Parallel Programming Using the Global Arrays Toolkit

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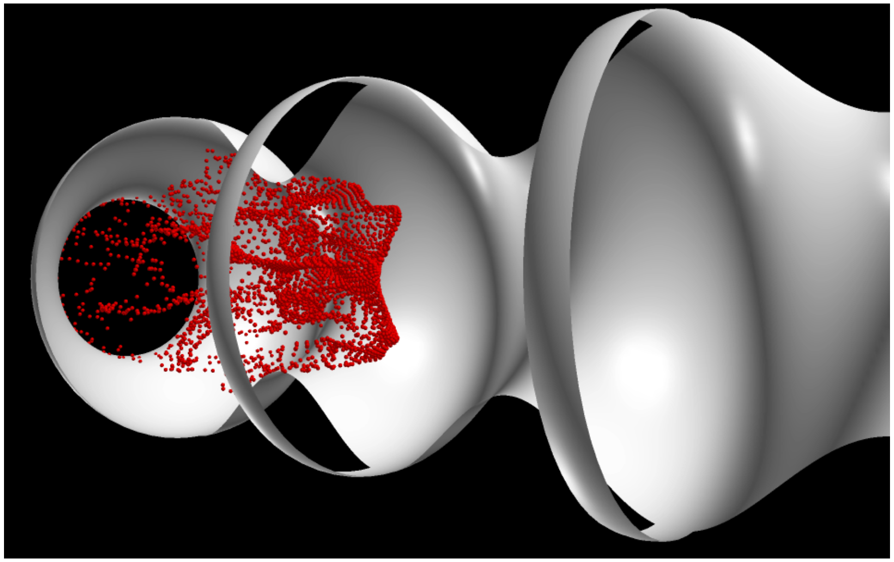
Global Arrays

- Developed over 20 years
- Under active development and focusing on preparing for future exascale platforms
- Available across platforms from PCs to leadership machines
- Easy access to distributed data on multiprocessor machines
  - High programmer productivity
- Library available from: http://www.emsl.pnl.gov/docs/global

Outline of the Tutorial

- Overview of parallel programming
- Introduction to Global Arrays programming model
- Basic GA commands
- Advanced features of the GA Toolkit
- Current and future developments in GA



Why Parallel?

- When to Parallelize:
  - Program takes too long to execute on a single processor
  - Program requires too much memory to run on a single processor
  - Program contains multiple elements that are executed or could be executed independently of each other
- Advantages of parallel programs:
  - Single processor performance is not increasing. The only way to improve performance is to write parallel programs.
  - Data and operations can be distributed amongst N processors instead of 1 processor. Codes execute potentially N times as quickly.
- Disadvantages of parallel programs:
  - They are bad for your mental health

Parallel vs Serial

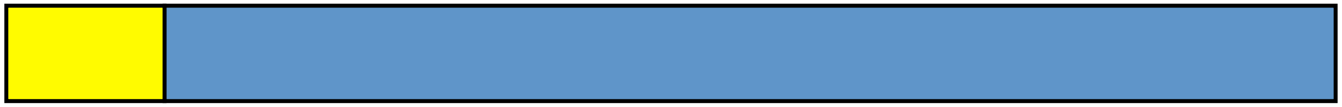
- Parallel codes can divide the work and memory required for application execution amongst multiple processors
- New costs are introduced into parallel codes:
  - Communication
  - Code complexity
  - New dependencies

Communication

- Parallel applications require data to be communicated from one processor to another at some point
- Data can be communicated by having processors exchanging data via messages (message-passing)
- Data can be communicated by having processors directly write or read data in another processors memory (onesided)

Data Transfers

- The amount of time required to transfer data consists of two parts
  - Latency: the time to initiate data transfer, independent of data size
  - Transfer time: the time to actually transfer data once the transfer is started, proportional to data size



Latency

Data Transfer

Because of latency costs, a single large message is preferred over many small messages

Parallel Efficiency

- Strong Scaling:

  For a given size problem, the time to execute is inversely proportional to the number of processors used. If you want to get your answers faster, you want a strong scaling program.

- Weak Scaling:

  If the problem size increases in proportion to the number of processors, the execution time is constant. If you want to run larger calculations, you are looking for weak scaling.

- Speedup:

  The ratio of the execution time on N processors to the execution time on 1 processor. If your code is linearly scaling (the best case) then speedup is equal to the number of processors.

- Strong Scaling and Weak Scaling are not incompatible. You can have both.

Sources of Parallel Inefficiency

- Communication
  - Message latency is a constant regardless of number of processors
  - Not all message sizes decrease with increasing numbers of processors
  - Number of messages per processor may increase with number of processors, particularly for global operations such as synchronizations, etc.
- Load Imbalance
  - Some processors are assigned more work than others resulting in processors that are idle

Note: parallel inefficiency is like death and taxes. It’s inevitable. The goal of parallel code development is to put off as long as possible the point at which the inefficiencies dominate.

Increasing Scalability

- Design algorithms to minimize communication
  - Exploit data locality
  - Aggregate messages
- Overlapping computation and communication
  - On most high end platforms, computation and communication use non-overlapping resources. Communication can occur simultaneously with computation
  - Onesided non-blocking communication and double buffering
- Load balancing
  - Static load balancing: partition calculation at startup so that each processor has approximately equal work
  - Dynamic load balancing: structure algorithm to repartition work while calculation is running. Note that dynamic load balancing generally increases the other source of parallel inefficiency, communication.

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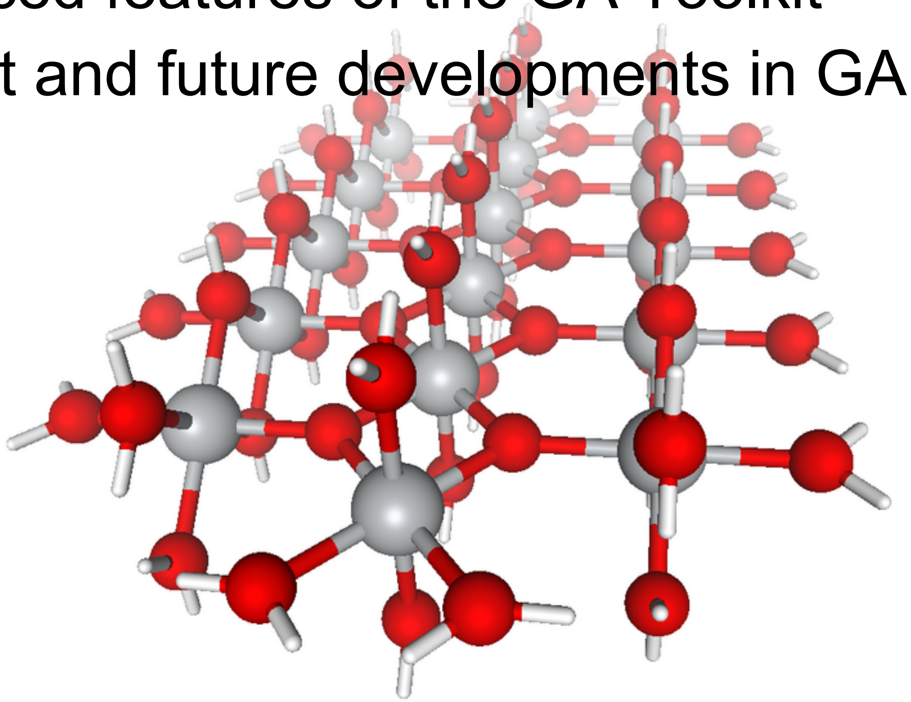

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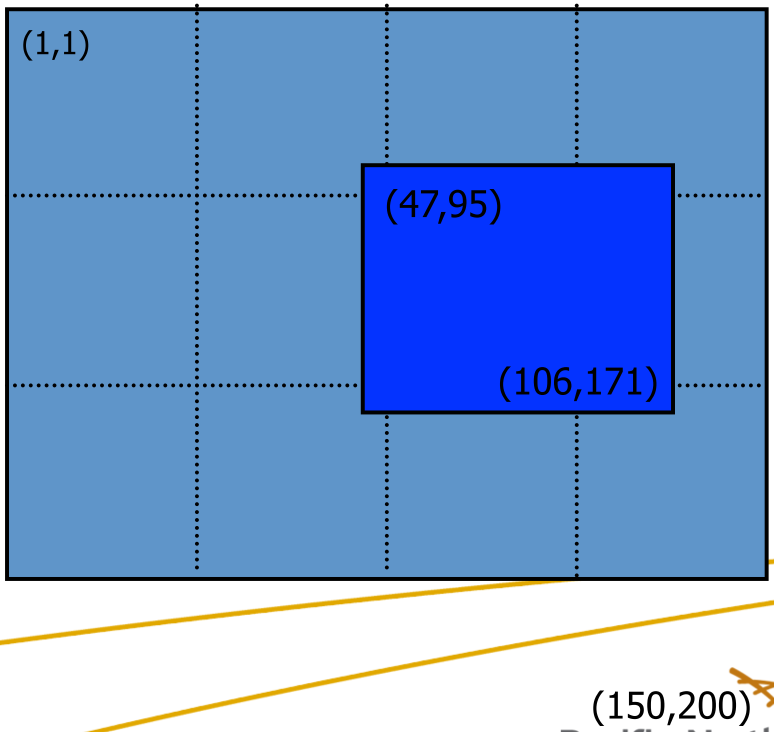
Distributed Data vs Shared Memory

Shared Memory:

Data is in a globally accessible address space, any processor can access data by specifying its location using a global index

Data is mapped out in a natural manner (usually corresponding to the original problem) and access is easy. Information on data locality is obscured and leads to loss of performance.

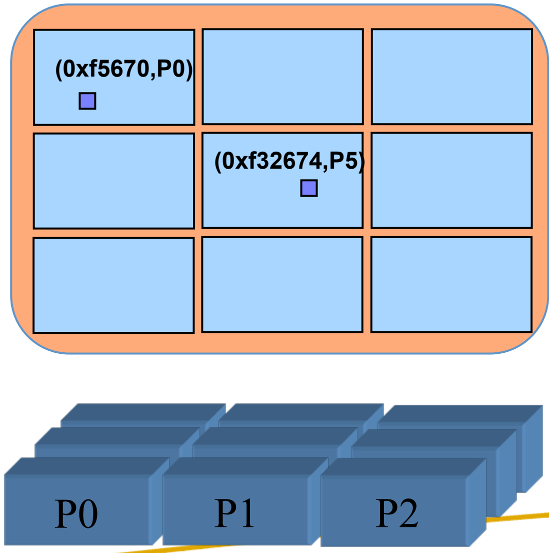


Distributed vs Shared Data View

Distributed Data:

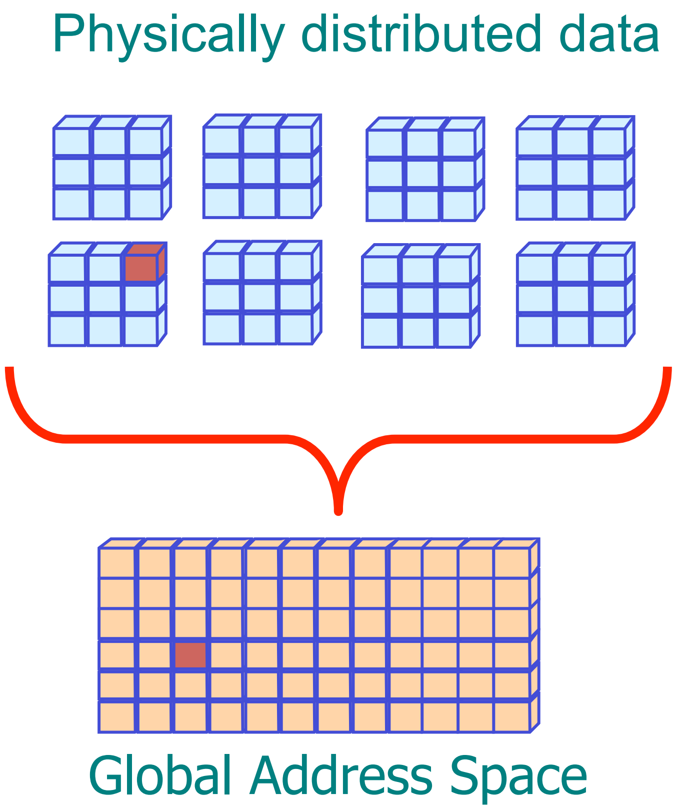
Data is explicitly associated with each processor, accessing data requires specifying the location of the data on the processor and the processor itself.

Data locality is explicit but data access is complicated. Distributed computing is typically implemented with message passing (e.g. MPI)



Global Arrays

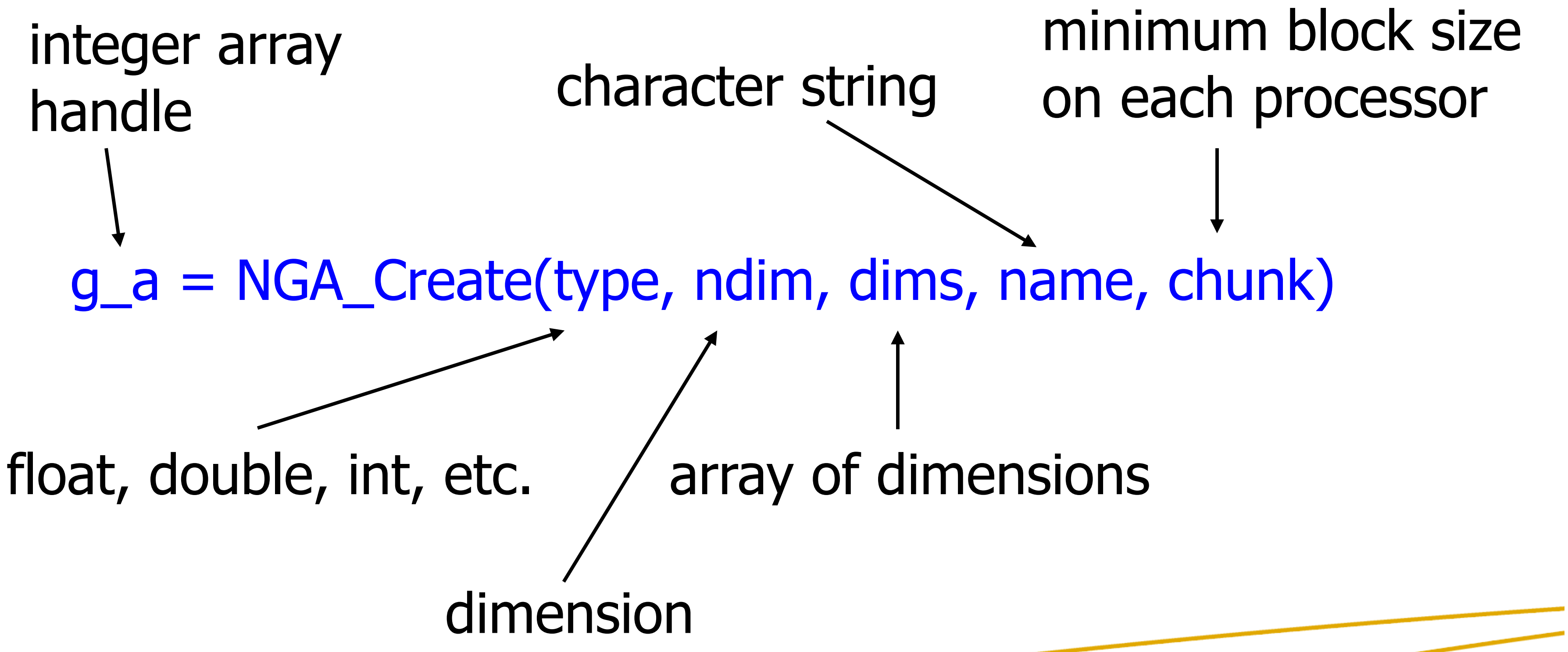
Distributed dense arrays that can be accessed through a shared memory-like style



single, shared data structure/ global indexing

e.g., access A(4,3) rather than buf(7) on task 2

Creating Global Arrays



integer array handle

character string

minimum block size on each processor

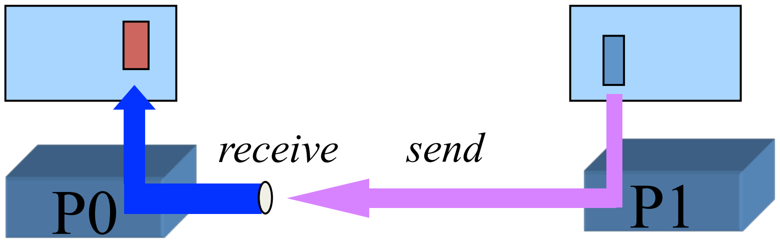
```
g_a = NGA_Create(type, ndim, dims, name, chunk)
```

float, double, int, etc.

array of dimensions

dimension

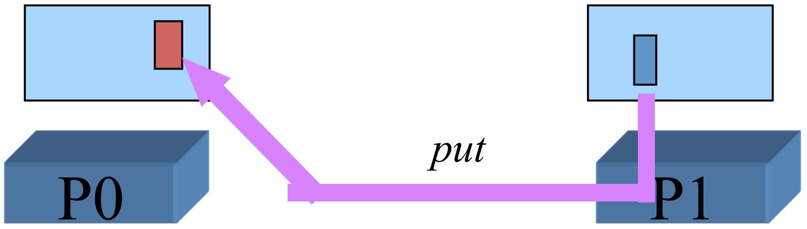
One-sided Communication



message passing
MPI

Message Passing:

Message requires cooperation on both sides. The processor sending the message (P1) and the processor receiving the message (P0) must both participate.



one-sided communication
SHMEM, ARMCI, MPI-2-1S

One-sided Communication:

Once message is initiated on sending processor (P1) the sending processor can continue computation. Receiving processor (P0) is not involved. Data is copied directly from switch into memory on P0.

Remote Data Access in GA vs MPI

Message Passing:

```
identify size and location of data
blocks

loop over processors:
    if (me = P_N) then
        pack data in local message
        buffer
        send block of data to
        message buffer on P0
    else if (me = P0) then
        receive block of data from
        P_N in message buffer
        unpack data from message
        buffer to local buffer
    endif
end loop

copy local data on P0 to local buffer
```

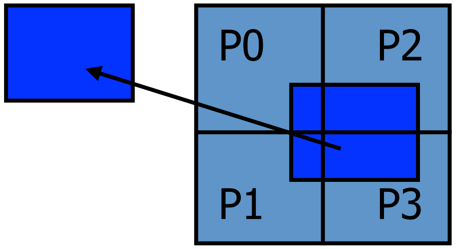
Global Arrays:

NGA_Get(g_a, lo, hi, buffer, ld);

Global Array handle

Global upper and lower indices of data patch

Local buffer and array of strides

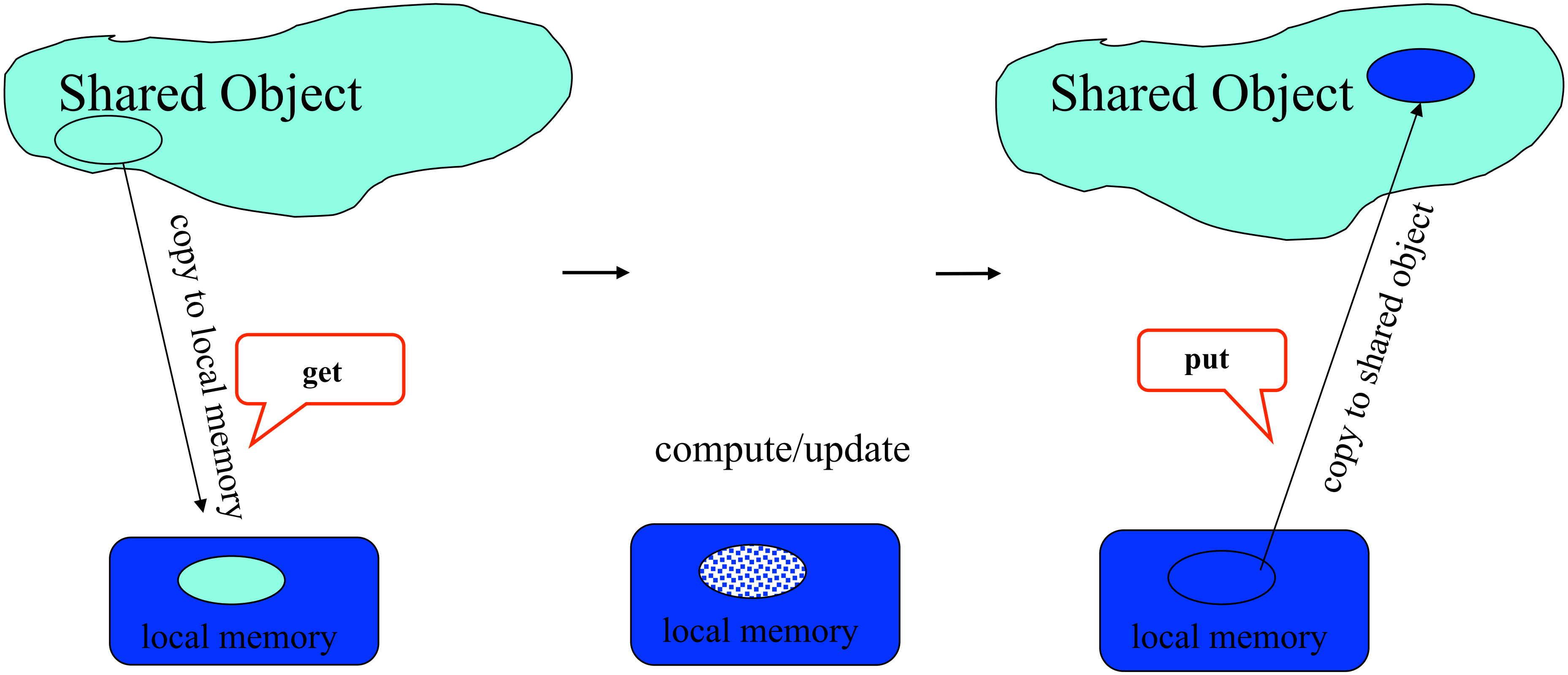


Onesided vs Message Passing

- Message-passing
  - Communication patterns are regular or at least predictable
  - Algorithms have a high degree of synchronization
  - Data consistency is straightforward

- One-sided
  - Communication is irregular
    - Load balancing
  - Algorithms are asynchronous
    - But also can be used for synchronous algorithms
  - Data consistency must be explicitly managed

GLOBAL ARRAY MODEL OF COMPUTATIONS



Global Arrays vs. Other Models

Advantages:

- Inter-operates with MPI
  - Use more convenient global-shared view for multi-dimensional arrays, but can use MPI model wherever needed
- Data-locality and granularity control is explicit with GA's get-compute-put model, unlike the non-transparent communication overheads with other models (except MPI)
- Library-based approach: does not rely upon smart compiler optimizations to achieve high performance

Disadvantage:

- Data consistency must be explicitly managed

Global Arrays (cont.)

