The Global Arrays User Manual

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Chapter 1

Introduction

1.1 Overview

The Global Arrays (GA) toolkit provides a shared memory style programming environment in the context of distributed array data structures (called "global arrays"). From the user perspective, a global array can be used as if it was stored in shared memory. All details of the data distribution, addressing, and data access are encapsulated in the global array objects. Information about the actual data distribution and locality can be easily obtained and taken advantage of whenever data locality is important. The primary target architectures for which GA was developed are massively-parallel distributed-memory and scalable shared-memory systems.

GA divides logically shared data structures into "local" and "remote" portions. It recognizes variable data transfer costs required to access the data depending on the proximity attributes. A local portion of the shared memory is assumed to be faster to access and the remainder (remote portion) is considered slower to access. These differences do not hinder the ease-of-use since the library provides uniform access mechanisms for all the shared data regardless where the referenced data is located. In addition, any processes can access a local portion of the shared data directly/in-place like any other data in process local memory. Access to other portions of the shared data must be done through the GA library calls.

GA was designed to complement rather than substitute the message-passing model, and it allows the user to combine shared-memory and message-passing styles of programming in the same program. GA inherits an execution environment from a message-passing library (w.r.t. processes, file descriptors etc.) that started the parallel program.

GA is implemented as a library with C and Fortran-77 bindings, and there have been also a Python and C++ interfaces (included starting with the release 3.2) developed. Therefore, explicit library calls are required to use the GA model in a parallel C/Fortran program.

A disk extension of the Global Array library is supported by its companion library called Disk Resident Arrays (DRA). DRA maintains array objects in secondary storage and allows transfer of data to/from global arrays.

1.2 Basic Functionality

The basic shared memory operations supported include *get*, *put*, *scatter* and *gather*. They are complemented by *atomic read-and-increment*, *accumulate* (reduction operation that combines data in local memory with data in the shared memory location), and *lock* operations. However, these operations can only be used to access data in global arrays rather than arbitrary memory locations. At least one global array has to be created before data transfer operations can be used. These GA operations are truly one-sided/unilateral and will complete regardless of actions taken by the remote process(es) that own(s) the referenced data. In particular, GA does not offer or rely on a polling operation or require inserting any other GA library calls to assure communication progress on the remote side.

A programmer in the GA program has a full control over the distribution of global arrays. Both regular and irregular distributions are supported, see Section 3 for details.

The GA data transfer operations use an array index-based interface rather than addresses of the shared data. Unlike other systems based on global address space that support remote memory (*put/get*) operations, GA does not require the user to specify the target process/es where the referenced shared data resides – it simply provides a global view of the data structures. The higher level array oriented API (application programming interface) makes GA easier to use, at the same time without compromising data locality control. The library internally performs global array index-to-address translation and then transfers data between appropriate processes. If necessary, the programmer is always able to inquire:

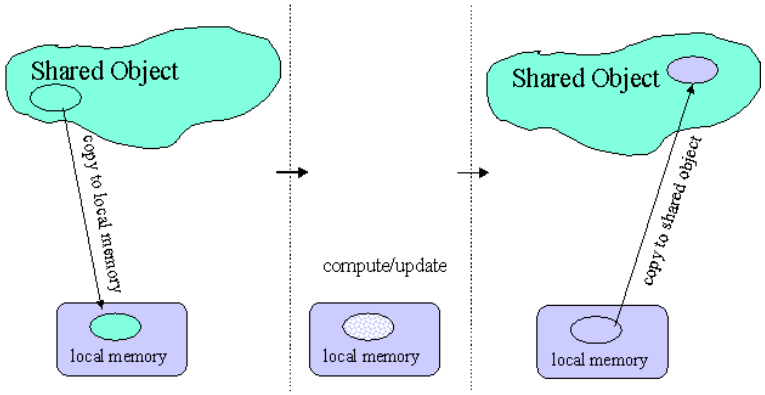
- where an an element or array section is located, and
- which process or processes own data in the specified array section.

The GA toolkit supports four data types in Fortran: integer, real, double precision, and double complex. In the C interface, int, long, float, double and struct double complex are available. Underneath, the library represents the data using C datatypes. For the Fortran users, it means that some arrays created in C for which there is no appropriate datatype mapping to Fortran (for example on the Cray T3E Fortran real is not implemented whereas C float is) might not be accessible. In all the other cases, the dataype representation is transparent.

The supported array dimensions range from one to seven. This limit follows the Fortran convention. The library can be reconfigured to support more than 7-dimensions but only through the C interface.

1.3 Programming Model

The Global Arrays library supports two programming styles: task-parallel and data-parallel. The GA task-parallel model of computations is based on the explicit remote memory copy: The remote portion of shared data has to be copied into the local memory area of a process before it can be used in computations by that process. Of course, the "local" portion of shared data can always be accessed directly thus avoiding the memory copy.



The data distribution and locality control are provided to the programmer. The data locality information for the shared data is also available. The library offers a set of operations for management of its data structures, one-sided data transfer operations, and supportive operations for data locality control and queries. The GA shared memory consistency model is a result of a compromise between the ease of use and a portable performance. The load and store operations are guaranteed to be *ordered* with respect to each other only if they target overlapping memory locations. The store operations (*put, scatter*) and *accumulate* complete locally before returning i.e., the data in the user local buffer has been copied out but not necessarily completed at the remote side. The memory consistency is only guaranteed for:

- multiple read operations (as the data does not change),
- multiple accumulate operations (as addition is commutative), and
- multiple disjoint put operations (as there is only one writer for each element).

The application can manage consistency of its data structures in other cases by using *lock, barrier*, and *fence* operations available in the library.

The data-parallel model is supported by a set of collective functions that operate on global arrays or their portions. Underneath, if any interprocessor communication is required, the library uses remote memory copy (most often) or collective message-passing operations.

1.4 Application Guidelines

These are some guidelines regarding suitability of the GA for different types of applications.

1.4.1 When to use GA:

Algorithmic Considerations

- applications with dynamic and irregular communication patterns
- for calculations driven by dynamic load balancing
- need 1-sided access to shared data structures
- need high-level operations on distributed arrays and/or for out-of-core array-based algorithms (GA + DRA)

Useability Considerations

- data locality must be explicitly available
- when coding in message passing becomes too complicated
- when portable performance is important
- need object orientation without the overhead of C++

1.4.2 When not to use GA

Algorithmic Considerations

- for systolic, or nearest neighbor communications with regular communication patterns
- when synchronization associated with cooperative point-to-point message passing is needed (e.g., Cholesky factorization in Scalapack)

Usability Considerations

- when interprocedural analysis and compiler parallelization is more effective
- a parallel language support is sufficient and robust compilers available

Chapter 2

Writing, Building and Running GA Programs

The GA build process has been improved by using the GNU autotools (autoconf, automake, and libtool) as well as by combining all of the historic GA libraries (`blacklinalg, armci, ma, pario`) into a single, monolithic `libga`. Details on configuring GA can be found by running "`configure --help`". The following sections explain some of the configure options a typical installation might require for configuring and building `libga`, its test programs, and how packages can link to and use GA.

The web page `www.emsl.pnl.gov/docs/global/support.html` contains information about using GA on different platforms. Please refer to this page frequently for most recent updates and platform information. Information on building GA on older systems is available in Appendix C, Global Arrays on Older Systems C.

2.1 Platform and Library Dependencies

The following platforms are supported by Global Arrays.

2.1.1 Supported Platforms

- BlueGene/L
- BlueGene/P
- Cray XT
- Cray XE
- Fujitsu
- IBM SP

- Linux Cluster with Ethernet, Myrinet, Infiniband, or Quadrics
- MAC
- NEC
- SGI Altix
- Solaris
- Windows (Cygwin)

For most of the platforms, there are two versions available: 32-bit and 64-bit. 64-bit is preferred and will automatically be selected by the configure script if the size of the C datatype `void*` is 8 bytes.

To aid the development of fully portable applications, in 64-bit mode the Fortran integer datatype is 64-bits. It is motivated by 1) the need of applications to use very large data structures, and 2) Fortran INTEGER*8 not being fully portable. The 64-bit representation of integer datatype is accomplished by using the appropriate Fortran compiler flag. The configure script will determine this flag as needed, but one can always override the configure script by supplying the environment variable `FFLAG_INT` e.g. `FFLAG_INT=-i8`.

Note: configure almost always does the right thing, so overriding this particular option is rarely needed. The best way to enforce the integer size of your choosing is to use the configure options `--enable-i4` or `--enable-i8`. These options will force the integer size to be 4 or 8 bytes in size, respectively.

