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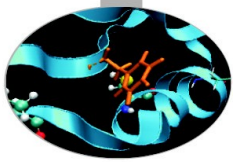
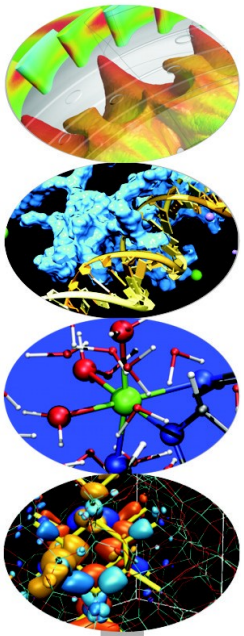
SuperComputing Applications and Innovation





Scalable Linear Algebra

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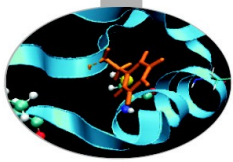
CINECA

Basic Linear Algebra Algorithms



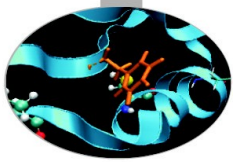
Linear algebra constitutes the core of most technical-scientific applications

Scalar products $$s = \sum_i a_i \cdot b_i$$

Linear Systems $$A_{ij} x_j = b_i$$

Eigenvalue Equations $$A_{ij} x_j = \alpha x_i$$

Algorithms and Libraries



Basic Linear Algebra algorithms are well known and largely available. See for instance:

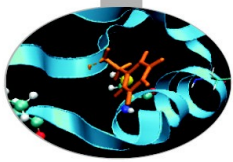
http://www.nr.com

Why should I use libraries?

- They are available on many platforms
- … and they are usually optimized by vendors
- In the case vendor libraries are not installed:

http://www.netlib.org

Standard Linear Algebra Libraries



BLACS

ACML

PETSc

LAPACK

PLASMA

MKL

PSBLAS

ATLAS

MAGMA

BLAS

… but not only

SPLEPc

TRILINOS

ESSL

ARPACK

SCALAPACK

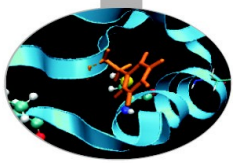
SCOTCH

CUBLAS

which library should I use?

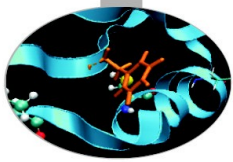
http://www.netlib.org/utk/people/JackDongarra/la-sw.html

Automaticcally Tuned Linear Algebra Software



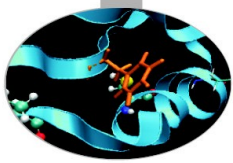
- ATLAS is both a research project and a software package.
- ATLAS's purpose is to provide portably optimal linear algebra software.
- The current version provides a complete BLAS API (for both C and Fortran77), and a very small subset of the LAPACK API.

(**P**arallel) **AR**noldi **PACK**age



- ARPACK is a collection of Fortran77 subroutines designed to solve large scale eigenvalue problems.
- It is most appropriate for large sparse or structured matrices. (Where structured means that a matrix-vector product requires order n rather than the usual order n^2 floating point operations.)
- ARPACK is dependent upon a number of subroutines from LAPACK and the BLAS.
- Main feature: reverse communication interface.
- A parallel version of the ARPACK library is availible. The message passing layers currently supported are BLACS and MPI .

TRILINOS

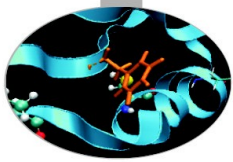


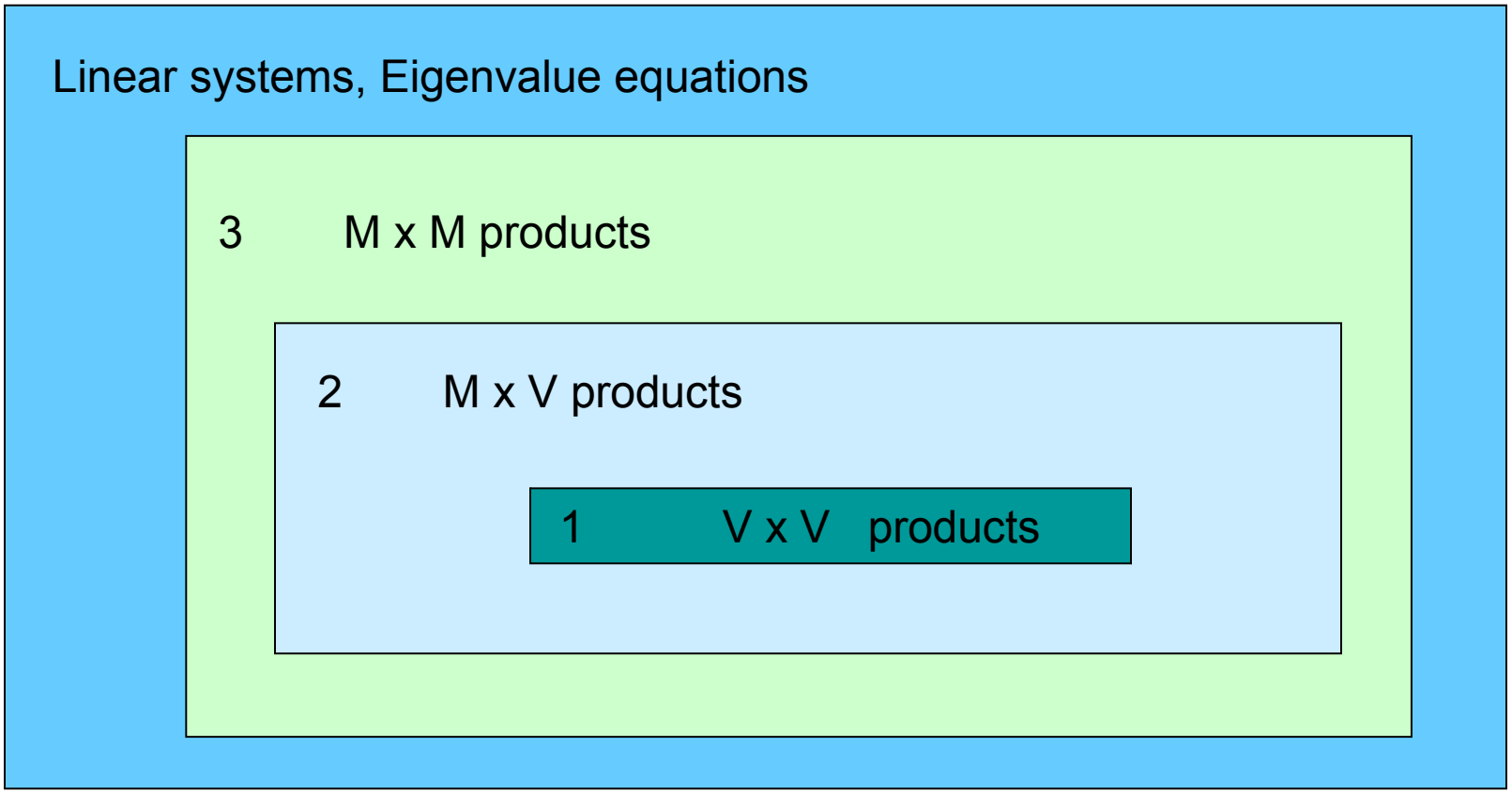
The Trilinos Project is an effort to develop algorithms and enabling technologies within an object-oriented software framework for the solution of large-scale, complex multi-physics engineering and scientific problems. A unique design feature of Trilinos is its focus on packages.