- Shared data model in context of distributed dense arrays
- Much simpler than message-passing for many applications
- Complete environment for parallel code development
- Compatible with MPI
- Data locality control similar to distributed memory/ message passing model
- Extensible
- Scalable

Data Locality in GA

What data does a processor own?

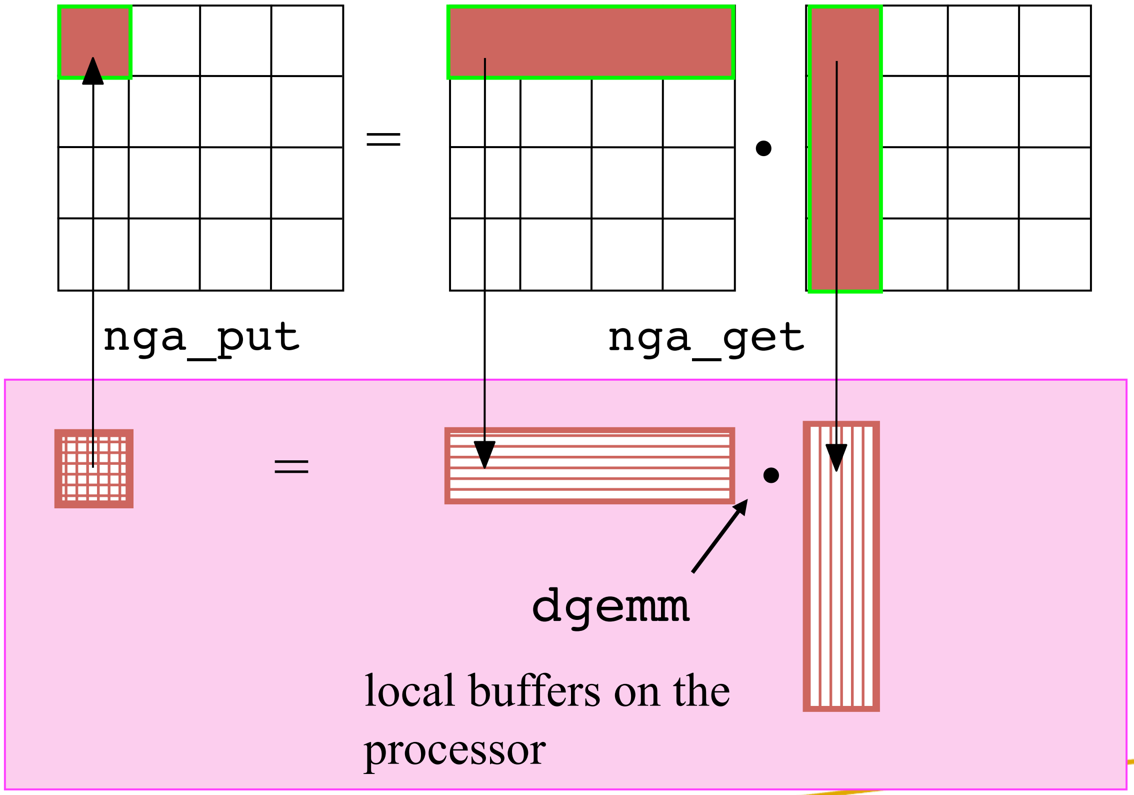
```
NGA_Distribution(g_a, iproc, lo, hi);
```

Where is the data?

```
NGA_Access(g_a, lo, hi, ptr, ld)
```

Use this information to organize calculation so that maximum use is made of locally held data

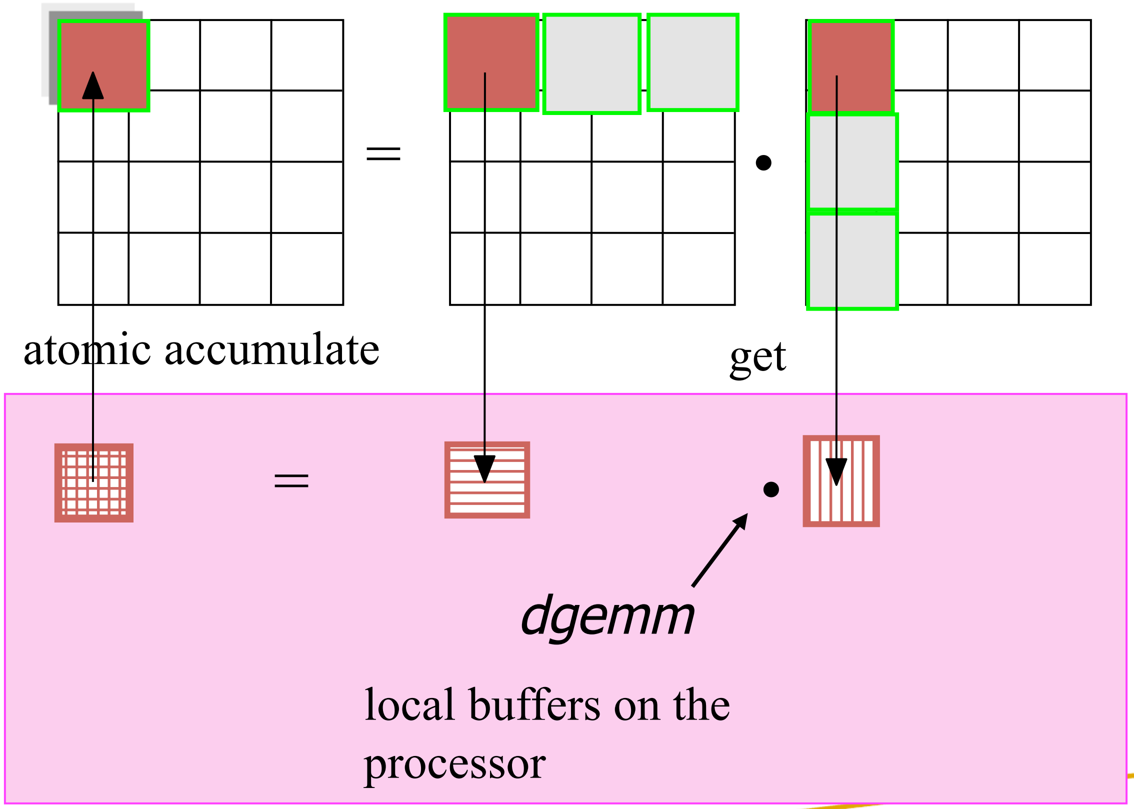
Example: Matrix Multiply



global arrays representing matrices

local buffers on the processor

Matrix Multiply
(a better version)



local buffers on the processor

more scalable!
(less memory,
higher parallelism)

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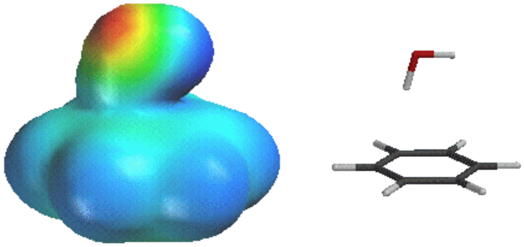
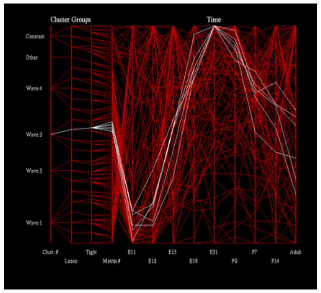
Application Areas

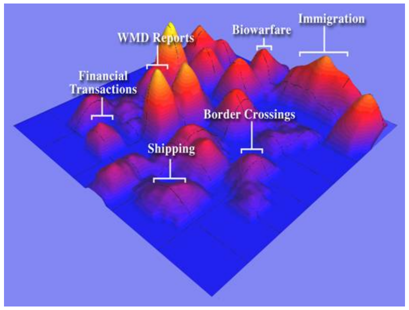


electronic structure chemistry

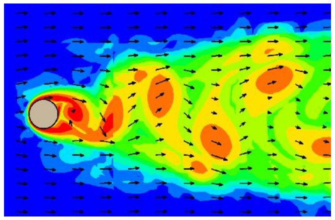
Major area



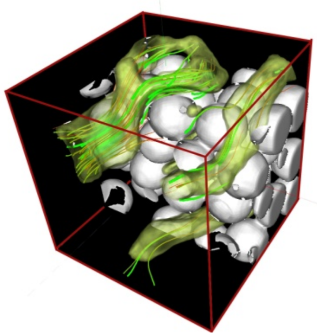
bioinformatics



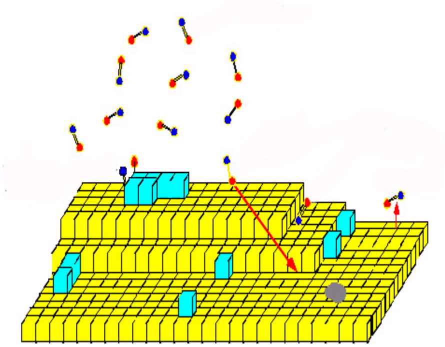
visual analytics



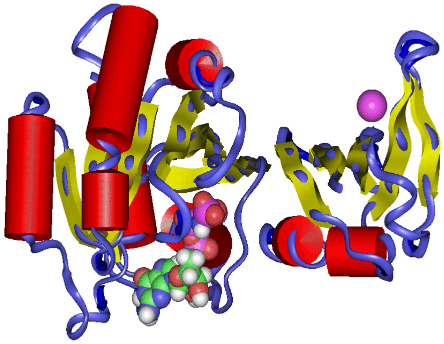
fluid dynamics



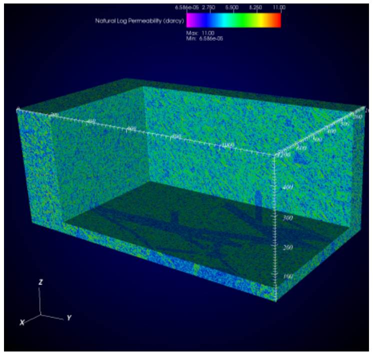
smoothed particle hydrodynamics



material sciences



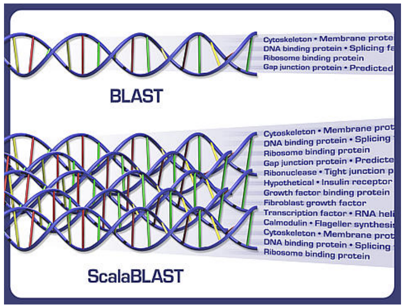
molecular dynamics



hydrology

Others: financial security forecasting, astrophysics, biology, climate analysis

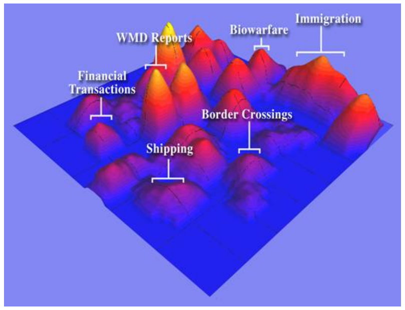
Recent Applications


Cytoskeleton • Membrane prote
DNA binding protein • Splicing fa
Ribosome binding protein
Gap junction protein • Predicted
BLAST
Cytoskeleton • Membrane prot
DNA binding protein • Splicing
Ribosome binding protein
Gap junction protein • Predicte
Ribonuclease • Tight junction p
Hypothetical • Insulin receptor
Growth factor binding protein
Fibroblast growth factor
Transcription factor • RNA heli
Calmodulin • Flageller synthesis
Cytoskeleton • Membrane prot
DNA binding protein • Splicing
Ribosome binding protein
ScalaBLAST

ScalaBLAST

C. Oehmen and J. Nieplocha. ScalaBLAST: "A scalable implementation of BLAST for high performance data-intensive bioinformatics analysis." IEEE Trans. Parallel

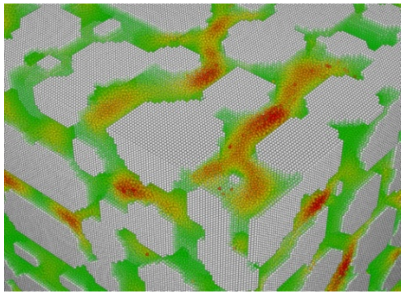
Distributed Systems, Vol. 17, No. 8, 2006



Parallel Inspire

Krishnan M, SJ Bohn, WE Cowley, VL Crow, and J Nieplocha, "Scalable Visual Analytics of Massive Textual Datasets", Proc. IEEE International Parallel and Distributed

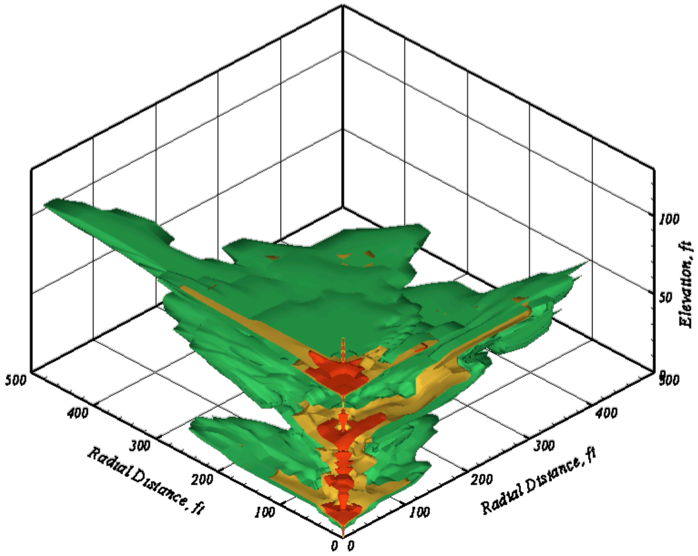
Processing Symposium, 2007.



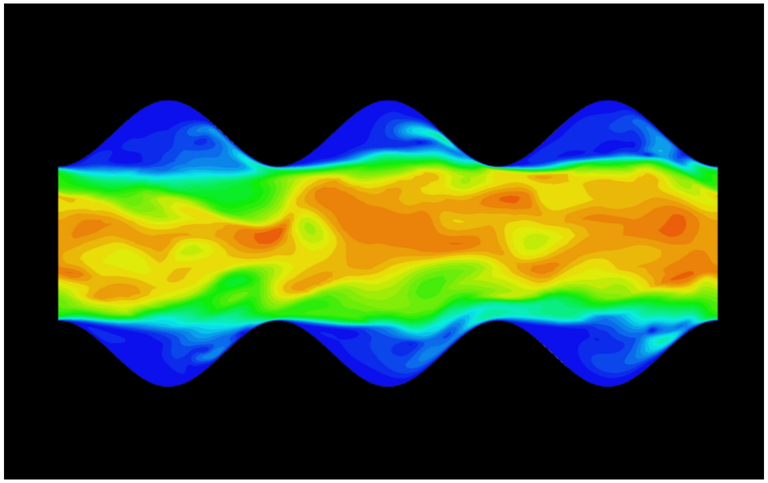
Smooth Particle Hydrodynamics

B. Palmer, V. Gurumoorthi, A. Tartakovsky, T. Scheibe, A Component-Based Framework for Smoothed Particle Hydrodynamics Simulations of Reactive Fluid Flow in Portous Media”, Int. J. High Perf. Comput. App., Vol 24, 2010

Recent Applications



Subsurface Transport Over Multiple Phases: STOMP



Transient Energy Transport Hydrodynamics Simulator: TETHYS

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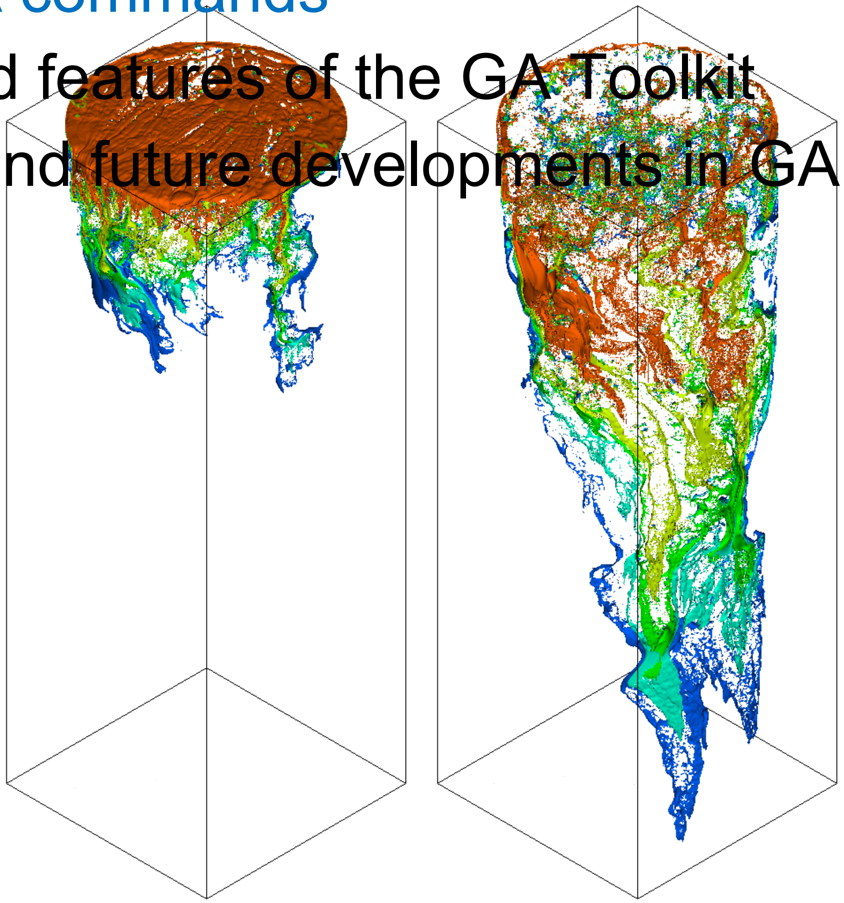

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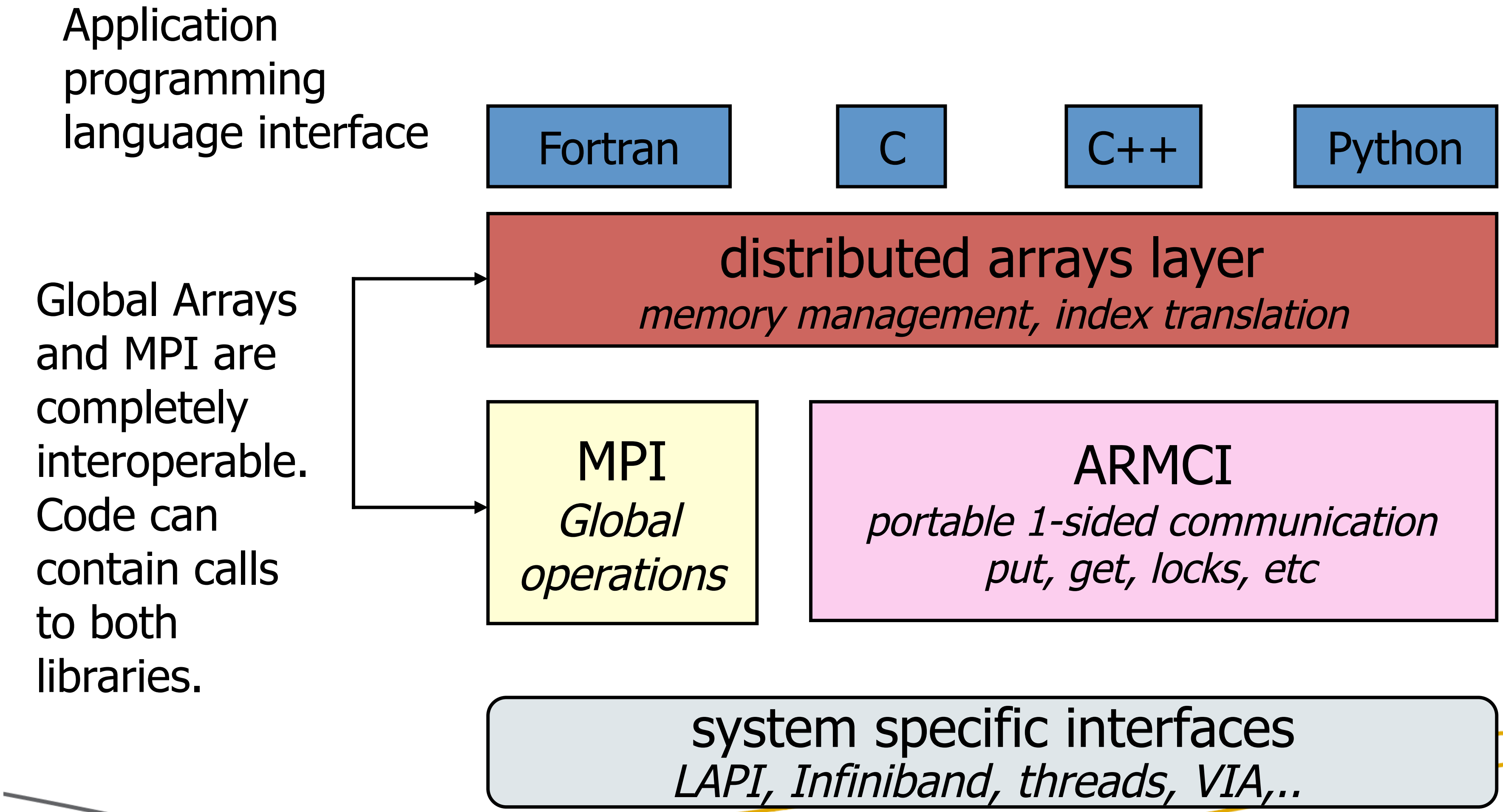
Structure of GA



Application programming language interface

Fortran

C

C++

Python

distributed arrays layer

memory management, index translation

Global Arrays and MPI are completely interoperable. Code can contain calls to both libraries.

MPI

Global operations

ARMCI

portable 1-sided communication put, get, locks, etc

system specific interfaces

LAPI, Infiniband, threads, VIA,..