Because of limited interest in heterogeneous computing among known us GA users, the Global Arrays library still does not support heterogeneous platforms. This capability can be added if required by new applications.

2.1.2 Selection of the communication network for ARMCI

Some cluster installations can be equipped with a high performance network which offer instead, or in addition to, TCP/IP some special communication protocol, for example GM on Myrinet network. To achieve high performance in Global Arrays, ARMCI must be built to use these protocols in its implementation of one-sided communication. Starting with GA 5.0, this is accomplished by passing an option to the configure script.

In addition, it might be necessary to provide a location for the header files and library path corresponding to the location of software supporting the appropriate protocol API.

Our ability to automatically locate the required headers and libraries is currently inadequate. Therefore, you will likely need to specify the optional ARG pointing to the necessary directories and/or libraries. Sockets is the default ARMCI network if nothing else is specified to configure. Note that the optional argument ARG takes a quoted string of any CPPFLAGS, LDFLAGS, or LIBS necessary for locating the headers and libraries of the given ARMCI network. On many systems it is simply necessary to specify the selected network:

```
./configure --with-openib
```

On others, you may need to specify the path to the network's installation if it is in a non-default location. The following will add -I/path/to/portals/install/include and -L/path/to/portals/install/lib to the CPPFLAGS and LDFLAGS if those directories are found to exist:

```
./configure --with-portals="/path/to/portals/install"
```

See section 2.3.1 for details of what you can pass as the quoted string to configure options.

Network	Protocol Name	Configure Option
IBM BG/L	BGML	--with-bgml
Cray shmem	Cray shmem	--with-cray-shmem
IBM BG/P	Deep Computing Message Framework	--with-dcmf
IBM LAPI	LAPI	--with-lapi
N/A	MPI Spawn - MPI-2 dynamic process management	--with-mpi-spawn
Infiniband	OpenIB	--with-openib
Cray XT	Portals	--with-portals
Ethernet	TCP/IP	--with-sockets (the default, so you don't need to specify this)

2.1.3 Selection of the message-passing library

As explained in Section 3, GA works with either MPI or TCGMSG message-passing libraries. That means GA applications can use either of these interfaces. Selection of the message-passing library takes place when GA is configured. Since the TCGMSG library is small and compiles fast, it is included with the GA distribution package but as of GA 5.0 it is no longer built by default. For GA 5.0, MPI is the default message-passing library. There are three possible configurations for running GA with the message-passing libraries:

1. GA with MPI (*recommended*): directly with MPI. In this mode, GA program should contain MPI initialization calls. Example: `./conifigure`
2. GA with TCGMSG-MPI (MPI and TCGMSG emulation library): TCGMSG-MPI implements functionality of TCGMSG using MPI. In this mode, the message passing library can be initialized using either TCGMSG PBEGIN(F) or MPI_Init. Example: `./configure --with-mpi --with-tcgmsg`
3. GA with TCGMSG: directly with TCGMSG. In this mode, GA program should contain TCGMSG initialization calls. Example: `./configure --with-tcgmsg`

For the MPI versions (1 and 2 above), the `--with-mpi` configure option can take parameters. If no parameters are specified, configure will search for the

MPI compilers. Using the MPI compilers is the recommended way to build GA. If the MPI compilers are not found, configure will exit with an error. The configure script will attempt to determine the underlying Fortran 77, C, and C++ compilers wrapped by the MPI compilers. This is necessary for other configure tests such as determining compiler-specific optimization flags or determining the Fortran 77 libraries needed when linking using the C++ linker.

If an argument is specified to `--with-mpi`, then configure will no longer use the MPI compilers. Instead, configure will attempt to located the MPI headers and libraries. The locations of the headers and the locations and names of the one or more MPI libraries can differ wildly. The argument to `--with-mpi` can be a quoted string of any install paths, include paths, library paths, and/or libraries required for compiling and linking MPI programs. See section 2.3.1 for details of the possible arguments.

2.1.4 Dependencies on other software

In addition to the message-passing library, GA requires (internally):

- MA (Memory Allocator), a library for managment of local memory;
- ARMCI, a one-sided communication library that GA uses as its run-time system;

GA optionally can use external:

- BLAS library is required for the eigensolver and `ga_dgemm` (a subset is included with GA, which is built into `libga.a`);
- LAPACK library is required for the eigensolver (a subset is included with GA, which is built into `libga.a`);

GA may also depend on other software depending on the functions being used.

- GA eigensolver, ga_diag, is a wrapper for the eigensolver from the PEIGS library; (Please contact George Fannabout PEIGS)
- SCALAPACK, PBBLAS, and BLACS libraries are required for *ga_ lu_ solve, ga_ cholesky, ga_ llt_ solve, ga_ spd_ invert, ga_ solve*. If these libraries are not installed, the named operations will not be available.

2.2 Writing GA Programs

C programs that use Global Arrays should include files *'ga.h'* and *'macdecls.h'*. Fortran programs should include the files *'mafdecls.fh'* and *'global.fh'*. Fortran source must be preprocessed as a part of compilation.

The GA program should look like:

- When GA runs with MPI

```
! Fortran MPI example
      program main
      include 'mpif.h'          ! MPI declarations
      integer ierror
      call mpi_init(ierror)     ! start MPI
      call ga_initialize()      ! start global arrays
      status = ma_init()        ! start memory allocator**
!     ...                       ! do work
      call ga_terminate()       ! tidy up global arrays call
      call mpi_finalize(ierror) ! tidy up MPI
      end program               ! exit program
```

```
/* C example */
int main(int argc, char **argv) {
  MPI_Init(&argc,&argv);    /* start MPI */
  GA_Initialize();          /* start global arrays */
  MA_Init(...);             /* start memory allocator** */
  /* ... */                 /* do work */
  GA_Terminate();           /* tidy up global arrays call */
  MPI_Finalize();           /* tidy up MPI */
}
```

- When GA runs with TCGMSG or TCGMSG-MPI

```
! Fortran TCGMSG example
      program main
      include 'tcgmsg.fh'       ! TCGMSG declarations
      call pbeginf()            ! start TCGMSG
      call ga_initialize()      ! start global arrays
      status = ma_init()        ! start memory allocator**
!     ...                       ! do work
      call ga_terminate()       ! tidy up global arrays call
      call pend()               ! tidy up TCGMSG
      end program               ! exit program
```

```
/* C TCGMSG example */
int main(int argc, char **argv) {
  tcg_pbegin(argc,argv);    /* start TCGMSG */
  GA_Initialize();          /* start global arrays */
  MA_Init(...);             /* start memory allocator** */
  /* ... */                 /* do work */
  GA_Terminate();           /* tidy up global arrays call */
  tcg_pend();               /* tidy up TCGMSG */
}
```

**The *ma_init* call looks like:

```
status = ma_init(type, stack_size, heap_size)
```

and it basically just goes to the OS and gets *stack_size+heap_size* elements of size *type*. The amount of memory MA allocates need to be sufficient for storing global arrays on some platforms. Please refer to section 3.2 for the details and information on more advanced usage of MA in GA programs.

2.3 Building GA

GNU Autotools (autoconf, automake, and libtool) are used to help build the GA library and example programs. GA follows the usual convention of:

```
./configure; make; make install
```

Before GA 5.0 the user was required to set a TARGET environment variable. This is no longer required - the configure script will determine the TARGET for the user. The configure script will also search for appropriate Fortran 77, C, and C++ compilers. To override the compilers, set the F77, CC, and/or CXX environment variables or specify them to configure:

```
./configure CC=gcc F77=ifort CFLAGS="-O2 -g -Wall"
```

For the complete list of environment variables which configure recognizes, see the output of running:

```
./configure --help
```

2.3.1 Building and Running GA Test and Example Programs

The GA distribution comes with a number of test and example programs located in ./global/testing and ./global/examples, respectively. To build these programs, after running configure and make, run the additional make target:

```
make checkprogs
```

To run the GA test suite, you must tell the make program how to run parallel programs. The following assumes either an interactive session on a queued system or a workstation:

```
make check MPIEXEC="mpirun -np 4"
```

Of course, replace the value of MPIEXEC to the appropriate command for the MPI implementation used to build GA. The test suite has not been tested with the TCGMSG message-passing library's parallel.x invoker.

