47 56 65 74 51 52 53 54 65 66 67 68 69 5 14 23 32 41 50 59 6 15 26 77 76 77 76 76 77 76 77 78 79 6 15 24 33 42 51 60 69 78 81 72 26 35 44 53 62 71 80

Standard Packed Storage Format

Rectangular Full Packed Storage Format

Matrix Indices Memory Placem 11 * <t< th=""><th>nent * * * * * * * * * * * * * 30 * * * * * 31 35 * * * 32 36 39 * * 33 37 40 42 * 34 38 41 43 44</th><th>Matrix Indices Memory Placement 11 66 76 86 96 21 22 77 87 97 1 10 19 28 37 31 32 33 88 98 2 11 20 29 38 41 42 43 44 99 3 12 21 30 39 51 52 53 55 4 13 22 31 40 61 62 63 64 65 5 14 23 32 41 71 72 73 74 75 6 15 24 33 42 81 82 83 84 85 7 16 25 34 43 91 92 93 94 95 8 17 26 35 44</th></t<>	nent * * * * * * * * * * * * * 30 * * * * * 31 35 * * * 32 36 39 * * 33 37 40 42 * 34 38 41 43 44	Matrix Indices Memory Placement 11 66 76 86 96 21 22 77 87 97 1 10 19 28 37 31 32 33 88 98 2 11 20 29 38 41 42 43 44 99 3 12 21 30 39 51 52 53 55 4 13 22 31 40 61 62 63 64 65 5 14 23 32 41 71 72 73 74 75 6 15 24 33 42 81 82 83 84 85 7 16 25 34 43 91 92 93 94 95 8 17 26 35 44
Matrix Indices * 12 23 * * * * * * * * * * * * * * * * * * *	ent 36 45 54 63 72 37 46 55 64 73 38 47 56 65 74 39 48 57 66 75	BLAS • Basic Linear Algebra Subroutines (BLAS) - http://www.netlib.org/blas/ Reference implementation - http://www.netlib.org/blas/ Auto-tuning HPC impl. - http://www.netlib.org/blas/gemm_based/ GEMM-based BLAS by Kågström et. al. - http://www.tacc.utexas.edu/resources/software/ GotoBLAS • Interfaces: - FORTRAN (official) - C, C++, Java, (unofficial) - C, assembler, FORTRAN, (depends on vendor)

BLAS - Content

- BLAS contains subroutines and functions for a number of basic linear algebra operations.
 - Dot product
 - Givens rotation generation and application
 - Vector updates
 - Matrix-vector product update
 - Triangular system solve (with single or multiple right hand sides)
 - Matrix-matrix product update
 - ...
- The routines operate on various storage formats and on four data types (single, double, complex, double complex).

Coding Conventions

_XXYYY _: Data type S, D, C, or Z XX: Type of matrix GE, GB: GEneral, General Banded HE, HB, HP: HErmitian, Hermitian Banded, Hermitian Packed SY, SB, SP: SYmmetric, Symmetric Banded, Symmetric Packed TR, TB, TP: TRiangular, Triangular Banded, Triangular Packed YY: Operation S: "Solve" M: "Matrix" V: "Vector" R: Rank-1 R2: Rank-2

- RK: Rank-k
- **R2K**: Rank-2k
- Example:
 - DTRSM:
 - Double precision
 - TRiangular
 Solve
 - Solve
 Multiple right hand sides

Memory Traffic - Limitations

- Memory bandwidth and latency can not match the high performance of floating point computations on the chip.
- Solution:
 - Exploit caches by data locality in space and time
- Solution requires:
 - An operation that has much inherent locality
- Metric for estimating inherent locality in linear algebra:
 - Number of floating point operations
 - Number of memory locations referenced
 - i.e., flop/memref

Locality - Examples

- Example of poor inherent locality: AXPY (a*x + y)
 - 2 vector loads (x, y)
 - 1 vector store (y)
 - 2 vector operations (*, +)
 - flop/memref = 2/3
- Example of good inherent locality: GEMM (a*A*B + b*C)
 - ~2*N^3 flops
 - ~3*N^2 loads
 - ~1*N^2 stores
 - flop/memref ~ N/2

