



The Global Arrays Toolkit

“Shared-Memory” Programming for “Distributed-Memory”
Computers

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The Global Arrays Toolkit

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Part I

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The Global Arrays Toolkit in a Sentence

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Definition

The Global Arrays (GA) Toolkit is an API for providing a portable “shared-memory” programming interface for “distributed-memory” computers.



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Shared-Memory Systems

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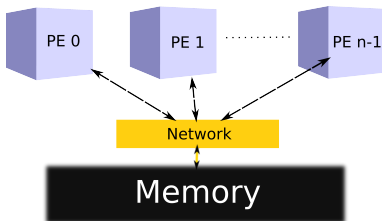
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Advantages

- 1 Global view of shared data (**global indexing**)
- 2 Data mapping usually corresponds to original problem
- 3 More intuitive and (arguably) simpler programming paradigm

Disadvantages

- 1 Details of data locality is obscured
- 2 Programmer needs to avoid race conditions and synchronise updates to shared resources



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Distributed-Memory Systems

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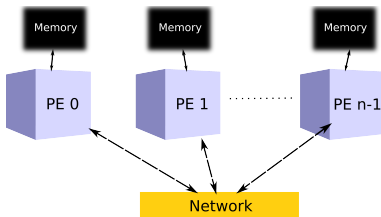
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Advantages

- 1 Data locality is explicit
- 2 Highly scalable
- 3 Generally requires less expensive hardware

Disadvantages

- 1 More difficult programming paradigm
- 2 More complicated data access
- 3 Programmer needs to manage all communication and synchronisation



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Global Arrays - The Best of Both Worlds?

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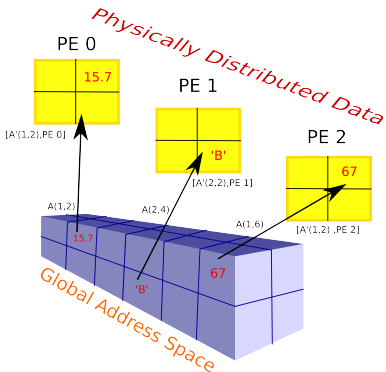
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Features

- 1 Distributed multidimensional arrays accessed through a shared-memory programming style
- 2 Single shared data structure (with **global indexing**)
- 3 Scalability of distributed-memory systems
- 4 Only useable for array data structures



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Global Arrays' Model of Computation

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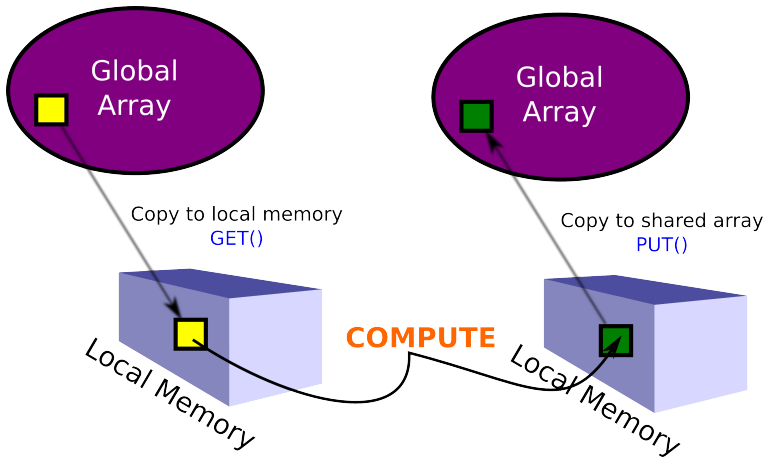
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- 1 Shared-memory model in context of distributed arrays
- 2 Much **simpler** than message-passing for many applications
- 3 Complete environment for parallel code development (including both **task-** and **data-parallelism**)
- 4 Compatible with MPI including packages such as PETSc
- 5 Data locality control similar to distributed-memory/message-passing model [▶ More Info](#)
- 6 Library-based; no special compiler required
- 7 Scalable
- 8 One-sided communication (i.e no co-operative hand-shaking) for point-point communications [▶ More Info](#)



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Global Arrays Toolkit ... continued

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Some Facts

- 1 Developed by Jarek Nieplochal et al. at Pacific Northwest National Laboratory (PNNL) [1]
- 2 The GA Toolkit has been public-domain since 1994
- 3 Employed in several large codes: NWChem, GAMESS-UK and MOLPRO
- 4 Language interfaces include: Fortran, C, C++ and Python (approx. 200 routines[4])
- 5 Implements both blocking and non-blocking local/remote memory access

▶ [More Info](#)



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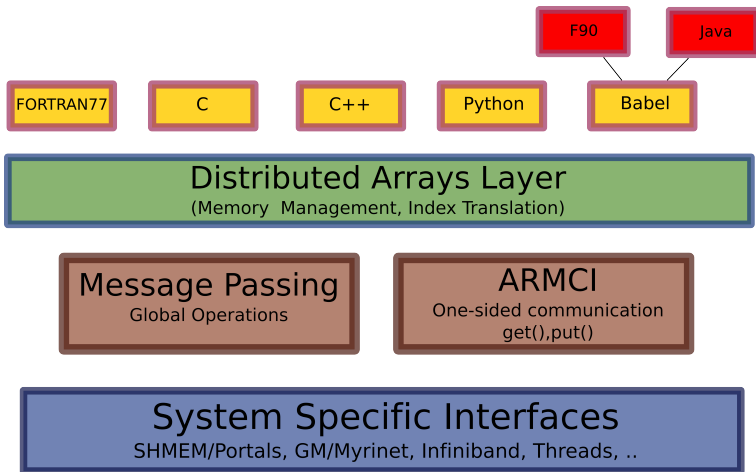
Structure of Global Arrays Toolkit

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Remote Data Access - Example

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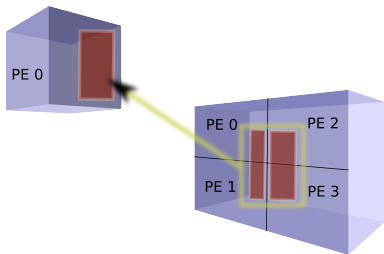
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Message-Passing

```
if (PID != 0) then
  pack data in message
  send message to PE(0)
else
  copy local data to array
  do message=1,3
    receive message from ID(n)
    unpack message to array
  end do
end if
```

GA Toolkit

```
if (ID == 0) then
  call NGA_GET(ga, lo, hi, array, stride)
end if
```





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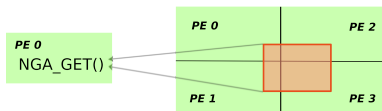
NGA_GET() Flowchart

The Global Arrays Toolkit

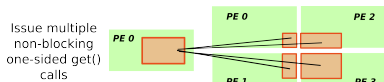
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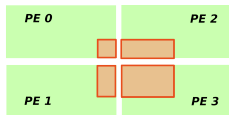


(a)



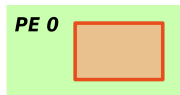
(c)

Determine ownership and locality



(b)

Wait for all data transfers to complete



(d)



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Source Code and Support

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- 1 Latest Stable Version (4.2)
- 2 Homepage at <http://www.emsl.pnl.gov/docs/global/>
- 3 Platforms supported (32-bit and 64-bit)
 - IBM SP, BlueGene
 - Cray X1, XD1, XT3 and XT4
 - Linux Clusters with Ethernet, Myrinet, Infiniband, or Quadrics
 - Solaris
 - Fujitsu
 - Hitachi
 - NEC
 - HP
 - Windows



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Supporting Libraries

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The GA Toolkit requires a number of lower-level libraries for operation:

- MPI[3] (e.g. job startup, run-time execution and collective communications)
- ARMCI (primary communication layer) [▶ More Info](#)
- Memory Allocator (MA) [▶ More Info](#)
- Disk Resident Arrays (DRA)[7] **optional** [▶ More Info](#)



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When To Use GA - Rules of Thumb

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Guidelines - When To Use GA

- 1 Applications with dynamic or irregular communication patterns
- 2 Calculations driven by dynamic load-balancing
- 3 Need one-sided access to shared data structures
- 4 Need high-level operations on distributed arrays and/or for out-of-core array-based algorithms (GA+DRA)
- 5 When message-passing coding becomes too complicated
- 6 Portability and performance is important



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When Not To GA Use - Rules of Thumb

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Guidelines - When Not To Use GA

- 1 Require nearest neighbour communications with regular communication patterns
- 2 When synchronisation with cooperative point-point communication is required (e.g. Cholesky Factorisation)
- 3 When compiler optimisation and parallelisation is more effective
- 4 Parallel language support and compiler tools are sufficient



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Part II

GA Programming Basics



GA Basics

Simplest GA Program Template

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Fortran Template

```
program GA_template

  use mpi

  implicit none

  ! Include GA Headers
#include "mafdecls.fh"
#include "global.fh"

  integer :: error

  ! Intitialize Message-Passing
  call mpi_init(error)

  ! Intitialize GA Library
  call ga_initialize()

  ... processing ...

  ! Terminate GA Library
  call ga_terminate()

  ! Terminate Message-Passing Lib
  call mpi_finalize(error)

end program GA_template
```

C Template

```
#include <stdio.h>

// Include GA Headers
#include "mpi.h"
#include "ga.h"
#include "macdecls.h"

int main(int argc, char **argv) {

  // Intitialize Message-Passing
  MPI_Init(&argc, &argv);

  // Intitialize GA Library
  GA_Initialize();

  ... processing ...

  // Terminate GA Library
  GA_Terminate();

  // Terminate Message-Passing
  MPI_Finalize();

  return 0;
}
```



GA Basics

GA.Initialize() - *Collective Operation*

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Important: The Message-Passing library (e.g. MPI) must be initialised before GA is initialised.

