21st Summer School of PARALLEL COMPUTING

July 2 - 13, 2012 (Italian)
September 3 - 14, 2012 (English)

Scalable Linear Algebra

Nicola Spallanzani – n.spallanzani@cineca.it
SuperComputing, Applications and Innovation Department
CINECA

Basic Linear Algebra Algorithms

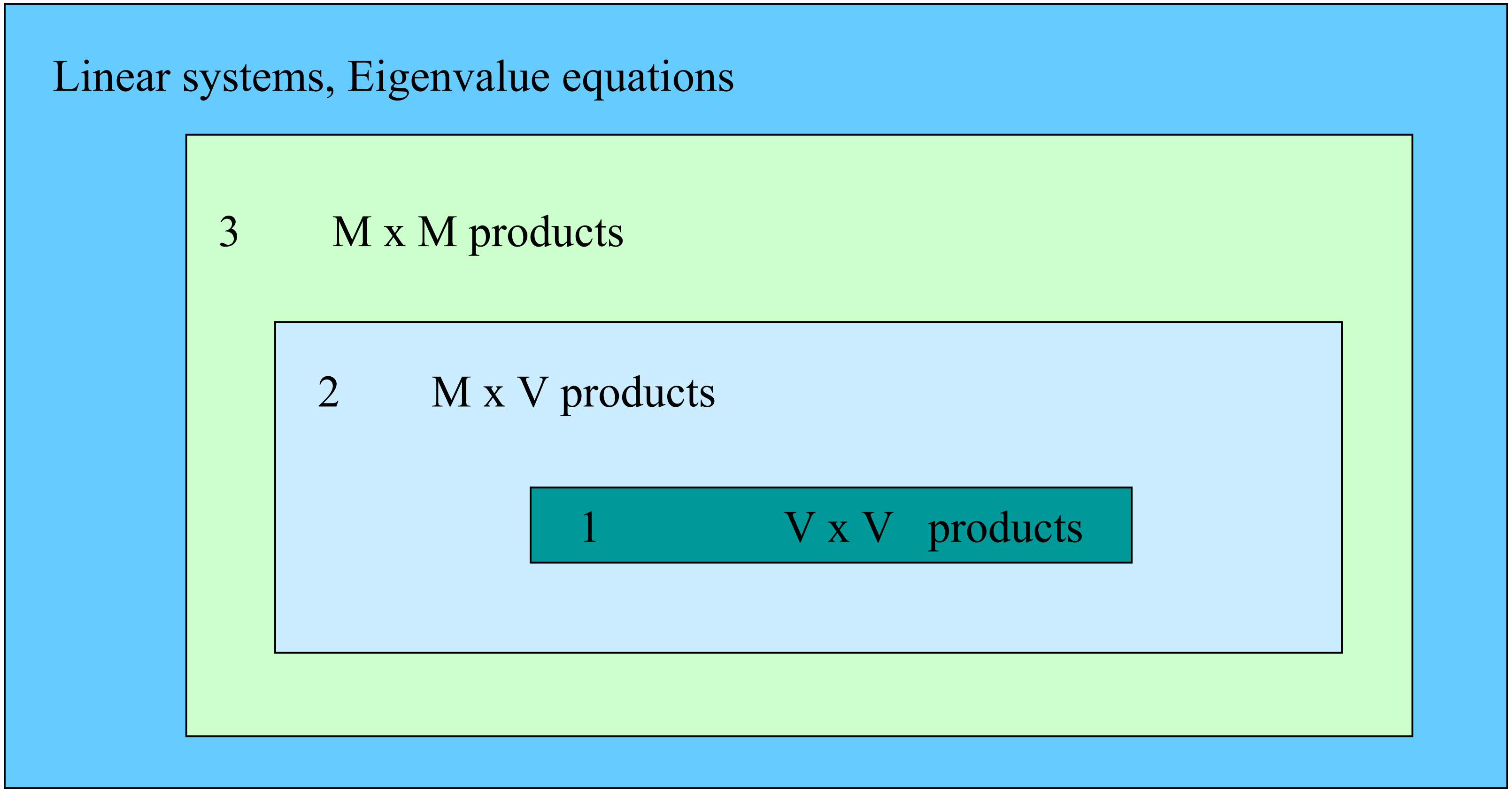
Linear algebra constitutes the core of most technical-scientific applications