Writing GA Programs

- GA requires the following functionalities from a message passing library (MPI/TCGMSG)
  - initialization and termination of processes
  - Broadcast, Barrier
  - a function to abort the running parallel job in case of an error
- The message-passing library has to be
  - initialized before the GA library
  - terminated after the GA library is terminated
- GA is compatible with MPI

```
#include <stdio.h>
#include "mpi.h"
#include "ga.h"
#include "macdecls.h"

int main( int argc, char **argv ) {
          MPI_Init( &argc, &argv );
          GA_Initialize();

          printf( "Hello world\n" );

          GA_Terminate();
          MPI_Finalize();
          return 0;
}
```

Source Code and More Information

- Version 5.0.2 available
- Homepage at http://www.emsl.pnl.gov/docs/global/
- Platforms
  - IBM SP, BlueGene
  - Cray XT, XE6 (Gemini)
  - Linux Cluster with Ethernet, Infiniband
  - Solaris
  - Fujitsu
  - Hitachi
  - NEC
  - HP
  - Windows

Documentation on Writing, Building and Running GA programs

- For detailed information
  - GA Webpage
    - GA papers, APIs, user manual, etc.
    - (Google: Global Arrays)
    - http://www.emsl.pnl.gov/docs/global/
  - GA User Manual
    - http://www.emsl.pnl.gov/docs/global/user.html
  - GA API Documentation
    - GA Webpage => User Interface
    - http://www.emsl.pnl.gov/docs/global/userinterface.html
  - GA Support/Help
    - hpctools@pnl.gov or hpctools@emsl.pnl.gov
  - 2 mailing lists: GA User Forum, and GA Announce

Installing GA

- GA 5.0 established autotools (configure && make && make install) for building
  - No environment variables are required
    - Traditional configure env vars CC, CFLAGS, CPPFLAGS, LIBS, etc
  - Specify the underlying network communication protocol
    - Only required on clusters with a high performance network
      - e.g. If the underlying network is Infiniband using OpenIB protocol use: configure --with-openib
  - GA requires MPI for basic start-up and process management
    - You can either use MPI or TCGMSG wrapper to MPI
      - MPI is the default: configure
      - TCGMSG-MPI wrapper: configure --with-mpi --with-tcgmsg
      - TCGMSG: configure --with-tcgmsg
- Various “make” targets
  - “make” to build GA libraries
  - “make install” to install libraries
  - “make checkprogs” to build tests and examples
  - “make check MPIEXEC=‘mpiexec -np 4’” to run test suite
- VPATH builds: one source tree, many build trees i.e. configurations

Compiling and Linking GA Programs

Your Makefile: Please refer to the CFLAGS, FFLAGS, CPPFLAGS, LDFLAGS and LIBS variables, which will be printed if you “make flags”.

```
# ===========================================================================
# Suggested compiler/linker options are as follows.
# GA libraries are installed in /Users/d3n000/ga/ga-5-0/bld_openmpi_shared/lib
# GA headers are installed in /Users/d3n000/ga/ga-5-0/bld_openmpi_shared/include
#
CPPFLAGS="-I/Users/d3n000/ga/ga-5-0/bld_openmpi_shared/include"
#
LDFLAGS="-L/Users/d3n000/ga/ga-5-0/bld_openmpi_shared/lib"
#
# For Fortran Programs:
FFLAGS="-fdefault-integer-8"
LIBS="-lga -framework Accelerate"
#
# For C Programs:
CFLAGS=""
LIBS="-lga -framework Accelerate -L/usr/local/lib/gcc/x86_64-apple-darwin10/4.6.0
-L/usr/local/lib/gcc/x86_64-apple-darwin10/4.6.0/../../.. -lgfortran"
# ===========================================================================
```

You can use these variables in your Makefile:
For example: gcc $(CPPLAGS) $(LDFLAGS) -o ga_test ga_test.c $(LIBS)

Writing GA Programs

- GA Definitions and Data types
  - C programs include files: ga.h, macdecls.h
  - Fortran programs should include the files: mafdecls.fh, global.fh.

```
#include <stdio.h>
#include "mpi.h“
#include "ga.h"
#include "macdecls.h"

int main( int argc, char **argv ) {
    /* Parallel program */
}
```

Running GA Programs

- Example: Running a test program “ga_test” on 2 processes for GA built using the MPI runtime
- mpirun -np 2 ga_test
- Running a GA program is same as MPI

11 Basic GA Operations

- GA programming model is very simple.
- Most of a parallel program can be written with these basic calls
  - **GA_Initialize, GA_Terminate**
  - **GA_Nnodes, GA_Nodeid**
  - **GA_Create, GA_Destroy**
  - **GA_Put, GA_Get**
  - **GA Distribution, GA_Access**
  - **GA_Sync**

GA Initialization/Termination

- There are two functions to *initialize* GA:
  - **Fortran**
    - subroutine ga_initialize()
    - subroutine ga_initialize_ltd(limit)
  - **C**
    - void GA_Initialize()
    - void GA_Initialize_ltd(size_t limit)
  - **Python**
    - import ga, then ga.set_memory_limit(limit)
- To *terminate* a GA program:
  - **Fortran** subroutine ga_terminate()
  - **C** void GA_Terminate()
  - **Python** N/A

```
      program main
      #include “mafdecls.fh”
      #include “global.fh”
      integer ierr
c
      call mpi_init(ierr)
      call ga_initialize()
c
      write(6,*) ‘Hello world’
c
      call ga_terminate()
      call mpi_finalize()
      end
```

Parallel Environment - Process Information

- **Parallel Environment:**
  - how many processes are working together (*size*)
  - what their IDs are (ranges from 0 to *size*-1)
- To return the process ID of the current process:
  - **Fortran** integer function ga_nodeid()
  - **C** int GA_Nodeid()
  - **Python** nodeid = ga.nodeid()
- To determine the number of computing processes:
  - **Fortran** integer function ga_nnodes()
  - **C** int GA_Nnodes()
  - **Python** nnodes = ga.nnodes()

Parallel Environment - Process Information (EXAMPLE)

```
 program main
 #include “mafdecls.fh”
 #include “global.fh”
 integer ierr,me,nproc

 call mpi_init(ierr)
 call ga_initialize()

 me = ga_nodeid()
 size = ga_nnodes()
 write(6,*) ‘Hello world: My rank is ’ +  me + ‘ out of ‘ +
&                size + ‘processes/nodes’

 call ga_terminate()
 call mpi_finilize()
 end
```

```
$ mpirun –np 4 helloworld
Hello world: My rank is 0 out of 4 processes/nodes
Hello world: My rank is 2 out of 4 processes/nodes
Hello world: My rank is 3 out of 4 processes/nodes
Hello world: My rank is 1 out of 4 processes/nodes
```

```
$ mpirun –np 4 python helloworld.py
Hello world: My rank is 0 out of 4 processes/nodes
Hello world: My rank is 2 out of 4 processes/nodes
Hello world: My rank is 3 out of 4 processes/nodes
Hello world: My rank is 1 out of 4 processes/nodes
```

GA Data Types

- C Data types

C_INT	- int
C_LONG	- long
C_FLOAT	- float
C_DBL	- double
C_SCPL	- single complex
C_DCPL	- double complex

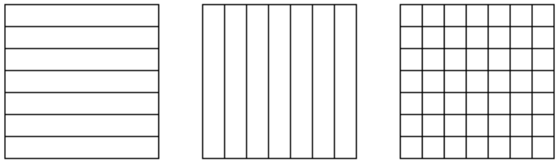
- Fortran Data types

MT_F_INT	- integer (4/8 bytes)
MT_F_REAL	- real
MT_F_DBL	- double precision
MT_F_SCPL	- single complex
MT_F_DCPL	- double complex

Creating/Destroying Arrays

- To *create* an array with a regular distribution:
  - **Fortran** logical function nga_create(type, ndim, dims, name, chunk, g_a)
  - **C** int NGA_Create(int type, int ndim, int dims[], char *name, int chunk[])
  - **Python** g_a = ga.create(type, dims, name="", chunk=None, int pgroup=-1)

character*(*)	name	- a unique character string	[input]
integer	type	- GA data type	[input]
integer	dims()	- array dimensions	[input]
integer	chunk()	- minimum size that dimensions should be chunked into	[input]
integer	g_a	- array handle for future references	[output]

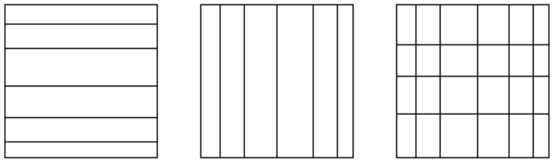


```
      dims(1) = 5000
      dims(2) = 5000
      chunk(1) = -1     !Use defaults
      chunk(2) = -1
      if (.not.nga_create(MT_F_DBL,2,dims,’Array_A’,chunk,g_a))
     +    call ga_error(“Could not create global array A”,g_a)
```

Creating/Destroying Arrays (cont.)

- To *create* an array with an irregular distribution:
  - **Fortran** logical function nga_create_irreg (type, ndim,
    dims, array_name, map, nblock, g_a)
  - **C** int NGA_Create_irreg(int type, int ndim, int dims[],
    char* array_name, nblock[], map[])
  - **Python** g_a = ga.create_irreg(int gtype, dims, block, map,
    name="", pgroup=-1)

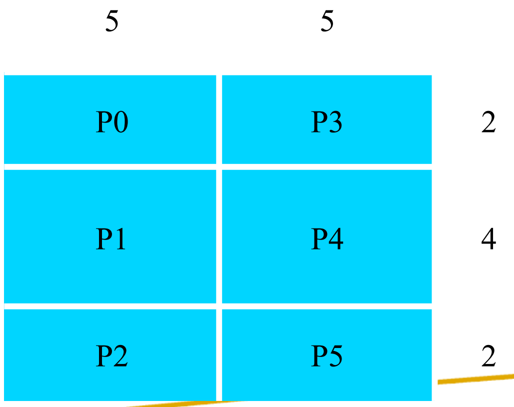
character*(*)	name	- a unique character string	[input]
integer	type	- GA datatype	[input]
integer	dims	- array dimensions	[input]
integer	nblock(*)	- no. of blocks each dimension is divided into	[input]
integer	map(*)	- starting index for each block	[input]
integer	g_a	- integer handle for future references	[output]



Creating/Destroying Arrays (cont.)

- Example of irregular distribution:
  - The distribution is specified as a Cartesian product of distributions for each dimension. The array indices start at 1.
    - The figure demonstrates distribution of a 2-dimensional array 8x10 on 6 (or more) processors. *block[2]*={3,2}, the size of *map* array is *s*=5 and array *map* contains the following elements *map*={1,3,7, 1, 6}.
    - The distribution is nonuniform because, P1 and P4 get 20 elements each and processors P0,P2,P3, and P5 only 10 elements each.

```
block(1) = 3
block(2) = 2
map(1) = 1
map(2) = 3
map(3) = 7
map(4) = 1
map(5) = 6
if (.not.nga_create_irreg(MT_F_DBL,2,dims, &
  ’Array_A’,map,block,g_a)) &
  call ga_error(“Could not create array A”,g_a)
```



Creating/Destroying Arrays (cont.)

- To *duplicate* an array:
  - **Fortran** logical function ga_duplicate(g_a, g_b, name)
  - **C** int GA_Duplicate(int g_a, char *name)
  - **Python** ga.duplicate(g_a, name)
- Global arrays can be *destroyed* by calling the function:
  - **Fortran** subroutine ga_destroy(g_a)
  - **C** void GA_Destroy(int g_a)
  - **Python** ga.destroy(g_a)

integer	g_a, g_b;	
character*(*)	name;	
name	- a character string	[input]
g_a	- Integer handle for reference array	[input]
g_b	- Integer handle for new array	[output]

```
 call nga_create(MT_F_INT,dim,dims,
+     'array_a',chunk,g_a)
 call ga_duplicate(g_a,g_b,'array_b')
 call ga_destroy(g_a)
```

Put/Get

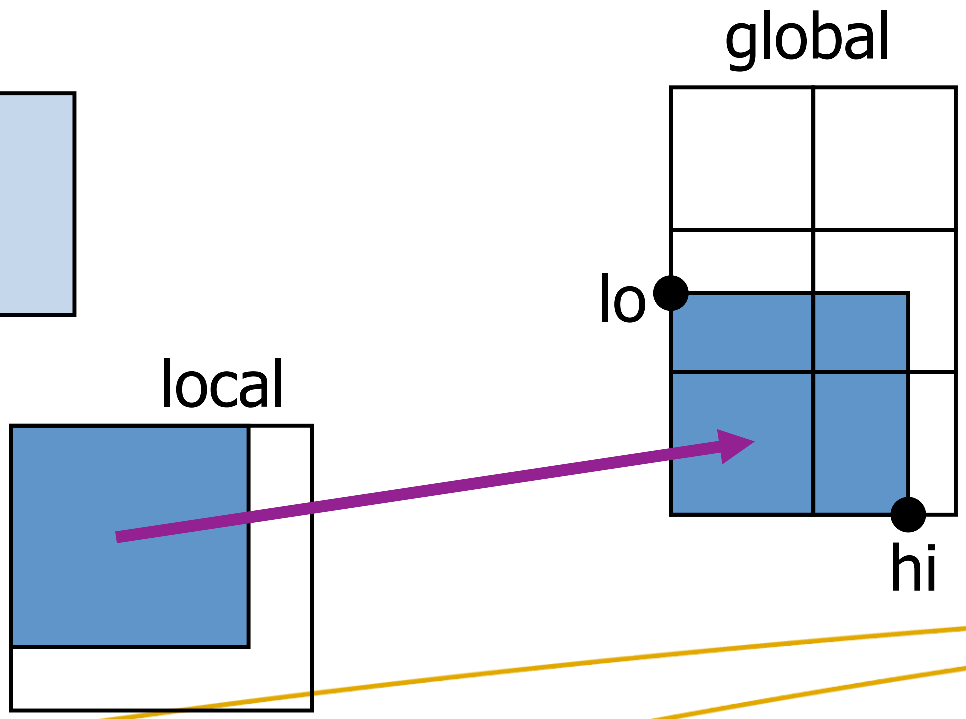
- *Put* copies data from a local array to a global array section:
  - **Fortran** subroutine nga_put(g_a, lo, hi, buf, ld)
  - **C** void NGA_Put(int g_a, int lo[], int hi[], void *buf, int ld[])
  - **Python** ga.put(g_a, buf, lo=None, hi=None)
- *Get* copies data from a global array section to a local array:
  - **Fortran** subroutine nga_get(g_a, lo, hi, buf, ld)
  - **C** void NGA_Get(int g_a, int lo[], int hi[], void *buf, int ld[])
  - **Python** buffer = ga.get(g_a, lo, hi, numpy.ndarray buffer=None)

integer	g_a	global array handle	[input]
integer	lo(),hi()	limits on data block to be moved	[input]
Double precision/complex/integer	buf	local buffer	[output]
integer	ld()	array of strides for local buffer	[input]

Put/Get (cont.)

- Example of *put* operation:
  - transfer data from a local buffer (10 x10 array) to (7:15,1:8) section of a 2-dimensional 15 x10 global array into *lo*={7,1}, *hi*={15,8}, ld={10}

```
double precision buf(10,10)
  :
  :
call nga_put(g_a,lo,hi,buf,ld)
```

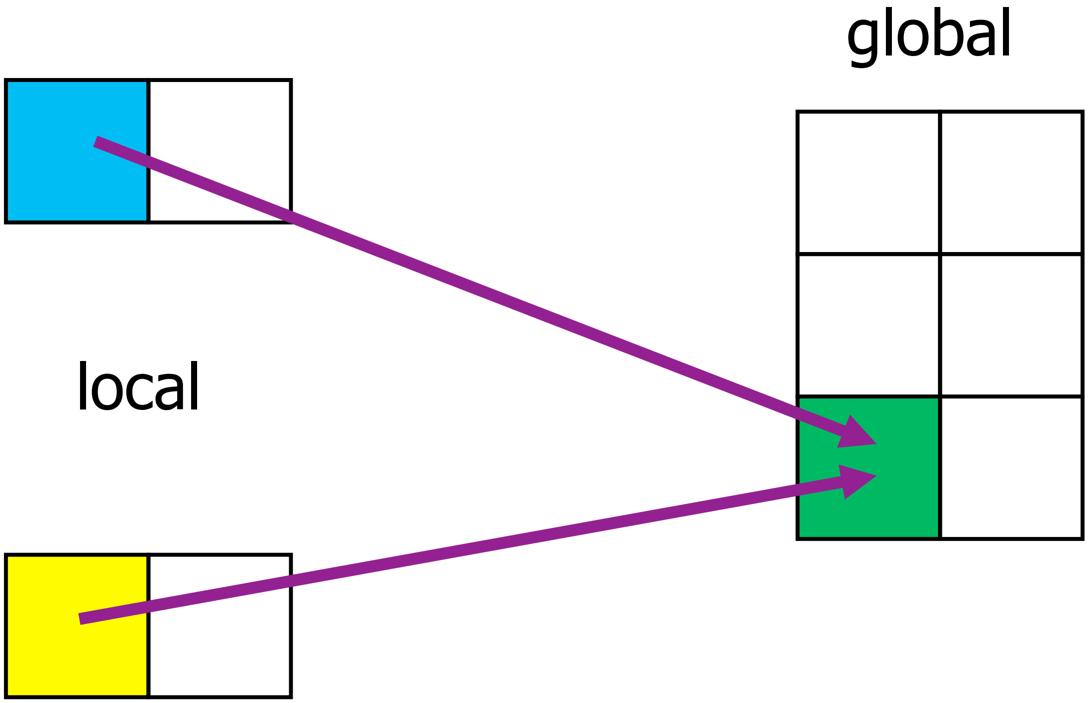


Atomic Accumulate

- *Accumulate* combines the data from the local array with data in the global array section:
  - **Fortran** subroutine nga_acc(g_a, lo, hi,
buf, ld, alpha)
  - **C** void NGA_Acc(int g_a, int lo[],
int hi[], void *buf, int ld[], void *alpha)
  - **Python** ga.acc(g_a, buffer, lo=None, hi=None,
alpha=None)

integer	g_a array handle	[input]
integer	lo(), hi() limits on data block to be moved	[input]
double	precision/complex buf local buffer	[input]
integer	ld() array of strides for local buffer	[input]
double	precision/complex alpha arbitrary scale factor	[input]

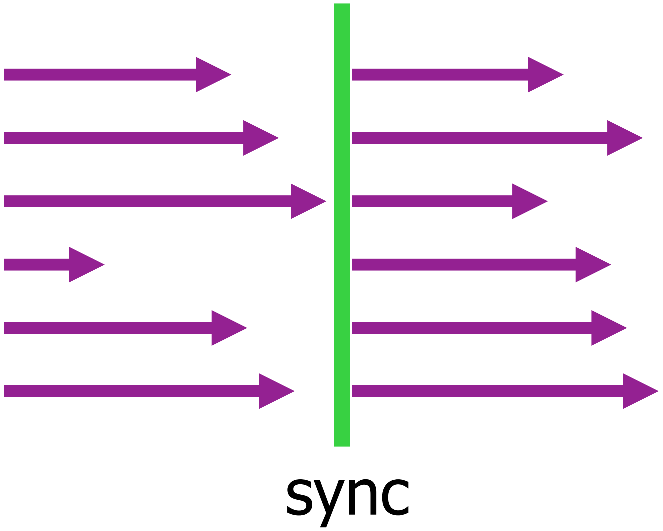
Atomic Accumulate (cont)



ga(i,j) = ga(i,j)+alpha*buf(k,l)

Sync

- *Sync* is a collective operation
- It acts as a barrier, which synchronizes all the processes and ensures that all outstanding Global Array operations are complete at the call
- The functions are:
  - **Fortran** subroutine ga_sync()
  - **C** void GA_Sync()
  - **Python** ga.sync()



GA_sync is the main mechanism in GA for guaranteeing data consistency

Global Operations

- Fortran

```
subroutine ga_brdcst(type, buf, lenbuf, root)
subroutine ga_igop(type, x, n, op)
subroutine ga_dgop(type, x, n, op)
```

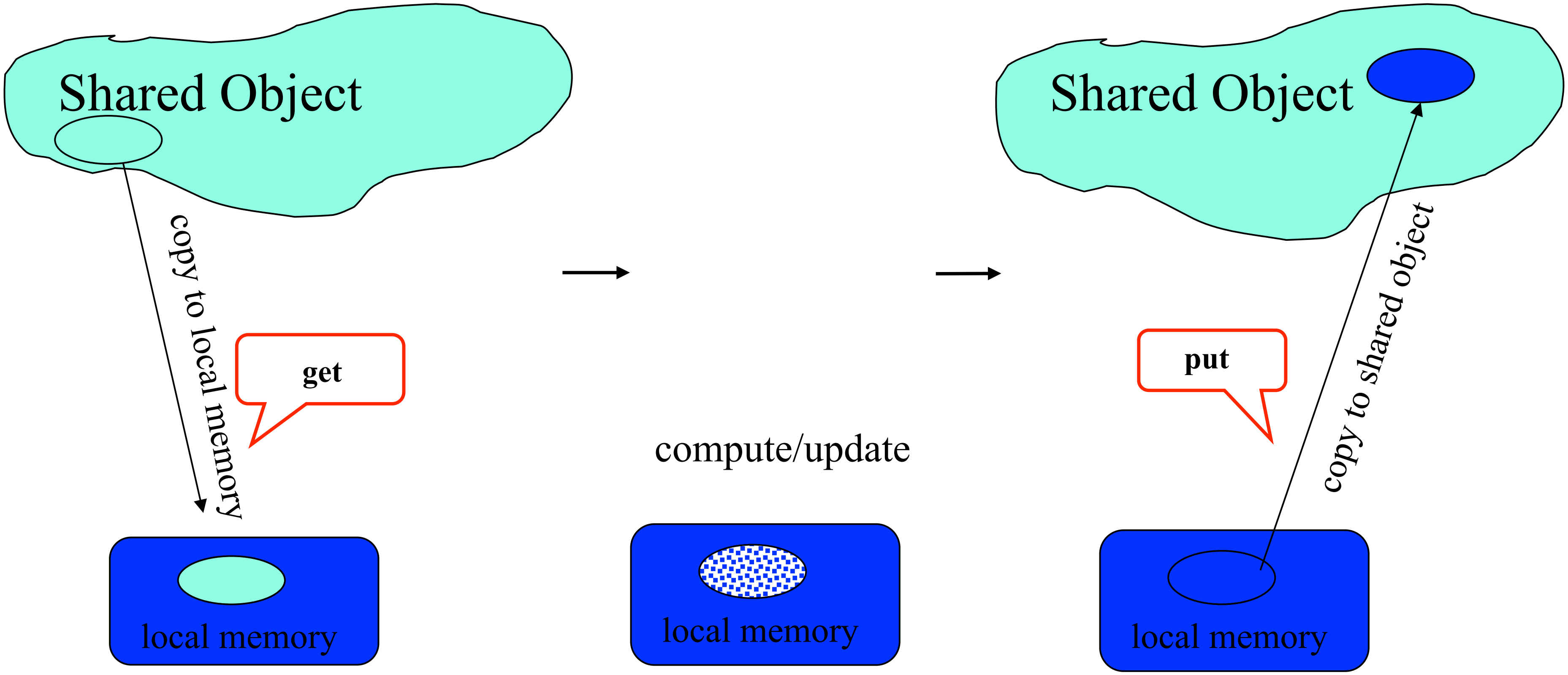
- C

```
void GA_Brdcst(void *buf, int lenbuf, int root)
void GA_Igop(long x[], int n, char *op)
void GA_Dgop(double x[], int n, char *op)
```

