Overview of the Global Arrays Parallel Software Development Toolkit: Introduction to Global Address Space Programming Models

P. Saddayappan\textsuperscript{2}, Bruce Palmer\textsuperscript{1}, Manojkumar Krishnan\textsuperscript{1}, Sriram Krishnamoorthy\textsuperscript{1}, Abhinav Vishnu\textsuperscript{1}, Daniel Chavarria\textsuperscript{1}, Patrick Nichols\textsuperscript{1}, Jeff Daily\textsuperscript{1}

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Outline of the Tutorial

- Parallel programming models
- Global Arrays (GA) programming model
- GA Operations
  - Writing, compiling and running GA programs
  - Basic, intermediate, and advanced calls
    - With C and Fortran examples
- GA Hands-on session
Performance vs. Abstraction and Generality

- Domain Specific Systems
- OpenMP
- Autoparallelized C/Fortran90
- MPI
- GA
- CAF

Scalability

Abstraction-M

Generality

“Holy Grail”
Parallel Programming Models

- **Single Threaded**
  - Data Parallel, e.g. HPF

- **Multiple Processes**
  - Partitioned-Local Data Access
    - MPI
  - Uniform-Global-Shared Data Access
    - OpenMP
  - Partitioned-Global-Shared Data Access
    - Co-Array Fortran
  - Uniform-Global-Shared + Partitioned Data Access
    - UPC, Global Arrays, X10
High Performance Fortran

- Single-threaded view of computation
- Data parallelism and parallel loops
- User-specified data distributions for arrays
- Compiler transforms HPF program to SPMD program
  - Communication optimization critical to performance
- Programmer may not be conscious of communication implications of parallel program

```fortran
HPF$ Independent
DO I = 1,N
  HPF$ Independent
  DO J = 1,N
    A(I,J) = B(J,I)
  END
END

s=s+1
A(1:100) = B(0:99)+B(2:101)
HPF$ Independent
Do I = 1,100
  A(I) = B(I-1)+B(I+1)
End Do
```
Message Passing Interface

- Most widely used parallel programming model today
- Bindings for Fortran, C, C++, MATLAB
- P parallel processes, each with local data
  - MPI-1: Send/receive messages for inter-process communication
  - MPI-2: One-sided get/put data access from/to local data at remote process
- Explicit control of all inter-processor communication
  - Advantage: Programmer is conscious of communication overheads and attempts to minimize it
  - Drawback: Program development/debugging is tedious due to the partitioned-local view of the data
OpenMP

- Uniform-Global view of shared data
- Available for Fortran, C, C++
- Work-sharing constructs (parallel loops and sections) and global-shared data view ease program development
- Disadvantage: Data locality issues obscured by programming model
Co-Array Fortran

- Partitioned, but global-shared data view
- SPMD programming model with local and shared variables
- Shared variables have additional co-array dimension(s), mapped to process space; each process can directly access array elements in the space of other processes
  - \( A(I,J) = A(I,J)[me-1] + A(I,J)[me+1] \)
- Compiler optimization of communication critical to performance, but all non-local access is explicit
Unified Parallel C (UPC)

- SPMD programming model with global shared view for arrays as well as pointer-based data structures.
- Compiler optimizations critical for controlling inter-processor communication overhead:
  - Very challenging problem since local vs. remote access is not explicit in syntax (unlike Co-Array Fortran).
  - Linearization of multidimensional arrays makes compiler optimization of communication very difficult.
- Performance study with NAS benchmarks (PPoPP 2005, Mellor-Crummey et. al.) compared CAF and UPC:
  - Co-Array Fortran had significantly better scalability.
  - Linearization of multi-dimensional arrays in UPC was a significant source of overhead.
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:
- Only useable for array data structures
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.
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

Physically distributed data

Global Address Space
Global Array Model of Computations

- Shared memory view for distributed dense arrays
- Get-Local/Compute/Put-Global model of computation
- MPI-Compatible; Currently usable with Fortran, C, C++, Python
- Data locality and granularity control similar to message passing model
Overview of the Global Arrays Parallel Software Development Toolkit: Global Arrays Programming Model

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Overview Of GA

- Programming model
- Structure of the GA toolkit
- Overview of interfaces
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)
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.
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

Physically distributed data

Global Address Space
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
Global Array Model of Computations

Shared Object

copy to local memory

get

local memory

Shared Object

compute/update

local memory

Shared Object

put

copy to shared object

local memory
Creating Global Arrays

```c
integer array handle
```

```c
character string
```

```c
float, double, int, etc.
```

```c
array of dimensions
```

```c
dimension
```

```c
minimum block size on each processor
```

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

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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

P0  P2
P1  P3
One-sided Communication

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:
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.