It is organized in Capability Areas:

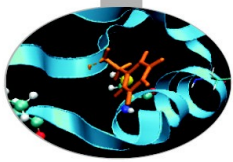
- User Experience
- Parallel Programming Environments
- Framework & Tools
- Software Engineering Technologies and Integration
- I/O Support
- Meshes, Geometry, & Load Balancing
- Discretizations
- Scalable Linear Algebra
- Linear & Eigen Solvers
- Embedded Nonlinear Analysis Tools

Linear Algebra is Hierarchical



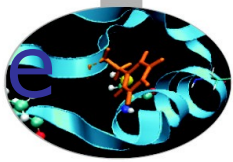


(Parallel) Basic Linear Algebra Subprograms (BLAS and PBLAS)



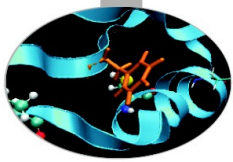
- **Level 1 : Vector - Vector operations**
- **Level 2 : Vector - Matrix operations**
- **Level 3 : Matrix - Matrix operations**

(Scalable) Linear Algebra PACKage (LAPACK and ScaLAPACK)



- **Matrix Decomposition**
- **Linear Equation Systems**
- **Eigenvalue Equations**
- **Linear Least Square Equations**
- **for dense, banded, triangular, real and complex matrices**

Levels of Routines

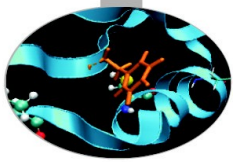


- ***Driver*** *routines*
  to solve a complete problem

- ***Computational*** *routines*
  to perform a distinct computational task

- ***Auxiliary*** *routines*
  to perform subtasks of block-partitioned algorithms or low-level computations

BLAS/LAPACK subroutines



Routines name scheme: XYYZZZ

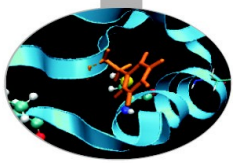
X data type → S = REAL
D = DOUBLE PRECISION
C = COMPLEX
Z = DOUBLE COMPLEX

YY matrix type (GE = general, SY = symmetric, HE = hermitian)

ZZZ algorithm used to perform computation

Some auxiliary functions don't make use of this naming scheme!

BLAS subroutines



matrix multiplication: C = A * B (level 3)

```
DGEMM( TRANSA, TRANSB, M, N, L, ALPHA, A, LDA, B, LDB, BETA, C, LDC )
```

'N' or 'T' max(1,M)

matrix times vector: Y = A * X (level 2)

```
DGEMV( TRANS, M, N, ALPHA, A, LDA, X, INCX, BETA, Y, INCY )
```

1.0d0 0.0d0

vector swap: X ⇔ Y (level 1)

```
DSWAP( N, X, INCX, Y, INCY )
```

scalar product: p = X′·Y (level 1)

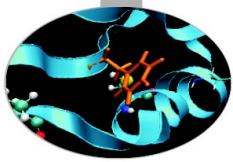
```
p = DDOT( N, X, INCX, Y, INCY )
```

Function Increment for elements

Quick Reference Guide to the BLAS

http://www.netlib.org/lapack/lug/node145.html

CBLAS subroutines

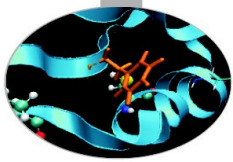


Instead of calling BLAS routines from a C-language program, you can use the CBLAS interface.

CBLAS is a C-style interface to the BLAS routines. You can call CBLAS routines using regular C-style calls. Use the ***mkl.h*** header file with the CBLAS interface. The header file specifies enumerated values and prototypes of all the functions.

```
matrix multiplication: C = A * B  (level 3)
cblas_dgemm(ORDER, TRANSA, TRANSB, M, N, L, ALPHA, A, LDA, B, LDB, BETA, C, LDC)
CblasRowMajor                      CblasNoTrans
matrix times vector: Y =  A * X   (level 2)
cblas_dgemv(ORDER, TRANS, M, N, ALPHA, A, LDA, X, INCX, BETA, Y, INCX)
```

LAPACK subroutines



Eigenvalues and, optionally, eigenvectors of a real symmetric matrix:

```
DSYEV( JOBZ, UPLO, N, A, LDA, W, WORK, LWORK, INFO )
```

'V' compute eigenvalues and eigenvectors
'N' compute eigenvalues only

'U' use upper triangular part of A
'L' use lower triangular part of A

Eigenvalues

Workspace

if `lwork = -1`, compute workspace dimension.
Return it in `work(1)`

```
void dsyev_( const char* jobz, const char* uplo, const MKL_INT* n,
             double* a, const MKL_INT* lda, double* w, double* work,
             const MKL_INT* lwork, MKL_INT* info );
```

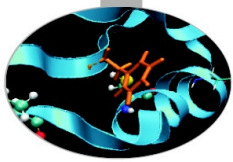
Index of Driver and Computational Routines:

http://www.netlib.org/lapack/lug/node142.html

Index of Auxiliary Routines:

http://www.netlib.org/lapack/lug/node144.html

How To Compile



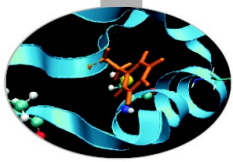
 # load these modules on Eurora

```
module load profile/advanced
module load gnu/4.6.3
module load blas/2011--gnu--4.6.3
module load lapack/3.5.0--gnu--4.6.3
```

FORTRAN:

```
LALIB="-L${LAPACK_LIB} -llapack -L${BLAS_LIB} -lblas"

gfortran -o program.x program.f90 ${LALIB}
```

How To Compile



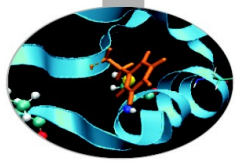
```
module load profile/advanced
module load intel/cs-xe-2013--binary
module load mkl/11.0.1--binary
```

C:

```
# remember to include the header file
#include "mkl.h"
# prefix for CBLAS (optional)
cblas_
LALIB="-I${MKL_INC} -L${MKL_LIB} -lmkl_intel_lp64 \
       -lmkl_sequential -lmkl_core"
icc -o program.x program.c ${LALIB}
icc -mkl -o program.x program.c
```

http://software.intel.com/en-us/articles/intel-mkl-link-line-advisor

Exercises:



1) Write a program that uses BLAS routines; at least one routine for each BLAS level. For example:

Level 1: DCOPY, DSCAL, DNRM2, DDOT

Level 2: DGEMV, DGER

Level 3: DGEMM

Print all matrices and vectors generated.

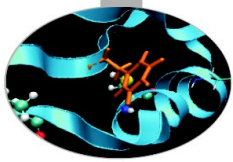
2) Write a program that uses the LAPACK routine DGESV. Print all matrices and vectors generated.

Ax=b ; b(i) = 207-i ;

A(i,j) = 10000 if i=j

A(i,j) = i+j/2 if i≠j

MAGMA



Matrix **A**lgebra for **G**PU and **M**ulticore **A**rchitecture

http://icl.cs.utk.edu/magma/

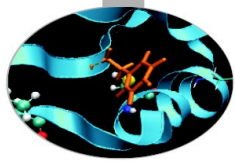
The MAGMA project aims to develop a dense linear algebra library similar to LAPACK but for heterogeneous/hybrid architectures, starting with current "Multicore+GPU" systems.

Methodology: CPU and GPU overlapping

MAGMA uses HYBRIDIZATION methodology based on

- Representing linear algebra algorithms as collections of TASKS and DATA DEPENDENCIES among them
- Properly SCHEDULING tasks' execution over multicore and GPU hardware components

MAGMA



CPU versus GPU interfaces

Why two different interfaces?