- Python

```
buffer = ga.brdcst(buffer, root)
buffer = ga.gop(x, op)
```

GLOBAL ARRAY MODEL OF COMPUTATIONS



Locality Information

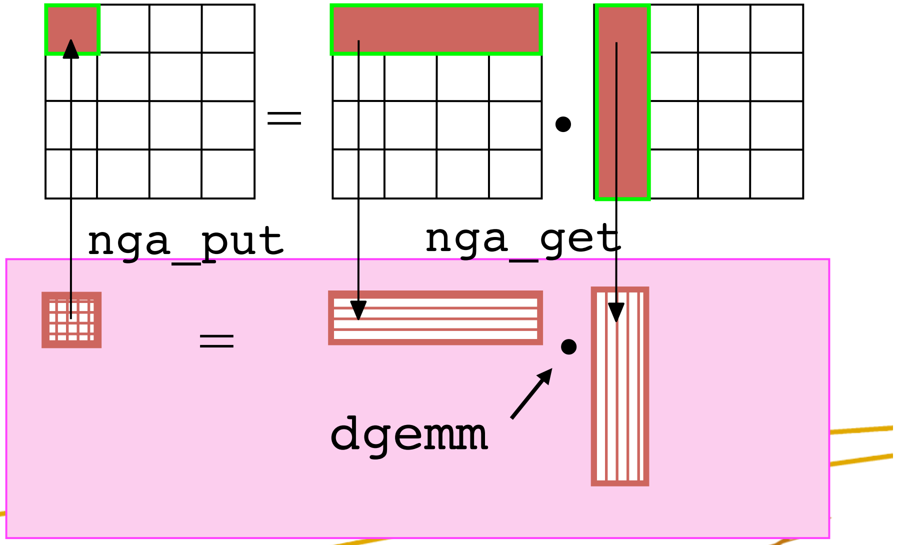
- Discover array elements held by each processor
  - **Fortran** nga_distribution(g_a,proc,lo,hi)
  - **C** void NGA_Distribution(int g_a, int proc, int *lo, int *hi)
  - **Python** lo,hi = ga.distribution(g_a, proc=-1)

integer	g_a	array handle	[input]
integer	proc	processor ID	[input]
integer	lo(ndim)	lower index	[output]
integer	hi(ndim)	upper index	[output]

```
do iproc = 1, nproc
  write(6,*) ‘Printing g_a info for processor’,iproc
  call nga_distribution(g_a,iproc,lo,hi)
  do j = 1, ndim
    write(6,*) j,lo(j),hi(j)
  end do
dnd do
```

Example: Matrix Multiply

```
/* Determine which block of data is locally owned. Note that
   the same block is locally owned for all GAs. */
NGA_Distribution(g_c, me, lo, hi);
/* Get the blocks from g_a and g_b needed to compute this block in
   g_c and copy them into the local buffers a and b. */
lo2[0] = lo[0]; lo2[1] = 0; hi2[0] = hi[0]; hi2[1] = dims[0]-1;
NGA_Get(g_a, lo2, hi2, a, ld);
lo3[0] = 0; lo3[1] = lo[1]; hi3[0] = dims[1]-1; hi3[1] = hi[1];
NGA_Get(g_b, lo3, hi3, b, ld);
/* Do local matrix multiplication and store the result in local
   buffer c. Start by evaluating the transpose of b. */
for(i=0; i < hi3[0]-lo3[0]+1; i++)
  for(j=0; j < hi3[1]-lo3[1]+1; j++)
     btrns[j][i] = b[i][j];
/* Multiply a and b to get c */
for(i=0; i < hi[0] - lo[0] + 1; i++) {
  for(j=0; j < hi[1] - lo[1] + 1; j++) {
    c[i][j] = 0.0;
    for(k=0; k<dims[0]; k++)
      c[i][j] = c[i][j] + a[i][k]*btrns[j][k];
  }
}
/* Copy c back to g_c */
NGA_Put(g_c, lo, hi, c, ld);
```



New Interface for Creating Arrays

- Developed to handle the proliferating number of properties that can be assigned to Global Arrays

Fortran

```
integer function ga_create_handle()
subroutine ga_set_data(g_a, dim, dims, type)
subroutine ga_set_array_name(g_a, name)
subroutine ga_set_chunk(g_a, chunk)
subroutine ga_set_irreg_distr(g_a, map, nblock)
subroutine ga_set_ghosts(g_a, width)
subroutine ga_set_block_cyclic(g_a, dims)
subroutine ga_set_block_cyclic_proc_grid(g_a,
                         dims, proc_grid)
logical function ga_allocate(g_a)
```

New Interface for Creating Arrays

C

```
 int  GA_Create_handle()
 void GA_Set_data(int g_a, int dim, int *dims,
                  int type)
 void GA_Set_array_name(int g_a, char* name)
 void GA_Set_chunk(int g_a, int *chunk)
 void GA_Set_irreg_distr(int g_a, int *map,
                         int *nblock)
 void GA_Set_ghosts(int g_a, int *width)
 void GA_Set_block_cyclic(int g_a, int *dims)
 void GA_Set_block_cyclic_proc_grid(int g_a, int
*dims,
                                    int *proc_grid)
 int  GA_Allocate(int g_a)
```

New Interface for Creating Arrays

Python

```
handle = ga.create_handle()
ga.set_data(g_a, dims, type)
ga.set_array_name(g_a, name)
ga.set_chunk(g_a, chunk)
ga.set_irreg_distr (g_a, map, nblock)
ga.set_ghosts(g_a, width)
ga.set_block_cyclic(g_a, dims)
ga.set_block_cyclic_proc_grid(g_a, dims,
            proc_grid)
bool ga.allocate(int g_a)
```

New Interface for Creating Arrays (Cont.)

```
      integer ndim,dims(2),chunk(2)
      integer g_a, g_b
      logical status
c
      ndim = 2
      dims(1)  = 5000
      dims(2)  = 5000
      chunk(1)  = 100
      chunk(2)  = 100
c
c Create global array A using old interface
c
      status = nga_create(MT_F_DBL, ndim, dims, chunk, ‘array_A’, g_a)
c
c Create global array B using new interface
C
      g_b = ga_create_handle()
      call ga_set_data(g_b, ndim, dims, MT_F_DBL)
      call ga_set_chunk(g_b, chunk)
      call ga_set_name(g_b, ‘array_B’)
      call ga_allocate(g_b)
```

Basic Array Operations

- Whole Arrays:
  - To set all the elements in the array to zero:

Fortran	subroutine ga_zero(g_a)
C	void GA_Zero(int g_a)
Python	ga.zero(g_a)

  - To assign a single value to all the elements in array:

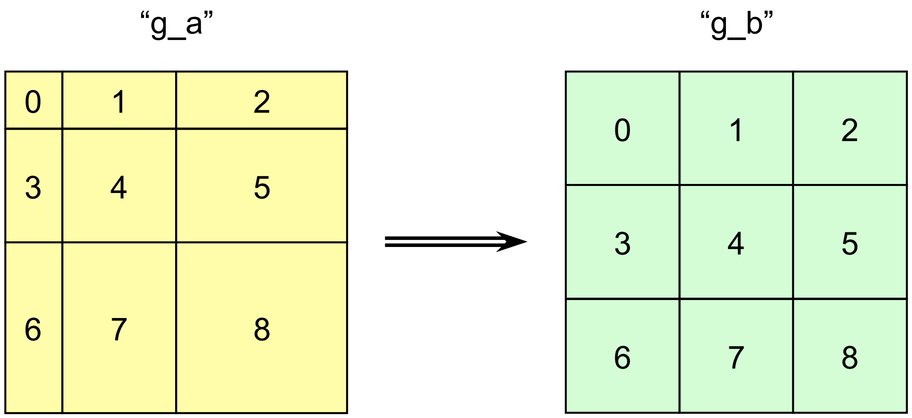
Fortran	subroutine ga_fill(g_a, val)
C	void GA_Fill(int g_a, void *val)
Python	ga.fill(g_a, val)

  - To scale all the elements in the array by factor*val*:

Fortran	subroutine ga_scale(g_a, val)
C	void GA_Scale(int g_a, void *val)
Python	ga.scale(g_a, val)

Basic Array Operations (cont.)

- Whole Arrays:
  - **To copy data between two arrays:**
    - **Fortran** subroutine ga_copy(g_a, g_b)
    - **C** void GA_Copy(int g_a, int g_b)
    - **Python** ga.copy(g_a, g_b)
  - Arrays must be same size and dimension
  - Distribution may be different



“g_a”

0	1	2
3	4	5
6	7	8

“g_b”

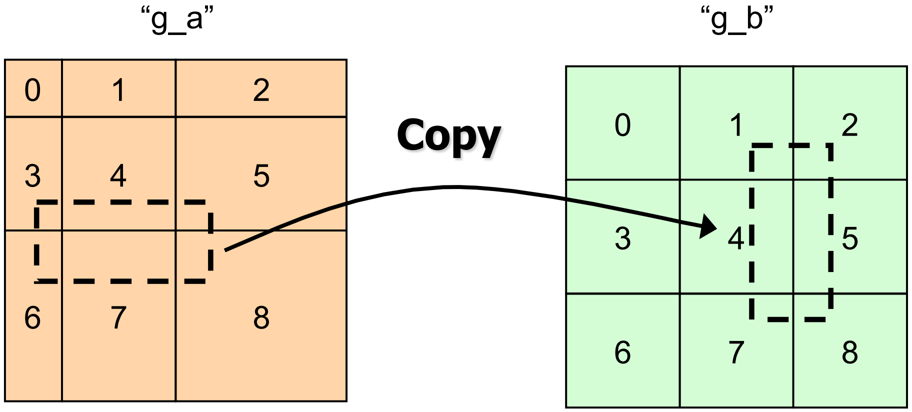
0	1	2
3	4	5
6	7	8

```
call ga_create(MT_F_INT,ndim,dims,
     'array_A',chunk_a,g_a)
call nga_create(MT_F_INT,ndim,dims,
     'array_B',chunk_b,g_b)

    ... Initialize g_a ....

call ga_copy(g_a, g_b)
```

Global Arrays g_a and g_b distributed on a 3x3 process grid

Basic Array Patch Operations

- Patch Operations:
  - The copy patch operation:
    - **Fortran** subroutine nga_copy_patch(trans, g_a, alo, ahi, g_b, blo, bhi)
    - **C** void NGA_Copy_patch(char trans, int g_a, int alo[], int ahi[], int g_b, int blo[], int bhi[])
    - **Python** ga.copy(g_a, g_b, alo=None, ahi=None, blo=None, bhi=None, bint trans=False)
  - Number of elements must match



Proudly Operated by Battelle Since 1965

Basic Array Patch Operations (cont.)

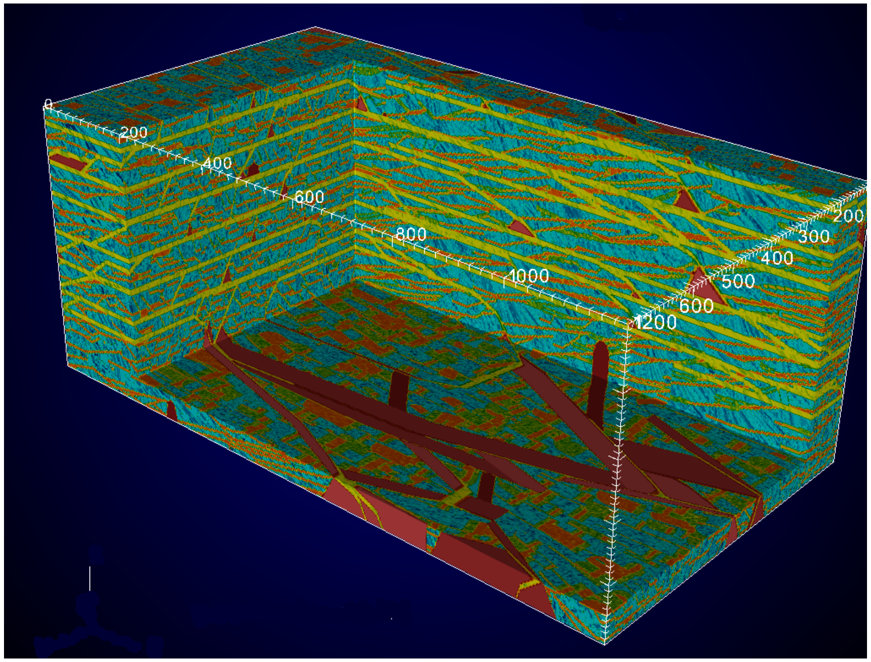
- Patches (Cont):
  - To set only the region defined by *lo* and *hi* to zero:
    - **Fortran** subroutine nga_zero_patch(g_a, lo, hi)
    - **C** void NGA_Zero_patch(int g_a, int lo[] int hi[])
    - **Python** ga.zero(g_a, lo=None, hi=None)
  - To assign a single value to all the elements in a patch:
    - **Fortran** subroutine nga_fill_patch(g_a, lo, hi, val)
    - **C** void NGA_Fill_patch(int g_a, int lo[], int hi[], void *val)
    - **Python** ga.fill(g_a, value, lo=None, hi=None)

Basic Array Patch Operations (cont.)

- Patches (Cont):
  - To scale the patch defined by lo and hi by the factor val:
    - **Fortran** subroutine nga_scale_patch(g_a, lo, hi, val)
    - **C** void NGA_Scale_patch(int g_a, int lo[], int hi[], void *val)
    - **Python** ga.scale(g_a, value, lo=None, hi=None)
  - The copy patch operation:
    - **Fortran** subroutine nga_copy_patch(trans, g_a, alo, ahi, g_b, blo, bhi)
    - **C** void NGA_Copy_patch(char trans, int g_a, int alo[], int ahi[], int g_b, int blo[], int bhi[])
    - **Python** ga.copy(g_a, g_b, alo=None, ahi=None, blo=None, bhi=None, bint trans=False)

Outline of the Tutorial

- Overview of parallel programming
- Introduction to Global Arrays programming model
- Basic GA commands
- Advanced features of the GA Toolkit
- Current and future developments in GA



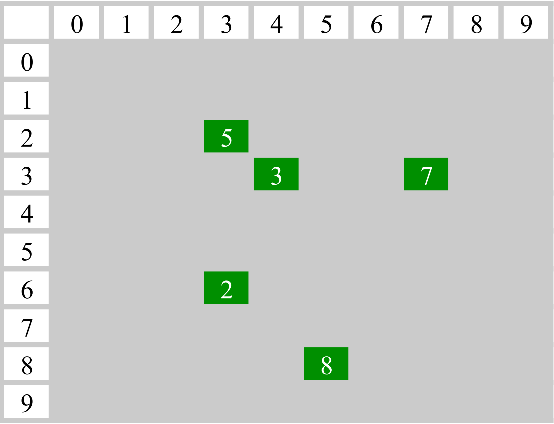
Scatter/Gather

- *Scatter* puts array elements into a global array:
  - **Fortran** subroutine nga_scatter(g_a, v, subscrpt_array, n)
  - **C** void NGA_Scatter(int g_a, void *v, int *subscrpt_array[], int n)
  - **Python** ga.scatter(g_a, values, subsarray)
- *Gather* gets the array elements from a global array into a local array:
  - **Fortran** subroutine nga_gather(g_a, v, subscrpt_array, n)
  - **C** void NGA_Gather(int g_a, void *v, int *subscrpt_array[], int n)
  - **Python** values = ga.gather(g_a, subsarray, numpy.ndarray values=None)

integer	g_a array handle	[input]
double precision	v(n) array of values	[input/output]
integer	n number of values	[input]
integer	subscrpt_array location of values in global array	[input]

Scatter/Gather (cont.)

- Example of *scatter* operation:
  - Scatter the 5 elements into a 10x10 global array
    - Element 1 v[0] = 5 subsArray[0][0] = 2
subsArray[0][1] = 3
    - Element 2 v[1] = 3 subsArray[1][0] = 3
subsArray[1][1] = 4
    - Element 3 v[2] = 8 subsArray[2][0] = 8
subsArray[2][1] = 5
    - Element 4 v[3] = 7 subsArray[3][0] = 3
subsArray[3][1] = 7
    - Element 5 v[4] = 2 subsArray[4][0] = 6
subsArray[4][1] = 3
  - After the *scatter* operation, the five elements would be scattered into the global array as shown in the figure.



	0	1	2	3	4	5	6	7	8	9
0										
1										
2				5						
3					3			7		
4										
5										
6				2						
7										
8						8				
9										

```
integer subscript(ndim,nlen)
    :
call nga_scatter(g_a,v,subscript,nlen)
```

Read and Increment

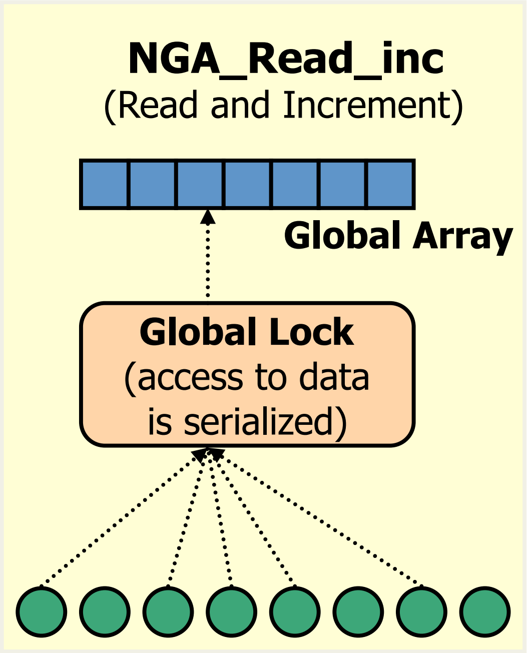
- *Read_inc* remotely updates a particular element in an integer global array and returns the original value:
  - **Fortran** integer function nga_read_inc(g_a, subscript, inc)
  - **C** long NGA_Read_inc(int g_a, int subscript[], long inc)
  - **Python** val = ga.read_inc(g_a, subscript, inc=1)
  - Applies to integer arrays only
  - Can be used as a global counter for dynamic load balancing

```
integer    g_a                        [input]
integer    subscript(ndim), inc       [input]
```

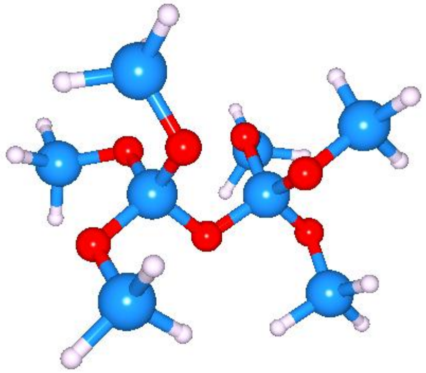
Read and Increment (cont.)

```
c  Create task counter
      status = nga_create(MT_F_INT,one,one,chunk,g_counter)
      call ga_zero(g_counter)
         :
      itask = nga_read_inc(g_counter,one,one)

      ... Translate itask into task ...
```

Every integer value is read once and only once by some processor



Hartree-Fock SCF



Obtain variational solutions to the electronic Schrödinger equation

$$H\Psi = E\Psi$$

within the approximation of a single Slater determinant.

Assuming the one electron orbitals are expanded as

$$\phi_i(\mathbf{r}) = \sum_{\mu} C_{i\mu}\chi_{\mu}(\mathbf{r})$$

the calculation reduces to the self-consistent eigenvalue problem

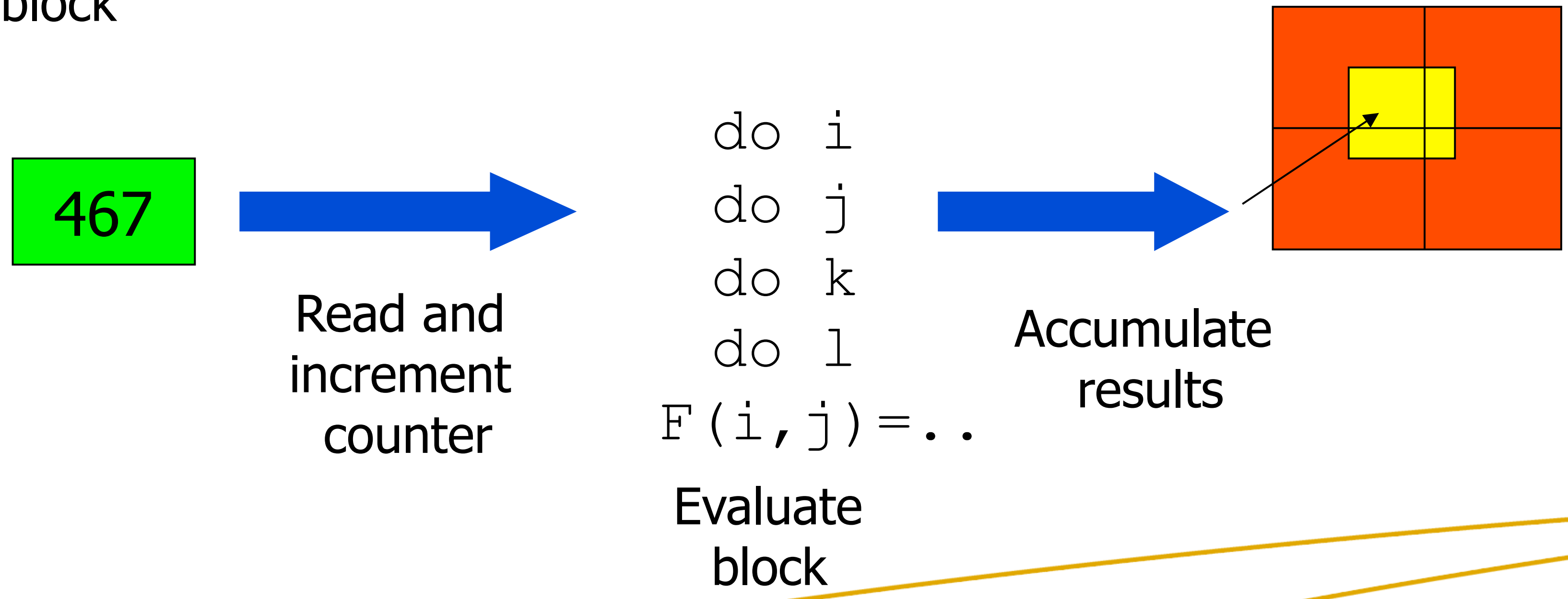
$$F_{\mu\nu}C_{k\nu} = \varepsilon D_{\mu\nu}C_{k\nu}$$

$$D_{\mu\nu} = \sum_{k} C_{\mu k}C_{\nu k}$$

$$F_{\mu\nu} = h_{\mu\nu} + \frac{1}{2}\sum_{\omega\lambda}\left[2(\mu\nu\,|\,\omega\lambda) - (\mu\omega\,|\,\nu\lambda)\right]D_{\omega\lambda}$$

Parallelizing the Fock Matrix

The bulk of the work involves computing the 4-index elements $(\mu\ \nu|\omega\ \lambda)$. This is done by decomposing the quadruple loop into evenly sized blocks and assigning blocks to each processor using a global counter. After each processor completes a block it increments the counter to get the next block