Message passing
MPI

one-sided communication
SHMEM, ARMCI, MPI-2-1S
Data Locality in GA

What data does a processor own?

\[
\text{NGA\_Distribution}(g\_a, \text{iproc}, \text{lo}, \text{hi});
\]

Where is the data?

\[
\text{NGA\_Access}(g\_a, \text{lo}, \text{hi}, \text{ptr}, \text{ld})
\]

Use this information to organize calculation so that maximum use is made of locally held data.
Example: Matrix Multiply

- Local buffers on the processor
- Global arrays representing matrices
- \( \text{nga\_put} \)
- \( \text{nga\_get} \)
- \( \text{dgemm} \)
Matrix Multiply (a better version)

more scalable!
(less memory, higher parallelism)

atomic accumulate

get

local buffers on the processor

dgemm
SUMMA 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

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

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SUMMA 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

- SRUMMA
- PBLAS/ScaLAPACK pdgemm
- Theoretical Peak
- Perfect Scaling

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

**Structure of GA**

- **Application programming language interface**
  - Fortran 77
  - C
  - C++
  - Python
  - Babel

- **Distributed arrays layer**
  - memory management
  - index translation

- **Execution layer**
  - task scheduling
  - load balancing
  - data movement

- ** MPI**
  - Global operations

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

- **System specific interfaces**
  - LAPI, GM/Myrinet, threads, VIA,..
Disk Resident Arrays

- Extend GA model to disk
  - system similar to Panda (U. Illinois) but higher level APIs
- Provide easy transfer of data between N-dim arrays stored on disk and distributed arrays stored in memory
- Use when
  - Arrays too big to store in core
  - checkpoint/restart
  - out-of-core solvers
TASCEL – Task Scheduling Library

- Dynamic Execution Models
  - 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, memory mgmt, comm. mgmt, locality optimization, etc.
- Extends Global Arrays’ execution model
Application Areas

bioinformatics

electronic structure chemistry
GA is the standard programming model

smoothed particle hydrodynamics

fluid dynamics

visual analytics

material sciences

molecular dynamics

hydrology

Others: financial security forecasting, astrophysics, climate analysis
ScalaBLAST


Parallel Inspire


Smooth Particle Hydrodynamics
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, Myrinet, Infiniband, or Quadrics
  - Solaris
  - Fujitsu
  - Hitachi
  - NEC
  - HP
  - Windows
Overview of the Global Arrays Parallel Software Development Toolkit: Getting Started, Basic Calls

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Outline

- Writing, Building, and Running GA Programs
- Basic Calls
- Intermediate Calls
- Advanced Calls
Writing, Building and Running GA programs

- Installing GA
- Writing GA programs
- Compiling and linking
- Running GA programs
- For detailed information
  - GA Webpage
    - GA papers, APIs, user manual, etc.
    - Google: Global Arrays
      - [http://www.emsl.pnl.gov/docs/global/](http://www.emsl.pnl.gov/docs/global/)
  - GA User Manual

- GA API Documentation
  - GA Webpage => User Interface
    - [http://www.emsl.pnl.gov/docs/global/userinterface.html](http://www.emsl.pnl.gov/docs/global/userinterface.html)

- GA Support/Help
  - [hpctools@googlegroups.com](mailto:hpctools@googlegroups.com)
  - [hpctools@ pnl.gov](mailto:hpctools@pnl.gov) and [hpctools@emsl.pnl.gov](mailto:hpctools@emsl.pnl.gov) forward to google group

- 2 mailing lists
  - Google group
  - 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
      - 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
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
  - Python programs import the ga module
- GA Initialize, GA_Terminate --> initializes and terminates GA library (C/Fortran only)

```c
/* C */
#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;
}
```

```python
# python
import mpi4py.MPI
import ga
print "Hello world"
```

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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

/* C */
#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;
}

# python
import mpi4py.MPI
import ga
print "Hello world"
Compiling and Linking GA Programs (cont.)

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

You can use these variables in your Makefile:

For example: gcc $(CPPLAGS) $(LDFLAGS) -o ga_test ga_test.c $(LIBS)
Example: Running a test program “ga_test” on 2 processes

mpirun -np 2 ga_test

Running a GA program is same as MPI
Writing, Building, and Running GA Programs

Basic Calls

Intermediate Calls

Advanced Calls
GA Basic 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_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

```fortran
program main
#include "mafdecls.h"
#include "global.fh"
integer ierr
  call mpi_init(ierr)
  call ga_initialize()
  call ga_terminate()
  call mpi_finalize()
end
```

```c
#include "mafdecls.h"
#include "global.fh"

c
int main(int argc, char *argv[])
{
  MPI_Init(&argc, &argv);
  ga_initialize();
  /* do stuff */
  ga_terminate();
  MPI_Finalize();
  return 0;
}
```
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()`
program main
#include "mafdecls.h"
#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_finalize()
end
GA Data Types

C/Python 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**

```python
g_a = ga.create(type, dims, name="", chunk=None, int pgroup=-1)
```

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>name</td>
<td>a unique character string</td>
<td>input</td>
</tr>
<tr>
<td>type</td>
<td>GA data type</td>
<td>input</td>
</tr>
<tr>
<td>dims()</td>
<td>array dimensions</td>
<td>input</td>
</tr>
<tr>
<td>chunk()</td>
<td>minimum size that dimensions should be chunked into</td>
<td>input</td>
</tr>
<tr>
<td>g_a</td>
<td>array handle for future references</td>
<td>output</td>
</tr>
</tbody>
</table>

```fortran
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**
  
  ```python
g_a = ga.create_irreg(int gtype, dims, block, map, name="", pgroup=-1)
  ```

<table>
<thead>
<tr>
<th>Name</th>
<th>Description</th>
<th>Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>character*(*) name</td>
<td>a unique character string</td>
<td>[input]</td>
</tr>
<tr>
<td>integer type</td>
<td>GA datatype</td>
<td>[input]</td>
</tr>
<tr>
<td>integer dims</td>
<td>array dimensions</td>
<td>[input]</td>
</tr>
<tr>
<td>integer nblock(*)</td>
<td>no. of blocks each dimension is divided into</td>
<td>[input]</td>
</tr>
<tr>
<td>integer map(*)</td>
<td>starting index for each block</td>
<td>[input]</td>
</tr>
<tr>
<td>integer g_a</td>
<td>integer handle for future references</td>
<td>[output]</td>
</tr>
</tbody>
</table>
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. $\text{block}[2]=\{3,2\}$, the size of $\text{map}$ array is $s=5$ and array $\text{map}$ contains the following elements $\text{map} = \{1,3,7,1,6\}$.

- The distribution is nonuniform because, P1 and P4 get 20 elements each and processors P0,P2,P3, and P5 only 10 elements each.

```fortran
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 global 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)

```plaintext
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)
```

```plaintext
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]
```
**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)

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<td>g_a</td>
<td>global array handle</td>
<td>integer</td>
</tr>
<tr>
<td>lo(), hi()</td>
<td>limits on data block to be moved</td>
<td>integer</td>
</tr>
<tr>
<td>buf</td>
<td>local buffer</td>
<td>Double precision/complex/integer</td>
</tr>
<tr>
<td>ld()</td>
<td>array of strides for local buffer</td>
<td>integer</td>
</tr>
</tbody>
</table>
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 \(lo=\{7,1\}, \ hi=\{15,8\}, \ ld=\{10\}\)

```plaintext
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)

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<td>Array of strides for local buffer</td>
<td>integer</td>
</tr>
<tr>
<td>alpha</td>
<td>Arbitrary scale factor</td>
<td>double</td>
</tr>
</tbody>
</table>

\[
\text{ga}(i,j) = \text{ga}(i,j) + \text{alpha} \ast \text{buf}(k,l)
\]
Sync is a collective operation
It acts as a barrier, which synchronizes all the processes and ensures that all the Global Array operations are complete at the call

The functions are:
- **Fortran** subroutine `ga_sync()`
- **C** `void GA_Sync()`
- **Python** `ga.sync()`
Global Operations

▶ Fortran

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

▶ C

```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

```python
buffer = ga.brdcst(buffer, root)
buffer = ga.gop(x, op)
```
Global Array Model of Computations

Shared Object

→

compute/update

→

put

Shared Object

↓

copy to shared object

local memory

get

↓

copy to local memory

Shared Object

local memory

local memory

local memory

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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)`