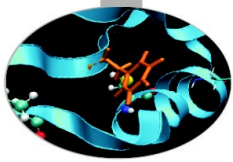
If data is already on the GPU

- pointer to GPU memory
- (some) additional memory allocation on CPU side

If data is already on the CPU

- no changes on the prototype
- internal overlap communication/computation (it uses pinned)
- (some) additional memory allocation on GPU side

MAGMA



How to compile/link

module load profile/advanced autoload magma/1.6.1--cuda--6.5.14

C/C++:

```
#include "magma.h"          #include "cublas.h"
magma_init();               magma_finalize();
```

FORTRAN:

```
USE magma
call magma_init()           call magma_finalize()
```

COMPILE:

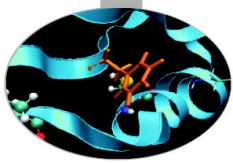
-I$MAGMA_INC -I$CUDA_INC -I$MKL_INC -fPIC -DHAVE_CUBLAS

LINKING:

-L$MAGMA_LIB -lmagma -L$CUDA_LIB -lcublas -lcudart -mkl

put MAGMA before CUDA and multi-threading library (like MKL)

MAGMA



How to use in the code

DGETRF: Computes an LU factorization of a general matrix A, using partial pivoting with row interchanges.

PROTOTYPE: **`DGETRF( M, N, A, LDA, IPIV, INFO )`**

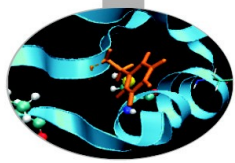
CPU interface:

```
FORTRAN:    call magmaf_dgetrf( M, N, A, lda, ipiv, info )
C:          magma_dgetrf( &M, &N, A, &lda, ipiv, &info );
```

GPU interface:

```
call cublas_set_matrix( M, N, size_of_elt, A, lda, d_A, ldda )
call magma_dgetrf_gpu( M, N, d_A, ldda, ipiv, info )
```

MKL on Intel Xeon Phi (MIC)



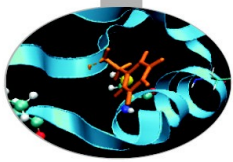
Intel released a version for Xeon Phi of the MKL mathematical libraries

MKL have three different usage models:

- Automatic offload (AO)
- Compiler assisted offload (CAO)
- Native execution

http://www.hpc.cineca.it/content/quick-guide-intel-mic-usage

MKL on Intel Xeon Phi (MIC)



Not all the MKL functions are enabled to AO. With this model offload is automatic and transparent. The library decides **when** to offload and **how much** to offload (workdivision).

Users can control parameters through environment variables or API. You can enable automatic offload with:

```
MKL_MIC_ENABLE=1
```

or

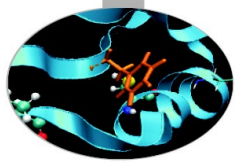
```
mkl_mic_enable()
```

MKL functions can be offloaded as other “ordinary” functions using the LEO pragmas.

All MKL functions can take advantage of the CAO model.

It's a more flexible option in terms of data management (you can use data persistence or mechanisms to hide the latency...)

MKL on MIC: CAO



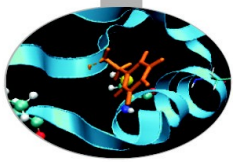
C/C++

```
#pragma offload target (mic) \
in (transa, transb, N, alpha, beta) \
in (A:length(matrix_elements)) in (B:length(matrix_elements)) \
inout (C:length(matrix_elements))
{
sgemm(&transa, &transb, &N, &N, &N, &alpha, A, &N, B, &N, &beta, C, &N);
}
```

Fortran

```
!dir$ attributes offload : mic : sgemm
!dir$ offload target(mic) &
!dir$ in (transa, transb, m, n, k, alpha, beta, lda, ldb, ldc), &
!dir$ in (a:length(ncola*lda)), in (b:length(ncolb*ldb)) &
!dir$ inout (c:length(n*ldc))
CALL sgemm (transa, transb,m,n,k,alpha,a,lda,b,ldb,beta,c,ldc)
```

MKL on MIC: Native mode



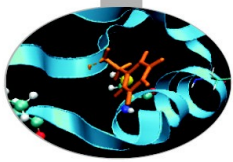
MKL libraries are also available when using the native mode. Tips:

- Use all the 240 threads: MIC_OMP_NUM_THREADS=240
- Set the thread affinity: MIC_KMP_AFFINITY = …

Compilation:

```
module load intel/cs-xe-2013--binary mkl/11.0.1--binary
source $INTEL_HOME/bin/compilervars.sh intel64

icc -o program.x program.c -openmp -mmic
    -I${MKLROOT}/include -L${MKLROOT}/lib/mic
    -lmkl_intel_lp64 -lmkl_core -lmkl_intel_thread
    -lpthread -lm
```

MKL on MIC: Native mode



MIC-native codes need to be executed inside the MIC card itself. In order to log into a MIC card you have to:

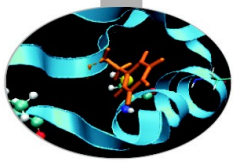
login to a MIC node with a PBS interactive session requesting at least 1 mic (nmics=1);

use the "qstat -f <job_id>" command in order to get the name of the specific MIC card assigned to you;

connect through ssh into the MIC card (in the example node018-mic1)

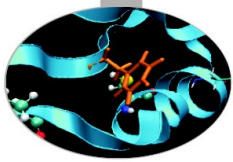
```
qsub -I -A <account_name> -l select=1:ncpus=1:nmics=1 -q debug
qsub: waiting for job 31085.node129 to start     (wait for long time)
 qsub: job 31085.node129 ready
...
qstat -f 31085.node129 | grep exec_vnode
...
exec_vnode = (node018:mem=1048576kb:ncpus=1+node018-mic1:nmics=1)
...
ssh node018-mic1
```

MKL on MIC: Native mode



For executing your native-MIC program, you need to set the LD_LIBRARY_PATH environment variable manually, by adding the path of the intel libraries specific for MIC execution:

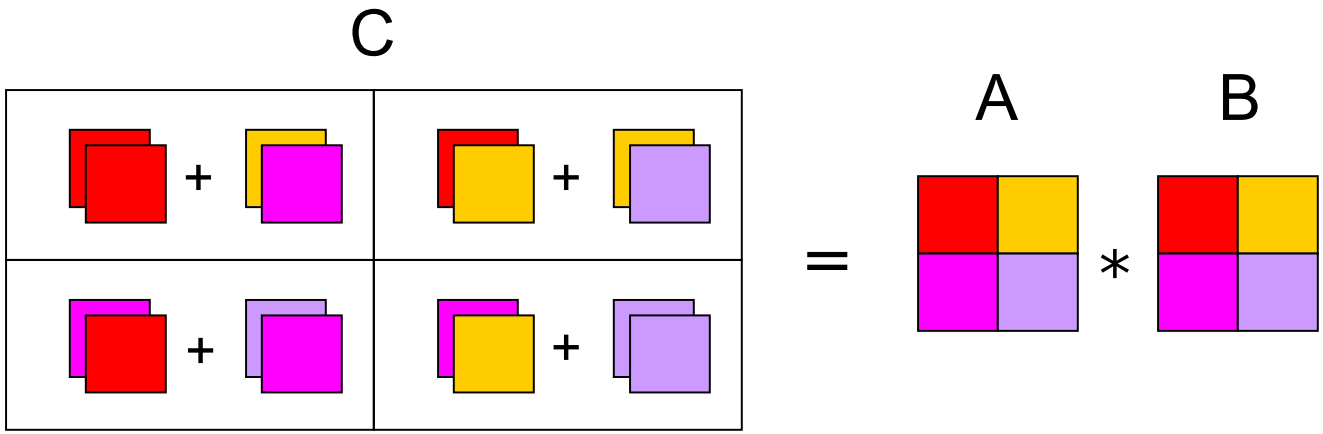
```
cd /path/to/the/working/directory/
export MIC_OMP_NUM_THREADS=60

export LD_LIBRARY_PATH=/cineca/prod/compilers/intel/cs-xe-2013/binary/lib/mic:${LD_LIBRARY_PATH}
export LD_LIBRARY_PATH=/cineca/prod/compilers/intel/cs-xe-2013/binary/mkl/lib/mic:${LD_LIBRARY_PATH}

./program.x > program.out
```