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Read and increment counter

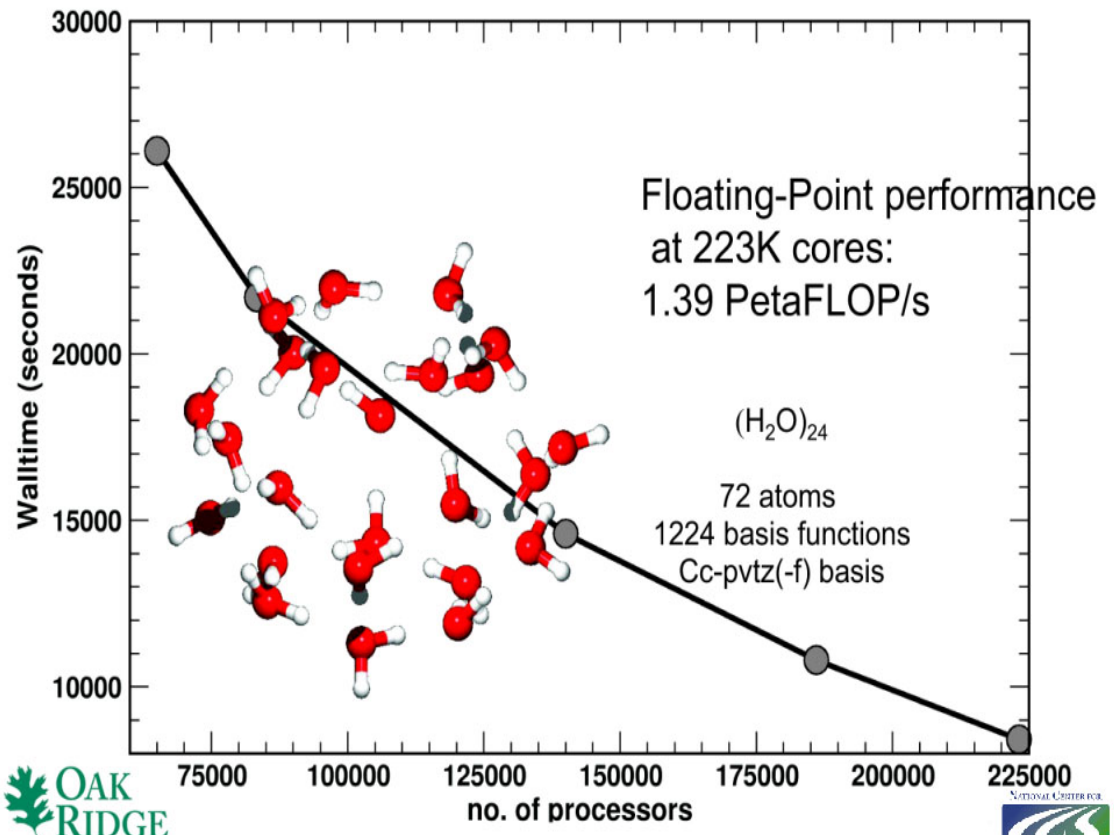
```
do i
do j
do k
do l
F(i,j)=..
```

Evaluate block

Accumulate results

Gorden Bell finalist at SC09 - GA Crosses the Petaflop Barrier

- GA-based parallel implementation of coupled cluster calculation performed at **1.39 petaflops using over 223,000 processes** on ORNL's Jaguar petaflop system
  - Apra et. al., "*Liquid water: obtaining the right answer for the right reasons*", SC 2009.
- Global Arrays is one of two programming models that have achieved this level of performance



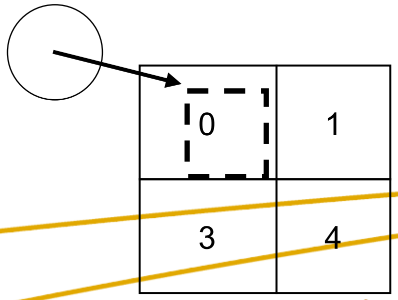
Floating-Point performance at 223K cores: 1.39 PetaFLOP/s

$(H_2O)_{24}$

72 atoms
1224 basis functions
Cc-pvtz(-f) basis

Direct Access to Local Data

- Global Arrays support abstraction of a distributed array object
- Object is represented by an integer handle
- A process can access its portion of the data in the global array
- To do this, the following steps need to be taken:
  - Find the distribution of an array, i.e. which part of the data the calling process owns
  - Access the data
  - Operate on the data: read/write
  - Release the access to the data

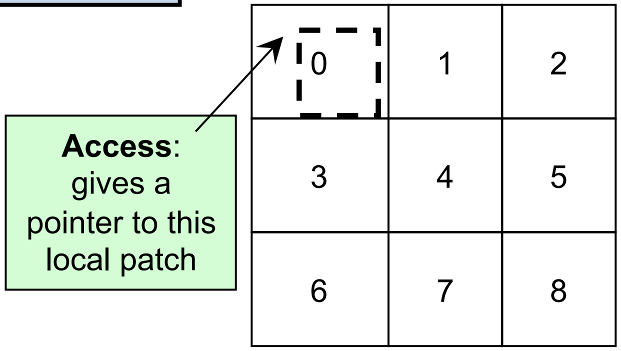


Access

- To provide direct access to local data in the specified patch of the array owned by the calling process:
  - **Fortran** subroutine nga_access(g_a, lo, hi, index, ld)
  - **C** void NGA_Access(int g_a, int lo[], int hi[],
    void *ptr, int ld[])
  - **Python** ndarray = ga.access(g_a, lo=None, hi=None)
  - Processes can access the local position of the global array
    - Process “0” can access the specified patch of its local position of the array
    - Avoids memory copy

Access (cont.)

```
status = nga_create(MT_F_DBL,2,dims,'Array',chunk,g_a)
  :
call nga_distribution(g_a,me,lo,hi)
call nga_access(g_a,lo,hi,index,ld)
call do_subroutine_task(dbl_mb(index),ld(1))
call nga_release(g_a,lo,hi)
subroutine do_subroutine_task(a,ld1)
double precision a(ld1,*)
```



Access: gives a pointer to this local patch

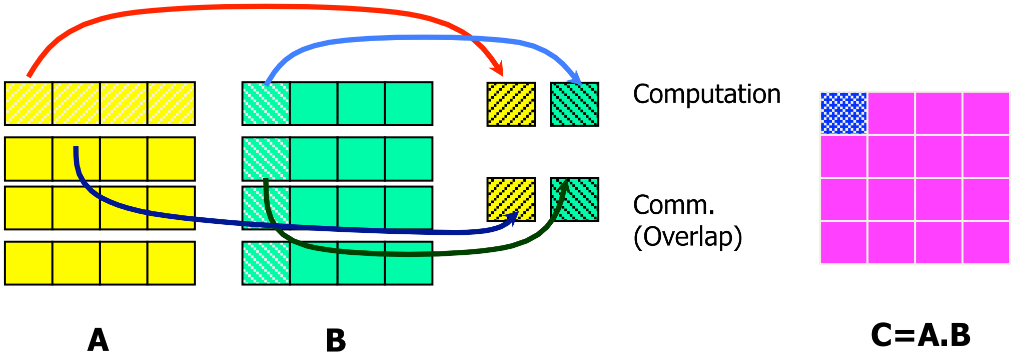
Non-blocking Operations

- The non-blocking APIs are derived from the blocking interface by adding a handle argument that identifies an instance of the non-blocking request.
  - **Fortran**
    - subroutine nga_nbput(g_a, lo, hi, buf, ld, nbhandle)
    - subroutine nga_nbget(g_a, lo, hi, buf, ld, nbhandle)
    - subroutine nga_nbacc(g_a, lo, hi, buf, ld, alpha, nbhandle)
    - subroutine nga_nbwait(nbhandle)
  - **C**
    - void NGA_NbPut(int g_a, int lo[], int hi[], void *buf, int ld[], ga_nbhdl_t* nbhandle)
    - void NGA_NbGet(int g_a, int lo[], int hi[], void *buf, int ld[], ga_nbhdl_t* nbhandle)
    - void NGA_NbAcc(int g_a, int lo[], int hi[], void *buf, int ld[], void *alpha,
      ga_nbhdl_t* nbhandle)
    - int NGA_NbWait(ga_nbhdl_t* nbhandle)
  - **Python**
    - handle = ga.nbput(g_a, buffer, lo=None, hi=None)
    - buffer,handle = ga.nbget(g_a, lo=None, hi=None, numpy.ndarray buffer=None)
    - handle = ga.nbacc(g_a, buffer, lo=None, hi=None, alpha=None)
    - ga.nbwait(handle)

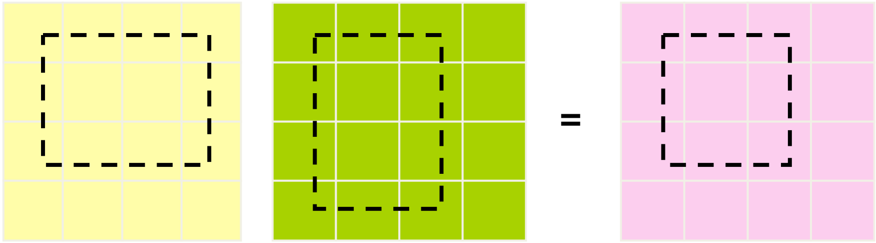
Non-Blocking Operations

```
double precision buf1(nmax,nmax)
double precision buf2(nmax,nmax)
   :
call nga_nbget(g_a,lo1,hi1,buf1,ld1,nb1)
ncount = 1
do while(.....)
  if (mod(ncount,2).eq.1) then
     ... Evaluate lo2, hi2
     call nga_nbget(g_a,lo2,hi2,buf2,nb2)
     call nga_wait(nb1)
     ... Do work using data in buf1
  else
     ... Evaluate lo1, hi1
     call nga_nbget(g_a,lo1,hi1,buf1,nb1)
     call nga_wait(nb2)
     ... Do work using data in buf2
  endif
  ncount = ncount + 1
end do
```

SRUMMA Matrix Multiplication



```
Issue NB Get A and B blocks
do (until last chunk)
    issue NB Get to the next blocks
    wait for previous issued call
    compute A*B (sequential dgemm)
    NB atomic accumulate into "C"
        matrix
done
```



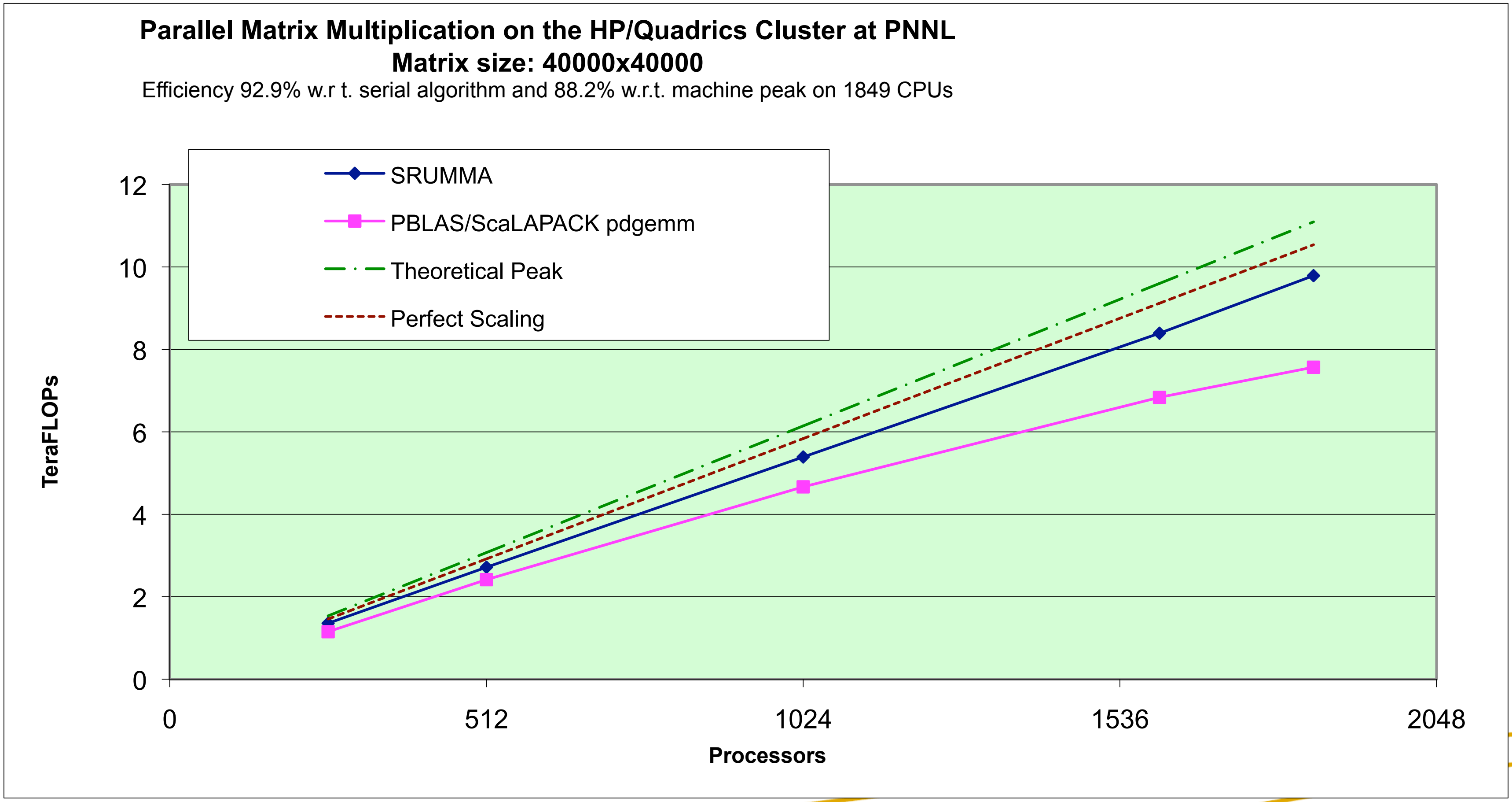
patch matrix multiplication

Advantages:

- Minimum memory
- Highly parallel
- Overlaps computation and communication
  - latency hiding
- exploits data locality
- patch matrix multiplication (easy to use)
- dynamic load balancing

http://hpc.pnl.gov/projects/srumma/

SRUMMA Matrix Multiplication: Improvement over PBLAS/ScaLAPACK



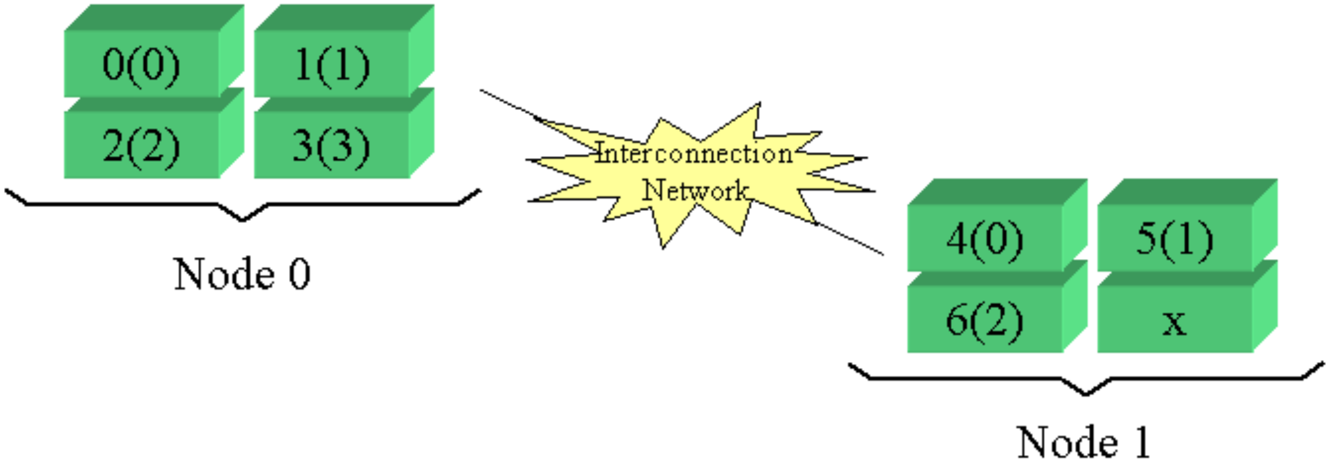
Parallel Matrix Multiplication on the HP/Quadrics Cluster at PNNL

Matrix size: 40000x40000

Efficiency 92.9% w.r t. serial algorithm and 88.2% w.r.t. machine peak on 1849 CPUs

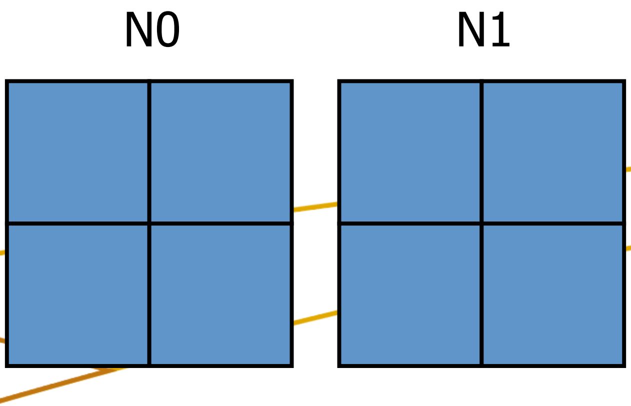
Cluster Information

- *Example:*
- 2 nodes with 4 processors each. Say, there are 7 processes created.
  - ga_cluster_nnodes returns 2
  - ga_cluster_nodeid returns 0 or 1
  - ga_cluster_nprocs(inode) returns 4 or 3
  - ga_cluster_procid(inode,iproc) returns a processor ID



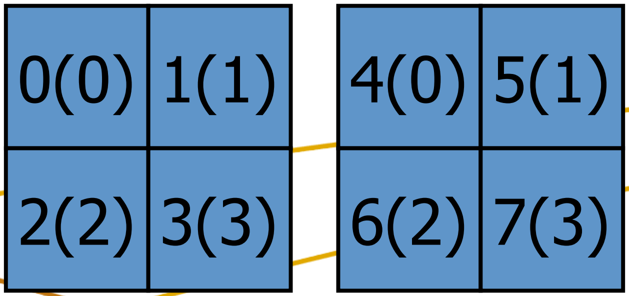
Cluster Information (cont.)

- To return the total number of nodes that the program is running on:
  - **Fortran** integer function ga_cluster_nnodes()
  - **C** int GA_Cluster_nnodes()
  - **Python** nnodes = ga.cluster_nnodes()
- To return the node ID of the process:
  - **Fortran** integer function ga_cluster_nodeid()
  - **C** int GA_Cluster_nodeid()
  - **Python** nodeid = ga.cluster_nodeid()



Cluster Information (cont.)

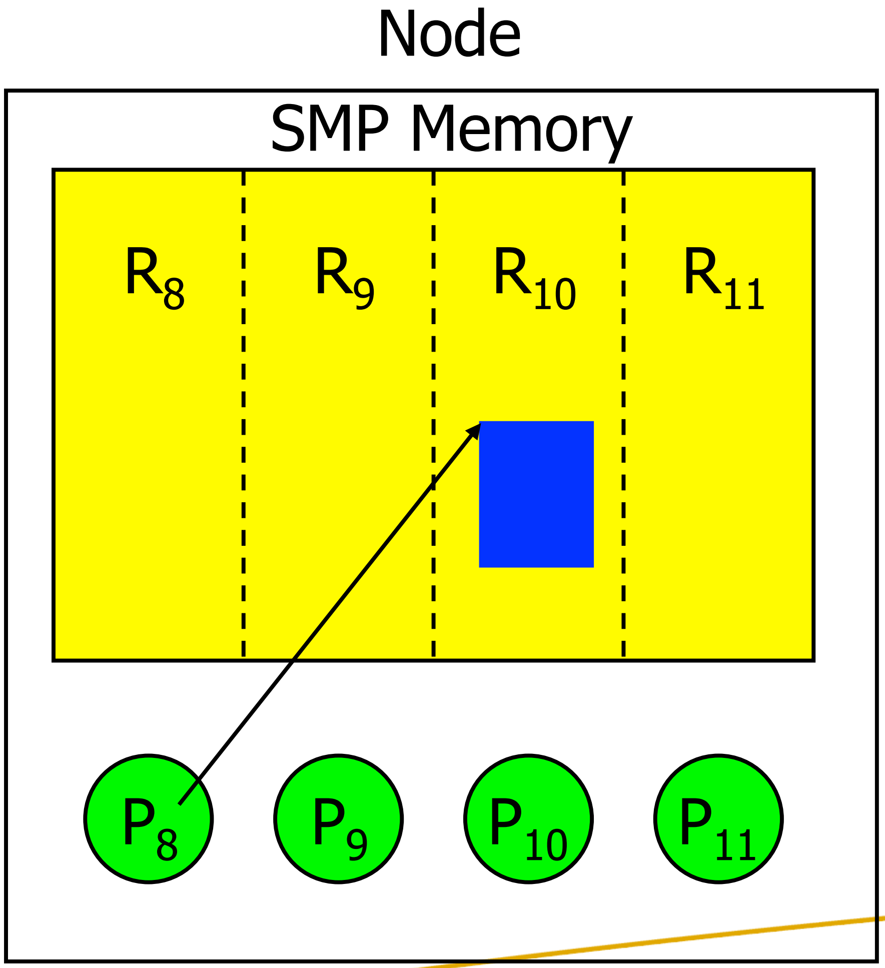
- To return the number of processors available on node inode:
  - **Fortran** integer function ga_cluster_nprocs(inode)
  - **C** int GA_Cluster_nprocs(int inode)
  - **Python** nprocs = ga.cluster_nprocs(inode)
- To return the processor ID associated with node inode and the local processor ID iproc:
  - **Fortran** integer function ga_cluster_procid(inode, iproc)
  - **C** int GA_Cluster_procid(int inode, int iproc)
  - **Python** procid = ga.cluster_procid(inode, iproc)



0(0) 1(1)
2(2) 3(3)

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

Accessing Processor Memory



ga_access

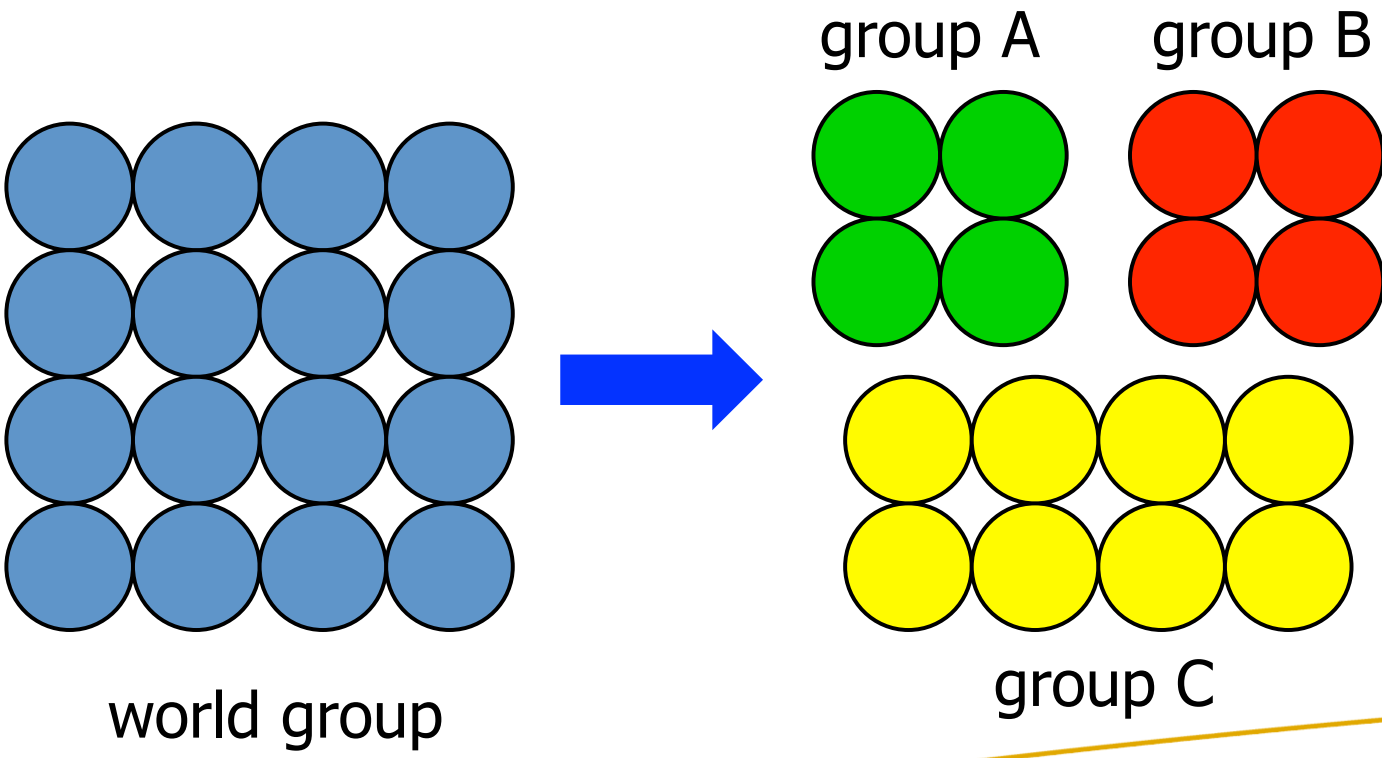
Processor Groups

- To create a new processor group:
  - **Fortran** integer function ga_pgroup_create(list, size)
  - **C** int GA_Pgroup_create(int *list, int size)
  - **Python** pgroup = ga.pgroup_create(list)
- To assign a processor groups:
  - **Fortran** logical function nga_create_config(
    type, ndim, dims, name, chunk, p_handle, g_a)
  - **C** int NGA_Create_config(int type, int ndim,
    int dims[], char *name, int p_handle, int chunk[])
  - **Python** g_a = ga.create(type, dims, name, chunk, pgroup=-1)

integer	g_a	- global array handle	[input]
integer	p_handle	- processor group handle	[output]
integer	list(size)	- list of processor IDs in group	[input]
integer	size	- number of processors in group	[input]

]

Processor Groups



Processor Groups (cont.)