There are two interfaces to initialise Global Arrays:

Interface 1

Fortran: `subroutine ga_initialize()`

C: `void GA_Initialize()`

GA can consume as much memory as application needs to allocate global arrays

Interface 2

Fortran: `subroutine ga_initialize_ltd(limit)`

C: `void GA_Initialize_ltd(size_t limit)`

Aggregate GA memory is limited to *limit* bytes when allocating global arrays



GA Basics

GA_Terminate() - *Collective Operation*

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The conventional way to terminate a GA program is to call the following function:

```
Fortran: subroutine ga_terminate()  
C:      void GA_Terminate()
```

The programmer can also **abort** a running program (e.g. within a error-handling routine) by calling the function:

```
Fortran: subroutine ga_error(message,code)  
C:      void GA_Error(char *message,int code)
```

message
code

User Error Message
Termination Error Code



Within a parallel programming environment there are two important questions to ask:

How many processes are working together?

This can be answered in a GA environment by calling the following function:

Fortran: `integer function ga_nnodes()`

C: `int GA_Nnodes()`

What is the ID of each process?

This can be answered in a GA environment by calling the following function:

Fortran: `integer function ga_nodeid()`

C: `int GA_Nodeid()`



GA Basics

Data Types

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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

Table: Fortran Data Types

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

Table: C Data Types



GA Basics

Compilation

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Fortran 90 Codes

Compile with:

```
mpif90 -I/path_to_GA/include -preprocess_flag \${OPT_Flags} -o foo foo.f90  
-L/path_to_GA/lib/ -lglobal -lma -lsci -llinalg -larmci -ltcgmsg-mpi -lmpich -lm
```

C Codes

```
mpicc -I/path_to_GA/include -preprocess_flag \${OPT_Flags} -o foo foo.c  
-L/path_to_GA/lib/ -lglobal -lma -lsci -llinalg -larmci -ltcgmsg-mpi -lmpich -lm -lm
```



GA Basics

Programming Exercise

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Exercise 1 (15 minutes)

Overview

Modify the GA code template given in the slides to develop a parallel “Hello World” program.

Requirements

- Your code should display a “Hello World” message for each participating process (test with 1,2 and 4 processes)
- Each process message should display it's ID along with the total number of participating processes

Sample Output

```
Hello World from process      1 of      4
Hello World from process      2 of      4
Hello World from process      3 of      4
Hello World from process      0 of      4
```




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Exercise 2

Part III

Creating and Destroying Global Arrays



Creating Global Arrays

Three Ways to Create Global Arrays

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Exercise 2

There are three (3) methods for creating global arrays:

- 1 The *original* interface supporting:
 - regular distributions
 - irregular distributions
- 2 Duplicating an existing global array
- 3 A *new* interface providing more explicit functionality



Creating Global Arrays

Original Interface - Regular Distributions

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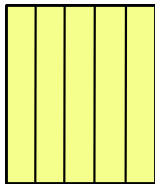
Exercise 2

Definition

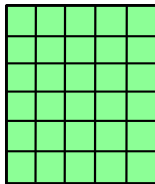
A *regular distribution* attempts to assign the same number of elements to each process. This allows for better **load-balancing** and overall **parallel efficiency**.



(a) Row Block-
ing



(b) Column
Blocking



(c) 2D Block-
ing

Figure: Regular Array Distributions



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Original Interface - Regular Distributions ... continued

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Exercise 2

To create global arrays with regular distributions, call the following function:

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[])`

type	GA Data Type e.g. <i>MT_F_DBL</i>
ndim	Number of Array Dimensions
dims	Vector of Array Dimension Sizes
name	Unique Character Identification String
chunk	Minimum Blocking Size for each Dimension
g_a	Array Handle Returned for Future Reference



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Original Interface - Regular Distributions ... continued

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Exercise 2

Creating a Global Array - Fortran Code Sample

```
integer,dimension(2) :: chunk,dims
integer               :: handle_A

! ... GA Initialization ...

! Set Global Array Dimensions
dims(1)=100000
dims(2)=100000

! Use Default Blocking
chunk(1)=-1
chunk(2)=-1

if (.not.nga_create(MT_F_DBL,2,dims,'Array_A',chunk,handle_A)) then
    call ga_error("Unable to create Global Array for Array A',handle_A")
end if

! ... GA Termination ...
```



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Original Interface - Irregular Distributions

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Exercise 2

Definition

In certain domains it can be beneficial to apply an **irregular distribution**, were the number of elements assigned per process is uneven.

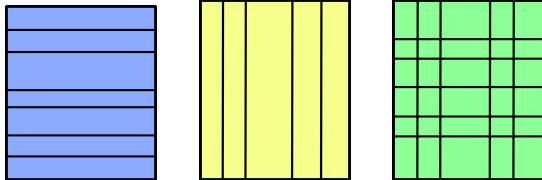


Figure: Irregular Array Distributions



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Original Interface - Irregular Distributions ... continued

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Exercise 2

To create global arrays with irregular distributions, call the following function:

```
Fortran: logical function nga_create_irreg(type, ndim, dims, name, map nblock,  
g-a)
```

```
C: int NGA_Create_irreg(int type, int ndim, int dims[], char *name, int nblock[],  
int map[])
```

type	GA Data Type e.g. <i>MT_F_DBL</i>
ndim	Number of Array Dimensions
dims	Vector of Array Dimension Sizes
name	Unique Character Identification String
map	Starting Index for Each Block
nblock	Number of Blocks Each Dimension is Divided Into
g_a	Array Handle Returned for Future Reference



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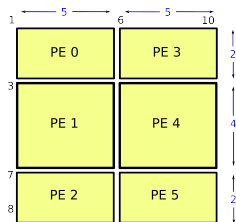
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Exercise 2

An Irregular Distribution Example

Consider the following irregular array distribution i.e. the distribution is non-uniform because processes $P1$ and $P4$ get 20 elements each and processes $P0$, $P2$, $P3$ and $P5$ receive only 10 elements each.



Fortran Code

```
integer :: map(5), nblock(2), dims(2), A

! Set Dimension Blocks
nblock(1)=3;nblock(2)=2

! Set Dimension Sizes
dims(1)=8;dims(2)=10

! Set Starting Indices
map(1)=1;map(2)=3;map(3)=7;map(4)=1;map(5)=6

nga_create_irreg(MT_F_DBL, 2, dims, 'Array_A', &
  map, nblock, A)
```




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Original Interface - Irregular Distributions ... continued

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Exercise 2

With an **irregular distribution**, the programmer specifies distribution points for every dimension using the **map** array argument.

- The GA library creates a distributed array that is a Cartesian product of distributions for each dimension

$nblock = \{3, 2\}$

Row Indices Column Indices

$map = \{1, 3, 7, 1, 6\}$

$product = \{(1,1), (1,6), (3,1), (3,6), (7,1), (7,6)\}$



Creating Global Arrays

Duplicating Global Arrays

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Exercise 2

Global arrays can be **duplicated** (i.e. inherit all the properties of an existing global array including distribution, type, dimensions etc.) with a call to the following function:

Fortran: `logical function ga_duplicate(g_a, g_b, name)`

C: `int GA_Duplicate(int g_a, char *name)`

<code>g_a</code>	Existing Global Array
<code>g_b</code>	New Duplicated Global Array
<code>name</code>	Unique Character Identification String



Creating Global Arrays

New Interface

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Exercise 2

Due to the increasingly varied ways in which global arrays can be configured, a new set of flexible interfaces has been recently developed for creating global arrays.

- The new interface supports all the configurations that were accessible with the old interfaces
- It is anticipated that a new range of global array properties will only be supported via the new interface

The creation of global arrays, using the new interface, progresses with calls to the following functions:

Step 1 - Mandatory

Fortran: `integer function ga_create_handle()`

C: `int GA_Create_handle()`

Step 1: Return a handle to the new global array



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New Interface ... continued

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Step 2 - Mandatory

Fortran: `subroutine ga_set_data(g_a, ndim, dims, type)`

C: `void GA_Set_data(int g_a, int ndim, int dims[], int type)`

Step 2: Set the required properties of the global array

Step 3: Optional properties of the global array can now be set using the following collection of individual `ga_set_XXX()` routines.