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

Linear Systems $A_{ij} x_j = b_i$

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

Linear Algebra is Hierarchical



Linear systems, Eigenvalue equations

3 M x M products

2 M x V products

1 V x V products

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

- blas
- lapack
- pblas
- scalapak
- arpack
- parpack
- PETSc

blas, lapack → Serial Linear Algebra Packages

essl	(IBM AIX)
mkl	(Intel)
acml	(AMD)
magma	(ICL – Univ. Tennessee)

pblas, scalapak → Parallel Linear Algebra Packages (dense matrices)

plasma	(ICL – Univ. Tennessee)

arpack, parpack → Eigenvalues Problems (sparse matrices)

PETSc → Sparse Linear Systems

(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

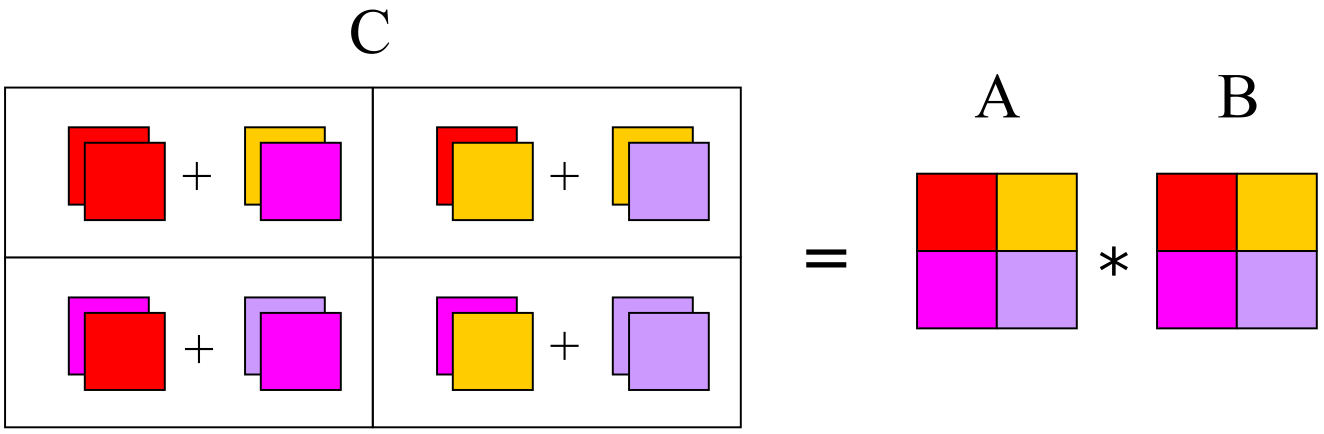
- **Computational** routines
  to perform a distinct computational task

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

Block Operations

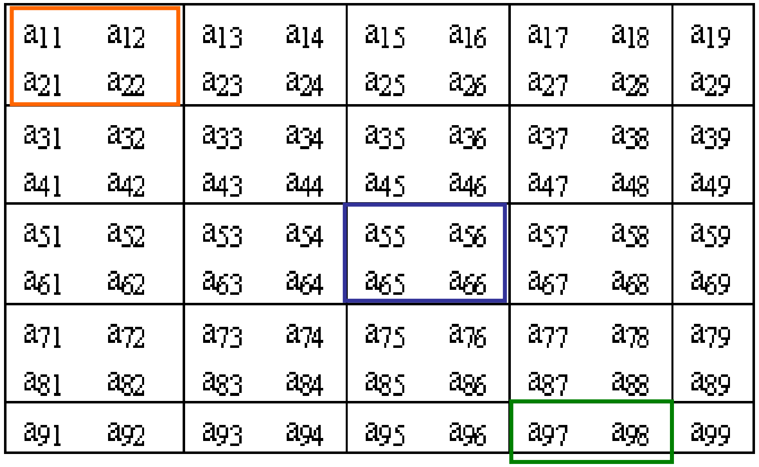
A block representation of a matrix operation constitutes the basic parallelization strategy for dense matrices.