2.3.2 Configure Options which Take Arguments

Certain configure options take arguments which help the configure script locate the headers and libraries necessary for the particular software. For example, when specifying the ARMCI network (see section 2.1.2), the location of the MPI installation (see section 2.1.3), or specifying the location of other external software such as BLAS, LAPACK, or ScaLAPACK.

You can put almost anything into the quoted argument to these configure options. For example, `-I*, -L*, -l*, -Wl*, -WL*, *.a, *.so` where the asterisk represents the usual arguments to those compiler and linker flags or paths to static or shared libraries. Here are some sample MPI uses to illustrate our point:

```
--with-mpi="/usr/local"
--with-mpi="-I/usr/local/include -L/usr/local/lib -lmpi"
--with-mpi="-lmpichf90 -lmpich"
```

2.3.3 BLAS and LAPACK

The GA distribution contains a subset of the BLAS and LAPACK routines necessary for successfully linking GA programs. However, those routines are not optimized. If optimized BLAS and LAPACK routines are available on your system, we recommend using them. The configure script will automatically attempt to locate external BLAS and LAPACK libraries.

Correctly determining the size of the Fortran INTEGER used when compiling external BLAS and LAPACK libraries is not automatic. Even on 64-bit platforms, external BLAS libraries are often compiled using 4-byte Fortran INTEGERs. The GA interface to the BLAS and LAPACK routines must match the Fortran INTEGER size used in the external BLAS and LAPACK routines. There are three options to configure:

- `--with-blas[=ARG]` is the default and will attempt to detect the size of the INTEGER, but if it fails (and it often will since this is no easy task), it will assume 4-byte INTEGERS. Automatic detection of the INTEGER size may improve in the future.
- `--with-blas4[=ARG]` assumes 4-byte INTEGERs
- `--with-blas8[=ARG]` assumes 8-byte INTEGERs

If LAPACK is in a separate library, you may need to specify `--with-lapack=ARG` where ARG is the path to the LAPACK library. See section 2.3.1 for details.

2.3.4 ScaLAPACK

GA interface routines to ScaLAPACK are only available when GA is built with MPI and ScaLAPACK. Before building GA, the user is required to configure --with-scalapack and pass the location of ScaLAPACK & Co. libraries passed

as arguments to those configure options. See section 2.3.2 (Configure Options which Take Arguments) for details.

2.3.5 GA C++ Bindings

The configure script automatically determines the Fortran 77 libraries required for linking a C++ application and places them in the FLIBS variable within the generated Makefile. Building the C++ bindings is then as simple as specifying:

```
./configure --enable-cxx
```

Running make will then link the libga++.a library in addition to the libga.a library. Both are then required for linking C++ GA applications, specifying libga++.a first and then libga.a (typically as -lga++ -lga).

2.3.6 Disabling Fortran

Fortran sources have typically been used by the GA and ARMCI distributions. For GA 5.0 and beyond, Fortran sources have been deprecated in the ARMCI distribution and are still used by default in the GA source. Therefore, ARMCI is free from Fortran dependencies while GA is not. The GA dependencies can be removed by specifying

```
./configure --disable-f77
```

Note that disabling Fortran 77 in GA is not well tested and doing so will also likely disable the use of external Fortran 77 libraries such as Fortran-based BLAS or ScaLAPACK. This also disables the use of the GA library in Fortran applications since the MA sources will no longer be compiled with Fortran 77 support. Use this option with care and only if developing C and/or C++ applications exclusively.

2.3.7 Python Bindings

GA 5.0 releases with Python bindings which were developed using the Cython package (http://www.cython.org/). At a minimum, GA must be configured with shared library support (which is disabled by default.) The configure script will automatically search for a python interpreter in the PATH environment variable, so make sure the appropriate Python interpreter can be found before configuring. For example:

```
./configure --enable-shared
```

should be all that is required to enable Python bindings. The Python bindings are not installed by default. You should run the following:

```
make python
```

in order to build and install the Python bindings. The python make target depends on the install target (i.e. "make install") and will pass the libga.so and ga.h library and header locations to the python setup.py invocation. Optionally, you can navigate to the python source directory and run:

```
python setup.py build_ext
```

or

```
python setup.py build_ext --inplace
```

to build the python bindings in a more manual way. The "make python" target is not well tested since specifying dependent libraries can be a difficult task.

If GA was built with external BLAS and LAPACK, those libraries must be specified when linking the Python shared library. Currently, users must edit the setup.py script within the python source directory in order to add these libraries to the standard distutils invocation of the linker. The BLAS and LAPACK libraries on OSX are particularly difficult to find, so this is done automatically for the user since the configure script will detect the vecLib framework on OSX automatically. Unforunately, at this time bulding the Python bindings is often a manual process but those fluent in Python and Python's `distutils` should have few problems editing the `setup.py` script.

2.3.8 Writing and Building New GA Programs

As of GA 5.0, the ability to place small single-file test programs into the global/testing directory of the distribution is no longer supported. Instead, you must install the GA headers and libraries using the "make install" target.

This will install the GA headers and libraries to the location specified by the --prefix configure option. If not specified, the default is `/usr/local/include` and `/usr/local/lib`. For our testing purposes, we often install GA into the same location as the build. Recall, GA can be configured from a separate build directory, keeping source and build trees separate. For example, from the top-level GA source distribution:

```
mkdir bld
cd bld
../configure --prefix=‘pwd‘
make
make install
```

will configure, build, and install the GA headers and library into the separate build directory "bld".

More specifically, you would find the GA library `libga` in `./bld/lib` and the GA headers in `./bld/include`. For packages using GA, you need to provide appropriate compiler and linker flags to indicate the locations of the GA header files and libraries.

2.4 Running GA Programs

Assume the GA program app.x had already been built. To run it,

Running on shared memory systems and clusters: (i.e., network of workstations/linux clusters)

If the app.x is built based on MPI, run the program the same way as any other MPI programs.

Example: to run on four processes on clusters, use

```
mpirun -np 4 app.x
```

Example: If you are using MPICH (or MPICH-like Implementations), and mpirun requires a machinefile or hostfile, then run the GA program same as any other MPI programs. *The only change required is to make sure the hostnames are specified in a consecutive manner in the machinefile.* Not doing this will prevent SMP optimizations and would lead to poor resource utilization.

```
mpirun -np 4 -machinefile machines.txt app.x
```

Contents of machines.txt: Let us say we have two 2-way SMP nodes (host1 and host2, and correct formats for a 4-processor machinefile is shown in the table below.

Correct	Correct	Incorrect
host1 host1 host2 host2	host2 host2 host1 host1	host1 host2 host1 (This is wrong, the same hosts should be specified together) host2

If app.x is built based on TCGMSG (not including Fujitsu, Cray J90, and Windows, because there are no native ports of TCGMSG), to execute the program on Unix workstations/servers, one should use the 'parallel.x' program. After building the application, a file called 'app.x.p' would also be generated (If there is not such a file, make it:

```
make app.x.p
```

This file can be edited to specify how many processors and tasks to use, and how to load the executables. Make sure that 'parallel.x' is accessible (you might copy it into your 'bin' directory). To execute, type:

```
parallel.x app.x
```

1. On MPPs, such as Cray XT3/XT4, or IMB SPs, use the appropriate system command to specify the number of processors, load and run the programs. Example:

   - to run on IBM SP, run as any other parallel programs (i.e., using *poe*)

- to run on Cray XT3/XT4, use *yod*.

2. On Microsoft NT, there is no support for TCGMSG, which means you can only build your application based on MPI. Run the application program the same way as any other MPI programs. For, WMPI you need to create the .pg file. Example:

```
R:\nt\g\global\testing> start /b test.x.exe
```

2.5 Building Intel Trace Analyzer (VAMPIR) Instrumented Global Arrays

Building GA for use with the intel trace analyzer is no loger supported. As of GA 5.1 allows the GA functions to be intercepted by user code.

TODO TODO TODO describe new pnga_ interfaces

Chapter 3

Initialization and Termination

For historical reasons (the 2-dimensional interface was developed first), many operations have two interfaces, one for two dimensional arrays and the other for arbitrary dimensional (one- to seven- dimensional, to be more accurate) arrays. The latter can definitely handle two dimensional arrays as well. The supported data types are integer,double precision, and double complex. Global Arrays provide C and Fortran interfaces in the same (mixed-language) program to the same array objects. The underlying data layout is based on the Fortran convention.

GA programs require message-passing and Memory Allocator (MA) libraries to work. Global Arrays is an extension to the message-passing interface. GA internally does not allocate local memory from the operating system - all dynamically allocated local memory comes from MA. We will describe the details of memory allocation later in this section.