- To set the default processor group
  - **Fortran** subroutine ga_pgroup_set_default(p_handle)
  - **C** void GA_Pgroup_set_default(int p_handle)
  - **Python** ga.pgroup_set_default(p_handle)
- To access information about the processor group:
  - **Fortran**
    - integer function ga_pgroup_nnodes(p_handle)
    - integer function ga_pgroup_nodeid(p_handle)
  - **C**
    - int GA_Pgroup_nnodes(int p_handle)
    - int GA_Pgroup_nodeid(int p_handle)
  - **Python**
    - nnodes = ga.pgroup_nnodes(p_handle)
    - nodeid = ga.pgroup_nodeid(p_handle)

integer p_handle - processor group handle [input]

Processor Groups (cont.)

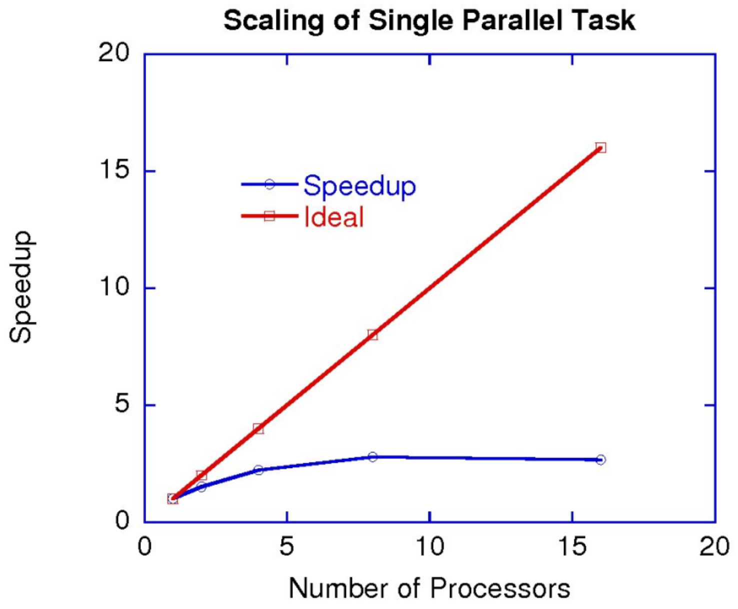
- To determine the handle for a standard group at any point in the program:
  - **Fortran**
    - integer function ga_pgroup_get_default()
    - integer function ga_pgroup_get_mirror()
    - integer function ga_pgroup_get_world()
  - **C**
    - int GA_Pgroup_get_default()
    - int GA_Pgroup_get_mirror()
    - int GA_Pgroup_get_world())
  - **Python**
    - p_handle = ga.pgroup_get_default()
    - p_handle = ga.pgroup_get_mirror()
    - p_handle = ga.pgroup_get_world()

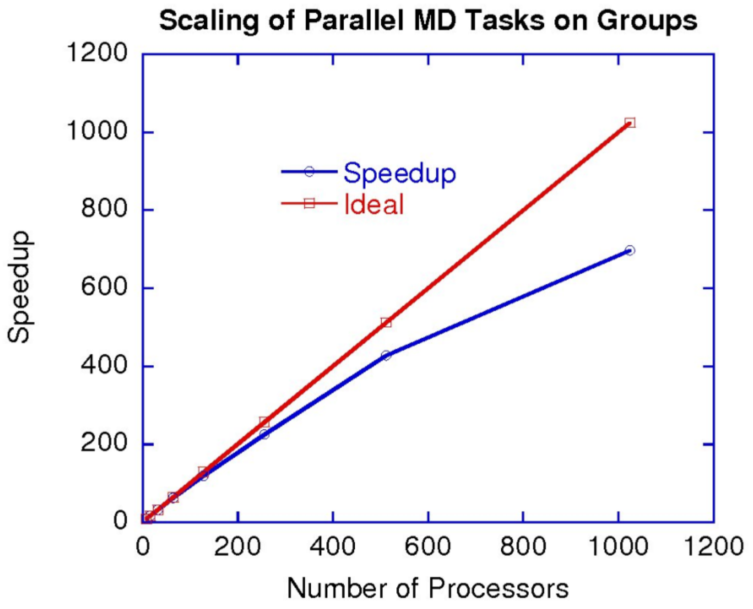
Default Processor Group

```
c
c  create subgroup p_a
c
      p_a = ga_pgroup_create(list, nproc)
      call ga_pgroup_set_default(p_a)
      call parallel_task()
      call ga_pgroup_set_default(ga_pgroup_get_world())
```

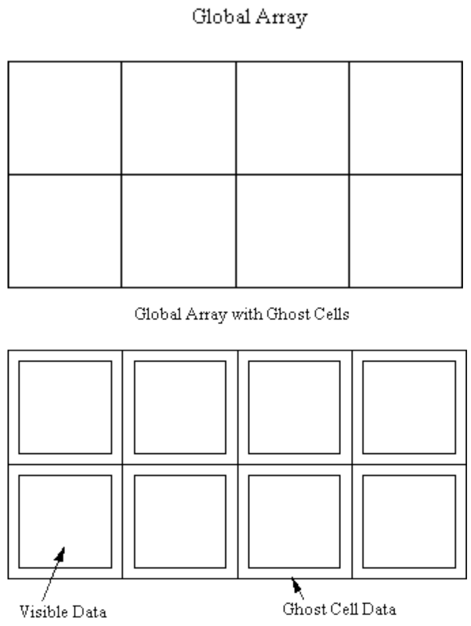
```
subroutine parallel_task()
p_b = ga_pgroup_create(new_list, new_nproc)
call ga_pgroup_set_default(p_b)
call parallel_subtask()
```

MD Application on Groups


Scaling of Single Parallel Task


Scaling of Parallel MD Tasks on Groups

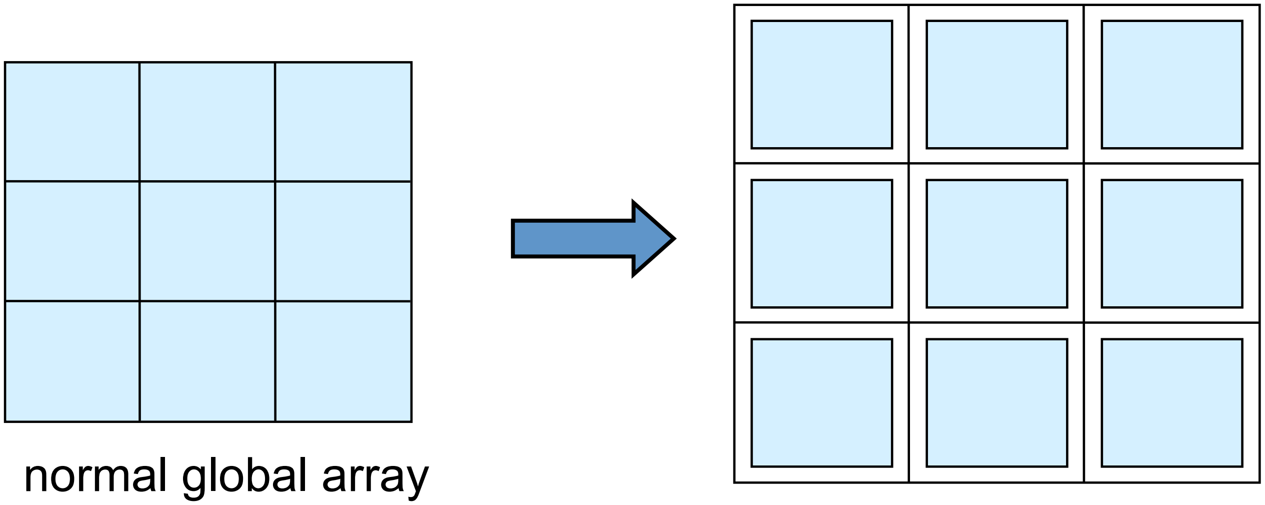
Creating Arrays with Ghost Cells



- To create arrays with ghost cells:
  - For arrays with regular distribution:
    - **Fortran** logical function nga_create_ghosts(type, dims, width, array_name, chunk, g_a)
    - **C** int int NGA_Create_ghosts(int type, int ndim, int dims[], int width[], char *array_name, int chunk[])
    - **Python** g_a = ga.create_ghosts(type, dims, width, name="", chunk=None, pgroup=-1)
  - For arrays with irregular distribution:
    - **n-d Fortran** logical function nga_create_ghosts_irreg(type, dims, width, array_name, map, block, g_a)
    - **C** int NGA_Create_ghosts_irreg(int type, int ndim, int dims[], int width[], char *array_name, int map[], int block[])
    - **Python** g_a = ga.create_ghosts_irreg(type, dims, width, block, map, name="", pgroup=-1)

integer width(ndim) - array of ghost cell widths [input]

Ghost Cells



normal global array

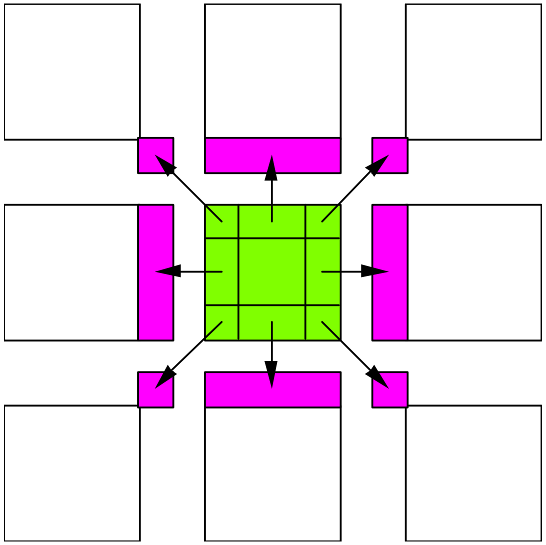
global array with ghost cells

Operations:

```
NGA_Create_ghosts   - creates array with ghosts cells
GA_Update_ghosts    - updates with data from adjacent processors
NGA_Access_ghosts   - provides access to “local” ghost cell
elements
NGA_Nbget_ghost_dir - nonblocking call to update ghosts cells
```

Ghost Cell Update

Automatically update ghost cells with appropriate data from neighboring processors. A multiprotocol implementation has been used to optimize the update operation to match platform characteristics.

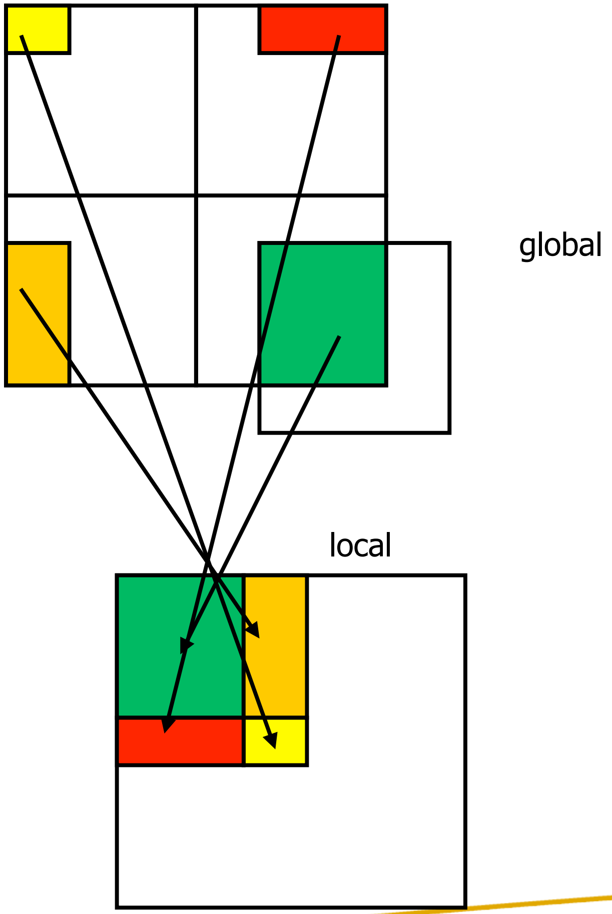


Periodic Interfaces

- Periodic interfaces to the one-sided operations have been added to Global Arrays in version 3.1 to support computational fluid dynamics problems on multidimensional grids.
- They provide an index translation layer that allows users to request blocks using put, get, and accumulate operations that possibly extend beyond the boundaries of a global array.
- The references that are outside of the boundaries are wrapped around inside the global array.
- Current version of GA supports three periodic operations:
  - *periodic get*
  - *periodic put*
  - *periodic acc*

Periodic Interfaces

```
ndim = 2
dims(1) = 10
dims(2) = 10
:
lo(1) = 6
lo(2) = 6
hi(1) = 11
hi(2) = 11
call nga_periodic_get(g_a,lo,hi,buf,ld)
```



Periodic Get/Put/Accumulate

- **Fortran** subroutine nga_periodic_get(g_a, lo, hi, buf, ld)
- **C** void NGA_Periodic_get(int g_a, int lo[], int hi[], void *buf, int ld[])
- **Python** ndarray = ga.periodic_get(g_a, lo=None, hi=None, buffer=None)

- **Fortran** subroutine nga_periodic_put(g_a, lo, hi, buf, ld)
- **C** void NGA_Periodic_put(int g_a, int lo[], int hi[], void *buf, int ld[])
- **Python** ga.periodic_put(g_a, buffer, lo=None, hi=None)

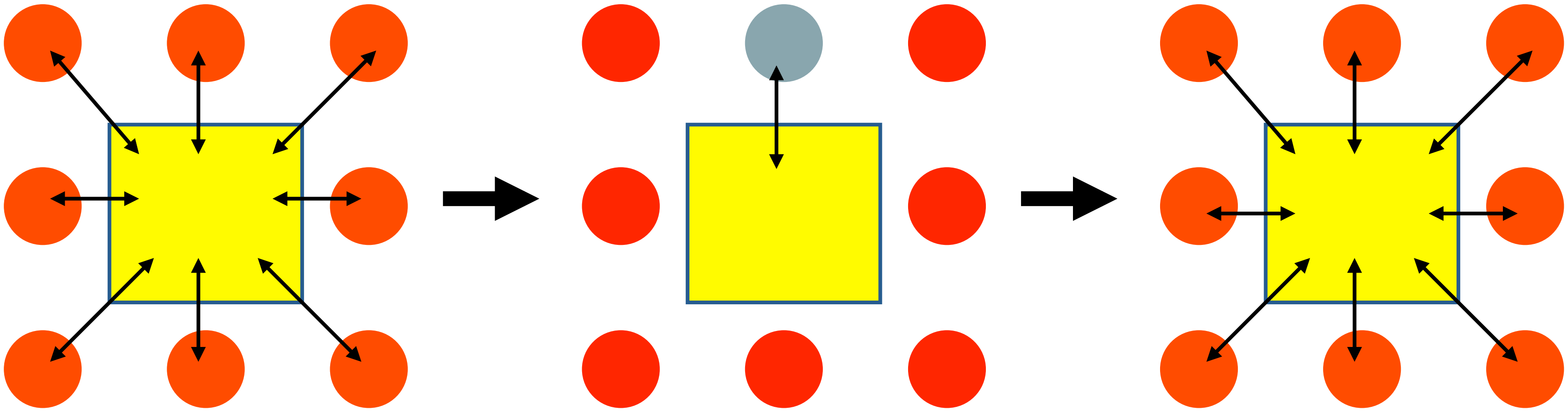
- **Fortran** subroutine nga_periodic_acc(g_a, lo, hi, buf, ld, alpha)
- **C** void NGA_Periodic_acc(int g_a, int lo[], int hi[], void *buf, int ld[], void *alpha)
- **Python** ga.periodic_acc(g_a, buffer, lo=None, hi=None, alpha=None)

Lock and Mutex

- *Lock* works together with *mutex*.
- Simple synchronization mechanism to protect a critical section
- To enter a critical section, typically, one needs to:
  - Create mutexes
  - Lock on a mutex
  - Do the exclusive operation in the critical section
  - Unlock the mutex
  - Destroy mutexes
- The *create mutex* functions are:

Fortran	logical function ga_create_mutexes(number)
C	int GA_Create_mutexes(int number)
Python	bool ga.create_mutexes(number)

Lock and Mutex (cont.)



Lock

Unlock

Lock and Mutex (cont.)

- The *destroy mutex* functions are:
  - **Fortran** logical function ga_destroy_mutexes()
  - **C** int GA_Destroy_mutexes()
  - **Python** bool ga.destroy_mutexes()
- The *lock* and *unlock* functions are:
  - **Fortran**
    - subroutine ga_lock(int mutex)
    - subroutine ga_unlock(int mutex)
  - **C**
    - void GA_lock(int mutex)
    - void GA_unlock(int mutex)
  - **Python**
    - ga.lock(mutex)
    - ga.unlock(mutex)

```
integer      mutex               [input]  ! mutex id
```

Fence

- *Fence* blocks the calling process until all the data transfers corresponding to the Global Array operations initiated by this process complete
- For example, since ga_put might return before the data reaches final destination, ga_init_fence and ga_fence allow process to wait until the data transfer is fully completed
  - ga_init_fence();
  - ga_put(g_a, ...);
  - ga_fence();
- The *initialize fence* functions are:

Fortran	subroutine ga_init_fence()
C	void GA_Init_fence()
Python	ga.init_fence()

- The *fence* functions are:

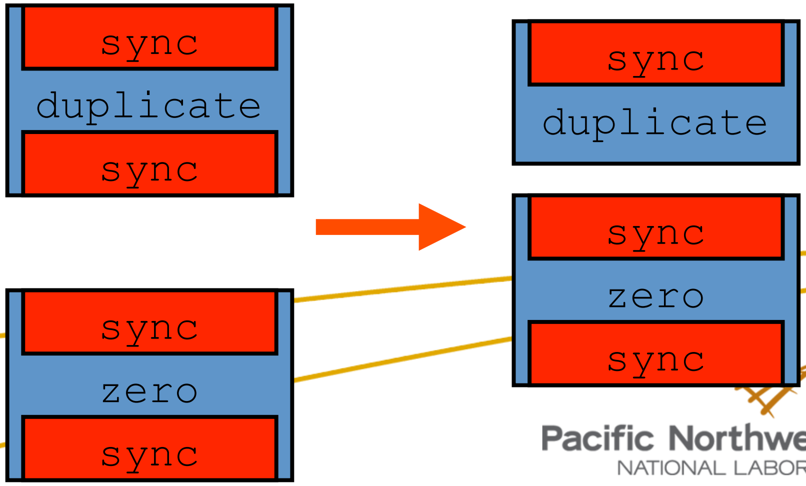
Fortran	subroutine ga_fence()
C	void GA_Fence()
Python	ga.fence()

Synchronization Control in Collective Operations

- To eliminate redundant synchronization points:
  - **Fortran** subroutine ga_mask_sync(prior_sync_mask, post_sync_mask)
  - **C** void GA_Mask_sync(int prior_sync_mask, int post_sync_mask)
  - **Python** ga.mask_sync(prior_sync_mask, post_sync_mask)

logical	first	- mask (0/1) for prior internal synchronization	[input]
logical	last	- mask (0/1) for post internal synchronization	[input]

```
status = ga_duplicate(g_a, g_b)
call ga_mask(0,1)
call ga_zero(g_b)
```



Linear Algebra

- To add two arrays:
  - **Fortran** subroutine ga_add(alpha, g_a, beta, g_b, g_c)
  - **C** void GA_Add(void *alpha, int g_a, void *beta, int g_b, int g_c)
  - **Python** ga.add(g_a, g_b, g_c, alpha=None, beta=None,
    alo=None, ahi=None, blo=None, bhi=None,
    clo=None, chi=None)
- To multiply arrays:
  - **Fortran** subroutine ga_dgemm(transa, transb, m, n, k, alpha, g_a, g_b,
    beta, g_c)
  - **C** void GA_Dgemm(char ta, char tb, int m, int n, int k, double alpha, int g_a, int g_b, double beta, int g_c)
  - **Python** def gemm(bool ta, bool tb, m, n, k, alpha, g_a, g_b, beta, g_c)

double precision/complex/integer	alpha, beta	- scale factor	[input]
integer	g_a, g_b, g_c	- array handles	[input]
character*1	transa, transb		[input]
integer	m, n, k		[input]

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Linear Algebra (cont.)