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

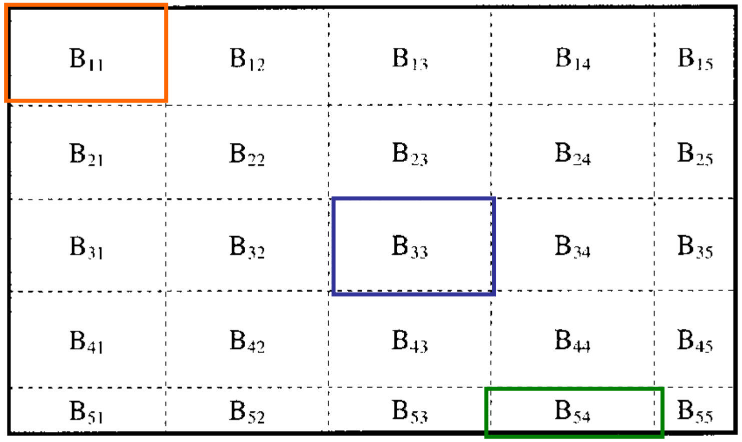


$$c_{ij} = \sum_{k=1}^{N} a_{ik} \cdot b_{kj}$$

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

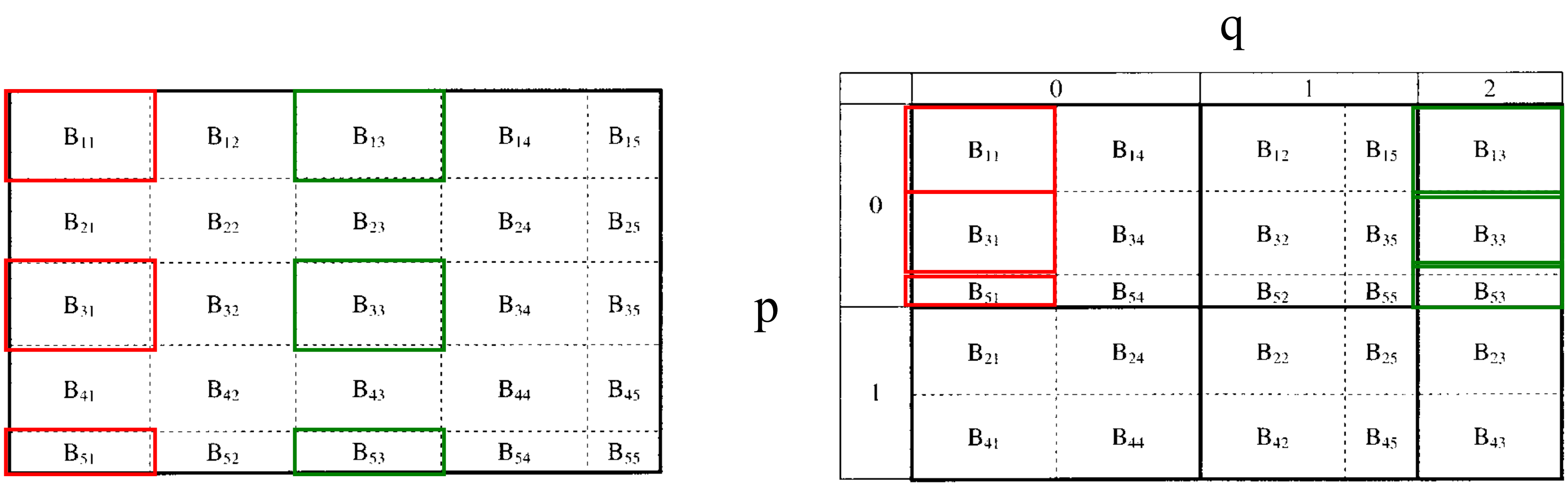
N processes are organized into a logical 2D mesh with p rows and q columns, such that p x q = N