3.1 Message Passing

The first version of Global Arrays was released in 1994 before robust MPI implementations became available. At that time, GA worked only with TCGMSG, a message-passing library that one of the GA authors (Robert Harrison) had developed before. In 1995, support for MPI was added. At the present time, the GA distribution still includes the TCGMSG library for backward compatibility purposes, and because it is small, fast to comple, and provides a minimal message-passing support required by GA programs. The MPI-compatible version of GA became the default as of version 5.0. See 2.1.3 for details.

The GA toolkit needs the following functionality from any message-passing library it runs with:

- initialization and termination of processes in an SPMD (single-program-multiple-data) program,
- synchronization,

- functions that return number of processes and calling process id,
- broadcast,
- reduction operation for integer and double datatypes, and
- 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 and terminated after the GA library is terminated.

GA provides two functions *ga_ nnodes* and *ga_ nodeid* that return the number of processes and the calling process id in a parallel program. Starting with release 3.0, these functions return the same values as their message-passing counterparts. In earlier releases of GA on clusters of workstations, the mapping between GA and message-passing process ids were nontrivial. In these cases, the *ga_ list_ nodeid* function (now obsolete) was used to describe the actual mapping.

Although message-passing libraries offer their own barrier (global synchronization) function, this operation does not wait for completion of the outstanding GA communication operations. The GA toolkit offers a *ga_ sync* operation that can be used for synchronization, and it has the desired effect of waiting for all the outstanding GA operations to complete.

3.2 Memory Allocation

GA uses a very limited amount of statically allocated memory to maintain its data structures and state. Most of the memory is allocated dynamically as needed, primarily to store data in newly allocated global arrays or as temporary buffers internally used in some operations, and deallocated when the operation completes.

There are two flavors of dynamically allocated memory in GA: shared memory and local memory. Shared memory is a special type of memory allocated from the operating system (UNIX and Windows) that can be shared between different user processes (MPI tasks). A process that attaches to a shared memory segment can access it as if it was local memory. All the data in shared memory is directly visible to every process that attaches to that segment. On shared memory systems and clusters of SMP (symmetritc multiprocessor) nodes, shared memory is used to store global array data and is allocated by the Global Arrays run-time system called ARMCI. ARMCI uses shared memory to optimize performance and avoid explicit interprocessor communication within a single shared memory system or an SMP node. ARMCI allocates shared memory from the operating system in large segments and then manages memory in each segment in response to the GA allocation and deallocation calls. Each segment can hold data in many small global arrays. ARMCI does not return shared memory segments to the operating system until the program terminates (calls *ga_ terminate*).

On systems that do not offer shared-memory capabilities or when a program is executed in a serial mode, GA uses local memory to store data in global arrays.

All of the dynamically allocated local memory in GA comes from its companion library, the Memory Allocator (MA) library. MA allocates and manages local memory using stack and heap disciplines. Any buffer allocated and deallocated by a GA operation that needs temporary buffer space comes from the MA stack. Memory to store data in global arrays comes from heap. MA has additional features useful for program debugging such as:

- left and right guards: they are stamps that detect if a memory segment was overwritten by the application,
- named memory segments, and
- memory usage statistics for the entire program.

Explicit use of MA by the application to manage its non-GA local data structures is not necessary but encouraged. Because MA is used implicitly by GA, it has to be initialized before the first global array is allocated. The *MA_init* function requires users to specify memory for heap and stack. This is because MA:

- allocates from the operating system only one segment equal in size to the sum of heap and stack,
- manages both allocation schemes using memory coming from opposite ends of the same segment, and
- the boundary between free stack and heap memory is dynamic.

It is not important what the stack and heap size argument values are as long as the aggregate memory consumption by a program does not exceed their sum at any given time.

MA is optional for C programs. You can replace GA's internal MA memory handling with `malloc()` and `free()` by using the function `GA_Register_stack_memory()`.

```
#include <mpi.h>     /* in this case we are using MPI */
#include <ga.h>      /* the global arrays declarations */
#include <stdlib.h> /* for malloc, free */

void* replace_malloc(size_t bytes, int align, char *name)
{
    return malloc(bytes);
}

void replace_free(void *ptr)
{
    free(ptr);
```

```
}

int main(int argc, char **agrv)
{
    MPI_Init(&argc,&argv);
    GA_Initialize();
    GA_Register_stack_memory(replace_malloc, replace_free);
    /* do work */
    GA_Terminate();
    MPI_Finalize();
}
```

3.2.1 Determining the Values of MA Stack and Heap Size

How can I determine what the values of MA stack and heap size should be?

The answer to this question depends on the run-time environment of the program including the availability of shared memory. A part of GA initialization involves initialization of the ARMCI run-time library. ARMCI dynamically determines if the program can use shared memory based on the architecture type and current configuration of the SMP cluster. For example, on uniprocessor nodes of the IBM SP shared memory is not used whereas on the SP with SMP nodes it is. This decision is made at run-time. GA reports the information about the type of memory used with the function *ga_uses_ma()*. This function returns false when shared memory is used and true when MA is used.

Based on this information, a programmer who cares about the efficient usage of memory has to consider the amount of memory per single process (MPI task) needed to store data in global arrays to set the heap size argument value in ma_init. The amount of stack space depends on the GA operations used by the program (for example *ga_mulmat_patch* or *ga_dgemm* need several MB of buffer space to deliver good performance) but it probably should not be less than 4MB. The stack space is only used when a GA operaion is executing and it is returned to MA when it completes.

3.3 GA Initialization

The GA library is initialized after a message-passing library and before MA. It is possible to initialize GA after MA but it is not recommended: GA must first be initialized to determine if it needs shared or MA memory for storing distributed array data. There are two alternative functions to initialize GA:

TODO

and

TODO

The first interface allows GA to consume as much memory as the application needs to allocate new arrays. The latter call allows the programmer to establish and enforce a limit within GA on the memory usage.

Note: In GA++, there is an additional functionality as follows:
TODO

3.3.1 Limiting Memory Usage by Global Arrays

GA offers an optional mechanism that allows a programmer to limit the aggregate memory consumption used by GA for storing Global Array data. These limits apply regardless of the type of memory used for storing global array data.They do not apply to temporary buffer space GA might need to use to execute any particular operation. The limits are given per process (MPI task) in bytes. If the limit is set, GA would not allocate more memory in global arrays that would exceed the specified value - any calls to allocate new arrays that would simply fail (return false). There are two ways to set the limit:

1. at initialization time by calling ga_initialize_ltd, or
2. after initialization by calling the function

TODO
It is encouraged that the user choose the first option, even though the user can intialize the GA normally and set the memory limit later.
Example: Initialization of MA and setting GA memory limits

```
call ga_initialize()
if (ga_uses_ma()) then
   status = ma_init(MT_DBL, stack, heap+global)
else
   status = ma_init(mt_dbl,stack,heap)
call ga_set_memory_limit(ma_sizeof(MT_DBL,global,MT_BYTE))
endif
if(.not. status) ... !we got an error condition here
```

In this example, depending on the value returned from ga_uses_ma(), we either increase the heap size argument by the amount of memory for global arrays or set the limit explicitly through ga_set_memory_limit(). When GA memory comes from MA we do not need to set this limit through the GA interface since MA enforces its memory limits anyway. In both cases, the maximum amount of memory acquired from the operating system is capped by the value *stack+heap+global*.

3.4 Termination

The normal way to terminate a GA program is to call the function
TODO
The programmer can also abort a running program for example as part of handling a programmatically detected error condition by calling the function
TODO

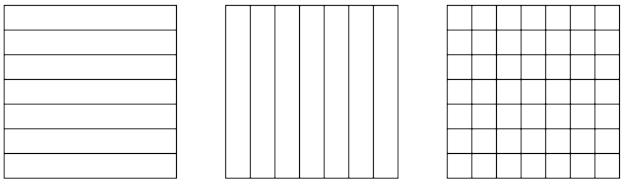


Figure 3.1: Regular Distribution

3.5 Creating Arrays - I

There are three ways to create new arrays:

1. From scratch, for regular distribution, using

   TODO

   or for regular distribution, using

   TODO

2. Based on a template (an existing array) with the function

   TODO

3. Refer to the "Creating Arrays - II" section.

In this case, the new array inherits all the properties such as distribution, datatype and dimensions from the existing array.