- To compute the element-wise dot product of two arrays:
  - Three separate functions for data types
    - Integer
      - **Fortran** ga_idot(g_a, g_b)
      - **C** GA_Idot(int g_a, int g_b)
    - Double precision
      - **Fortran** ga_ddot(g_a, g_b)
      - **C** GA_Ddot(int g_a, int g_b)
    - Double complex
      - **Fortran** ga_zdot(g_a, g_b)
      - **C** GA_Zdot(int g_a, int g_b)
  - Python has only one function: ga_dot(g_a, g_b)

integer	g_a, g_b	[input]
integer	GA_Idot(int g_a, int g_b)	
long	GA_Ldot(int g_a, int g_b)	
float	GA_Fdot(int g_a, int g_b)	
double	GA_Ddot(int g_a, int g_b)	
DoubleComplex	GA_Zdot(int g_a, int g_b)	

Linear Algebra (cont.)

- To symmetrize a matrix:

Fortran	subroutine ga_symmetrize(g_a)
C	void GA_Symmetrize(int g_a)
Python	ga.symmetrize(g_a)

- To transpose a matrix:

Fortran	subroutine ga_transpose(g_a, g_b)
C	void GA_Transpose(int g_a, int g_b)
Python	ga.transpose(g_a, g_b)

Linear Algebra on Patches

- To add element-wise two patches and save the results into another patch:
  - **Fortran** subroutine nga_add_patch(alpha, g_a, alo, ahi, beta,
    g_b, blo, bhi, g_c, clo, chi)
  - **C** void NGA_Add_patch(void *alpha, int g_a, int alo[], int ahi[],
    void *beta, int g_b, int blo[], int bhi[], int g_c, int clo[], int chi[])
  - **Python** ga.add(g_a, g_b, g_c, alpha=None, beta=None,
    alo=None, ahi=None, blo=None, bhi=None,
    clo=None, chi=None)

integer	g_a, g_b, g_c		[input]
dbl prec/comp/int	alpha, beta	scale factors	[input]
integer	ailo, aihi, ajlo, ajhi	g_a patch coord	[input]
integer	bilo, bihi, bjlo, bjhi	g_b patch coord	[input]
integer	cilo, cihi, cjlo, cjhi	g_c patch coord	[input]

Linear Algebra on Patches (cont.)

- To perform matrix multiplication:
  - **Fortran**

    ```
    subroutine ga_matmul_patch(transa, transb, alpha, beta,
            g_a, ailo, aihi, ajlo, ajhi,
            g_b, bilo, bihi, bjlo, bjhi,
            g_c, cilo, cihi, cjlo, cjhi)
    ```

  - **C**

    ```
    void GA_Matmul_patch(char *transa, char* transb,
            void* alpha, void *beta,
            int g_a, int ailo, int aihi, int ajlo, int ajhi,
            int g_b, int bilo, int bihi, int bjlo, int bjhi,
            int g_c, int cilo, int cihi, int cjlo, int cjhi)
    ```

  - **Fortran**

    ```
    subroutine ga_matmul_patch(bool transa, bool transb,
            alpha, beta,
            g_a, ailo, aihi, ajlo, ajhi,
            g_b, bilo, bihi, bjlo, bjhi,
            g_c, cilo, cihi, cjlo, cjhi)
    ```

integer	g_a, ailo, aihi, ajlo, ajhi	patch of g_a	[input]
integer	g_b, bilo, bihi, bjlo, bjhi	patch of g_b	[input]
integer	g_c, cilo, cihi, cjlo, cjhi	patch of g_c	[input]
dbl prec/comp	alpha, beta	scale factors	[input]
character*1	transa, transb	transpose flags	[input]

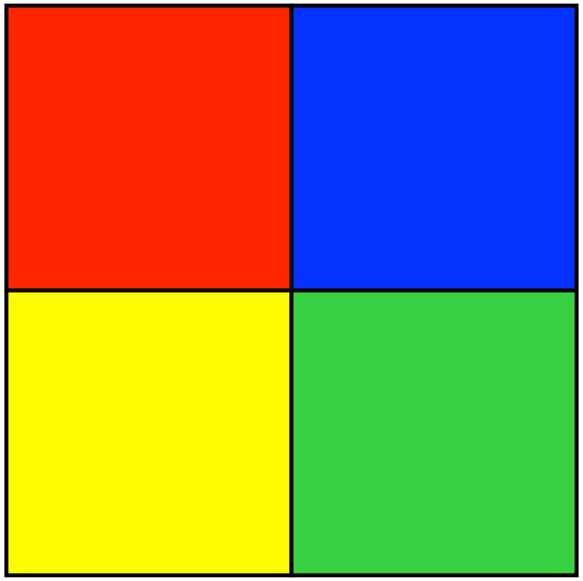
Linear Algebra on Patches (cont.)

- To compute the element-wise dot product of two arrays:
  - Three separate functions for data types
    - Integer
      - **Fortran** nga_idot_patch(g_a, ta, alo, ahi, g_b, tb, blo, bhi)
      - **C** NGA_Idot_patch(int g_a, char* ta,
        int alo[], int ahi[], int g_b, char* tb, int blo[], int bhi[])
    - Double precision
      - **Fortran** nga_ddot_patch(g_a, ta, alo, ahi, g_b, tb, blo, bhi)
      - **C** NGA_Ddot_patch(int g_a, char* ta,
        int alo[], int ahi[], int g_b, char* tb, int blo[], int bhi[])
    - Double complex
      - **Fortran** nga_zdot_patch(g_a, ta, alo, ahi, g_b, tb, blo, bhi)
      - **C** NGA_Zdot_patch(int g_a, char* ta,
        int alo[], int ahi[], int g_b, char* tb, int blo[], int bhi[])
  - Python has only one function: ga.dot(g_a, g_b,
    alo=None, ahi=None, blo=None, bhi=None, bint ta=False, bint tb=False)

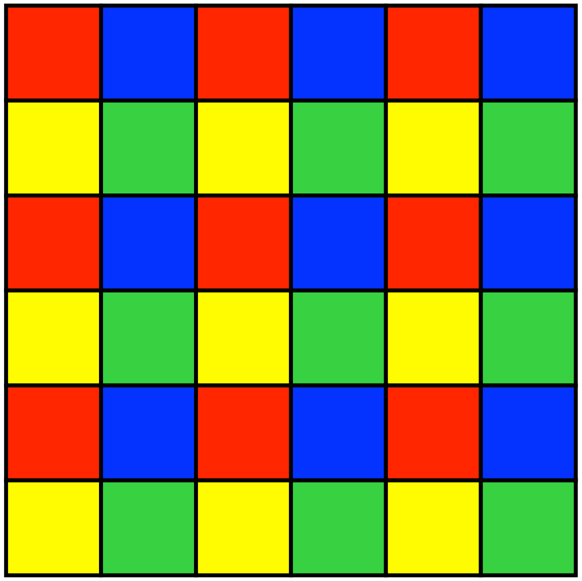
integer	g_a, g_b	[input]
integer	GA_Idot(int g_a, int g_b)	
long	GA_Ldot(int g_a, int g_b)	
float	GA_Fdot(int g_a, int g_b)	
double	GA_Ddot(int g_a, int g_b)	
DoubleComplex	GA_Zdot(int g_a, int g_b)	

Block-Cyclic Data Distributions

Normal Data Distribution

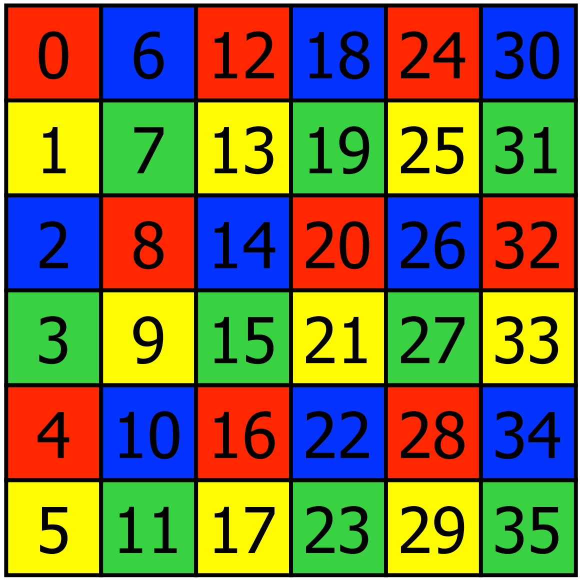


Block-Cyclic Data Distribution



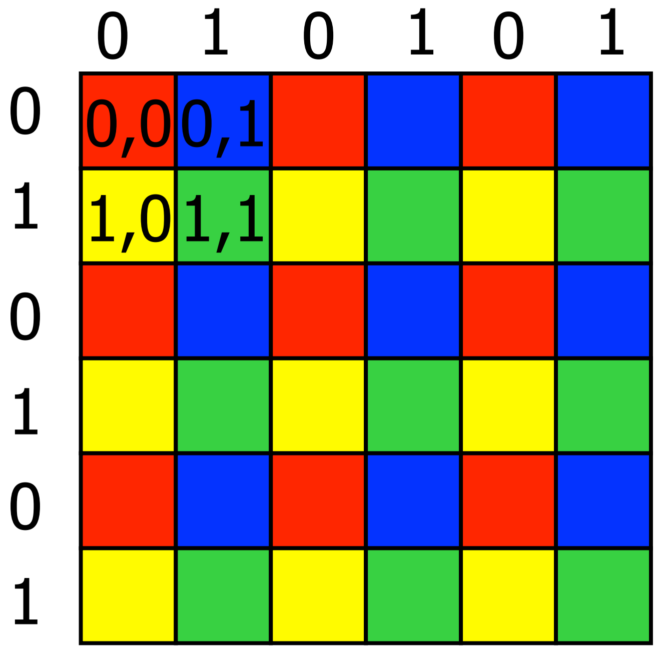
Block-Cyclic Data (cont.)

Simple Distribution



0	6	12	18	24	30
1	7	13	19	25	31
2	8	14	20	26	32
3	9	15	21	27	33
4	10	16	22	28	34
5	11	17	23	29	35

Scalapack Distribution



	0	1	0	1	0	1
0	0,0	0,1	🟥	🟦	🟥	🟦
1	1,0	1,1	🟨	🟩	🟨	🟩
0	🟥	🟦	🟥	🟦	🟥	🟦
1	🟨	🟩	🟨	🟩	🟨	🟩
0	🟥	🟦	🟥	🟦	🟥	🟦
1	🟨	🟩	🟨	🟩	🟨	🟩

2 x 2 processor grid

Block-Cyclic Data (cont.)

- Most operations work exactly the same, data distribution is transparent to the user
- Some operations (matrix multiplication, non-blocking put, get) not implemented
- Additional operations added to provide access to data associated with particular sub-blocks
- You need to use the new interface for creating Global Arrays to get create block-cyclic data distributions

Creating Block-Cyclic Arrays

- Must use new API for creating Global Arrays
  - Fortran subroutine ga_set_block_cyclic(g_a, dims)
    subroutine ga_set_block_cyclic_proc_grid(g_a, dims,
    proc_grid)
  - C void GA_Set_block_cyclic(int g_a, int dims[])
    void GA_Set_block_cyclic_proc_grid(g_a, dims[], proc_grid
    [])
  - Python ga.set_block_cyclic(g_a, dims)
    ga.set_block_cyclic_proc_grid(g_a, block, proc_grid)

integer dims[] - dimensions of blocks
integer proc_grid[] - dimensions of processor grid (note that product of all proc_grid dimensions

Block-Cyclic Methods

- Methods for accessing data of individual blocks
  - **Fortran**
    - subroutine ga_get_block_info(g_a, num_blocks, block_dims)
    - integer function ga_total_blocks(g_a)
    - subroutine nga_access_block_segment(g_a, iproc, index, length)
    - subroutine nga_access_block(g_a, idx, index, ld)
    - subroutine nga_access_block_grid(g_a, subscript, index, ld)
  - **C**
    - void GA_Get_block_info(g_a, num_blocks[], block_dims[])
    - int GA_Total_blocks(int g_a)
    - void NGA_Access_block_segment(int g_a, int iproc, void *ptr, int *length)
    - void NGA_Access_block(int g_a, int idx, void *ptr, int ld[])
    - void NGA_Access_block_grid(int g_a, int subscript[], void *ptr, int ld[])
  - **Python**
    - num_blocks,block_dims = ga.get_block_info(g_a)
    - blocks = ga.total_blocks(g_a)
    - ndarray = ga.access_block_segment(g_a, iproc)
    - ndarray = ga.access_block(g_a, idx)
    - ndarray = ga.access_block_grid(g_a, subscript)

integer length	- total size of blocks held on processor
integer idx	- index of block in array (for simple block-cyclic distribution)
integer subscript[]	- location of block in block grid (for Scalapack distribution)

Interfaces to Third Party Software Packages

- Scalapack
  - Solve a system of linear equations
  - Compute the inverse of a double precision matrix

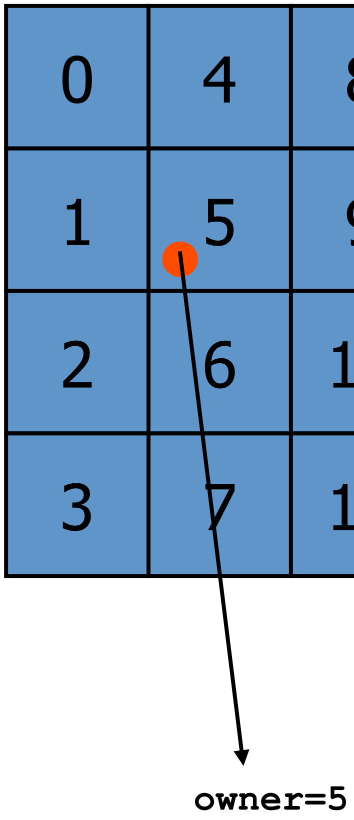
- TAO
  - General optimization problems

- Interoperability with Others
  - PETSc
  - CUMULVS

Data Mapping Information

- To determine the process ID that owns the element defined by the array subscripts:
  - **Fortran** logical function nga_locate(g_a, subscript, owner)
  - **C** int NGA_Locate(int g_a,
    int subscript[])
  - **Python** proc = ga.locate(g_a, subscript)

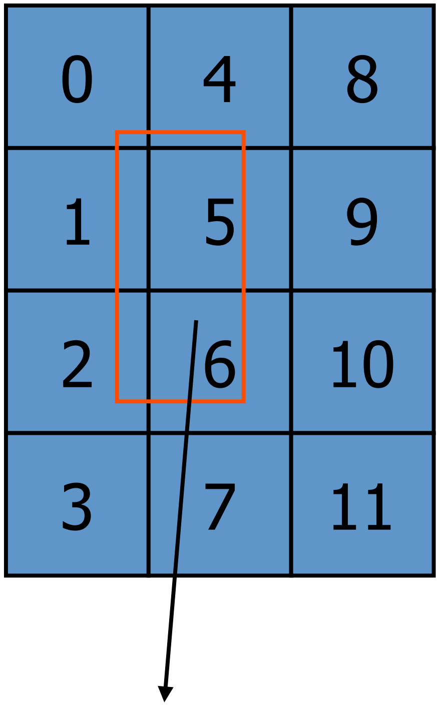
integer	g_a	array handle	[input]
Integer	subscript(ndim)	element subscript	[input]
integer	owner	process id	[output]



Data Mapping Information (cont.)

- To return a list of process IDs that own the patch:
  - **Fortran** logical function nga_locate_region(g_a, lo, hi, map, proclist, np)
  - **C** int NGA_Locate_region(int g_a, int lo[], int hi[], int *map[], int procs[])
  - **Python** map,procs = ga.locate_region(g_a, lo, hi)

integer	np	- number of processors that own a portion of block	[output]
integer	g_a	- global array handle	[input]
integer	ndim	- number of dimensions of the global array	
integer	lo(ndim)	- array of starting indices for array section	[input]
integer	hi(ndim)	- array of ending indices for array section	[input]
integer	map(2*ndim,*)	- array with mapping information	[output]
integer	procs(np)	- list of processes that own a part of array section	[output]

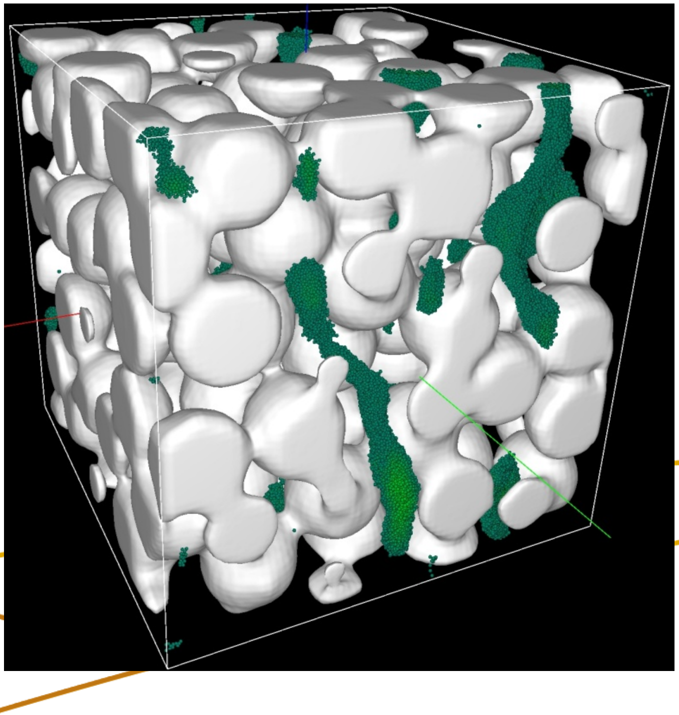


procs = {0,1,2,4,5,6}

map = {lo_{01},lo_{02},hi_{01},hi_{02},
lo_{11},lo_{12},hi_{11},hi_{12},
lo_{21},lo_{22}’hi_{21},hi_{22},
lo_{41},lo_{42},hi_{41},hi_{42},
lo_{51},lo_{52},hi_{51},hi_{52}’
lo_{61}’lo_{62},hi_{61},hi_{62}}

Outline of the Tutorial

- Overview of parallel programming
- Introduction to Global Arrays programming model
- Basic GA commands
- Advanced features of the GA Toolkit
- Current and future developments in GA



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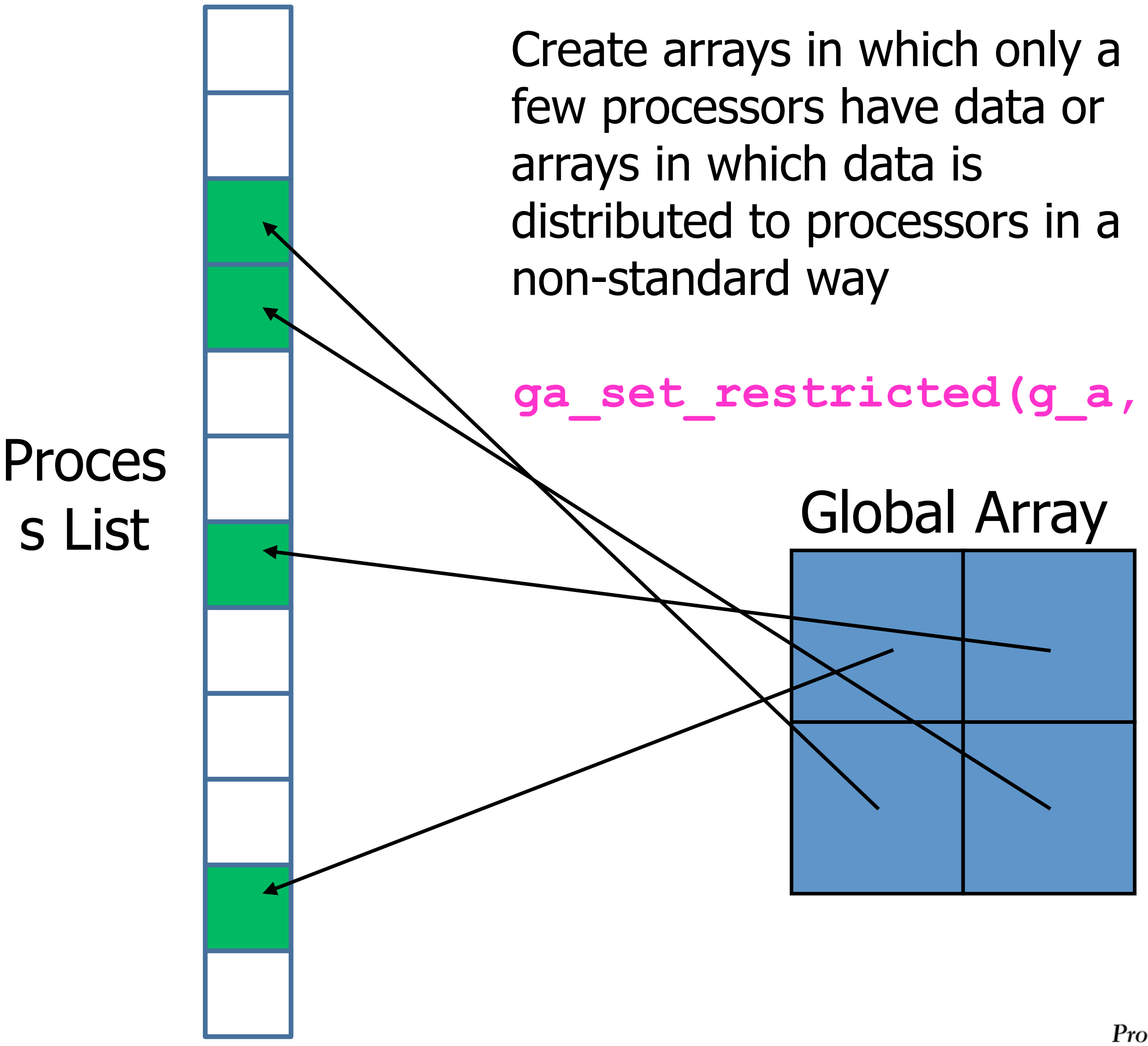
Profiling Capability

- Weak bindings for ARMCI and GA API
  - Enable custom user wrappers to intercept these calls
- ARMCI/GA support in TAU
  - On par with support for MPI
  - Available in current stable TAU release
- Performance patterns for ARMCI in SCALASCA
  - Analysis of traces from ARMCI/GA programs
  - Available in an upcoming SCALASCA release
- Consistent naming convention (NGA_)

Restricted Arrays

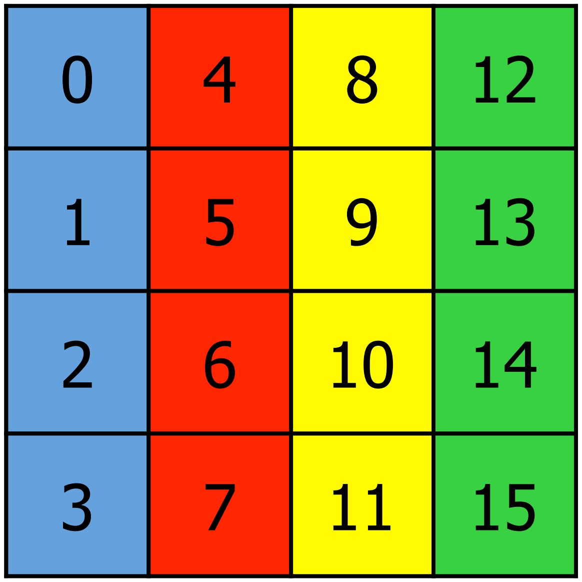
Create arrays in which only a few processors have data or arrays in which data is distributed to processors in a non-standard way

```
ga_set_restricted(g_a, list, nproc)
```