Step 3 - Optional

Fortran: `subroutine ga_set_array_name(g_a, name)`

C: `void GA_Set_array_name(int g_a, char *name)`



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Exercise 2

Step 3 - Optional

Fortran: `subroutine ga_set_chunk(g_a, chunk)`

C: `void GA_Set_chunk(int g_a, int chunk[])`

Note: The default setting of chunk is -1 along all dimensions

Step 3 - Optional

Fortran: `subroutine ga_set_irreg_distr(g_a, map, nblocks)`

C: `void GA_Set_irreg_distr(int g_a, int map[], int nblock[])`



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Exercise 2

Step 4: After all the array properties have been set, memory for the global array is allocated by a call to the following function:

Step 4 - Mandatory

Fortran: `logical function ga_allocate(g_a)`

C: `int GA_Allocate(int g_a)`

After this (successful) call, the global array is ready for use.



Destroying Global Arrays

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Exercise 2

Global arrays can be **destroyed** with a call to the following function:

Fortran: **logical function ga_destroy(g_a)**

C: **void GA_Destroy(int g_a)**

g_a Global Array to be Destroyed



Creating/Destroying Global Arrays

Programming Exercise

The Global
Arrays Toolkit

CSCS

Creating and
Destroying
Global Arrays

Creating Global
Arrays

The Simple
Interface

Duplicating
Global Arrays

The New
Interface

Destroying
Global Arrays

Exercise 2

Exercise 2 (30 minutes)

Requirements

Modify your GA Template to **create** and **destroy** four (4) global arrays with the following requirements: (test your solution with 6 processes)

- 1 Create a 5000x5000 Integer Global Array using a column-striped regular distribution
- 2 Create the irregular distributed Global Array given in the slides
 - Look up the GA routine `ga_print_distribution()` in the Interface Documentation[4] and use it to verify the correct creation of the array
- 3 Duplicate the Global Arrays given in part (1) and part (2)
- 4 Create a fourth global array (with the same properties given in part (1)) using the new interface creation methods
- 5 Destroy all the created global arrays



Part IV

One-Sided Communications



One-Sided Communications

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tions

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Put

Get

Atomic

Accumulate

Scatter/Gather

One-Sided, Non-Collective Communications

The Global Arrays Toolkit provides the programmer with *one-sided*, *non-collective* communication operations for accessing data in global arrays without the cooperation of the process or processes that store the referenced data.

Benefits

- 1 The processes containing the referenced data are oblivious to other processes accessing and/or updating their data items
- 2 Since global array indices are still used to reference non-local data items, the calling process does not need to specify process IDs and remote address information



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Remote Blockwise Read/Write	<code>ga_put()</code> , <code>ga_get()</code>
Remote Atomic Update	<code>ga_acc()</code> , <code>ga_read_inc()</code> <code>ga_scatter_acc()</code>
Remote Elementwise Read/Write	<code>ga_scatter()</code> , <code>ga_gather()</code>

Table: The Three Categories of One-Sided Operations in GA



One-Sided Communications

NGA_Put() - Local Communication

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To place data from a local buffer into a section of a global array, use the following function:

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[])`

<code>g_a</code>	Global Array Handle
<code>lo</code>	Array of Starting Patch Indices
<code>hi</code>	Array of Ending Patch Indices
<code>buf</code>	Local Buffer containing Data Values
<code>ld</code>	Leading Dimensions for Buffer



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NGA.Put() - Local Communication

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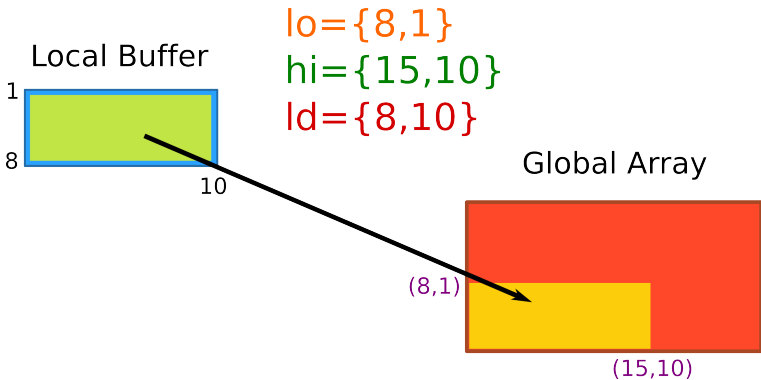


Figure: GA Put() One-Sided Operation



One-Sided Communications

NGA_Get() - Local Communication

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To place data from a section of a global array into a local buffer, use the following function:

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[])`

<code>g_a</code>	Global Array Handle
<code>lo</code>	Array of Starting Patch Indices
<code>hi</code>	Array of Ending Patch Indices
<code>buf</code>	Local Buffer to Receive Data Values
<code>ld</code>	Leading Dimensions for Buffer



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Atomic Accumulate

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Accumulation

Frequently, data moved in a **put** operation has to be combined with the data at the target process, rather than replace it i.e. **accumulation**.

The Global Arrays Toolkit provides two operations **accumulate()** and **read_inc()** which allows a global array patch (**array section**) or element to be remotely updated, with the following benefits:

- 1 **Operations are atomic** i.e. the same patch of global array can be updated by multiple processes without loss of correctness or consistency
- 2 The processes owning the data are not involved in the atomic updates



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Atomic Accumulate ... continued

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Global Array



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



Local
Buffer

Figure: GA Atomic Accumulate Operation



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NGA_Acc()

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To perform an atomic accumulate on a global array patch, call the following function:

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)`

<code>g_a</code>	Global Array Handle
<code>lo</code>	Array of Starting Patch Indices
<code>hi</code>	Array of Ending Patch Indices
<code>buf</code>	Local Buffer containing Data Values
<code>ld</code>	Leading Dimensions for Buffer
<code>alpha</code>	The Scaling Factor



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NGA_Read_inc() - Local Communication

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To perform an atomic accumulate on a single global array element, call the following function:

Fortran: `integer function nga_read_inc(g_a, subscript,inc)`

C: `long NGA_Read_inc(int g_a, int subscript[], long inc)`

<code>g_a</code>	Global Array Handle
<code>subscript</code>	Vector of Element Indices
<code>inc</code>	Increment Value

Notes

- 1 The original global array element is returned
- 2 Only applies to Integer Global Arrays
- 3 Can be used to implement global counters for dynamic balancing



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NGA_Read_inc() ... continued

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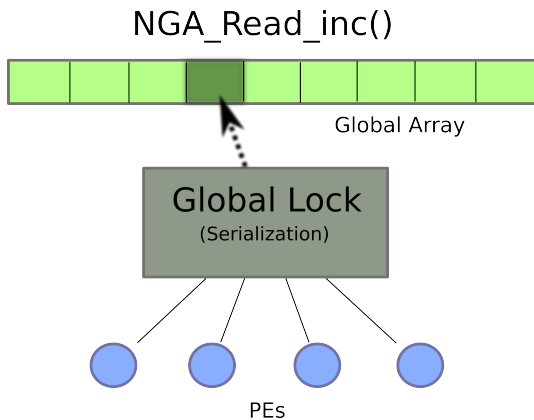


Figure: GA Atomic Read-Increment Operation



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NGA_Scatter() - Local Communication

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Definition

Scatter allows a set of values to be scattered (distributed) to non-contiguous positions in a global array.

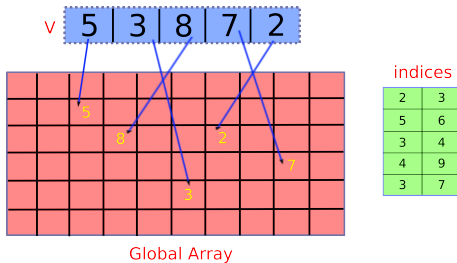


Figure: Scattering Five Elements to a Global Array



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NGA_Scatter() ... continued

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To perform a scatter operation, call the following function:

Fortran: `subroutine nga_scatter(g_a, v, indices,n)`

C: `void NGA_Scatter(int g_a, void *v, int indices[], int n)`

`g_a` Global Array Handle

`v` Vector of Values

`indices` Array of Scatter Indices

`n` Number of Values



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Definition

Gather allows a set of values to be gathered (collected) from non-contiguous global array positions to a local buffer.