With the regular distribution shown in Figure 3.1, the programmer can specify block size for none or any dimension. If block size is not specified the library will create a distribution that attempts to assign the same number of elements to each processor (for static load balancing purposes). The actual algorithm used is based on heuristics.

With the irregular distribution shown in Figure 3.2, the programmer specifies distribution points for every dimension using map array argument. The library creates an array with the overall distribution that is a Cartesian product of distributions for each dimension. A specific example is given in the documentation.

If an array cannot be created, for example due to memory shortages or an enforced memory consumption limit, these calls return failure status. Otherwise an integer handle is returned. This handle represents a global array object in all operations involving that array. This is the only piece of information the programmer needs to store for that array. All the properties of the object (data type, distribution data, name, number of dimensions and values for each dimension) can be obtained from the library based on the handle at any time, see Section 7.4. It is not necessary to keep track of this information explicitly in the application code.

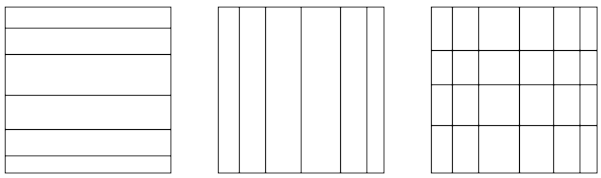


Figure 3.2: Irregular Distribution

Note that regardless of the distribution type at most one block can be owned/assigned to a processor.

3.5.1 Creating Arrays with Ghost Cells

Individual processors ordinarily only hold the portion of global array data that is represent by the lo and hi index arrays returned by a call to nga_distribution or that have been set using the nga_create_irreg call. However, it is possible to create global arrays where this data is padded by a boundary region of array elements representing portions of the global array residing on other processors. These boundary regions can be updated with data from neighboring processors by a call to a single GA function. To create global arrays with these extra data elements, referred to in the following as ghost cells, the user needs to call either the functions:

TODO

These two functions are almost identical to the `nga_create` and `nga_create_irreg` functions described above. The only difference is the parameter array width. This is used to control the width of the ghost cell boundaries in each dimension of the global array. Different dimensions can be padded with different numbers of ghost cells, although it is expected that for most applications the widths will be the same for all dimensions. If the width has been set to zero for all dimensions, then these two functions are completely equivalent to the functions `nga_create` and `nga_create_irreg`.

To illustrate the use of these functions, an ordinary global array is shown in Figure 3.3. The boundaries represent the data that is held on each processor.

For a global array with ghost cells, the data distribution can be visualized as shown in Figure 3.4:

Each processor holds "visible" data, corresponding to the data held on each processor of an ordinary global array, and "ghost cell" data, corresponding to neighboring points in the global array that would ordinarily be held on other processors. This data can be updated in a single call to `nga_update`, described under the collective operations section of the user documentation. Note that the ghost cell data duplicates some portion of the data in the visible portion of the global array. The advantage of having the ghost cells is that this data ordinarily

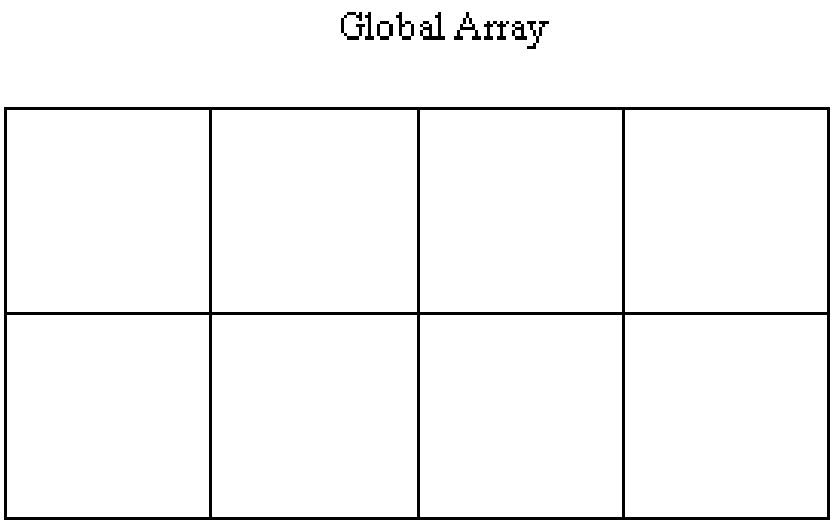


Figure 3.3: Ordinary Global Array

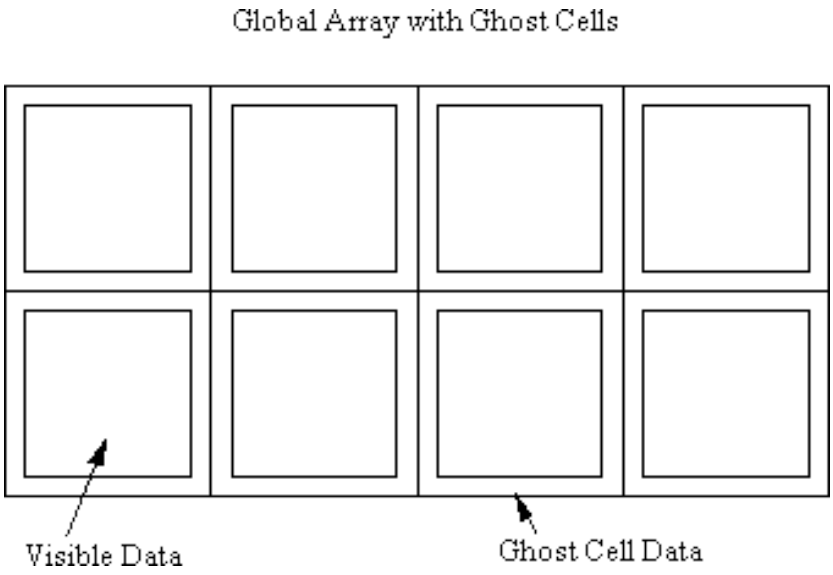


Figure 3.4: Global Array with Ghost Cells

resides on other processors and can only be retrieved using additional calls. To access the data in the ghost cells, the user must use the `nga_access_ghosts` function described in Section 6.1.

3.6 Creating Arrays - II

As mentioned in the previous section ("Creating arrays - I"), there are 3 ways to create arrays. This section describes method #3 to create arrays. Because of the increasingly varied ways that global arrays can be configured, a set of new interfaces for creating global arrays has been created. This interface supports all the configurations that were accessible via the old ga_create_XXX calls, as well as new options that can only be accessed using the new interface. Creating global arrays using the new interface starts by a call to ga_create_handle that returns the user a new global array handle. The user then calls several ga_set_XXX calls to assign properties to this handle. These properties include the dimension of the array, the data type, the size of the array, and any other properties that may be relevant. At present, the available ga_set_XXX calls largely reflect properties that are accessible via the nga_create_XXX calls, however, it is anticipated that the range of properties that can be set using these calls will expand considerably in the future. After all the properties have been set, the user calls ga_allocate on the array handle and memory is allocated for the array. The array can now be used in exactly the same way as arrays created using the traditional ga_create_XXX calls. The calls for obtaining a new global array handle are

TODO

Properties of the global arrays can be set using the ga_set_XXX calls. Note that the only required call is to ga_set_data. The others are all optional.

TODO

The argument *g_a* is the global array handle, *ndim* is the dimension of the array, *dims* is an array of *ndim* numbers containing the dimensions of the array, and *type* is the data type as defined in either the macdecls.h or mafdecls.h files. Other options that can be set using these subroutines are:

TODO

This subroutine assigns a character string as an array name to the global array.

TODO

The chunk array contains the minimum size dimensions that should be allocated to a single processor. If the minimum size is set to -1 for some of the dimensions, then the minimum size allocation is left to the GA toolkit. The default setting of the chunk array is -1 along all dimensions.

TODO

The ga_set_irreg_distr subroutine can be used to specify the distribution of data among processors. The block array contains the processor grid used to lay out the global array and the map array contains a list of the first indices of each block along each of the array axes. If the first value in the block array is

M, then the first M values in the map array are the first indices of each data block along the first axis in the processor grid. Similarly, if the second value in the block array is N, then the values in the map array from M+1 to M+N are the first indices of the each data block along the second axis and so on through the D dimensions of the global array.

TODO

This call can be used to set the ghost cell width along each of the array dimensions.

TODO

This call assigns a processor group to the global array. If no processor group is assigned to the global array, it is assumed that the global array is created on the default processor group.

After all the array properties have been set, memory for the global array is allocated by a call to ga_allocate. After this call, the global array is ready for use inside the parallel application.