p

		0	1	2
q	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}

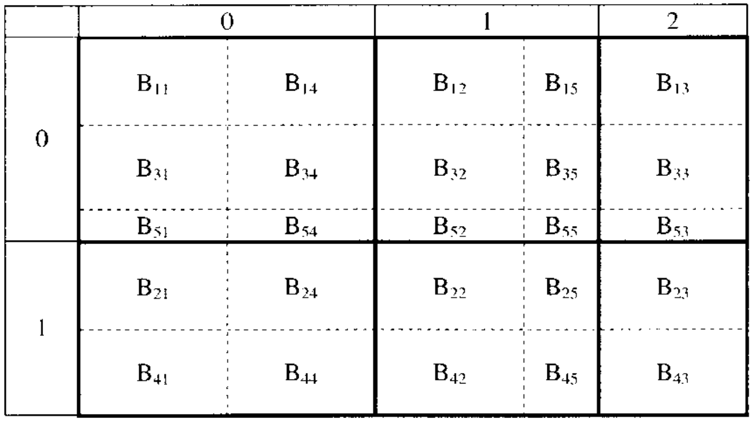
	0		1		2
0	B_{11}	B_{14}	B_{12}	B_{15}	B_{13}
	B_{31}	B_{34}	B_{32}	B_{35}	B_{33}
	B_{51}	B_{54}	B_{52}	B_{55}	B_{53}
1	B_{21}	B_{24}	B_{22}	B_{25}	B_{23}
	B_{41}	B_{44}	B_{42}	B_{45}	B_{43}

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

$$q = MOD(N_q + k - 1, N_q)$$

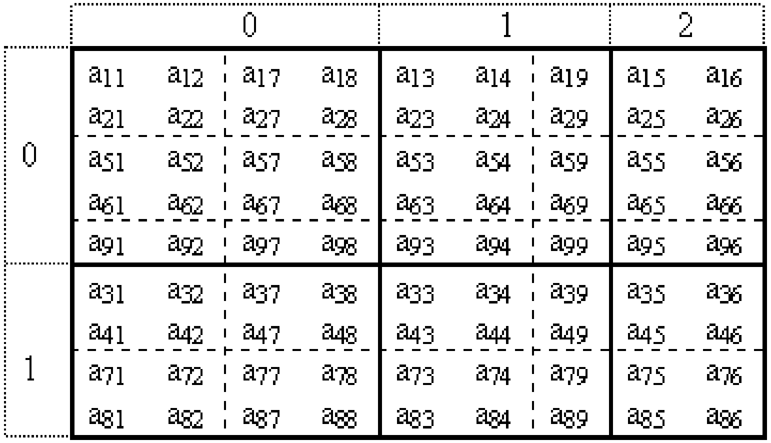
Blocks are distributed on processors in a cyclic manner on each index

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}

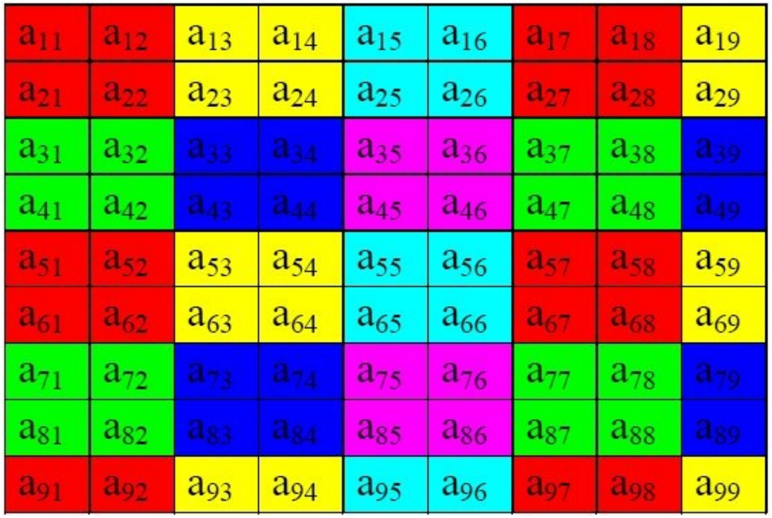
The indexes of a single element can be traced back to the processor