To perform a gather operation, call the following function:

Fortran: `subroutine nga_gather(g_a, v, indices,n)`

C: `void NGA_Gather(int g_a, void *v, int indices[], int n)`

<code>g_a</code>	Global Array Handle
<code>v</code>	Local Vector of Values
<code>indices</code>	Array of Gather Indices
<code>n</code>	Number of Values



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Utility Operations



Locality Information

NGA_Locate() - *Local Operation*

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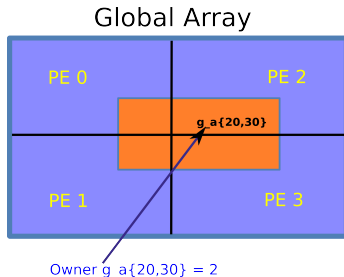
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To determine the **ID** of the process that stores a given **Global Array Index**, the following routine can be used:

```
Fortran: logical function nga_locate(g_a, subscript, owner)
C:        int NGA_Locate(int g_a, int subscript[])
```



subscript
owner

Array containing Global Index
Process ID of Owner

Figure: NGA_Locate() Operation



Locality Information

NGA_Locate_region() - *Local Operation*

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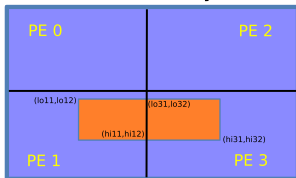
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Other Routines

To determine the **ID(s)** of the process(es) that store a given **Global Array Patch**, the following routine can be used:

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[])

Global Array



proclist={1,3}, map={lo11,lo12,hi11,hi12,
np={2} lo31,lo32,hi31,hi32}

lo Starting Indices for Patch
hi Ending Indices for Patch
map Process Map Info
proclist List of Patch Owners
np Number of Patch Owners

Figure: NGA_Locate_region()



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Frequently a process will want to modify a patch of a global array that is stored locally. To provide direct access to this patch (**and improve overall performance**) the following procedure is required:

Procedure For Direct Access to Local Patch

- 1 Determine the local patch of the Global Array
i.e. Which Part of the Global Array does the Process Own?
- 2 Access the Local Data Patch
- 3 Operate on the Data Patch
- 4 Release Access to the Data Patch



Locality Information

NGA_Distribution() - *Local Operation*

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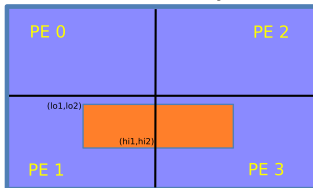
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To determine the **index range** of a Global Array that a process owns, call the following routine:

Fortran: `subroutine nga_distribution(g_a, process, lo, hi)`

C: `void NGA_Distribution(int g_a, int process, int lo[], int hi[])`

Global Array



lo Starting Indices for Patch
hi Ending Indices for Patch
process Process ID

`process={1}, lo={lo1,lo2}, hi={hi1,hi2}`

Figure: GA Distribution Operation



Locality Information

NGA_Access() - *Local Operation*

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Other Routines

To obtain **read/write access** to the local patch data owned by the calling process, call the following routine:

Fortran: `subroutine nga_access(g_a, lo, hi, index, ld)`

C: `void NGA_Access(int g_a, int lo[], int hi[], void *index, int ld[])`

NGA_Access() - Fortran Example

```
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 foo(dbl_mb(index), ld(1))
call nga_release(g_a, lo, hi)

subroutine foo(a, ld1)
  double precision a(ld1,*)
end subroutine
```

lo Starting Indices for Patch
hi Ending Indices for Patch
index Patch Starting Address
ld Leading Dimension of Patch



Locality Information

NGA_Release() - *Local Operation*

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To **release access** to a Global Array patch (which was only used for **reading**), call the following routine:

Fortran: `subroutine nga_release(g_a, lo, hi)`

C: `void NGA_Access(int g_a, int lo[], int hi[])`

To **release access** to a Global Array patch (which was **modified**), call the following routine:

Fortran: `subroutine nga_release_update(g_a, lo, hi)`

C: `void NGA_Access_update(int g_a, int lo[], int hi[])`



Printing Global Arrays

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Other Routines

Global Array Display Options

The Global Arrays Toolkit provides routines to print:

- 1 the contents of a Global Array
- 2 the contents of a Global Array patch
- 3 the status of array operations
- 4 a summary of allocated arrays



Printing

GA_Print()/GA_Print_patch() - *Collective Operations*

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To print an entire Global Array to standard output (**with formatting**) call the following routine:

```
Fortran: subroutine ga_print(g_a)
C:       void GA_Print(int g_a)
```

To print a Global Array patch to standard output call the following routine:

```
Fortran: subroutine ga_print_patch(g_a, lo, hi, pretty)
C:       void GA_Print_patch(int g_a, int lo[], int hi[], int pretty)
```

- 1 pretty=0 - dump all elements of patch without formatting
- 2 pretty=1 - display labelled array with formatted rows and columns



Printing

GA_Print_stats() - *Local Operation*

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Other Routines

To print **global statistics** about array operations for the calling process, call the following routine:

```
Fortran: subroutine ga_print_stats()
C:       void GA_Print_stats()
```

This routine will print:

- 1 the number of calls to the GA **create()**, **duplicate()**, **destroy()**, **get()**, **put()**, **scatter()**, **gather()** and **read_and_inc()** operations
- 2 the total amount of data moved in the GA primitive operations
- 3 the amount of data moved in the primitive GA operations to logically remote locations
- 4 the maximum memory consumption of Global Arrays (high-water mark)



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To print distribution information ([array mapping to processes](#)) for a Global Array, call the following routine:

```
Fortran: subroutine ga_print_distribution(g_a)
C:       void GA_Print_distribution(int g_a)
```

To display summary information on allocated arrays call the following routine:

```
Fortran: subroutine ga_summarize(verbose)
C:       void GA_Summarize(int verbose)
```

① `verbose = 0 or 1`



Further Utility Routines

The Global Arrays Toolkit provides other utility routines that are described further in the GA documentation. They include routines for:

- 1 Memory Availability
- 2 Cluster Topology and Details
- 3 Broadcast/Reduction
- 4 Array Dimension, Type and Name Inquiry



Part VI

Collective Communications



Collective Communications

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Definition

The Global Arrays Toolkit provides **collective operations** which can be applied to **whole** global arrays or **patches** of global arrays.

- Collective operations require that **all** processes initiate the collective call (although in general they only operate on their local array data)

GA collective operations span the following categories:

- 1 Basic Array Operations
- 2 Linear Algebra Operations
- 3 Interfaces to 3rd Party Software Packages



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Since GA doesn't specifically initialise newly created arrays, a global array can be [set to 0](#) with the the following routine:

```
Fortran: subroutine ga_zero(g_a)
C:       void GA_Zero(int g_a)
```

If a global array is required to be initialised with a [non-zero](#) value, the following routine can be called:

```
Fortran: subroutine ga_fill(g_a, value)
C:       void GA_Fill(int g_a, void *value)
```

Note: The type of `value` should match the type of the global array `g_a`.



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GA_Scale()

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To **scale** all the elements in a global array by the factor s , call the following routine:

```
Fortran: subroutine ga_scale(g_a, s)
C:       void GA_Scale(int g_a, void *s)
```

Note: The type of s should match the type of the global array g_a .



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Copying Arrays

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To **copy** the contents of one global array to another, call the following routine:

```
Fortran: subroutine ga_copy(g_a, g_b)
```

```
C: void GA_Copy(int g_a, g_b)
```

- 1 The global arrays **g_a** and **g_b** should be of the same type
- 2 The global arrays **g_a** and **g_b** should have the same number of elements and dimensions (but can be copied to an array with a different shape and/or distribution)



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Copying Arrays ... continued

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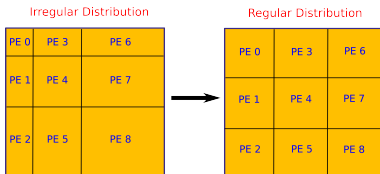


Figure: Copying Global Arrays on 3x3 Process Grid

Array Copy - Fortran Example

```
! Create Irregular Distribution
status=nga_create_irreg(MT_F_DBL, 2, dims, 'A', map, nblocks, A)

! Create Regular Distribution
status=nga_create(MT_F_DBL, 2, dims, 'B', chunks, B)

... Initialise A ...

! Copy global array A to global array B
call ga_copy(A, B)
```




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Initialising Array Patches

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GA also provides analogous routines for initialising array **patches** (as opposed to whole arrays):

Fortran: `subroutine nga_zero_patch(g_a, lo, hi)`

C: `void GA_Zero_patch(int g_a, int lo[], int hi[])`

lo Starting Indices of Array Patch

hi Ending Indices of Array Patch

Fortran: `subroutine nga_fill_patch(g_a, lo, hi, value)`

C: `void GA_Fill_patch(int g_a, int lo[], int hi[], void *value)`



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NGA_Copy_patch()

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One of the most fundamental GA operations is `nga_copy_patch()`. This operation copies a patch in one global array to a patch in another global array.