Block Operations

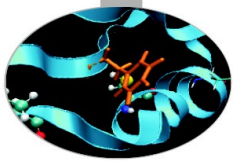
A block representation of a matrix operation constitutes the basic parallelization strategy for dense matrices.

For instance, a matrix-matrix product can be split in a sequence of smaller operations of the same type acting on subblocks of the original matrix



$$c_{ij} = \sum_{k=1}^{N} a_{ik} \cdot b_{kj}$$

Example: Partitioning into 2x2 Blocks



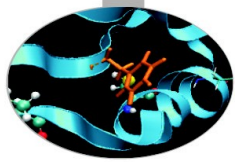
a_{11}	a_{12}	a_{13}	a_{14}	a_{15}	a_{16}	a_{17}	a_{18}	a_{19}
a_{21}	a_{22}	a_{23}	a_{24}	a_{25}	a_{26}	a_{27}	a_{28}	a_{29}
a_{31}	a_{32}	a_{33}	a_{34}	a_{35}	a_{36}	a_{37}	a_{38}	a_{39}
a_{41}	a_{42}	a_{43}	a_{44}	a_{45}	a_{46}	a_{47}	a_{48}	a_{49}
a_{51}	a_{52}	a_{53}	a_{54}	a_{55}	a_{56}	a_{57}	a_{58}	a_{59}
a_{61}	a_{62}	a_{63}	a_{64}	a_{65}	a_{66}	a_{67}	a_{68}	a_{69}
a_{71}	a_{72}	a_{73}	a_{74}	a_{75}	a_{76}	a_{77}	a_{78}	a_{79}
a_{81}	a_{82}	a_{83}	a_{84}	a_{85}	a_{86}	a_{87}	a_{88}	a_{89}
a_{91}	a_{92}	a_{93}	a_{94}	a_{95}	a_{96}	a_{97}	a_{98}	a_{99}

B_{11}	B_{12}	B_{13}	B_{14}	B_{15}
B_{21}	B_{22}	B_{23}	B_{24}	B_{25}
B_{31}	B_{32}	B_{33}	B_{34}	B_{35}
B_{41}	B_{42}	B_{43}	B_{44}	B_{45}
B_{51}	B_{52}	B_{53}	B_{54}	B_{55}

Block Representation

Next Step: distribute blocks among processors

Process Grid

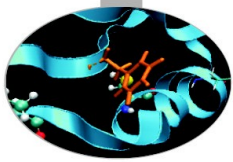


N processes are organized into a logical 2D mesh with p rows and q columns, such that p x q = N

q \ p	0	1	2
0	rank = 0	rank = 1	rank = 2
1	rank = 3	rank = 4	rank = 5

A process is referenced by its coordinates within the grid rather than a single number

Cyclic Distribution of Blocks



B_{11}	B_{12}	B_{13}	B_{14}	B_{15}
B_{21}	B_{22}	B_{23}	B_{24}	B_{25}
B_{31}	B_{32}	B_{33}	B_{34}	B_{35}
B_{41}	B_{42}	B_{43}	B_{44}	B_{45}
B_{51}	B_{52}	B_{53}	B_{54}	B_{55}

q

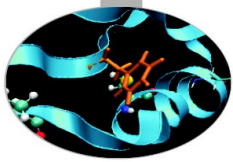
p

	0		1		2
0	B_{11}	B_{14}	B_{12}	B_{15}	B_{13}
	B_{31}	B_{34}	B_{32}	B_{35}	B_{33}
	B_{51}	B_{54}	B_{52}	B_{55}	B_{53}
1	B_{21}	B_{24}	B_{22}	B_{25}	B_{23}
	B_{41}	B_{44}	B_{42}	B_{45}	B_{43}

$$B_{h,k} \rightarrow (p,q) \qquad p = MOD(N_p + h - 1, N_p)$$
$$q = MOD(N_q + k - 1, N_q)$$

Blocks are distributed on processors in a cyclic manner on each index

Distribution of matrix elements



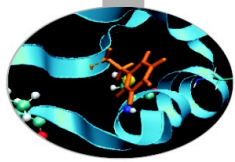
	0		1		2
0	B_{11}	B_{14}	B_{12}	B_{15}	B_{13}
	B_{31}	B_{34}	B_{32}	B_{35}	B_{33}
	B_{51}	B_{54}	B_{52}	B_{55}	B_{53}
1	B_{21}	B_{24}	B_{22}	B_{25}	B_{23}
	B_{41}	B_{44}	B_{42}	B_{45}	B_{43}

The indexes of a single element can be traced back to the processor

	0				1			2	
0	a_{11}	a_{12}	a_{17}	a_{18}	a_{13}	a_{14}	a_{19}	a_{15}	a_{16}
	a_{21}	a_{22}	a_{27}	a_{28}	a_{23}	a_{24}	a_{29}	a_{25}	a_{26}
	a_{51}	a_{52}	a_{57}	a_{58}	a_{53}	a_{54}	a_{59}	a_{55}	a_{56}
	a_{61}	a_{62}	a_{67}	a_{68}	a_{63}	a_{64}	a_{69}	a_{65}	a_{66}
	a_{91}	a_{92}	a_{97}	a_{98}	a_{93}	a_{94}	a_{99}	a_{95}	a_{96}
1	a_{31}	a_{32}	a_{37}	a_{38}	a_{33}	a_{34}	a_{39}	a_{35}	a_{36}
	a_{41}	a_{42}	a_{47}	a_{48}	a_{43}	a_{44}	a_{49}	a_{45}	a_{46}
	a_{71}	a_{72}	a_{77}	a_{78}	a_{73}	a_{74}	a_{79}	a_{75}	a_{76}
	a_{81}	a_{82}	a_{87}	a_{88}	a_{83}	a_{84}	a_{89}	a_{85}	a_{86}

myid=0	myid=1	myid=2	myid=3	myid=4	myid=5
p=0 q=0	p=0 q=1	p=0 q=2	p=1 q=0	p=1 q=1	p=1 q=2

Distribution of matrix elements



a_{11}	a_{12}	a_{13}	a_{14}	a_{15}	a_{16}	a_{17}	a_{18}	a_{19}
a_{21}	a_{22}	a_{23}	a_{24}	a_{25}	a_{26}	a_{27}	a_{28}	a_{29}
a_{31}	a_{32}	a_{33}	a_{34}	a_{35}	a_{36}	a_{37}	a_{38}	a_{39}
a_{41}	a_{42}	a_{43}	a_{44}	a_{45}	a_{46}	a_{47}	a_{48}	a_{49}
a_{51}	a_{52}	a_{53}	a_{54}	a_{55}	a_{56}	a_{57}	a_{58}	a_{59}
a_{61}	a_{62}	a_{63}	a_{64}	a_{65}	a_{66}	a_{67}	a_{68}	a_{69}
a_{71}	a_{72}	a_{73}	a_{74}	a_{75}	a_{76}	a_{77}	a_{78}	a_{79}
a_{81}	a_{82}	a_{83}	a_{84}	a_{85}	a_{86}	a_{87}	a_{88}	a_{89}
a_{91}	a_{92}	a_{93}	a_{94}	a_{95}	a_{96}	a_{97}	a_{98}	a_{99}