TODO

This function returns a logical variable that is true if the global array was successfully allocated and false otherwise.

3.7 Destroying Arrays

Global arrays can be destroyed by calling the function

TODO

that takes as its argument a handle representing a valid global array. It is a fatal error to call ga_destroy with a handle pointing to an invalid array.

All active global arrays are destroyed implicitly when the user calls `ga_terminate`.

Chapter 4

One-sided Communication Operations

Global Arrays provide one-sided, noncollective communication operations that allow to access data in global arrays without cooperation with the process or processes that hold the referenced data. These processes do not know what data items in their own memory are being accessed or updated by remote processes. Moreover, since the GA interface uses global array indices to reference nonlocal data, the calling process does not even have to know process ids and location in memory where the refernenced data resides.

The one-sided operations that Global Arrays provide can be summarized into three categories:

Operation	Process
Remote blockwise write/read	`ga_put, ga_get`
Remote atomic update	`ga_acc, ga_read_inc, ga_scatter_acc`
Remote elementwise write/read	`ga_scatter, ga_gather`

4.1 Put/Get

Put and *get* are two powerful operations for interprocess communication, performing remote write and read. Because of their one-sided nature, they don't need cooperation from the process(es) that owns the data. The semantics of these operations do not require the user to specify which remote process or processes own the accessed portion of a global array. The data is simply accessed as if it were in shared memory.

Put copies data from the local array to the global array section, which is

```
\textcolor{green}{n-D}~\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/do
```

```
\textcolor{green}{2-D}~\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/do

\textcolor{blue}{C}~~~~~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\

~~~~~~~~~~~~~~~~~~~~~~~~int~ld{[}{]})~

\textcolor{blue}{C++}~~~~~~~~~void~GA::GlobalArray::put(int~lo{[}{]},~int~hi{[}{]},~

~~~~~~~~~~~~~~~~~~~~~~~~void~{*}buf,~int~ld{[}{]})
```

All the arguments are provided in one call: `lo` and ***hi*** specify where the data should go in the global array; ***ld*** specifies the stride information of the local array ***buf***. The local array should have the same number of dimensions as the global array; however, it is really required to present the n-dimensional view of the local memory buffer, that by itself might be one-dimensional.

The operation is transparent to the user, which means the user doesn't have to worry about where the region defined by ***lo*** and ***hi*** is located. It can be in the memory of one or many remote processes, owned by the local process, or even mixed (part of it belongs to remote processes and part of it belongs to a local process).

Get is the reverse operation of *put*. It copies data from a global array section to the local array. It is

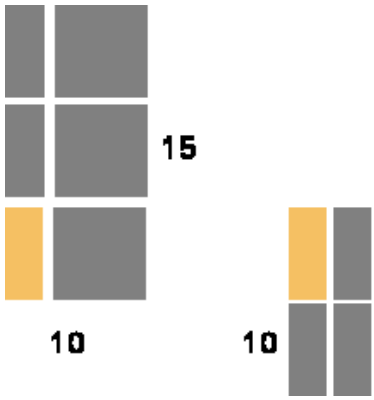
```
\textcolor{green}{n-D}~\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/do

\textcolor{green}{2-D}~\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/do

\textcolor{blue}{C}~~~~~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\

~~~~~~~~~~~~~~~~~~~~~~~~void~{*}buf,~int~ld{[}{]})~

\textcolor{blue}{C++}~~~~~~~~~void~GA::GlobalArray::get(int~lo{[}{]},~int~hi{[}{]},~

~~~~~~~~~~~~~~~~~~~~~~~~~void~{*}buf,~int~ld{[}{]})
```

Similar to *put*, ***lo*** and ***hi*** specify where the data should come from in the global array, and ***ld*** specifies the stride information of the local array ***buf***. The local array is assumed to have the same number of dimensions as the global array. Users don't need to worry about where the region defined by ***lo*** and ***hi*** is physically located.

Example:

For a ***ga_get*** operation transferring data from the (11:15,1:5) section of a 2-dimensional 15 x10 global array into a local buffer 5 x10 array we have: (In Fortran notation)

$$lo=\{11,1\},\ hi=\{15,5\},\ ld=\{10\}$$



4.2 Accumulate and Read-and-increment

It is often useful in a put operation to combine the data moved to the target process with the data that resides at that process, rather then replacing the data there. *Accumulate* and *read_inc* perform an *atomic* remote update to a patch (a section of the global array) in the global array and an element in the global array, respectively. They don't need the cooperation of the process(es) who owns the data. Since the operations are atomic, the same portion of a global array can be referenced by these operations issued by multiple processes and the GA will assure the correct and consistent result of the updates.

Accumulate combines the data from the local array with data in the global array section, which is

```
\textcolor{green}{n-D}~\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/do

\textcolor{green}{2-D}~\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/do

~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~ld,~alpha)~

\textcolor{blue}{C}~~~~~~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\

~~~~~~~~~~~~~~~~~~~~~~~~~~int~ld{[}{]},~void~{*}alpha)~

\textcolor{blue}{C++}~~~~~~~~~~void~NGA::GlobalArray::acc(int~lo{[}{]},~int~hi{[}{]},~

~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~void~{*}buf,~int~ld{[}{]},~v

~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~oid~{*}alpha)
```

The local array is assumed to have the same number of dimensions as the global array. Users don't need to worry about where the region defined by lo and hi is physically located. The function performs

*global array section (lo[], hi[]) += alpha * buf*

Read_inc remotely updates a particular element in the global array, which is

```
\textcolor{green}{n-D}~\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/do

\textcolor{green}{2-D}~\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/do

\textcolor{blue}{C}~~~~~~~~~~~long~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\

\textcolor{blue}{C++}~~~~~~~~~long~GA::GlobalArray::readInc(int~subscript{[}{]},~long~inc)
```

This function applies to integer arrays only. It atomically reads and increments an element in an integer array. It performs

a(subsripts) += *inc*

and returns the original value (before the update) of *a(subscript)*.

4.3 Scatter/Gather

Scatter and *gather* transfer a specified set of elements to and from global arrays. They are one-sided: that is they don't need the cooperation of the process(es) who own the referenced elements in the global array.

Scatter puts array elements into a global array, which is

```
\textcolor{green}{n-D}~\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/do

\textcolor{green}{2-D}~\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/do

\textcolor{blue}{C}~~~~~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\

~~~~~~~~~~~~~~~~~~~~~~{*}subsarray{[}{]},~int~n)~

\textcolor{blue}{C++~}~~~~~~~~void~GA::GlobalArray::scatter(void~{*}v,~

~~~~~~~~~~~~~~~~~~~~~~int~{*}subsarray{[}{]},~int~n)
```

It performs (in C notation)

```
for(k=0;~k<=~n;~k++)~\{

a{[}subsArray{[}k{]}{[}0{]}{]}{[}subsArray{[}k{]}{[}1{]}{]}{[}subsArray{[}k{]}{[}2{]}{]}...~

\}
```

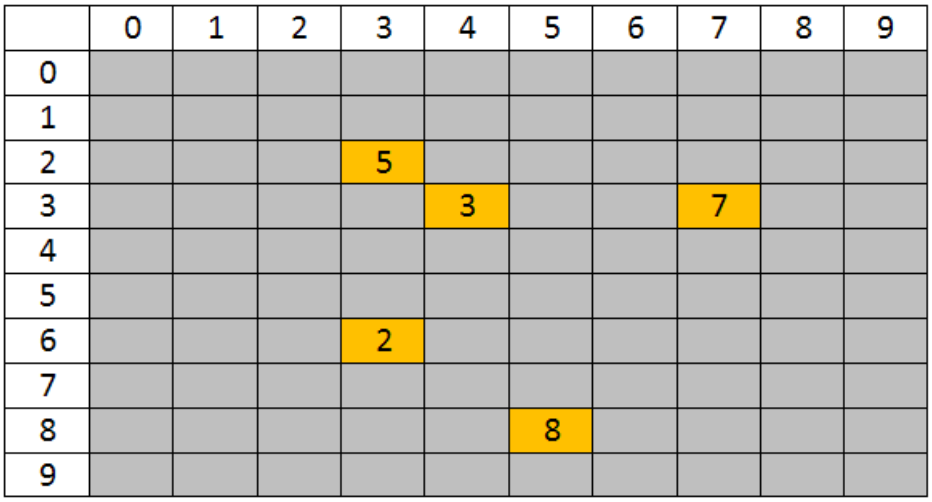
Example:

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 following figure.



Gather is the reverse operation of scatter. It gets the array elements from a global array into a local array.