Fortran: `subroutine nga_copy_patch(trans, g_a, lo1, hi1, g_b, lo2, hi2)`

C: `void GA_Zero_patch(char trans, int g_a, int lo1[], int hi1[], int g_b, int lo2[], int hi2[])`

trans Transpose Patch ('Y' or 'N')

Notes:

- 1 The source patch must be on a **different** global array than the destination patch
- 2 Array patches must be the **same type**
- 3 Array patches must have the **same number of elements** (but not necessarily the same shape)



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Copying Array Patches

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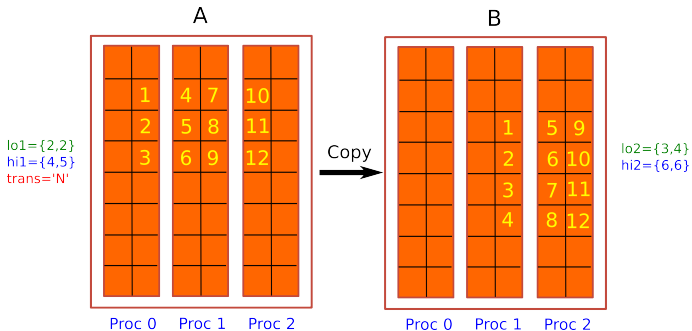


Figure: Global Array Patch Copy with Reshape



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Copying Array Patches ... continued

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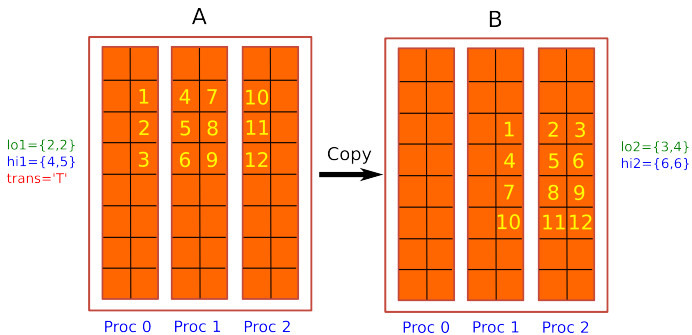


Figure: Global Array Patch Copy with Reshape and Transpose



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Matrix Addition

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GA provides a range of routines for performing **linear algebra operations** on Global Arrays (routines are available for both whole array and patches).

To **add** two global arrays A and B (element-wise) with the result placed into array C , call the following routine:

Whole 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)`

$$C = \alpha A + \beta B$$



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Matrix Addition ... continued

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Fortran: `subroutine ga_add_patch(alpha, g_a, lo1, hi1, beta, g_b, lo2, hi2, g_c, lo3, hi3)`

C: `void GA_Add(void *alpha, int g_a, int lo1[], int hi1[], void *beta, int g_b, int lo2[], int hi2[], int g_c, int lo3[], int hi3[])`



Collective Communications

Matrix Multiplication

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To perform **matrix multiplication** between two global arrays A and B (with the result placed in global array C), call the following operation:

```
Fortran: subroutine nga_matmul_patch(transa, transb, alpha, beta, g_a, alo, ahi,  
g_b, blo, bhi, g_c, clo, chi)
```

```
C: void NGA_Matmul_patch(char transa, char transb, void* alpha, void *beta, int  
g_a, int alo[], int ahi[], int g_b, int blo[], int bhi[], int g_c, int clo[], int chi[])
```

$$C = \alpha A * B + \beta C$$

Note:

- 1 A , B and C must be 2D Global Arrays



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Other 2D Collective Operations

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There are two other GA operations that can only be applied to 2D Global Arrays:

Fortran: `subroutine ga_symmetrize(g_a)`

C: `void GA_Symmetrize(int g_a)`

$$A = \frac{1}{2}(A + A')$$

Fortran: `subroutine ga_transpose(g_a, g_b)`

C: `void GA_Transpose(int g_a, int g_b)`

$$B = A'$$



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Further Operations

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GA provides a wealth of whole array and patch array routines for many linear operations (please see [4] for more detailed information):

Further operations include:

- 1 **Dot Products**
- 2 **Elemental Operations**
 - Element Addition, Multiplication, Division, Reciprocals
 - Maximum/Minimum Elements
- 3 **Diagonal Operations**
 - Diagonal Shifts
 - Diagonal Initialisation/Updates
 - Diagonal Addition
- 4 **Row/Column Scaling**
- 5 **Norms**
- 6 **Medians**



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ScaLAPACK

ScaLAPACK[5] is a well known software library for linear algebra computations on distributed-memory architectures. GA interfaces with this library to solve systems of linear equations and also to invert matrices.

PeIGS

The PeIGS library contains routines for solving standard and generalized real symmetric eigensystems. For more information about the availability of PeIGS with GA contact: fanngi@ornl.gov.

PETSc

GA can be intermixed with PETSc[6] routines (a library for the parallel scalable solution of scientific applications modelled by partial differential equations). Instructions for using PETSC with GA can be found at:

<http://www.emsl.pnl.gov/docs/global/petsc.html>



Collective Communications

GA_Solve()

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To solve the system of linear equations $AX = B$, call the following routine:

```
Fortran: integer function ga_solve(g_a, g_b)
```

```
C: int GA_Solve(int g_a, int g_b)
```

Notes:

- 1 In the first instance, a **Cholesky factorisation** and **Cholesky solve** will be performed
 - If a Cholesky factorisation is not successful, then a *LU* factorisation will be performed with a forward/backward substitution
- 2 On exit, B will contain the solution X



Collective Communications

GA_Llt_solve()

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To solve a system of linear equations $AX = B$ using the Cholesky factorisation of an NxN double precision **symmetric positive definite matrix** A , call the following routine:

```
Fortran: integer function ga_llt_solve(g_a, g_b)
```

```
C: int GA_Llt_solve(int g_a, int g_b)
```

Notes:

- 1 On exit, B will contain the solution X



Collective Communications

GA_Lu_solve()

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To solve a system of linear equations $op(A)X = B$ (where $op(A) = A$ or A') using a **LU factorisation** of a general real matrix A , call the following routine:

```
Fortran:  subroutine ga.lu_solve(g_a, g_b)
```

```
C:        int GA_Lu_solve(int g_a, int g_b)
```

Notes:

- 1 On exit, B will contain the solution X (possibly multiple RHS vectors)



Collective Communications

GA_Spd_inverse()

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To compute the **inverse** of a double precision matrix using the Cholesky factorisation of an $N \times N$ double precision symmetric positive definite matrix A , call the following routine:

```
Fortran: integer function ga_spd_inverse(g_a)
C:       int GA_Spd_inverse(int g_a)
```

Notes:

- 1 On exit, A will contain the inverse



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Improving Synchronisation Control of Collective Operations

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Redundant Synchronisation

In some cases it may be possible (if you are careful) to remove **redundant implicit synchronisation** within collective GA operations (and improve performance).

- 1 Collective operations exploit implicit synchronisation to ensure local data is in a consistent state before it is accessed locally i.e. no outstanding communication operations
- 2 In many cases the **internal synchronisation points**, within back-back collective communications (or if the user calls an explicit synchronisation operation before the collective communication), can be removed:



Collective Communications

GA_Mask_sync()

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To set the implicit synchronisation points for the next collective operation, call the following routine:

```
Fortran:  subroutine ga_mask_sync(prior_sync_mask, post_sync_mask)
C:        void GA_Mask_sync(int prior_sync_mask, int post_sync_mask)
```

`prior_sync_mask` When false, disables synchronisation at start of next collective call

`post_sync_mask` When false, disables synchronisation at end of next collective call



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Improving Synchronisation Control of Collective Operations ... continued

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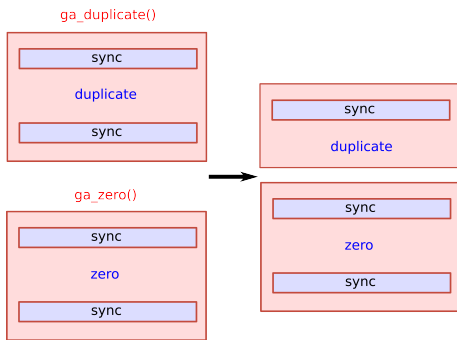
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Synchronisation Mask - Fortran Example

```
! Mask Implicit Synchronisation
call ga_duplicate(g_a, g_b)
call ga_mask_sync(0,1)
call ga_zero(g_b)
```



Part VII

Inter-Process Synchronisation



Synchronisation

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Definition

Process *synchronisation* refers to the coordination of simultaneous processes to complete a task in order to get correct runtime order and avoid unexpected race conditions.

Classification of GA Synchronisation

The Global Arrays Toolkit provides three (3) types of synchronisation operations:

- 1 Lock with Mutex
- 2 Fence
- 3 Sync



Synchronisation

Lock and Mutex

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Background

A *lock* and *mutex* are useful primitives in shared-memory programming. A mutex can be locked to exclusively protect access to a **critical section** of code e.g. to avoid the simultaneous use of a common resource, such as a **global variable**.

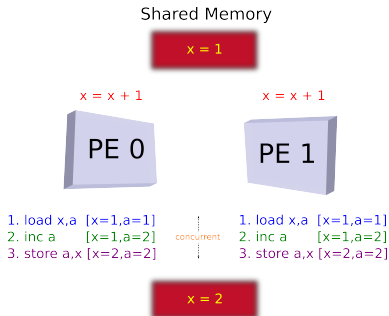


Figure: Conflict with Shared Resource Update



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Lock and Mutex ... continued

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Critical Section Algorithm

1. Create Mutexes
- ...
2. Lock on a Mutex
3. Perform Critical Section Operation
4. Unlock the Mutex
- ...
5. Destroy Mutexes

Notes

A mutex is a lock that can be obtained ([set](#)) by a process (if it is free), prior to a [critical section](#) of code. If a lock is set by a given process (and the process enters the critical section) no other processes can obtain the lock and therefore enter the critical section at the same time.