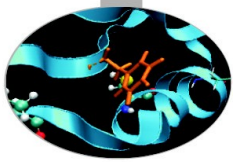
Logical View (Matrix)

a_{11}	a_{12}	a_{17}	a_{18}	a_{13}	a_{14}	a_{19}	a_{15}	a_{16}
a_{21}	a_{22}	a_{27}	a_{28}	a_{23}	a_{24}	a_{29}	a_{25}	a_{26}
a_{51}	a_{52}	a_{57}	a_{58}	a_{53}	a_{54}	a_{59}	a_{55}	a_{56}
a_{61}	a_{62}	a_{67}	a_{68}	a_{63}	a_{64}	a_{69}	a_{65}	a_{66}
a_{91}	a_{92}	a_{97}	a_{98}	a_{93}	a_{94}	a_{99}	a_{95}	a_{96}
a_{31}	a_{32}	a_{37}	a_{38}	a_{33}	a_{34}	a_{39}	a_{35}	a_{36}
a_{41}	a_{42}	a_{47}	a_{48}	a_{43}	a_{44}	a_{49}	a_{45}	a_{46}
a_{71}	a_{72}	a_{77}	a_{78}	a_{73}	a_{74}	a_{79}	a_{75}	a_{76}
a_{81}	a_{82}	a_{87}	a_{88}	a_{83}	a_{84}	a_{89}	a_{85}	a_{86}

Local View (CPUs)

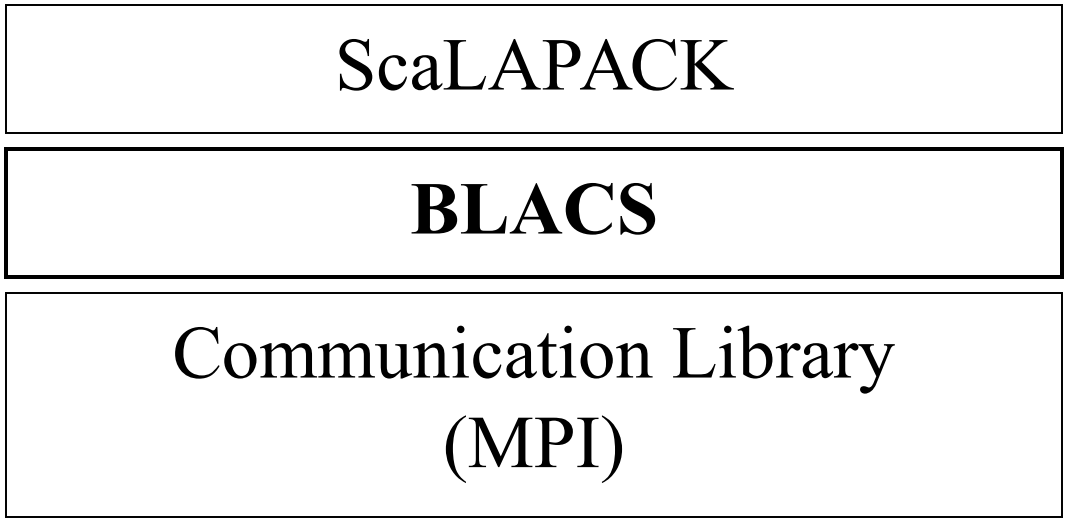
http://acts.nersc.gov/scalapack/hands-on/datadist.html
http://acts.nersc.gov/scalapack/hands-on/addendum.html

BLACS

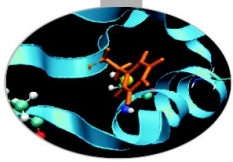


(**B**asic **L**inear **A**lgebra **C**ommunication **S**ubprograms)

The BLACS project is an ongoing investigation whose purpose is to create a linear algebra oriented message passing interface that may be implemented efficiently and uniformly across a large range of distributed memory platforms



BLACS Process Grid



Processes are distributed on a 2D mesh using row-order or column-order (ORDER='R' or 'C'). Each process is assigned a row/column ID as well as a scalar ID

column ID

row ID

	0	1	2	3
0	0	1	2	3
1	4	5	6	7

COMM_ROW
Communications along rows

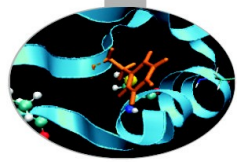
COMM_COL
Communications along columns

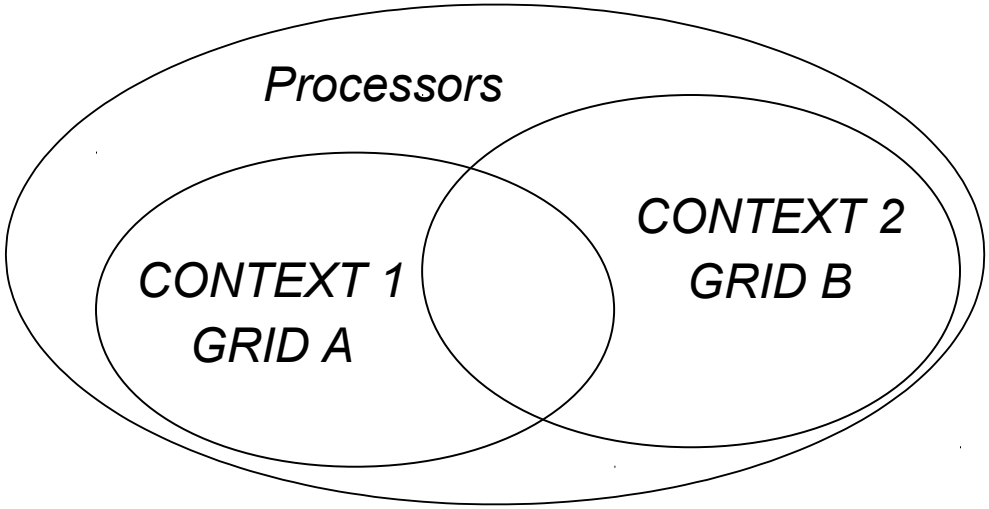
MPI task ID (rank)

BLACS_GRIDINIT(CONTEXT, ORDER, NPROW, NPCOL)

Initialize a 2D grid of NPROW x NPCOL processes with an order specified by ORDER in a given CONTEXT

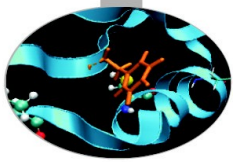
CONTEXT





Context ⟷ *MPI Communicators*

BLACS: Subroutines



BLACS_PINFO(MYPNUM, NPROCS)

Query the system for process ID MYPNUM (output) and number of processes NPROCS (output).