	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}

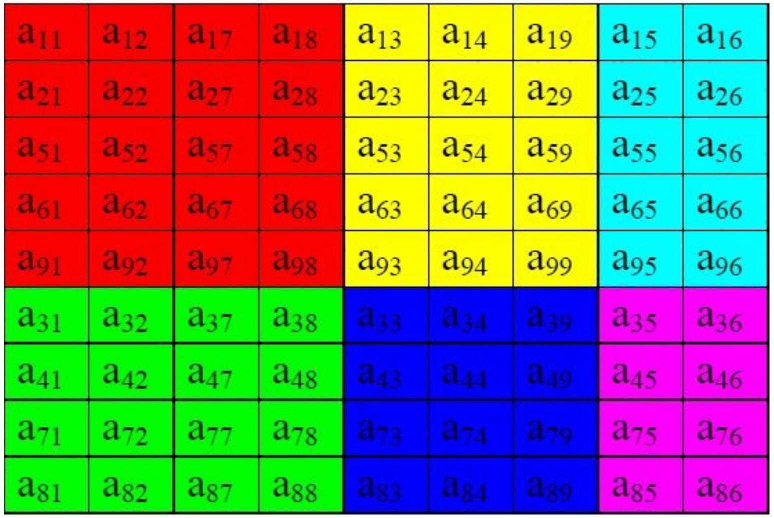
myid=0	myid=1	myid=2	myid=3	myid=4	myid=5
p=0 q=0	p=0 q=1	p=0 q=2	p=1 q=0	p=1 q=1	p=1 q=2

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}

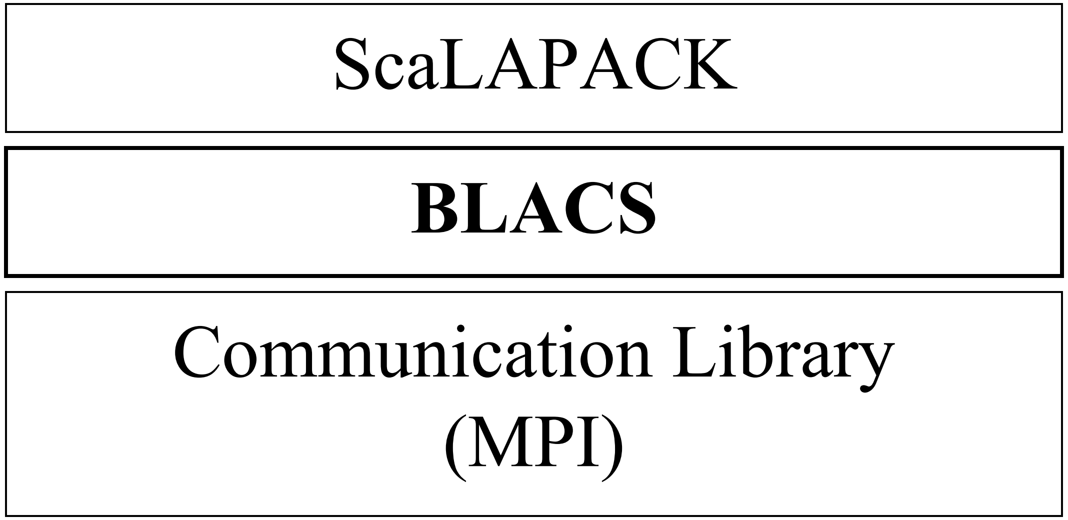
Local View (CPUs)