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Lock and Mutex ... continued

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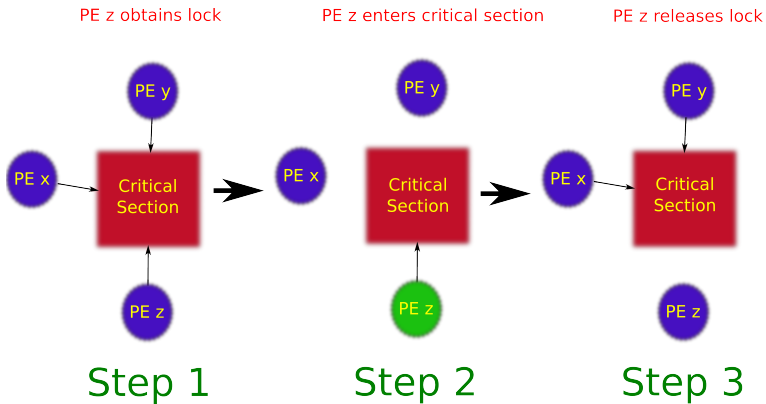


Figure: Mutual Exclusion Using Locks



Synchronisation

GA_Create_mutexes() - *Collective Operation*

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To create a **mutex set** in GA, call the following function:

```
Fortran: logical function ga_create_mutexes(number)
C:       int GA_Create_mutexes(int number)
```

`number` **Number of Mutexes in Mutex Array**

Note:

- 1 Only one set of mutexes can exist at one time
- 2 Mutexes are numbered $[0 \dots number - 1]$
- 3 GA_Create_mutexes() is a collective operation



Synchronisation

GA_Destroy_mutexes() - *Collective Operation*

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To destroy a **mutex set** in GA, call the following function:

```
Fortran: logical function ga_destroy_mutexes()  
C:       int GA_Destroy_mutexes()
```

Note:

- 1 Mutexes can be created and destroyed as many times as is needed
- 2 GA_Destroy_mutexes() is a collective operation



Synchronisation

GA.Lock()

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To **lock** a mutex object in GA, call the following function:

```
Fortran: subroutine ga_lock(mutex)
```

```
C:      int GA_Lock(int mutex)
```

mutex **Mutex Number**

Note:

- 1 It is a fatal error for a process to lock a mutex object that has already been locked by this process



Synchronisation

GA_Unlock()

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To **unlock** a mutex object in GA, call the following function:

```
Fortran: subroutine ga_unlock(mutex)
```

```
C:      int GA_Unlock(int mutex)
```

mutex **Mutex Number**

Note:

- 1 It is a fatal error for a process to unlock a mutex object that has not been locked by this process



Synchronisation

Lock and Mutex ... continued

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Lock and Mutex Fortran Example

```
! Create Mutex Set (with one mutex)
status = ga_create_mutexes(1)

! Check if Mutex Creation Successful
if (.not. status) then
  call ga_error("ga_create_mutexes failed",0)
end if

! Obtain Lock
call ga_lock(0)

! Now do something in Critical Section
call ga_put(g_a, ... )
...

! Release Lock
call ga_unlock(0)

! Destroy Mutexes
status = ga_destroy_mutexes(1)
if (.not. status) then
  call ga_error("ga_destroy_mutexes failed",0)
end if
```



Synchronisation

Fence

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Definition

A **fence** operation blocks the calling process until all the data transfers corresponding to the Global Array operations initiated by this process are complete.

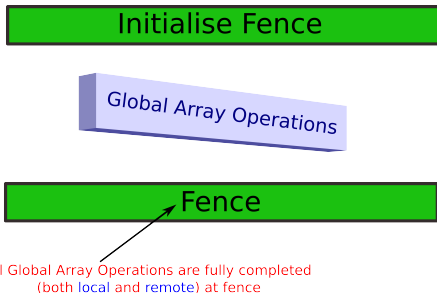


Figure: GA Fence Operation



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GA_Init_fence()

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To **initiate** a fence in GA, call the following function:

Fortran: `subroutine ga_init_fence()`

C: `void GA_Init_fence()`

Note:

- 1 GA_Init_fence() initialises tracing of the completion status of global array data movement operations



Synchronisation

GA_Init_Fence() ... continued

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A **fence** can be called in GA with the following function:

```
Fortran: subroutine ga_fence()  
C:      void GA_Fence()
```

Note:

- 1 GA_Fence() blocks the calling process until all Global Array data transfers called after GA_Init_fence() are fully completed.
- 2 GA_Fence() must be called after a GA_Init_fence() (i.e. called in pairs)
- 3 GA_Init_fence()/GA_Fence() pairs can be nested



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Fence Examples

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Fortran Example 1

```
call ga_init_fence()  
call ga_put(g_a, ...)  
call ga_fence()
```

GA_Put() can return before the data reaches its final destination. A **GA_Init_fence()/GA_Fence()** pair allows the process to wait until the data transfer is complete

Fortran Example 2

```
call ga_init_fence()  
call ga_put(g_a, ...)  
call ga_scatter(g_a, ...)  
call ga_put(g_b, ...)  
call ga_fence()
```

The calling process will be blocked until the data movements of two **GA_Puts()** and one **GA_Scatter()** are completed.



Synchronisation

GA_Sync()

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Definition

The GA **sync** operation is a collective barrier operation which synchronises all the processes and ensures all Global Array operations are complete after the call.

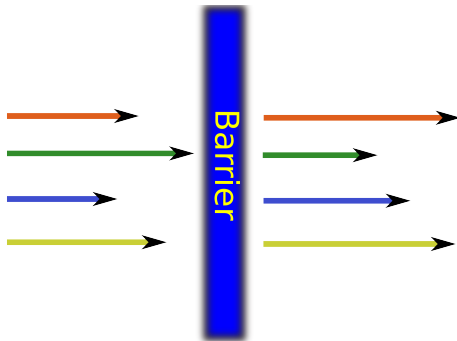


Figure: Barrier Synchronisation



Synchronisation

GA_Sync() ... continued

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A GA **synch** operation can be called with the following function:

```
Fortran: subroutine ga_sync()  
C:      void GA_Sync()
```

Note:

- 1 GA Sync operations should be inserted where necessary
- 2 Increased synchronisation can result in reduced application performance



Part VIII

Processor Groups



Processor Groups

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Definition

Processor Groups can be a useful technique for dividing the default domain (**world**) of processes into separate subgroups of processes.

Benefits for applying group management include:

- 1 Global Arrays created in a group are only distributed among the processes in the group
- 2 Collective operations on the subgroup are restricted to the processes in the group
- 3 A Synchronisation operation applied to a group will not affect the processes residing outside the group
- 4 Independent parallel operations can be applied to different subgroups concurrently



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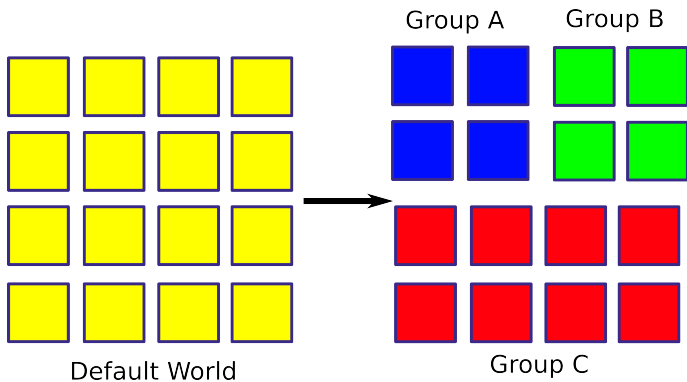


Figure: Decomposition of World into Subgroups



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Important Notes

- 1 When applying subgroups, it is a good idea to ensure that the default world is divided into a complete covering of non-overlapping subgroups
- 2 Global Arrays are only created on the **default group** (usually the **world group**), and most global array operations are restricted to the default group:
 - Typically you change the default group prior to applying a Global Array operation (the global array operation will subsequently be applied to the new current default group)
 - Or use the GA routines that specifically accept **subgroup array handles**



Processor Groups

GA_Pgroup_create()

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A new processor group can be created in GA with the following function:

```
Fortran: integer function ga_pgroup_create(proclist,size)
C:        int GA_Pgroup_create(int *proclist, int size)
```

proclist Vector of Processes
size Number of Processes in Group

- This call must be executed by **all processes in the new subgroup**.
- The integer handle of the newly created process group will be returned on completion of the call



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Assigning Process Groups

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A processor group can be applied to a Global Array using both **original** and **new** interfaces:

Original Interface

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[])`

`p_handle` Handle of Process Group

New Interface

Fortran: `logical function ga_set_pgroup(g_a, p_handle)`

C: `int NGA_Create_config(int g_a, int p_handle)`



Processor Groups

Setting Default Process Group

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The default process group can be set with the following routine:

```
Fortran: subroutine ga_pgroup_set_default(p_handle)
C:       void GA_Pgroup_set_default(int p_handle)
```

- This routine can set the default group to something other than the default **world group**
- This routine must be called by all processes within the process group represented by **p_handle**
- Once the default process group is set, all subsequent operations will be applied to the new default group.