BLACS_GET(ICONTEXT, WHAT, VAL)

Query to BLACS environment based on WHAT (input) and ICONTEXT (input)
If WHAT=0, ICONTEX is ignored and the routine returns in VAL (output) a value indicating the default system context

BLACS_GRIDINIT(CONTEXT, ORDER, NPROW, NPCOL)

Initialize a 2D mesh of processes

BLACS_GRIDINFO(CONTEXT, NPROW, NPCOL, MYROW, MYCOL)

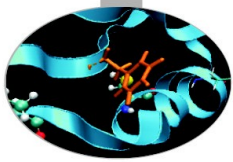
Query CONTEXT for the dimension of the grid of processes (NPROW, NPCOL) and for row-ID and col-ID (MYROW, MYCOL)

BLACS_GRIDEXIT(CONTEXT)

Release the 2D mesh associated with CONTEXT

BLACS_EXIT(CONTINUE) Exit from BLACS environment

BLACS: Subroutines



Point to Point Communication

DGESD2D(ICONTEX,M,N,A,LDA,RDEST,CDEST)

Send matrix A(M,N) to process (RDEST,CDEST)

DGERV2D(ICONTEX,M,N,A,LDA,RSOUR,CSOUR)

Receive matrix A(M,N) from process (RSOUR,CSOUR)

Broadcast

DGEBS2D(ICONTEX,SCOPE,TOP,M,N,A,LDA)

Execute a Broadcast of matrix A(M,N)

DGEBR2D(ICONTEX,SCOPE,TOP,M,N,A,LDA,RSRC,CSRC)

Receive matrix A(M,N) sent from process (RSRC,CSRC) with a broadcast operation

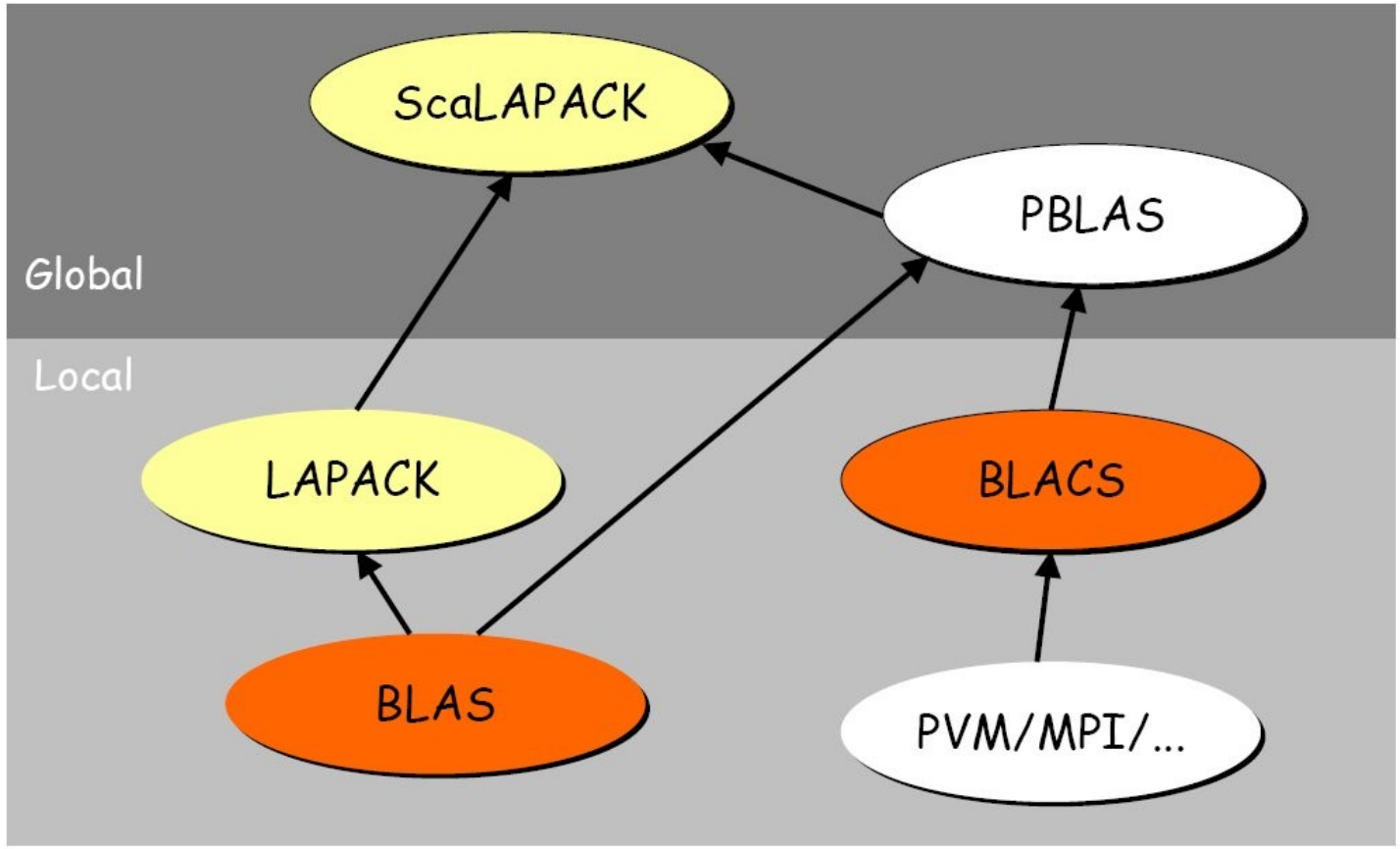
Global reduction

DGSUM2D(ICONTXT,SCOPE,TOP,M,N,A,LDA,RDST,CDST)

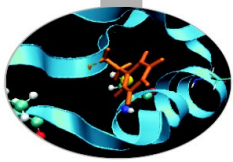
Execute a parallel element-wise sum of matrix A(M,N) and store the result in process (RDST,CDST) buffer

http://www.netlib.org/blacs/BLACS/QRef.html

Dependencies

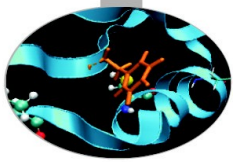


ScaLAPACK and PBLAS: template



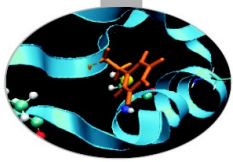
1. *Initialize BLACS*
2. *Initialize BLACS grids*
3. *Distribubute matrix among grid processes (cyclic block distribution)*
4. *Calls to ScaLAPACK/PBLAS routines*
5. *Harvest results*
6. *Release BLACS grids*
7. *Close BLACS environment*

Example:



```
      !     Initialize the BLACS

      CALL BLACS_PINFO( IAM, NPROCS )

      !     Set the dimension of the 2D processors grid

      CALL GRIDSETUP( NPROCS, NPROW, NPCOL ) ! User defined

      write (*,100) IAM, NPROCS, NPROW, NPCOL
100   format(' MYPE ',I3,', NPE ',I3,', NPE ROW ',I3,', NPE COL ',I3)

      !     Initialize a single BLACS context

      CALL BLACS_GET( -1, 0, CONTEXT )
      CALL BLACS_GRIDINIT( CONTEXT, 'R', NPROW, NPCOL )
      CALL BLACS_GRIDINFO( CONTEXT, NPROW, NPCOL, MYROW, MYCOL )
      .....
      .....
      CALL BLACS_GRIDEXIT( CONTEXT )
      CALL BLACS_EXIT( 0 )
```

Descriptor

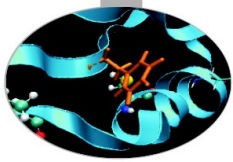


The Descriptor is an integer array that stores the information required to establish the mapping between each global array entry and its corresponding process and memory location.