<table>
<thead>
<tr>
<th>Type</th>
<th>Name</th>
<th>Description</th>
<th>Input/Output</th>
</tr>
</thead>
<tbody>
<tr>
<td>integer</td>
<td><code>g_a</code></td>
<td>array handle</td>
<td>[input]</td>
</tr>
<tr>
<td>integer</td>
<td><code>proc</code></td>
<td>processor ID</td>
<td>[input]</td>
</tr>
<tr>
<td>integer</td>
<td><code>lo(ndim)</code></td>
<td>lower index</td>
<td>[output]</td>
</tr>
<tr>
<td>integer</td>
<td><code>hi(ndim)</code></td>
<td>upper index</td>
<td>[output]</td>
</tr>
</tbody>
</table>

```fortran
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)'))
dnd do
```

Proudly Operated by Battelle Since 1965
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);
Overview of the Global Arrays Parallel Software Development Toolkit: Intermediate and Advanced APIs

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\textsuperscript{1}Pacific Northwest National Laboratory
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Outline

➢ Writing, Building, and Running GA Programs
➢ Basic Calls
➢ Intermediate Calls
➢ Advanced Calls
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)`
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

Global Arrays `g_a` and `g_b` distributed on a 3x3 process grid
Basic Array Operations (cont.)

- 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
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)
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)
Scatter/Gather

- **Scatter** puts array elements into a global array:
  - **Fortran** subroutine nga_scatter(g_a, v, subscript_array, n)
  - **C** `void NGA_Scatter(int g_a, void *v, int *subscript_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, subscript_array, n)
  - **C** `void NGA_Gather(int g_a, void *v, int *subscript_array[], int n)`
  - **Python** `values = ga.gather(g_a, subsarray, numpy.ndarray(values=None)`

<table>
<thead>
<tr>
<th>Data Type</th>
<th>Description</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>integer</td>
<td>g_a array handle</td>
<td>[input]</td>
</tr>
<tr>
<td>double precision</td>
<td>v(n) array of values</td>
<td>[input/output]</td>
</tr>
<tr>
<td>integer</td>
<td>n number of values</td>
<td>[input]</td>
</tr>
<tr>
<td>integer</td>
<td>subscript_array location of values in global array</td>
<td>[input]</td>
</tr>
</tbody>
</table>
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.

```fortran
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

<p>| | | |</p>
<table>
<thead>
<tr>
<th></th>
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</thead>
<tbody>
<tr>
<td><strong>g_a</strong></td>
<td>[input]</td>
<td></td>
</tr>
<tr>
<td>subscript(ndim), inc</td>
<td>[input]</td>
<td></td>
</tr>
</tbody>
</table>

```c
fun
    nga_create(MT_F_INT,one,one,chunk,g_counter)
    ga_zero(g_counter)
    itask = nga_read_inc(g_counter,one,one)

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

► Writing, Building, and Running GA Programs
► Basic Calls
► Intermediate Calls
► Advanced Calls
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

```plaintext
call 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,*)
```
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.
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)
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

A \times B = C

Computation
Comm. (Overlap)

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

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/sruminma/
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

- SRUMMA
- PBLAS/ScaLAPACK pdgemm
- Theoretical Peak
- Perfect Scaling

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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()
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)
Accessing Processor Memory

Node

SMP Memory

R_8  R_9  R_{10}  R_{11}

P_8  P_9  P_{10}  P_{11}

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)

<table>
<thead>
<tr>
<th>Type</th>
<th>Description</th>
<th>Input/Output</th>
</tr>
</thead>
<tbody>
<tr>
<td>integer</td>
<td>g_a</td>
<td>- global array handle [input]</td>
</tr>
<tr>
<td>integer</td>
<td>p_handle</td>
<td>- processor group handle [output]</td>
</tr>
<tr>
<td>integer</td>
<td>list(size)</td>
<td>- list of processor IDs in group [input]</td>
</tr>
<tr>
<td>integer</td>
<td>size</td>
<td>- number of processors in group [input]</td>
</tr>
</tbody>
</table>
Processor Groups

world group

group A

group B

group C
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)

**p_handle** - processor group handle  [input]
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()
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
Creating Arrays with Ghost Cells

To create arrays with ghost cells:

- For arrays with regular distribution:
  - **Fortran**
    ```fortran
    logical function nga_create_ghosts(type, dims, width, array_name, chunk, g_a)
    ```
  - **C**
    ```c
    int int NGA_Create_ghosts(int type, int ndim, int dims[], int width[], char *array_name, int chunk[])
    ```
  - **Python**
    ```python
g_a = ga.create_ghosts(type, dims, width, name="", chunk=None, pgroup=-1)
    ```

- For arrays with irregular distribution:
  - **n-d Fortran**
    ```fortran
    logical function nga_create_ghosts_irreg(type, dims, width, array_name, map, block, g_a)
    ```
  - **C**
    ```c
    int int NGA_Create_ghosts_irreg(int type, int ndim, int dims[], int width[], char *array_name, int map[], int block[])
    ```
  - **Python**
    ```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

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
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`

```c
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)`

  `number` - number of mutexes in mutex array. [input]
Lock and Mutex (cont.)

Lock

Unlock
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()`
To eliminate redundant synchronization points:

- **Fortran** subroutine \texttt{ga\_mask\_sync(prior\_sync\_mask, post\_sync\_mask)}
- **C** \texttt{void GA\_Mask\_sync(int prior\_sync\_mask, int post\_sync\_mask)}
- **Python** \texttt{ga.mask\_sync(prior\_sync\_mask, post\_sync\_mask)}

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

\begin{verbatim}
call ga_duplicate(g_a, g_b)
call ga_mask_sync(0,1)
call ga_zero(g_b)
\end{verbatim}
Linear Algebra – Whole Arrays

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)`

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Type/Example</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>alpha</code></td>
<td>double precision/complex/integer</td>
</tr>
<tr>
<td><code>beta</code></td>
<td>integer</td>
</tr>
<tr>
<td><code>g_a</code>, <code>g_b</code>, <code>g_c</code></td>
<td>integer</td>
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<tr>
<td><code>*alpha</code></td>
<td>double/complex/int</td>
</tr>
<tr>
<td><code>*beta</code></td>
<td>double/complex/int</td>
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<tr>
<td><code>transa</code>, <code>transb</code></td>
<td>character*1</td>
</tr>
<tr>
<td><code>m</code>, <code>n</code>, <code>k</code></td>
<td>integer</td>
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<td><code>alpha</code>, <code>beta</code></td>
<td>double precision</td>
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<tr>
<td><code>alpha</code>, <code>beta</code></td>
<td>double complex</td>
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<tr>
<td><code>g_a</code>, <code>g_b</code></td>
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<tr>
<td><code>g_c</code></td>
<td>integer</td>
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<td>- array handles</td>
<td>[input]</td>
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<tr>
<td>- input</td>
<td>[output]</td>
</tr>
</tbody>
</table>
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)
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)
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)

<table>
<thead>
<tr>
<th>Type</th>
<th>Variables</th>
<th>Description</th>
<th>Notes</th>
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<tr>
<td>integer</td>
<td>g_a, g_b, g_c</td>
<td>[input]</td>
<td></td>
</tr>
<tr>
<td>dbl prec/comp/int</td>
<td>alpha, beta</td>
<td>scale factors</td>
<td>[input]</td>
</tr>
<tr>
<td>integer</td>
<td>ailo, aihi, ajlo, ajhi</td>
<td>g_a patch coord</td>
<td>[input]</td>
</tr>
<tr>
<td>integer</td>
<td>bilo, bihi, bjlo, bjhi</td>
<td>g_b patch coord</td>
<td>[input]</td>
</tr>
<tr>
<td>integer</td>
<td>cilo, cihi, cjlo, cjhi</td>
<td>g_c patch coord</td>
<td>[input]</td>
</tr>
</tbody>
</table>
To perform matrix multiplication:

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