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



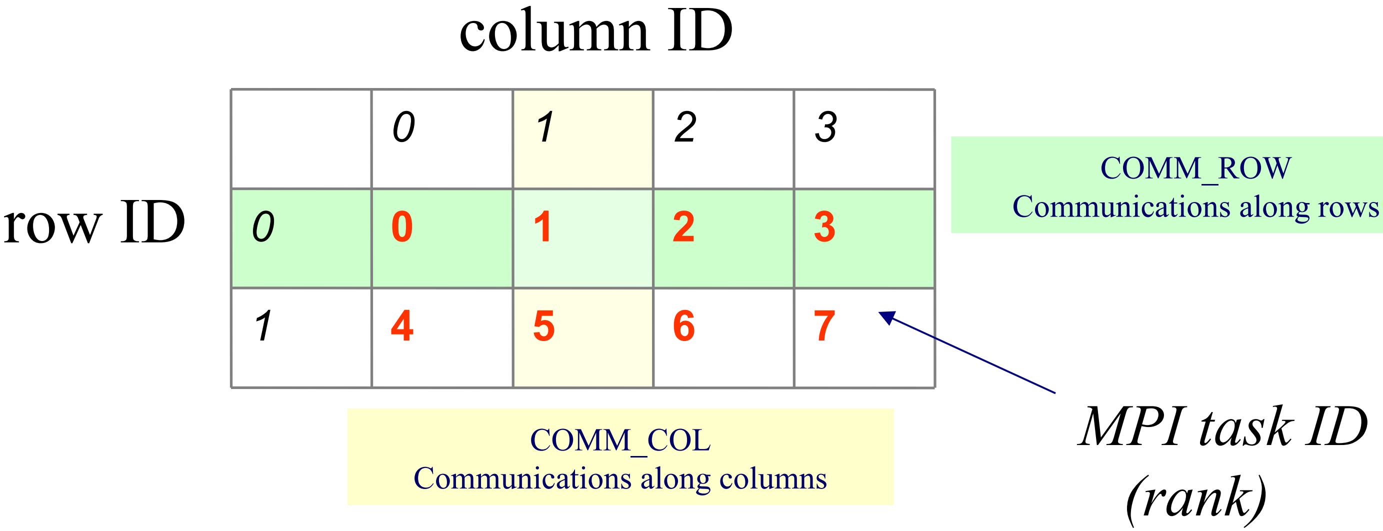
ScaLAPACK

BLACS

Communication Library (MPI)