Each matrix MUST be associated with a Descriptor. Anyhow it's responsibility of the programmer to distribute the matrix coherently with the Descriptor.

```
DESCA( 1 ) = 1          DESCA( 2 ) = ICTXT
DESCA( 3 ) = M          DESCA( 4 ) = N
DESCA( 5 ) = MB         DESCA( 6 ) = NB
DESCA( 7 ) = RSRC       DESCA( 8 ) = CSRC
DESCA( 9 ) = LDA
```

Descriptor Initialization



DESCINIT(DESCA, M, N, MB, NB, RSRC, CSRC, ICTXT, LDA, INFO)

DESCA(9) (global output) matrix A ScaLAPACK Descriptor

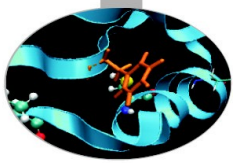
M, N (global input) global dimensions of matrix A

MB, NB (global input) blocking factors used to distribute matrix A

RSRC, CSRC (global input) process coordinates over which the first element of A is distributed

ICTXT (global input) BLACS context handle, indicating the global context of the operation on matrix

LDA (local input) leading dimension of the local array (depends on process!)



ScaLAPACK tools

http://www.netlib.org/scalapack/tools

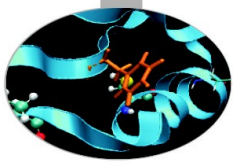
Computation of the local matrix size for a M x N matrix distributed over processes in blocks of dimension MB x NB

```
Mloc = NUMROC( M, MB, ROWID, 0, NPROW )
Nloc = NUMROC( N, NB, COLID, 0, NPCOL )
allocate( Aloc( Mloc, Nloc ) )
```

Computation of local and global indexes

```
iloc = INDXG2L( i, MB, ROWID, 0, NPROW )
jloc = INDXG2L( j, NB, COLID, 0, NPCOL )

i = INDXL2G( iloc, MB, ROWID, 0, NPROW )
j = INDXL2G( jloc, NB, COLID, 0, NPCOL )
```

ScaLAPACK tools



Compute the process to which a certain global element `(i,j)` belongs

```
iprow = INDXG2P( i, MB, ROWID, 0, NPROW )
jpcol = INDXG2P( j, NB, COLID, 0, NPCOL )
```

Define/read a local element, knowing global indexes

```
CALL PDELSET( A, i, j, DESCA, aval )
```

local array

input value

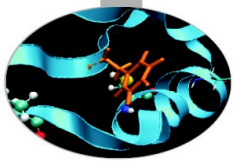
```
CALL PDELGET( SCOPE, TOP, aval, A, i, j, DESCA )
```

output value

character*1 topology of the broadcast ‘D’ or ‘I’

character*1 scope broadcast ‘R’, ‘C’ or ‘A’

PBLAS/ScaLAPACK subroutines



Routines name scheme: PXYYZZZ

Parallel

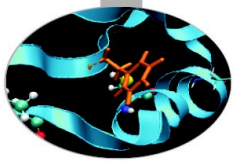
X data type → S = REAL
D = DOUBLE PRECISION
C = COMPLEX
Z = DOUBLE COMPLEX

YY matrix type (GE = general, SY = symmetric, HE = hermitian)

ZZZ algorithm used to perform computation

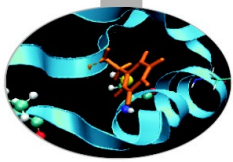
Some auxiliary functions don't make use of this naming scheme!

Calls to ScaLAPACK routines



- It's responsibility of the programmer to correctly distribute a global matrix before calling ScaLAPACK routines
- ScaLAPACK routines are written using a message passing paradigm, therefore each subroutine access directly ONLY local data
- Each process of a given CONTEXT must call the same ScaLAPACK routine...
- … providing in input its local portion of the global matrix
- Operations on matrices distributed on processes belonging to different contexts are not allowed

PBLAS subroutines



matrix multiplication: C = A * B (level 3)

```
PDGEMM('N', 'N', M, N, L, 1.0d0, A, 1, 1, DESCA, B, 1, 1, DESCB, 0.0d0, C, 1,
       1, DESCC)
```

matrix transposition: C = A′ (level 3)

```
PDTRAN( M, N, 1.0d0, A, 1, 1, DESCA, 0.0d0, C, 1, 1, DESCC )
```

matrix times vector: Y = A * X (level 2)

```
PDGEMV('N', M, N, 1.0d0, A, 1, 1, DESCA, X, 1, JX, DESCX, 1, 0.0d0, Y, 1, JY,
       DESCY, 1)
```

X(1:N,JX:JX)

Y(1:M,JY:JY)

row / column swap: X ⇔ Y (level 1)

```
PDSWAP( N, X, IX, JX, DESCX, INCX, Y, IY, JY, DESCY, INCY )
```

X(IX,JX:JX+N-1) if INCX = M_X, X(IX:IX+N-1,JX) if INCX = 1 and INCX <> M_X,

Y(IY,JY:JY+N-1) if INCY = M_Y, Y(IY:IY+N-1,JY) if INCY = 1 and INCY <> M_Y.

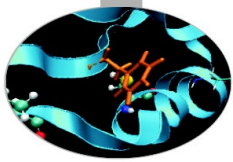
scalar product: p = X′·Y (level 1)

```
PDDOT( N, p, X, IX, JX, DESCX, INCX, Y, IY, JY, DESCY, INCY )
```

X(IX,JX:JX+N-1) if INCX = M_X, X(IX:IX+N-1,JX) if INCX = 1 and INCX <> M_X,

Y(IY,JY:JY+N-1) if INCY = M_Y, Y(IY:IY+N-1,JY) if INCY = 1 and INCY <> M_Y.

ScaLAPACK subroutines



Eigenvalues and, optionally, eigenvectors: A Z = w Z

```
PDSYEV( 'V', 'U', N, A, 1, 1, DESCA, W, Z, 1, 1, DESCZ, WORK, LWORK, INFO )
```

'U' use upper triangular part of A
'L' use lower triangular part of A

'V' compute eigenvalues and eigenvectors
'N' compute eigenvalues only

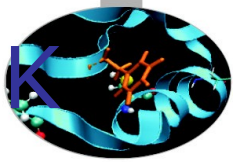
if **lwork = -1**, compute workspace dimension.
Return it in **work(1)**

Print matrix

```
PDLAPRNT( M, N, A, 1, 1, DESCA, IR, IC, CMATNM, NOUT, WORK)
```

M	global first dimension of A	**IR, IC**	coordinates of the printing process
N	global second dimension of A	**CMATNM**	character*(*) title of the matrix
A	local part of matrix A	**NOUT**	output fortran units (0 stderr, 6 stdout)
DESCA	descriptor of A	**WORK**	workspace

BLAS/LAPACK vs. PBLAS/ScaLAPACK



- **"P" prefix for parallel routines!**
- **The "Leading dimension" turns into a "Descriptor"**
- **Global indexes are additional parameters of the subroutine**

BLAS routine:

```
DGEMM('N', 'N', M, N, L, 1.0, A(1,1), LDA, B(1,1), LDB, 0.0, C(1,1),LDC)
```

PBLAS routine:

```
PDGEMM('N', 'N', M, N, L, 1.0, A, 1, 1, DESCA, B, 1, 1, DESCB, 0.0, C,
       1, 1, DESCC)
```

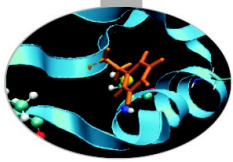
LAPACK routine:

```
DGESV(N, NRHS, A(I,J), LDA, IPIV, B(I,1), LDB, INFO)
```

SCALAPACK routine:

```
PDGESV(N, NRHS, A, I, J, DESCA, IPIV, B, I, 1, DESCB, INFO)
```

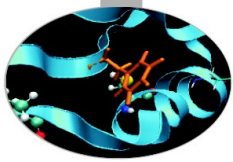
ScaLAPACK Users' Guide



http://www.netlib.org/scalapack/slug/

At the end of the “Contents” you can find the “Quick Reference Guides” for ScaLAPACK, PBLAS and BLACS routines

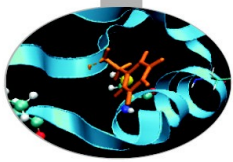
BLACS/ScaLAPACK + MPI



It is quite tricky to write a program using BLACS as a communication library, therefore:

→ MPI and BLACS must be used consistently!