```
\textcolor{green}{n-D}~\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/do

\textcolor{green}{2-D}~\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/do

\textcolor{blue}{C}~~~~~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\

~~~~~~~~~~~~~~~~~~~~~~~~~~~int~{*}subsarray{[}{]},~int~n)~
```

```
\textcolor{blue}{C++}~~~~~~~~~~void~GA::GlobalArray::gather(void~{*}v,~int~

~~~~~~~~~~~~~~~~~~~~~~~~~~~~{*}subsarray{[}{]},~int~n)
```

It performs (in C notation)

```
for(k=0;~k<=~n;~k++)\{~

~~~~~v{[}k{]}~=~a{[}subsArray{[}k{]}{[}0{]}{]}{[}subsArray{[}k{]}{[}1{]}{]}{[}subsArray{[}k{

\}~
```

4.4 Periodic Interfaces

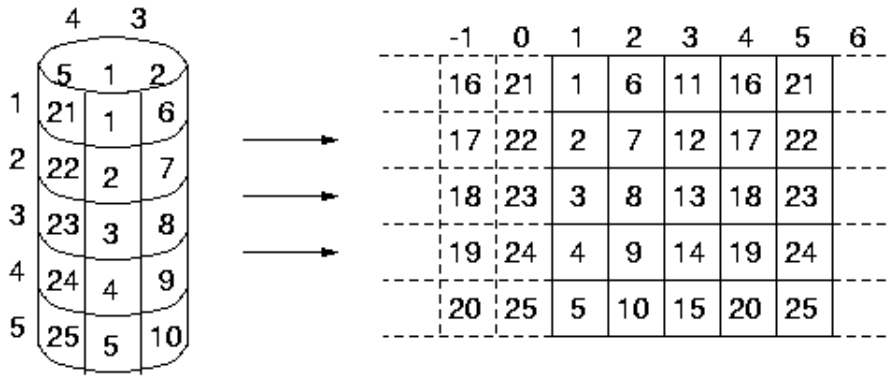
Periodic interfaces to the one-sided operations have been added to Global Arrays in version 3.1 to support some computational fluid dynamics problems on multidimensional grids. They provide an index translation layer that allows you to use put, get, and accumulate operations, possibly extending beyond the boundaries of a global array. The references that are outside of the boundaries are wrapped up inside the global array. To better illustrate these operations, look at the following example:

Example:

Assume a two dimensional global array g_a with dimensions 5 X 5.

	1	2	3	4	5
1	1	6	11	16	21
2	2	7	12	17	22
3	3	8	13	18	23
4	4	9	14	19	24
5	5	10	15	20	25

To access a patch [2:4,-1:3], one can assume that the array is wrapped over in the second dimension, as shown in the following figure



Therefore the patch [2:4, -1:3] is

```
17~22~2~7~12~

18~23~3~8~13~

19~24~4~9~14
```

Periodic operations extend the boudary of each dimension in two directions, toward the lower bound and toward the upper bound. For any dimension with lo(i) to hi(i), where 1 < i < ndim, it extends the range from

```
{[}lo(i)~:~hi(i){]}~
```

to

```
{[}(lo(i)-1-(hi(i)-lo(i)+1))~:~(lo(i)-1){]},~{[}lo(i)~:~hi(i){]},~
```

and

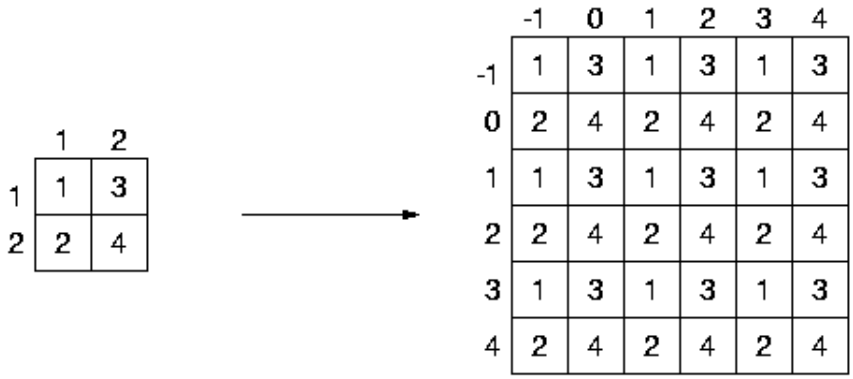
```
{[}(hi(i)+1)~:~(hi(i)+1+(hi(i)-lo(i)+1)){]},~
```

or

```
{[}(lo(i)-1-(hi(i)-lo(i)+1))~:~(hi(i)+1+(hi(i)-lo(i)+1)){]}.
```

Even though the patch spans in a much large range, the length must always be less, or equal to (hi(i)-lo(i)+1)).

Example: For a 2 x 2 array as shown in the following figure, where the dimensions are [1:2, 1:2], periodic operations would look at the range of each of the dimensions as [-1:4, -1:4].



Current version of GA supports three periodic operations. They are

- periodic get,
- periodic put, and
- periodic accumulate

Periodic Get copies data from a global array section to a local array, which is almost the same as regular get, except the indices of the patch can be outside the boundaries of each dimension.

```
\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_

~~~~~~~~~~~~~void~{*}buf,~int~ld{[}{]})~

\textcolor{blue}{C++}~~~~~void~GA::GlobalArray::periodicGet(int~lo{[}{]},~

~~~~~~~~~~~~~int~hi{[}{]},~void~{*}buf,~int~ld{[}{]})
```

Similar to regular *get*, ***lo*** and ***hi*** specify where the data should come from in the global array, and ***ld*** specifies the stride information of the local array ***buf***.

Example: Let us look at the first example in this section. It is 5 x 5 two dimensional global array. Assume that the local buffer is an 4x3 array.

Also assume that

```
lo{[}0{]}~=~-1,~hi{[}0{]}~=~2,~

lo{[}1{]}~=~4,~hi{[}1{]}~=~6,~and~

ld{[}0{]}~=~4.
```

	1	2	3	4	5
1	1	6	11	16	21
2	2	7	12	17	22
3	3	8	13	18	23
4	4	9	14	19	24
5	5	10	15	20	25

The local buffer *buf* is

```
19~~~~24~~~~4~

20~~~~25~~~~5~~

16~~~~21~~~~1~

17~~~~22~~~~2~
```

Periodic Put is the reverse operations of Periodic Get. It copies data from the local array to the global array section, which is

```
\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_

~~~~~~~~~~~~~void~{*}buf,~int~ld{[}{]})~

\textcolor{blue}{C++}~~~~~void~GA::GlobalArray::periodicPut(int~lo{[}{]},~

~~~~~~~~~~~~~int~hi{[}{]},~void~{*}buf,~int~ld{[}{]})
```

Similar to regular *put*, *lo* and *hi* specify where the data should go in the global array; *ld* specifies the stride information of the local array *buf*.

Periodic Put/Get (also include the *Accumulate*, which will be discussed later in this section) divide the patch into several smaller patches. For those smaller patches that are outside the global aray, adjust the indices so that they rotate back to the original array. After that call the regular *Put/Get/Accumulate*, for each patch, to complete the operations.