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

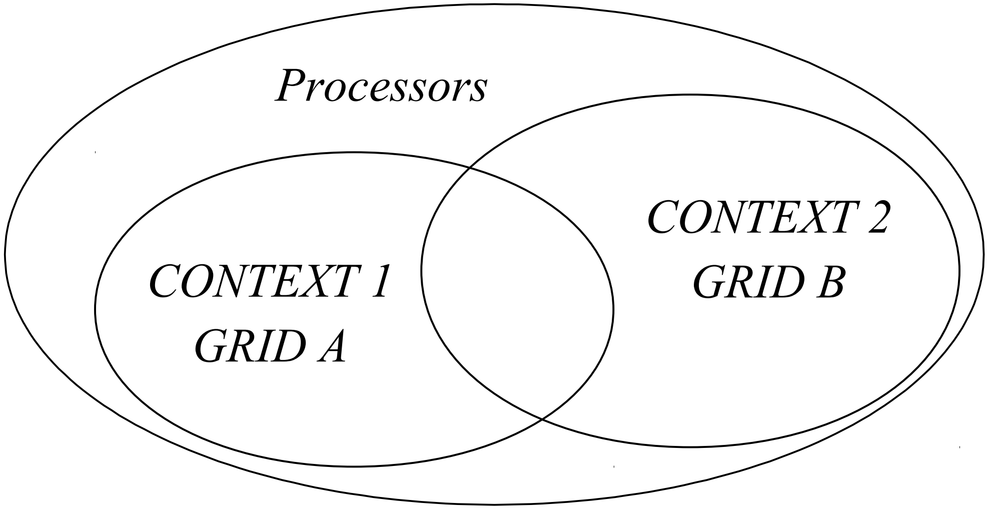
COMM_COL
Communications along columns

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



Processors

CONTEXT 1
GRID A

CONTEXT 2
GRID B

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

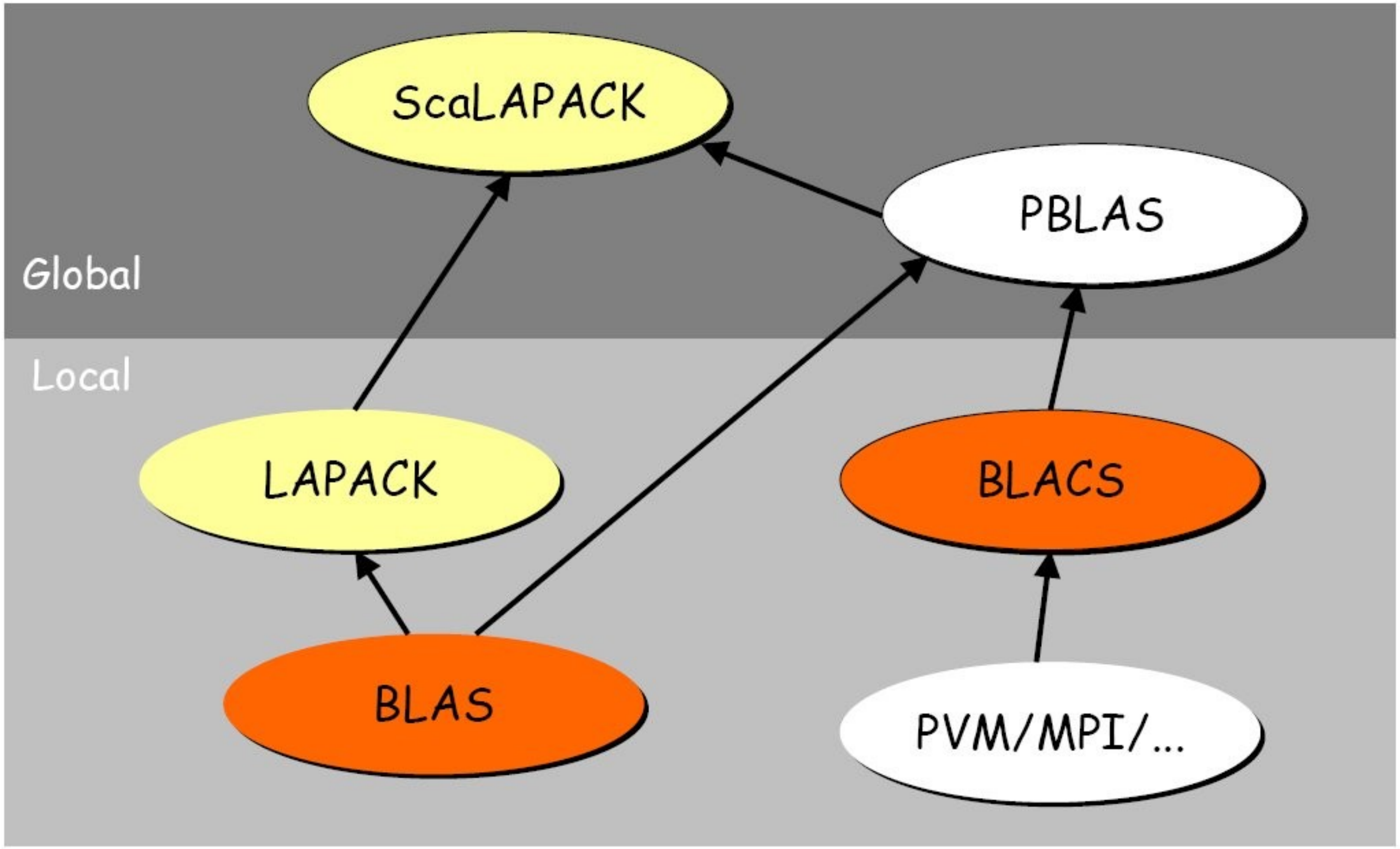
Global reduction

`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 )

      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( Nloc, Mloc ) )
```

Computation of 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

Schema del nome delle routines: 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

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

‘V’ compute eigenvalues and eigenvectors
‘N’ compute eigenvalues only

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

SCALAPACK routine:

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

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
!
```

Initialize MPI environment

```
ndims = 2
dims  = 0
CALL MPI_DIMS_CREATE( NPROC, ndims, dims, IERR)

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

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

```
!     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)
```

Initialize BLACS process grid of size nprow x npcol

```
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)
```

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 ) )
```

MAGMA

Matrix Algebra for GPU and Multicore Architecture

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

Hybridization means...

- Panels (Level 2 BLAS) are factored on CPU using LAPACK
- Trailing matrix updates (Level 3 BLAS) are done on the GPU using “look-ahead”

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

C/C++:

```
#include "magma.h"
```

FORTRAN:

```
USE magma
```

COMPILE:

```
-I$(MAGMADIR)/include -I$(CUDADIR)/include
```

LINKING:

```
-L$(MAGMADIR)/lib -lmagma -lmagmablas
$(MAGMADIR)/lib/libmagma.a $(MAGMADIR)/lib/libmagma
```

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:

```
call 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 )
```