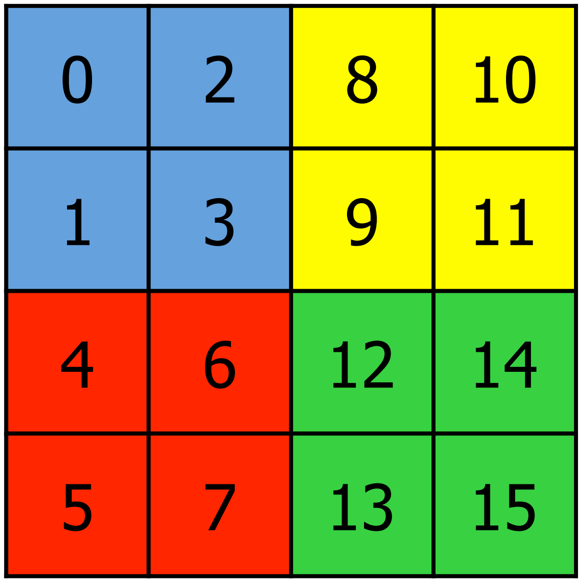
Restricted Arrays

4 nodes, 16 processors



0	4	8	12
1	5	9	13
2	6	10	14
3	7	11	15

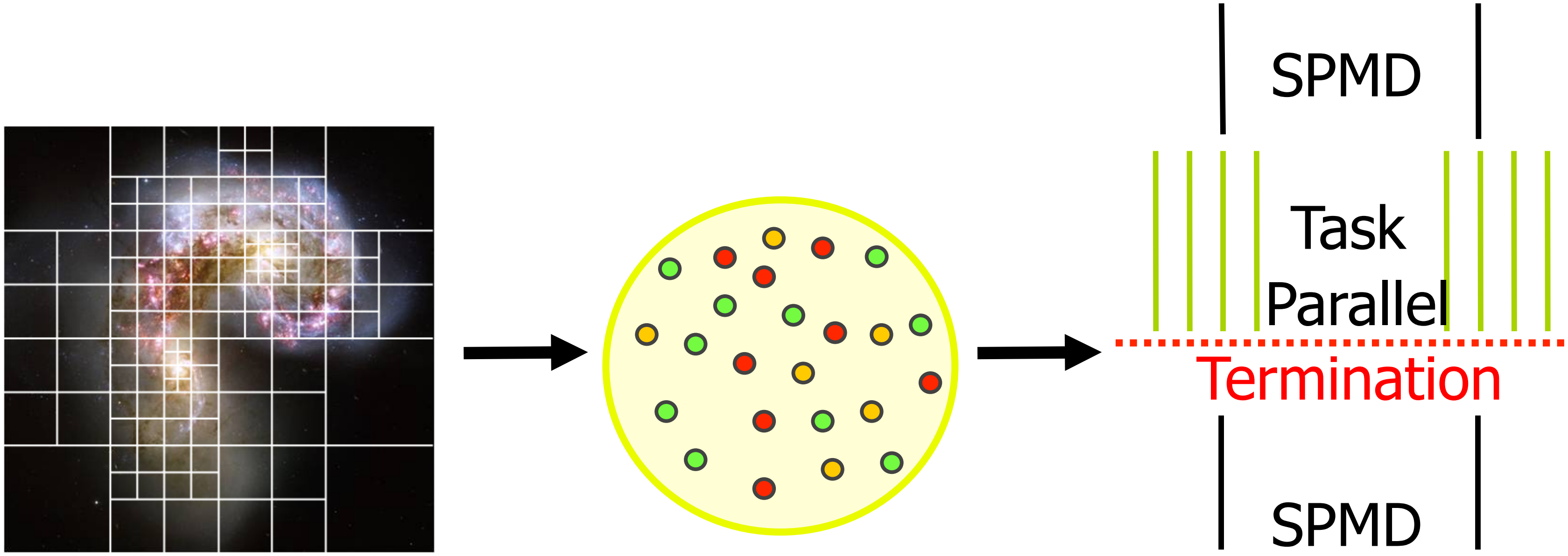
Standard data distribution



0	2	8	10
1	3	9	11
4	6	12	14
5	7	13	15

User-specified distribution

TASCEL-Dynamic Load Balancing



SPMD

Task Parallel

Termination

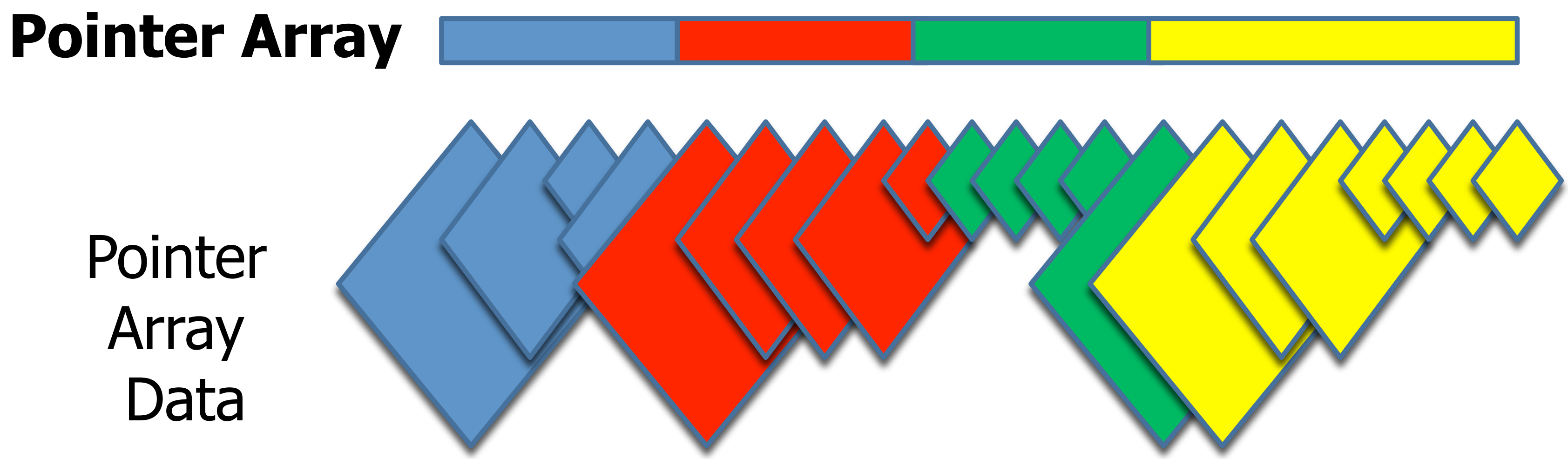
SPMD

- Express computation as collection of tasks
  - Tasks operate on data stored in PGAS (Global Arrays)
  - Executed in collective task parallel phases
- TASCEL runtime system manages task execution
  - Load balancing, locality optimization, etc.
- Extends Global Arrays’ execution model

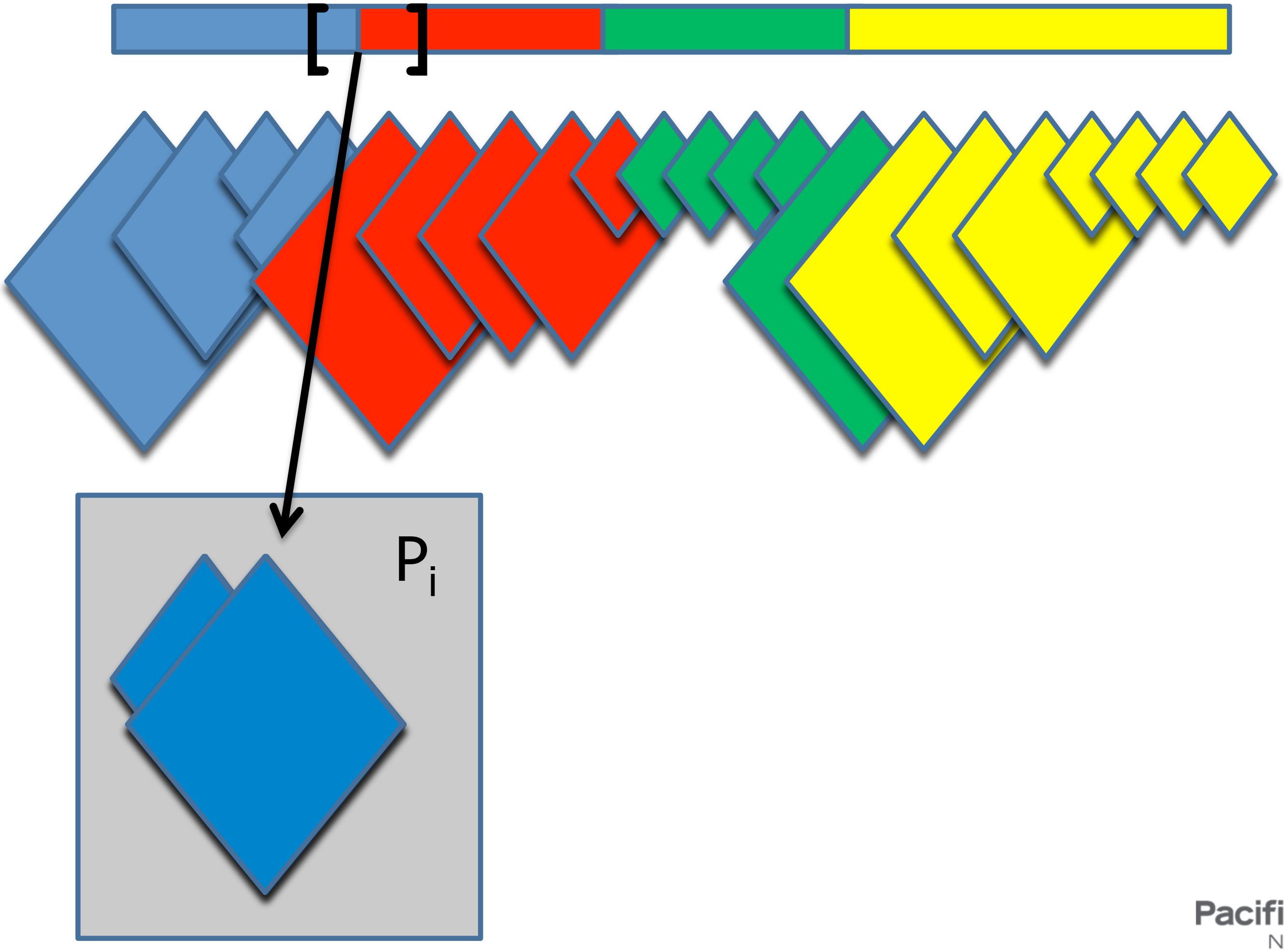
Global Pointer Arrays

- Create arrays where each array element can be an arbitrary data object
  - May be more limited in Fortran where each array object might need to be restricted to an arbitrarily sized array of some type
- Access blocks of array elements or single elements and copy them into local buffers using standard put/get syntax
- Potential Applications
  - Block sparse matrix
  - Embedded refined grids
  - Recursive data structures

Global Pointer Arrays (cont.)



Global Pointer Arrays (cont.)



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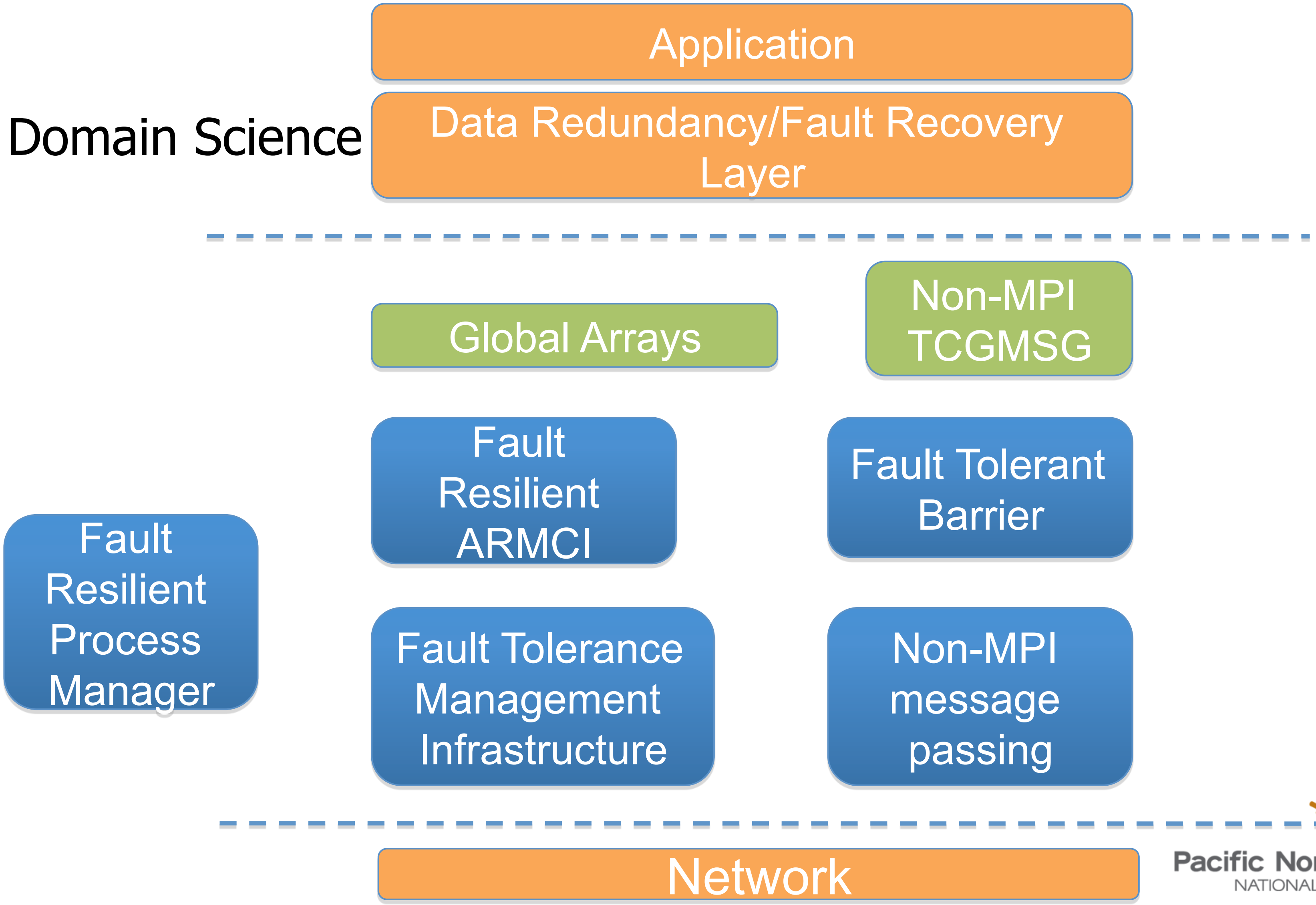
Fault Tolerance



Fault Tolerance (cont.)

- Exploration of multiple data redundancy models for fault tolerance
- Recent demonstrations of fault tolerance with
  - Global Arrays and ARMCI
- Design and implementation of CCSD(T) using this methodology
  - Ongoing Demonstrations at PNNL booth
- Future ongoing developments for leading platforms
  - Cray and IBM based systems

Exascale Challenges

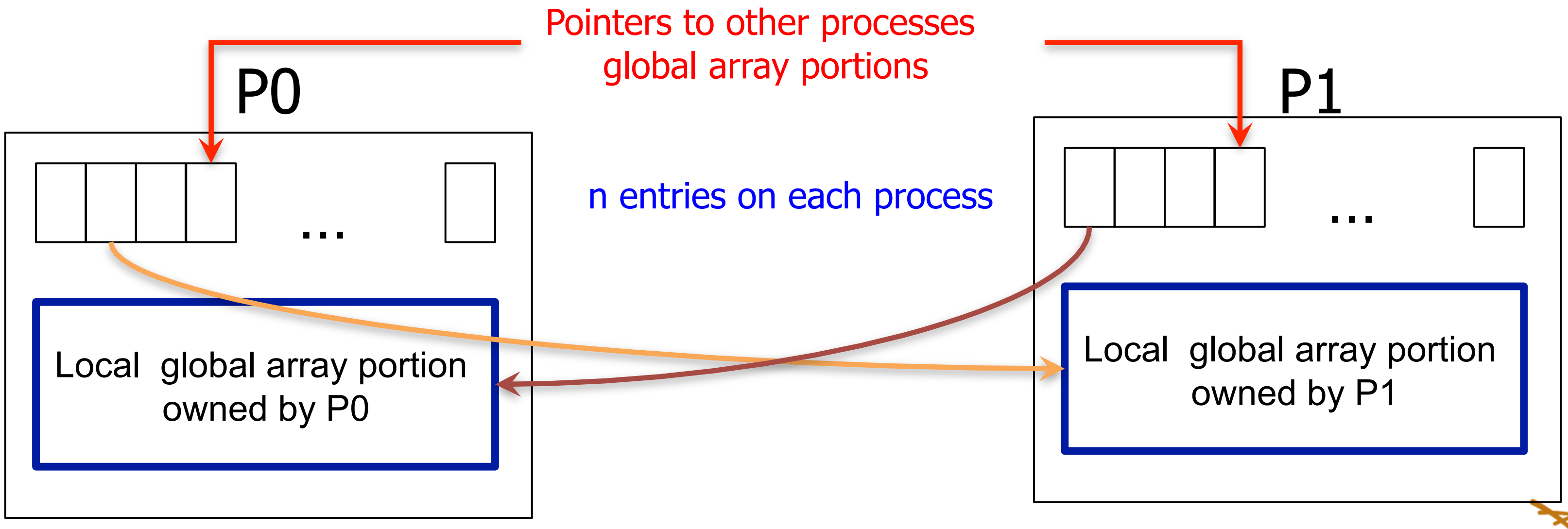
- Node architecture will change significantly
  - Multiple memory and program spaces
    - Develop GA support for Hybrid Platforms
  - Small amounts of memory per core forces the use of non-SPMD programming/execution models
    - Thread safety - support for multithreaded execution
  - There's not enough memory (or memory bandwidth) to fully replicate data in private process spaces
    - Distributing GA metadata within nodes
  - Greater portability challenges
    - Refactoring ARMCI

Exascale Challenges

- Much shorter mean time between failures
  - Fault tolerant GA and ARMCI
- Likely traditional SPMD execution will not be feasible
- Programming models with *intrinsic* parallelism will be needed
  - MPI & GA in their current incarnations only have *external* parallelism
- Data consistency will be more of a challenge at extreme scales

Scalability – GA Metadata is a key component

- GA currently allocates metadata for each global array in a replicated manner on each process
- OK for now on petascale systems with O(10^5) processes
  - 200,000 × 8 bytes = 1.5 MB per global array instance
  - Not that many global arrays in a typical application


Pointers to other processes global array portions
P0
P1
...
n entries on each process
...
Local global array portion owned by P0
Local global array portion owned by P1

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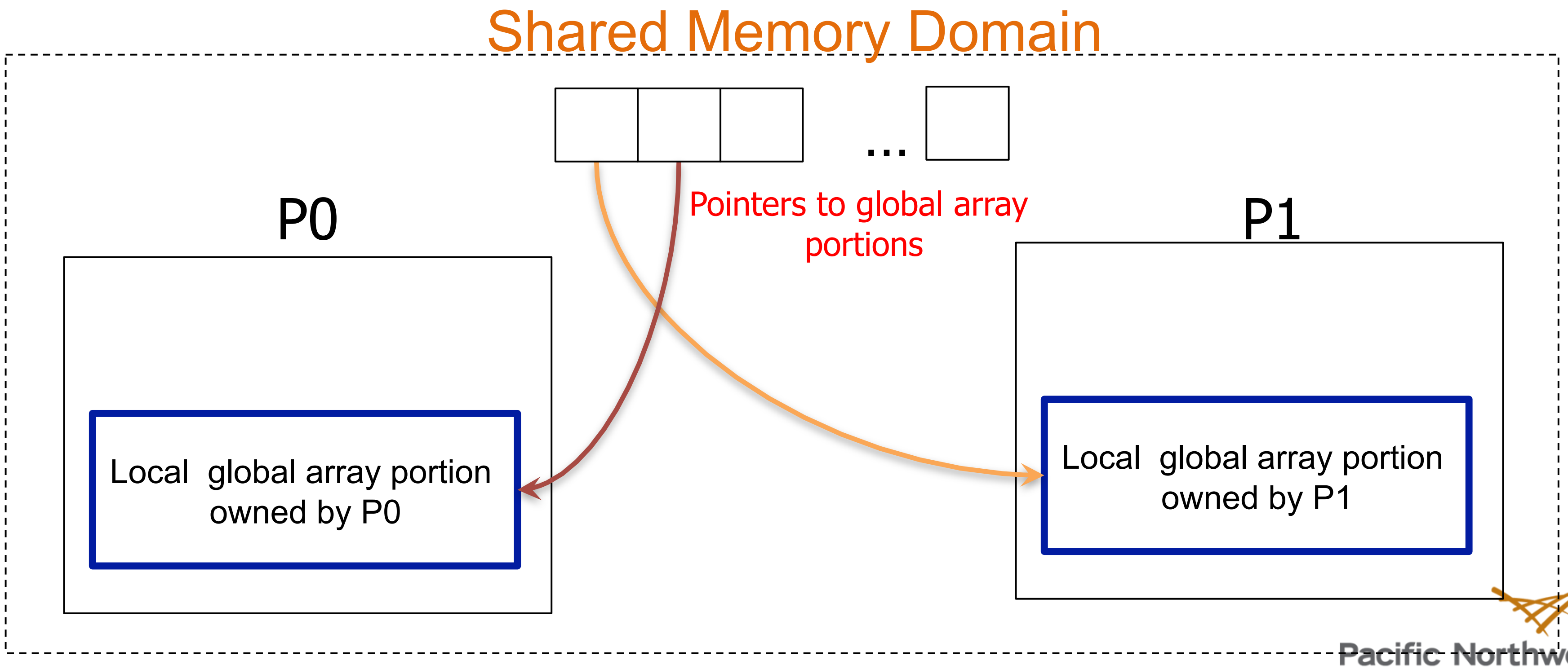
Scalability – Proposed Metadata Overhead Reduction

- Share metadata between processes on the same shared memory domain (today's "node")
- Reduce metadata storage by the number of processes per shared memory domain


Shared Memory Domain
…
P0
P1
Pointers to global array portions
Local global array portion owned by P0
Local global array portion owned by P1

Summary

- Global Arrays supports a global address space
  - Easy mapping between distributed data and original problem formulation
- One-sided communication
  - No need to coordinate between sender and receiver
  - Random access patterns are easily programmed
    - Load balancing
- High Performance
  - Demonstrated scalability to 200K+ cores and greater than 1 Petaflop performance
- High programmer productivity
  - Global address space and one-sided communication eliminate many programming overheads

Thanks

- DOE Office of Advanced Scientific and Computing Research
- PNNL Extreme Scale Computing Initiative

Discussion