Processor Groups

Process Group Inquiry Functions

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To inquire about the number of nodes in a process group, call the following routine:

Fortran: `integer function ga_pgroup_nnodes(p_handle)`

C: `int GA_Pgroup_nnodes(int p_handle)`

To inquire about the local ID of the calling process within the group, call the following routine:

Fortran: `integer function ga_pgroup_nodeid(p_handle)`

C: `int GA_Pgroup_nodeid(int p_handle)`



Processor Groups

Process Group Inquiry Functions

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To determine the handle for the current default process group, call the following routine:

Fortran: `integer function ga_pgroup_get_default()`

C: `int GA_Pgroup_get_default()`

To determine the handle for the current world process group, call the following routine:

Fortran: `integer function ga_pgroup_get_world()`

C: `int GA_Pgroup_get_world()`



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Process Group Example

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Default Process Group Example

```
! Create Subgroup A
A = ga_pgroup_create(listA,nprocA)
call ga_pgroup_set_default(A)

! Perform some parallel work
call parallel_work()

! Reset Default Process Group to World Group
call ga_pgroup_set_default(ga_pgroup_get_world())

contains

  subroutine parallel_work()

    ! Create Subgroup B
    B = ga_pgroup_create(listB,nprocB)
    call ga_pgroup_set_default(B)
    call more_parallel_work

  end subroutine
```



Part IX

Advanced Topics



Ghost Cells

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Definition

Ghost cells are a common technique to reduce communication in parallel applications that exploit domain decomposition, where the data required by a given process to complete a calculation resides on a neighbouring process e.g. codes that employ finite-difference and finite-element methods.

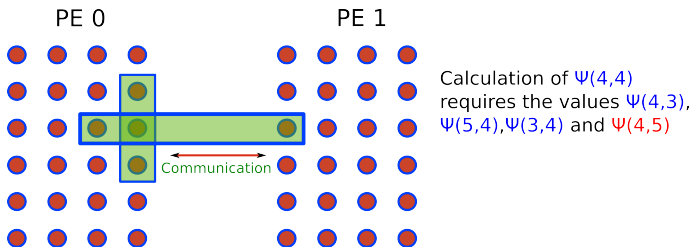


Figure: Domain Decomposition - Data Exchange



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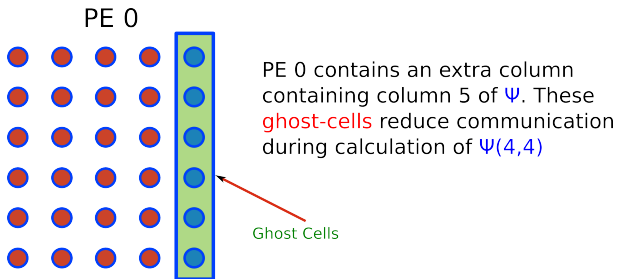


Figure: Domain Decomposition With Ghost-Cells

- 1 Ghost cells need to be updated when they are modified on the neighbouring process. GA allows the programmer to perform this update with a single function.



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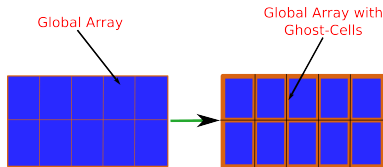
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Ghost cells can be automatically created for a global array (with regular distribution) using the following functions:

Fortran: logical function nga_create_ghosts(type, ndim, dims, width, name, chunk, g_a)

C: int NGA_Create_ghosts(int type, int ndim, int dims[], int width[], char *name, int chunk[])

width Vector of Ghost Cell Widths in each Dimension



```
nga_create_ghosts(MT_F_DBL,2,dims,width,'Array_A',chunk,g_a)
```



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Ghost cells can be automatically created for a global array (with **irregular distribution**) using the following functions:

Fortran: `logical function nga_create_ghosts_irreg(type, ndim, dims, width, name, map, nblocks, g-a)`

C: `int NGA_Create_ghosts_irreg(int type, int ndim, int dims[], int width[], char *name, int map[], int nblocks[])`

width **Vector of Ghost Cell Widths in each Dimension**



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Ghost cells can be updated with values from their adjacent neighbours using the following functions:

```
Fortran: subroutine ga_update_ghosts(g_a)
C:       void GA_Update_ghosts(int g_a)
```

Note:

- 1 The update operation assumes **periodic** (wrap-around) boundary conditions (see **Periodic Interfaces**)



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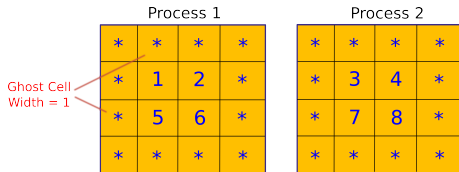


Figure: Global Array With Uninitialised Ghost Cells

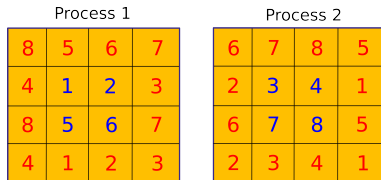


Figure: Global Array After Ghost Cell Update



Ghost Cells

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GA also provides a routine to update ghost cells in **individual directions** (most useful when updates can be overlapped with computation).

Fortran: `logical function nga_update_ghosts_dir(g_a, dimension, direction, corner)`

C: `int NGA_Update_ghosts_dir(int g_a, int dimension, int direction, int corner)`

- dimension** Coordinate direction is to be updated
 (e.g. `dimension=2` corresponds to *y*-axis in *2D* or *3D* system)
- direction** Updated side is in positive or negative direction?
- flag** Should corners on updated side be included?



Ghost Cells

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```
status = NGA_Update_ghost_dir(g_a, 0, -1, 1)
status = NGA_Update_ghost_dir(g_a, 0, 1, 1)
status = NGA_Update_ghost_dir(g_a, 1, -1, 0)
status = NGA_Update_ghost_dir(g_a, 1, 1, 0)
```

Figure: Equivalent Calls for 2D GA_Update_ghosts Call



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The values of **local** ghost cells can be accessed using the following functions:

Fortran: `subroutine nga_access_ghosts(g_a, dims, index, ld)`

C: `void NGA_Access_ghosts(int g_a, int dims[], void *index, int ld[])`

dims Array of Local Dimensions Including Ghost Cells

index Index Corresponding to the Local Global Array Patch

ld Dimensions of the Local Array Patch including Ghost Cells



Periodic Interfaces

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Definition

One-sided **Periodic Interfaces** have been added to GA to support computational fluid dynamics problems on multi-dimensional grids .

- 1 They provide an index translation layer that allows `put()`, `get()` and `accumulate()` operations to extend beyond the boundaries of the global array
- 2 The references outside the boundaries are wrapped around the global array like a torus



Periodic Interfaces

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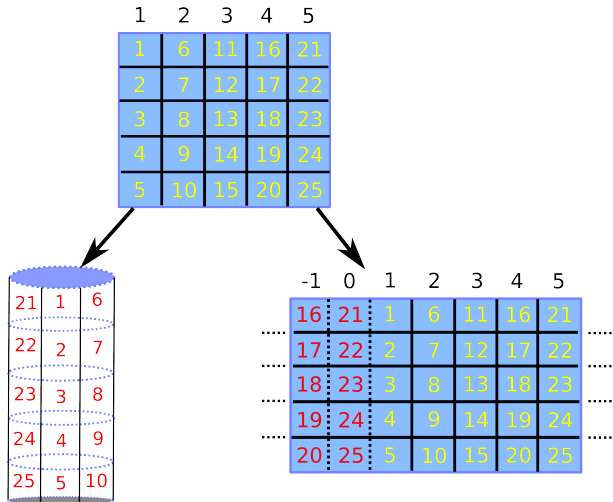


Figure: Horizontal Boundary Wrapping with Periodic Interface



Periodic Interfaces

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	-1	0	1	2	3
2	17	22	2	7	12
3	18	23	3	8	13
4	19	24	4	9	14

Figure: The Global Array Patch $[2 : 4, -1 : 3]$



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To perform periodic operations, call the following functions:

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[])`

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[])`

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)`

lo	Array of Starting Patch Indices
hi	Array of Ending Patch Indices
buf	Local Buffer to Send/Receive Data Values
ld	Leading Dimensions for Buffer
alpha	The Scaling Factor



Non-blocking Operations

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Definition

Improved performance can be obtained with **non-blocking communications**

- were the communication operation completes before the data buffer is ready to be overwritten

By returning from the communication operation after the data transfer has been initiated, **overlapping** of computation and communication can be performed.



Non-blocking Operations

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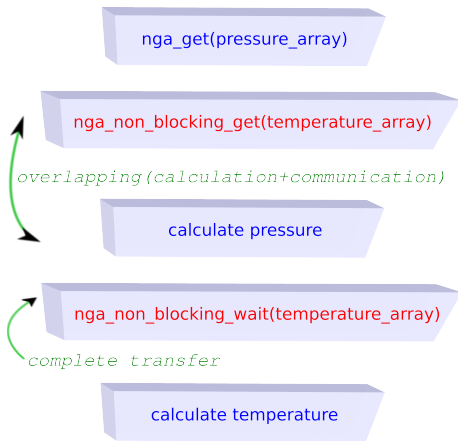


Figure: Non-blocking Communication Example



Non-blocking Operation

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Notes:

- 1 GA non-blocking communications (`get/put/accumulate`) are derived from the standard blocking interface by adding an **extra `handle request`** argument .
- 2 The **`wait`** function completes a non-blocking operation **locally**
- 3 Waiting on a non-blocking `put()/accumulate()`
 - ensures the data was injected into network and the user buffer is ready to be reused
- 4 Waiting on a non-blocking `get()`
 - ensures the data has arrived and the user buffer is ready to be used
- 5 Unlike blocking communications, non-blocking communications are not ordered with respect to the destination
 - If ordering is required, a **`fence`** operation can be used to confirm remote completion



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Non-blocking operations can be called with the following routines:

Fortran Routines