```
integer g_a, ailo, aih, 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]
```
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)`
Block-Cyclic Data Distributions

Normal Data Distribution

Block-Cyclic Data Distribution

Proudly Operated by Battelle Since 1965
## Simple Distribution

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## Scalapack Distribution

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<td>1,1</td>
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</tbody>
</table>
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 must equal total number of processors)
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
Locality Information

To determine the process ID that owns the element defined by the array subscripts:

- **n-Dfortran**
  
  logical function nga_locate(g_a, subscript, owner)

- **C**
  
  int NGA_Locate(int g_a, int subscript[])

- **Python**
  
  proc = ga.locate(g_a, subscript)

<p>| | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
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</tr>
</thead>
<tbody>
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</table>

<p>| |</p>
<table>
<thead>
<tr>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>owner=5</td>
</tr>
</tbody>
</table>
Locality 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 [input]
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}

Proudly Operated by Battelle Since 1965
New Interface for Creating Arrays – Fortran

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

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)
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)
integer ndim, dims(2), chunk(2)
  integer g_a, g_b
logical status

ndim = 2
 dims(1) = 5000
dims(2) = 5000
chunk(1) = 100
chunk(2) = 100

Create global array A using old interface

status = nga_create(MT_F_DBL, ndim, dims, chunk, 'array_A', g_a)

Create global array B using new interface

  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)
Example Code

- 1-D Transpose (Fortran)
- 1-D Transpose (C)
- Matrix Multiply (Fortran)
- Matrix Multiply (C)
Example: 1-D Transpose
```c
int ndim, dims[1], chunk[1], ld[1], lo[1], hi[1];
int lo1[1], hi1[1], lo2[1], hi2[1];
int g_a, g_b, a[MAXPROC*TOTALELEMS], b[MAXPROC*TOTALELEMS];
int nelem, i;

/* Find local processor ID and number of processors */
ext me=GA_Nodeid(), nprocs=GA_Nnodes();

/* Configure array dimensions. Force an unequal data distribution */
ext ndim = 1; /* 1-d transpose */
dims[0] = nprocs*TOTALELEMS + nprocs/2;
ld[0] = dims[0];
chunk[0] = TOTALELEMS; /* minimum data on each process */

/* create a global array g_a and duplicate it to get g_b */
g_a = NGA_Create(C_INT, 1, dims, "array A", chunk);
if (!g_a) GA_Error("create failed: A", 0);
if (me==0) printf(" Created Array A\n");