Initialize MPI + BLACS



```
CALL MPI_INIT(IERR)
CALL MPI_COMM_SIZE(MPI_COMM_WORLD,NPROC,IERR)
CALL MPI_COMM_RANK(MPI_COMM_WORLD,MPIME,IERR)
!
comm_world = MPI_COMM_WORLD
!
ndims = 2
dims  = 0
CALL MPI_DIMS_CREATE( NPROC, ndims, dims, IERR)

NPROW = dims(1)   !  cartesian direction 0
NPCOL = dims(2)   !  cartesian direction 1

!     Get a default BLACS context
!
CALL BLACS_GET( -1, 0, ICONTEXT )

!     Initialize a default BLACS context
CALL BLACS_GRIDINIT(ICONTEXT, 'R', NPROW, NPCOL)
CALL BLACS_GRIDINFO(ICONTEXT, NPROW, NPCOL, ROWID, COLID)

CALL MPI_COMM_SPLIT(comm_world, COLID, ROWID, COMM_COL, IERR)
CALL MPI_COMM_RANK(COMM_COL, coor(1), IERR)
!
CALL MPI_COMM_SPLIT(comm_world, ROWID, COLID, COMM_ROW, IERR)
CALL MPI_COMM_RANK(COMM_ROW, coor(2), IERR)
```

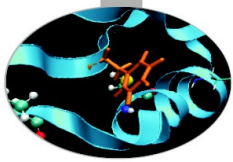
Initialize MPI environment

Compute the dimensions of a 2D mesh compatible with NPROCS processes

Initialize BLACS process grid of size nprow x npcol

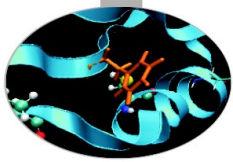
Create a row and a column communicator using BLACS indexes rowid and colid

Matrix redistribution



```
! Distribute matrix A0 (M x N) from root node to all processes in context ictxt.
!
call SL_INIT(ICTXT, NPROW, NPCOL)
call SL_INIT(rootNodeContext, 1, 1) ! create 1 node context
                                    ! for loading matrices
call BLACS_GRIDINFO( ICTXT, NPROW, NPCOL, MYROW, MYCOL)
!
! LOAD MATRIX ON ROOT NODE AND CREATE DESC FOR IT
!
if (MYROW == 0 .and. MYCOL == 0) then
   NRU = NUMROC( M, M, MYROW, 0, NPROW )
   call DESCINIT( DESCA0, M, N, M, N, 0, 0, rootNodeContext, max(1, NRU), INFO )
else
   DESCA0(1:9) = 0
   DESCA0(2) = -1
end if
!
!  CREATE DESC FOR DISTRIBUTED MATRIX
!
NRU = NUMROC( M, MB, MYROW, 0, NPROW )
CALL DESCINIT( DESCA, M, N, MB, NB, 0, 0, ICTXT, max(1, NRU), INFO )
!
!  DISTRIBUTE DATA
!
if (debug) write(*,*) "node r=", MYROW, "c=", MYCOL, "M=", M, "N=", N
call PDGEMR2D( M, N, A0, 1, 1, DESCA0, A, 1, 1, DESCA, DESCA( 2 ) )
```

How To Compile (GNU)

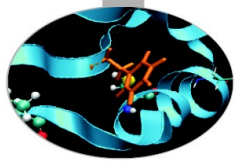


```
# load these modules on Eurora
module load autoload profile/advanced
module load scalapack/2.0.2--openmpi--1.6.5--gnu--4.6.3

LALIB="-L${SCALAPACK_LIB} -lscalapack \
       -L${LAPACK_LIB} -llapack -L${BLAS_LIB} -lblas"
```

FORTRAN:

```
mpif90 -o program.x program.f90 ${LALIB}
```

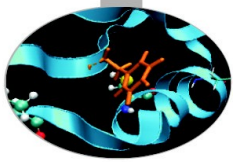
How To Compile (GNU)



C:

```
// CBLACS PROTOTYPES
extern void Cblacs_pinfo( int* mypnum, int* nprocs );
extern void Cblacs_get( int context, int request, int* value );
extern int  Cblacs_gridinit( int* context, char* order, int np_row,
                             int np_col );
extern void Cblacs_gridinfo( int context, int* np_row, int* np_col,
                             int* my_row, int* my_col );
extern void Cblacs_gridexit( int context );
extern void Cblacs_exit( int error_code );
extern void Cblacs_barrier( int context, char* scope );
```

How To Compile (GNU)

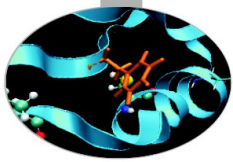


C:

```
// BLACS/SCALAPACK PROTOTYPES
int numroc_( int* n, int* nb, int* iproc, int* isrcproc, int* nprocs );
void descinit_( int * desca, int * m, int * n, int * mb, int * nb,
     int * irsrc, int * icsrc, int * context,int * llda, int * info );
void pdgesv_( int * n, int * nrhs, double * A, int * ia, int * ja,
     int * desca, int * ipiv, double * b, int * ib, int * jb, int * descb,
     int * info );
void pdelset_( double * A, int * i, int * j, int * desca, double * alpha );
void pdlaprnt_( int * m, int * n, double * A, int * ia, int * ja,
     int * desca, int * irprnt, int * icprn, char * cmatnm, int * nout,
     double * work );
```

```
mpicc -o program.x program.c ${LALIB} -lgfortran
```

How To Compile (INTEL, MKL)



 # load these modules on Eurora

```
module load autoload intelmpi/4.1.1—binary
module load mkl/11.0.1--binary
```

C:

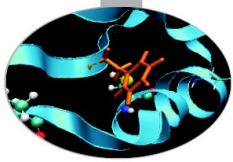
(remember to include mkl.h, mkl_scalapack.h, mkl_blacs.h)

```
mpicc -o program.x program.c -mkl -lmkl_scalapack_lp64 \
      -lmkl_blacs_intelmpi_lp64 -lpthread -lm
```

FORTRAN:

```
mpif90 -o program.x program.f90 -mkl -lmkl_scalapack_lp64 \
       -lmkl_blacs_intelmpi_lp64 -lpthread -lm
```

Exercises:



1) Write a program that initializes the BLACS environment, define a matrix and write it to file. Then modifies the program to read the matrix from the previous file and rewrite it to standard output. For I/O use ScaLAPACK routines.

2) Write a program that uses PBLAS routines; at least one routine for each PBLAS level. For example:

Level 1: PDCOPY, PDSCAL, PDNRM2, PDDOT

Level 2: PDGEMV, PDGER

Level 3: PDGEMM

3) Write a program that uses the ScaLAPACK routine PDGESV. Print in files all matrices and vectors generated.

Ax=b ; b(i) = 207-i ;

A(i,j) = 10000 if i=j

A(i,j) = i+j/2 if i≠j

Thanks for your attention!