```
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)
```

nbhandle Handle for Non-Blocking Request



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C Routines

```
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)
```

```
subroutine nga_NbWait(ga_nbhdl_t* nbhandle)
```

nbhandle Handle for Non-Blocking Request



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Non-Blocking GA Fortran Example

```
double precision buf1(nmax,nmax)
double precision buf2(nmax,nmax)

! Evaluate lo1, hi1
call nga_nbaget(g_a,lo1,hi1,buf1,ld1,nb1)
ncount=1
do while (...)
  if (mod(ncount,2) .eq. 1) then
    ! Evaluate lo2, hi2
    call nga_nbaget(g_a,lo2,hi2,buf2,ld2,nb2)
    call nga_nbwait(nb1)
    ! Do work with data in buf1
  else
    ! Evaluate lo1, hi1
    call nga_nbaget(g_a,lo1,hi1,buf1,ld1,nb1)
    call nga_nbwait(nb2)
    ! Do work with data in buf2
  endif
  ncount=ncount+1
end do
```



Part X

Supplemental Information



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Message-Passing Communication

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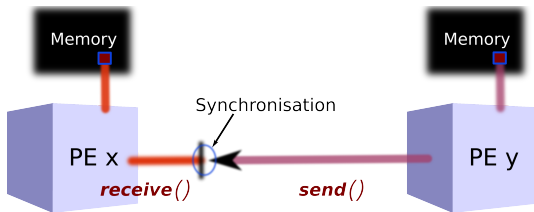
ARMCi

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- Message-passing requires cooperation on both sides



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One-Sided Communication

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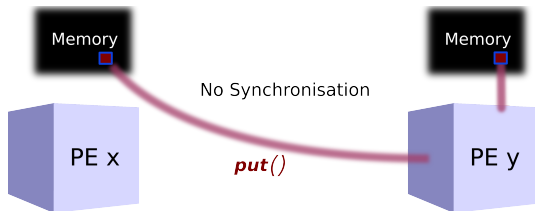
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- Once the message is initiated on PE y the sending processor can continue with computation. PE x is never involved in the communication
- One-sided communications can be implemented with shared-memory, threads, network hardware, Remote Direct Memory Access (RDMA) and vendor-specific mechanisms
- Common one-sided communication libraries: ARMCI, SHMEM and MPI-2



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ScaLAPACK Interface - Solving a Linear System using LU Factorisation

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GA Interface

```
call ga_lu_solve(gA, gB)
```

instead of ...

```
call pdgetrf(n, m, locaA, p, q, dA, ind, info)
call pdgetrs(trans, n, mb, locA, p, q, dA, dB, info)
```

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Aggregate Remote Method Copy Interface (ARMCI)

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A general, portable, efficient one-sided communication interface

ARMCI offers an extensive set of Remote Memory Access (RMA) communication functionality utilising network interfaces on clusters and supercomputers[2]:

- 1 data transfer operations optimised for contiguous and noncontiguous (strided, scatter/gather, I/O vector) data transfers
 - 2 atomic operations
 - 3 memory management and synchronisation
 - 4 locks
- GA's **primary** communication interfaces combine the ARMCI interfaces with a global-array index translation.



Performance Notes:

- 1 On cluster connects, ARMCI achieves bandwidth close to the underlying network protocols
 - Similarly, latency is comparable if the native platform protocol supports an equivalent remote memory operation (e.g. *elan_get()* on Quadrics).
- 2 For systems that do not support a native remote *get()* the latency can include the cost of interrupt processing that is used by ARMCI to implement the *get()* operation.
- 3 Check www.emsl.pnl.gov/docs/parsoft/armci/performance.htm for further details.

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Data Distribution and Data Locality

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- 1 GA can support the programmer in controlling data distribution when creating global arrays:
 - You can allow GA to determine the array distribution
 - You can specify the decomposition of one array dimension and allow GA to determine the others
 - You can specify the block size for all dimensions
 - You can specify an irregular distribution as a Cartesian product of irregular distributions for each dimension
- 2 GA maintains locality information for all global arrays which can be accessed via query functions to find:
 - the array data portion held by a given processor
 - which process owns a particular array element
 - block lists owned by each process for a given global array section

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Blocking and Non-Blocking Operations

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Blocking Store Operations

There are two types of completion for store operations (**local** and **remote**):

- 1 The blocking store operation completes after the operation is completed locally i.e. the user buffer containing the source data can be **overwritten**
- 2 The blocking store operation completes remotely after either:
 - a fence operation
 - a barrier synchronisation



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Blocking and Non-Blocking Operations ... continued

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Ordered Blocking

- 1 Blocking loads/store operations are ordered **only** if they target overlapping sections of a global array
- 2 Blocking loads/stores that target different array sections complete arbitrarily

Non-Blocking Operations

- 1 Non-blocking load/store operations complete in arbitrary order. Wait/Test operations can be used to order completion of these operations, if required.

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Local Memory Allocation

The Global Arrays Toolkit requires the **Memory Allocator** (MA) library, which is a collection of routines for performing dynamic memory allocation for C, Fortran and mixed-language applications. GA uses MA to provide all its dynamically allocated **local** memory (global memory is allocated via ARMCI using operating system shared memory operations) .

- MA provides both stack and heap memory management operations
- MA provides memory availability and utilisation information and statistics
- MA supports both C and Fortran data types
- MA offers both debugging and verification mechanisms (memory boundary guards)

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Disk Resident Arrays (DRAs)

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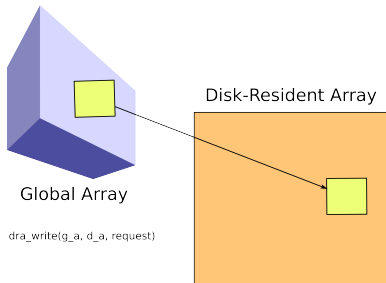
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- Data transferred between disk and global memory using simple read/write commands.
- I/O operations have nonblocking interface to allow computation overlapping.
- Whole or sections of global arrays can be transferred (using global indexing).



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Disk Resident Arrays (DRAs) ... continued

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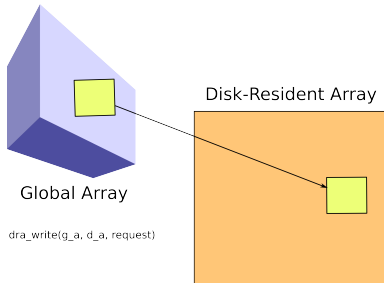
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Data Locality and Distribution

Blocking and Non-Blocking Operations

The Memory Allocator (MA)

Disk Resident Arrays (DRAs)



- Reshaping and transpose operations allowed during the transfer.
- Disk arrays can be accessed by arbitrary number of processors.
- Distribution on the disk is optimised for large data transfer.
- Hints provided by the user allow improved performance for specific I/O patterns.



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Disk Resident Arrays (DRAs) ... continued

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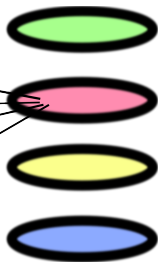
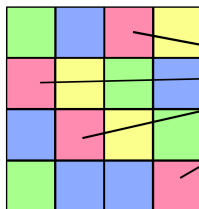
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Parallel
File-System
(Disks)

Disk-Resident Arrays
automatically decomposed
into multiple files

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[J. Nieplocha et al.]

Disk Resident Arrays

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