  g_b = GA_Duplicate(g_a, "array B");
if (! g_b) GA_Error("duplicate failed", 0);
if (me==0) printf(" Created Array B\n");
```

---

Transverse Example – C
/* initialize data in g_a */
if (me==0) {
    printf(" Initializing matrix A\n");
    for(i=0; i<dims[0]; i++) a[i] = i;
    lo[0]  = 0;
    hi[0] = dims[0]-1;
    NGA_Put(g_a, lo, hi, a, ld);
}

/* Synchronize all processors to guarantee that everyone has data before proceeding to the next step. */
GA_Sync();

/* Start initial phase of inversion by inverting the data held locally on each processor. Start by finding out which data each processor owns. */
NGA_Distribution(g_a, me, lol, hil);

/* Get locally held data and copy it into local buffer a */
NGA_Get(g_a, lol, hil, a, ld);

/* Invert data locally */
nelem = hil[0] - lol[0] + 1;
for (i=0; i<nelem; i++) b[i] = a[nelem-1-i] ;
/* Invert data globally by copying locally inverted blocks into
* their inverted positions in the GA */
lo2[0] = dims[0] - hi1[0] -1;
hi2[0] = dims[0] - lo1[0] -1;
NGA_Put(g_b,lo2,hi2,b,ld);

/* Synchronize all processors to make sure inversion is complete */
GA_Sync();

/* Check to see if inversion is correct */
if(me == 0) verify(g_a, g_b);

/* Deallocate arrays */
GA_Destroy(g_a);
GA_Destroy(g_b);
integer dims(3), chunk(3), nprocs, me, i, lo(3), hi(3), lo1(3)
integer hi1(3), lo2(3), hi2(3), ld(3), nelem
integer g_a, g_b, a(MAXPROC*TOTALELEMS), b(MAXPROC*TOTALELEMS)
integer heap, stack, ichk, ierr
logical status

heap = 300000
stack = 300000

c Initialize communication library
c
#ifdef USE_MPI
    call mpi_init(ierr)
#else
    call pbeginf
#endif

c Initialize GA library
c
    call ga_initialize()
c
c Find local processor ID and number of processors
  
  me = ga_nodeid()
  nprocs = ga_nnodes()
  if (me.eq.0) write(6,101) nprocs
  101 format('Using ',i4,' processors')
  
  Allocate memory for GA library
  
  status = ma_init(MT_F_DBL, stack/nprocs, heap/nprocs)
  
  Configure array dimensions. Force an unequal data distribution.
  
  dims(1) = nprocs*TOTALELEMS + nprocs/2
  ld(1) = MAXPROC*TOTALELEMS
  chunk(1) = TOTALELEMS ! Minimum data on each processor
  
  Create global array g_a and then duplicate it to get g_b
  
  status = nga_create(MT_F_INT, NDIM, dims, "Array A", chunk, g_a)
  status = ga_duplicate(g_a, g_b, "Array B")
c  c  Initialize data in g_a
c  
do  i = 1, dims(1)
   a(i) = i  
end do
lo1(1) = 1
hi1(1) = dims(1)

c  Copy data from local buffer a to global array g_a. Only do this for
  c  processor 0.
c  if  (me.eq.0) call nga_put(g_a, lo1, hil, a, ld)

  Synchronize all processors to guarantee that everyone has data
  before proceeding to the next step.
  call ga_sync
Start initial phase of inversion by inverting the data held locally on each processor. Start by finding out which data each processor owns.

call nga_distribution(g_a, me, lo, hi)

cGet locally held data and copy it into local buffer a
call nga_get(g_a, lo, hi, a, ld)

cInvert local data
nelem = hi(1) - lo(1) + 1
    do i = 1, nelem
        b(i) = a(nelem - i + 1)
    end do

cDo global inversion by copying locally inverted data blocks into their inverted positions in the GA
lo2(1) = dims(1) - hi(1) + 1
hi2(1) = dims(1) - lo(1) + 1
call nga_put(g_b, lo2, hi2, b, ld)
c

Synchronize all processors to make sure inversion is complete

c
    call ga_sync()

c
Check to see if inversion is correct. Start by copying g_a into local
buffer a, and g_b into local buffer b.

c
    call nga_get(g_a, lo1, hi1, a, ld)
    call nga_get(g_b, lo1, hi1, b, ld)
    ichk = 0
    do i = 1, dims(1)
        if (a(i).ne.b(dims(1)-i+1) .and. me.eq.0) then
            write(6,111) i,a(i),b(dims(1)-i+1)
        endif
    end do
    if (ichk.eq.0.and.me.eq.0) write(6,*) 'Transpose OK'
c
Deallocate memory for arrays and clean up GA library

if (me.eq.0) write(6,*) 'Terminating…'
status = ga_destroy(g_a)
status = ga_destroy(g_b)
call ga_terminate

#ifdef USE_MPI
   call mpi_finalize
#else
   call pend
#endif
stop
end
int dims[NDIM], chunk[NDIM], ld[NDIM];
int lo[NDIM], hi[NDIM], lo1[NDIM], hi1[NDIM];
int lo2[NDIM], hi2[NDIM], lo3[NDIM], hi3[NDIM];
int g_a, g_b, g_c, i, j, k, l;

/* Find local processor ID and the number of processors */
int me=GA_Nodeid(), nprocs=GA_Nnodes();

/* Configure array dimensions. Force an unequal data distribution */
for(i=0; i<NDIM; i++) {
    dims[i] = TOTALElems;
    ld[i]= dims[i];
    chunk[i] = TOTALElems/nprocs-1; /*minimum block size on each process*/
}
/* create a global array g_a and duplicate it to get g_b and g_c*/
g_a = NGA_Create(C_DBL, NDIM, dims, "array A", chunk);
if (!g_a) GA_Error("create failed: A", NDIM);
if (me==0) printf("  Created Array A\n");

g_b = GA_Duplicate(g_a, "array B");
g_c = GA_Duplicate(g_a, "array C");
if (!g_b || !g_c) GA_Error("duplicate failed",NDIM);
if (me==0) printf("  Created Arrays B and C\n");

/* initialize data in matrices a and b */
if (me==0) printf("  Initializing matrix A and B\n");
k = 0; l = 7;
for (i=0; i<dims[0]; i++) {
    for (j=0; j<dims[1]; j++) {
        a[i][j] = (double)(++k%29);
        b[i][j] = (double)(++l%37);
    }
}
/* Copy data to global arrays g_a and g_b */
lo1[0] = 0;
lo1[1] = 0;
hi1[0] = dims[0]-1;
hi1[1] = dims[1]-1;
if (me==0) {
    NGA_Put(g_a, lo1, hi1, a, ld);
    NGA_Put(g_b, lo1, hi1, b, ld);
}

/* Synchronize all processors to make sure everyone has data */
GA_Sync();

/* 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);
Matrix Multiply Example – C (cont.)

/* 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);
verify(g_a, g_b, g_c, lo1, hi1, ld);

/* Deallocate arrays */
GA_Destroy(g_a);
GA_Destroy(g_b);
GA_Destroy(g_c);