Level 1, 2, 3	LAPACK
 Level-1 BLAS: Vector operations (~1 flop/memref) dot axpy swap copy scal Level-2 BLAS: Matrix-Vector operations (~1 flop/memref) gemv symv trsv Level-3 BLAS: Matrix-Matrix operations (~N flop/memref) gemm syrk trsm 	 Linear Algebra PACKage (LAPACK) http://www.netlib.org/lapack/ Official LAPACK releases http://www.netlib.org/lapack/lanws/ Publications related to LAPACK and DLA Some vendors provide their own optimized LAPACK routines as well as BLAS routines: IBM: ESSL (Proprietary) AMD: ACML (Free?) Intel: MKL (Proprietary?) Cray: libsci (Proprietary?) Interfaces: FORTRAN (official) C, C++, Java, (unofficial) Language: FORTRAN 77+
 LAPACK - Content Compared with BLAS, the high level algorithms and tricky numerical algorithms go into LAPACK. Factorizing matrices LU, Cholesky, QR, QL, RQ, LQ, Applying factored-form orthogonal matrices Solving linear equations Solving linear least squares problems Decomposing matrices SVD, Schur, Computing eigenvalues and eigenvectors Symmetric, non-symmetric, Error bounds, condition estimation 	 Workspace Management Many routines in LAPACK require auxilliary workspace to function and/or run faster. Users must provide this storage. Routines take workspace via their arguments, typically: work: Workspace Lwork: Length of workspace allow workspace queries. Workspace query:

Error Reporting LAPACK - Examples LAPACK routines have an extra INTEGER argument at the Solving a linear system after LU factorization end of their argument lists: INFO - DGETRS(TRANS, N, NRHS, A, LDA, IPIV, B, LDB, INFO) - The value of **INFO** tells what went wrong (if anything): • 0: Success • Computing QR factorization • < 0: Argument number -INFO contained an illegal value (fatal, - DGEQRF(M, N, A, LDA, TAU, WORK, LWORK, INFO) programming error) • > 0: Something went wrong during computation (exact interpretation is routine specific) - Example: **DGETRF** (LU factorization) **INFO > 0: U(INFO, INFO)** is exactly zero

BLACS

Basic Linear Algebra Communication Subroutines **Official BLACS releases**

- http://www.netlib.org/blacs/
- Purpose:
 - Communication of submatrices appropriate for dense linear algebra algorithms (e.g., ScaLAPACK)
- Objection:
 - "I know MPI inside out, why should I learn BLACS?"
- Answer:
 - It will hopefully be apparent at the end of this segment.
- Interfaces:
 - FORTRAN, C (official)
- Language:
 - C

2D-Grid, Scope, Context

- Processes are arranged in a logical 2D-grid.
- Each process is a member of three scopes:
 - 'All': All processes in the grid
 - 'Row': All processes on the same row of the grid
 - 'Column': All processes on the same column of the grid
- BLACS communication is tied to a context (think of MPI communicators) which is an integer.

Submatrix Communication	Point-to-Point
 The BLACS unit of communication is a submatrix of some specified size and shape. Two types of submatrices: General submatrices: Parameters: M, N, A, LDA Trapezoidal submatrices (generalization of triangular): Parameters: M, N, A, LDA, UPLO, DIAG Packing of matrices hidden from user Types supported: I: Integer Single precision D: Double precision C: Complex single precision z: Complex double precision 	 Send: xGESD2D(CTXT, M, N, A, LDA, RDST, CDST) xTRSD2D(CTXT, UPLO, DIAG, M, N, A, LDA, RDST, CDST) Receive: xGERV2D(CTXT, M, N, A, LDA, RSRC, CSRC) xTRRV2D(CTXT, UPLO, DIAG, M, N, A, LDA, RSRC, CSRC)
Collectives	Collectives: Topology
 Broadcast (send): xGEBS2D(CTXT, SCOPE, TOP, M, N, A, LDA) xTRBS2D(CTXT, SCOPE, TOP, UPLO, DIAG, M, N, A, LDA) Broadcast (receive): xGEBR2D(CTXT, SCOPE, TOP, M, N, A, LDA, RSRC, CSRC) xTRBR2D(CTXT, SCOPE, TOP, UPLO, DIAG, M, N, A, LDA, RSRC, CSRC) Combine operations (SUM, MAX, MIN): xGSUM2D(CTXT, SCOPE, TOP, M, N, A, LDA, RDST, CDST) xGAMX2D(CTXT, SCOPE, TOP, M, N, A, LDA, RA, CA, RCFLAG, RDST, CDST) 	 Topologies (TOP) specify the communication pattern. 'I': Increasing ring 'D': Decreasing ring 'S': Split ring 'M': Multi-ring 'I': 1-tree 'B': Bidirectional exchange ' ': Default (may use MPI_Bcast)

BLACS – Setup (FORTRAN)	PBLAS
 Initializing BLACS: CALL BLACS_PINFO(ME, NP) Initializing context: CALL BLACS_GET(0, 0, CTXT) CALL BLACS_GRIDINIT(CTXT, 'Row', P, Q) CALL BLACS_GRIDINFO(CTXT, P, Q, MYROW, MYCOL) Getting someones rank from coordinates RANK = BLACS_PNUM(CTXT, ROW, COL) Getting someones coordinates from rank CALL BLACS_PCOORD(CTXT, RANK, ROW, COL) Exiting BLACS CALL BLACS_EXIT(0) 	 Parallel BLAS http://www.netlib.org/scalapack/ PBLAS reference impl. is part of ScaLAPACK Interfaces: FORTRAN C? Language: C
2D Block Cyclic Distribution	Matrix Descriptors
 PBLAS operates on data distributed using the 2D block cyclic distribution. Recall: 0 11 12 13 14 15 15 14 15 15 15 15 14 15 12 13 14 15 15 16 17 11 12 15 16 17 11 12 15 16 17 11 12 15 15 16 17 11 12 15 15 16 17 17 17 11 12 15 13 14 14 14 15 14 14 15 15 15 15 14 14 14 14 14 14 14 14 15 14 14 14 15 15 15 14 14 14 14 14 14	 Descriptors are used in PBLAS and ScaLAPACK to encapsulate information on a distributed matrix. A descriptor is a 9-item integer vector: INTEGER DESCA(9) DESCA(1): (DTYPE) DESCA(2): (CTXT) BLACS context DESCA(3): (M) Number of rows in global matrix DESCA(4): (N) Number of columns in global matrix DESCA(5): (MB) Row blocking factor DESCA(6): (NB) Column blocking factor DESCA(6): (RSRC) Row index of owner of A(1, 1) DESCA(9): (LLD)

 PBLAS - Example Parallel version of DGEMM CALL PDGEMM(TRANSA, TRANSB, M, N, K, ALPHA, A, IA, JA, DESC_A, B, IB, JB, DESC_B, BETA, C, IC, JC, DESC_C) Notice: PBLAS has interfaces that take descriptions of submatrices BLAS, on the other hand, takes submatrices implicitly 	ScaLAPACK • SCAlable LAPACK (distributed memory) - http://www.netlib.org/scalapack/ Official ScaLAPACK releases
 ScaLAPACK - Content Most of LAPACK No support for band and packed matrices Missing some more advanced algorithms SVD and QR w/ pivoting least squares Generalized least squares Non-symmetric eigenvalue problems D&C SVD 	 ScaLAPACK – Coding Conventions Symbols are similar to LAPACK (just add p) Submatrices are referenced explicitly in interface: A(I, J), LDA LAPACK submatrix reference A, I, J, DESCA ScaLAPACK submatrix reference

Utilities: DESCINIT

- SUBROUTINE DESCINIT(DESC, M, N, MB, NB, RSRC, CSRC, CTXT, LLD, INFO)
- Initializes all elements of a descriptor.

• Arguments:

- DESC Descriptor to initialize (output)
- M, N Size of global matrix
- MB, NB Blocking factors
- **RSRC**, **CSRC** Coordinates of owner of (1, 1) matrix element
- CTXT BLACS context
- LLD Leading dimension of local matrix (use NUMROC to find)
- INFO Error reporting, 0: success (output)

Utilities: NUMROC

- INTEGER FUNCTION NUMROC(N, NB, ME, SRC, NP)
 Finds the number of rows (or columns) mapped to a specific grid row (or column).
 Arguments:

 N Extent of matrix dimension
 NB Blocking factor in matrix dimension
 ME Row (or column) index of processor of interest
 SRC Row (or column) index of source
 - NP Number of processes in grid dimension

Utilities: INFOG2L

- SUBROUTINE INFOG2L(GRINDX, GCINDX, DESC, NPROW, NPCOL, MYROW, MYCOL, LRINDX, LCINDX, RSRC, CSRC)
- Given a global matrix element (GRINDX, GCINDX), returns the corresponding local matrix element (LRINDX, LCINDX) and coordinates of processor that owns that element (RSRC, CSRC).

• Arguments:

- GRINDX, GCINDX Global matrix element
- DESC Descriptor
- NPROW, NPCOL
- MYROW, MYCOL
- LRINDX, LCINDX
- RSRC, CSRC

- Global matrix elemen Descriptor of matrix Grid size
- My coordinates
- CINDXLocal matrix element (output)
- CSRC Owner of element (output)