Example: Look at the example for periodic get. Because it is a 5 x 5 global array, the valid indices for each dimension are

```
dimension~0:~{[}1~:~5{]}~
```

```
dimension~1:~{[}1~:~5{]}
```

The specified lo and hi are apparently out of the range of each dimension:

```
dimemsion~0:~{[}-1~:~2{]}~-{}->~{[}-1~:~0{]}~-{}-~wrap~back~-{}->~{[}4~:~5{]}~{[}~1~:~2{]}~c
```

```
dimension~1:~{[}~4~:~6{]}~-{}->~{[}~4~:~5{]}~ok~{[}~6~:~6{]}~-{}-~wrap~back~-{}->~{[}1~:~1{]
```

Hence, there will be four smaller patches after the adjustment. They are

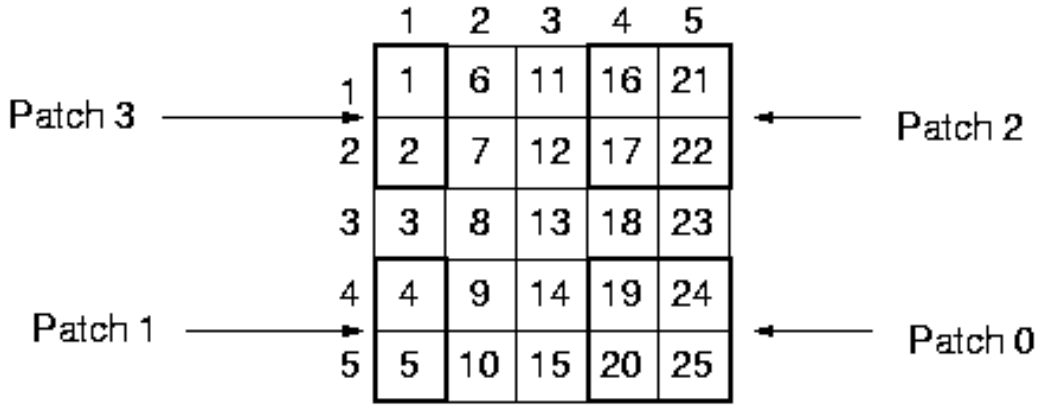
```
patch~0:~{[}4~:~5,~4~:~5{]}~
```

```
patch~1:~{[}4~:~5,~1~:~1{]}~
```

```
patch~2:~{[}1~:~2,~4~:~5{]}~
```

```
patch~3:~{[}1~:~2,~1~:~1{]}
```

as shown in the following figure



Of course the destination addresses of each samller patch in the local buffer also need to be calculated.

Similar to regular *Accumulate, Periodic Accumulate* combines the data from the local array with data in the global array section, which is

```
\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#
```

```
\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_
```

```
~~~~~~~~~~~~~~~~~~~void~{*}buf,~int~ld{[}{]},~void~{*}alpha)~
```

```
\textcolor{blue}{C++~}~~~~void~GA::GlobalArray::periodicAcc(int~lo{[}{]},~int~hi{[}{]},~

~~~~~~~~~~~~~~~~~~~void~{*}buf,~int~ld{[}{]},~void~{*}alpha)
```

The local array is assumed to have the same number of dimensions as the global array. Users don't need to worry about where the region defined by *lo* and *hi* is physically located. The function performs

*global array section (lo[], hi[]) += alpha * buf*

Example: Let us look at the same example as above. There is a 5 x 5 two dimensional global array. Assume that the local buffer is an 4x3 array.

Also assume that

```
lo{[}0{]}~=~-1,~hi{[}0{]}~=~2,~

lo{[}1{]}~=~4,~hi{[}1{]}~=~6,~and~

ld{[}0{]}~=~4.
```

	1	2	3	4	5
1	1	6	11	16	21
2	2	7	12	17	22
3	3	8	13	18	23
4	4	9	14	19	24
5	5	10	15	20	25

The local buffer buf is

```
1~~5~~9~

4~~6~~5~

3~~2~~1~

7~~8~~2
```

and the *alpha = 2*.

After the Periodic Accumulate operation, the global array will be

	1	2	3	4	5
1	3	6	11	22	25
2	6	7	12	24	38
3	3	8	13	18	23
4	22	9	14	21	34
5	15	10	15	28	37

4.5 Non-blocking operations

The non-blocking operations (get/put/accumulate) are derived from the blocking interface by adding a handle argument that identifies an instance of the non-blocking request. Nonblocking operations initiate a communication call and then return control to the application. A return from a nonblocking operation call indicates a mere initiation of the data transfer process and the operation can be completed locally by making a call to the wait (e.g. nga_nbwait) routine.

The wait function completes a non-blocking one-sided operation locally. Waiting on a nonblocking put or an accumulate operation assures that data was injected into the network and the user buffer can be now be reused. Completing a get operation assures data has arrived into the user memory and is ready for use. Wait operation ensures only local completion. Unlike their blocking counterparts, the nonblocking operations are not ordered with respect to the destination. Performance being one reason, the other reason is that by ensuring ordering we incur additional and possibly unnecessary overhead on applications that do not require their operations to be ordered. For cases where ordering is necessary, it can be done by calling a fence operation. The fence operation is provided to the user to confirm remote completion if needed.

Example: Let us take a simple case for illustration. Say, there are two global arrays i.e. one array stores pressure and the other stores temperature. If there are two computation phases (first phase computes pressure and second phase computes temperature), then we can overlap communication with computation, thus hiding latency.

```
.~.~.~.~.~.~.~.~.~.~

nga\_get~(get\_pressure\_array)

nga\_nbget(initiates~data~transfer~to~get~temperature\_array,~

~~~~~and~returns~immediately)

compute\_pressure()~/{*}~hiding~latency~-~communication~

~~~~~is~overlapped~with~computation~{*}/

nga\_nbwait(temperature\_array~-~completes~data~transfer)

compute\_temperature()~

.~.~.~.~.~.~.~.
```

The non-blocking APIs are derived from the blocking interface by adding a handle argument that identifies an instance of the non-blocking request.

```
\textcolor{green}{n-D}~\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/do

\textcolor{green}{n-D}~Fortran~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.h

\textcolor{green}{n-D}~\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/do

~~~~~~~~~~~~~~~~~~~~~nbhandle)~

\textcolor{green}{n-D}~\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/do

\textcolor{green}{2-D}~\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/do

~~~~~~~~~~~~~~~~~~~~ld,~nbhandle)~

\textcolor{green}{2-D}~\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/do

~~~~~~~~~~~~ld,~nbhandle)~

\textcolor{green}{2-D}~\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/do
```

```
~~~~~~~~~~~~ld,~alpha,~nbhandle)~

\textcolor{green}{2-D}~\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/do

\textcolor{blue}{C}~~~~~~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\

~~~~~~~~~~~~~~~~~~~~~void~{*}buf,~int~ld{[}{]},~ga\_nbhdl\_t{*}~nbhandle)~

\textcolor{blue}{C}~~~~~~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\

~~~~~~~~~~~~~~~~~~~~~void~{*}buf,~int~ld{[}{]},~ga\_nbhdl\_t{*}~nbhandle)~

\textcolor{blue}{C}~~~~~~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\

~~~~~~~~~~~~~~~~~~~~~void~{*}buf,~int~ld{[}{]},~void~{*}alpha,~

~~~~~~~~~~~~~~~~~~~~ga\_nbhdl\_t{*}~nbhandle)~

\textcolor{blue}{C}~~~~~~~~~~~~int~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#

\textcolor{blue}{C++}~~~~~~~~~~void~GA::GlobalArray::nbPut(int~lo{[}{]},~int~hi{[}{]},~

~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~void~{*}buf,~

~~~~~~~~~~~~~~int~ld{[}{]},~ga\_nbhdl\_t{*}~nbhandle)~

\textcolor{blue}{C++}~~~~~~~~~~void~GA::GlobalArray::nbGet(int~lo{[}{]},~int~hi{[}{]},~

~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~void~{*}buf,~

~~~~~~~~~~~~~~int~ld{[}{]},~ga\_nbhdl\_t{*}~nbhandle)~

\textcolor{blue}{C++}~~~~~~~~~~void~GA::GlobalArray::nbAcc(int~lo{[}{]},~int~hi{[}{]},~

~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~void~{*}buf,~

~~~~~~~~~~~~~~int~ld{[}{]},~void~{*}alpha,~ga\_nbhdl\_t{*}~nbhandle)~

\textcolor{blue}{C++}~~~~~~~~~~int~GA::GlobalArray::NbWait(ga\_nbhdl\_t{*}~nbhandle)
```

Chapter 5

Interprocess Synchronization

Global Arrays provide three types of synchronization calls to support different synchronization styles.

Lock with mutex:	is useful for a shared memory model. One can lock a mutex, to exclusively access a critical section.
Fence:	guarantees that the Global Array operations issued from the calling process are complete. The fence operation is local.
Sync:	is a barrier. It synchronizes processes and ensures that all Global Array operations are completed. Sync operation is collective.

5.1 Lock and Mutex

Lock works together with mutex. It is a simple synchronization mechanism used to protect a critical section.To enter a critical section, typically, one needs to do:

```
1.~~Create~mutexes~

2.~~Lock~on~a~mutex~

3.~~...~

~~~~Do~the~exclusive~operation~in~the~critical~section~~

~~~~...~

4.~~Unlock~the~mutex~
```

```
5.~~Destroy~mutexes
```

The function

```
\textcolor{blue}{Fortran}~logical~function~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.

\textcolor{blue}{C}~~~~~~~int~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_c

\textcolor{blue}{C++~}~~~~int~GA::GAServices::createMutexes(int~number)
```

creates a set containing the number of mutexes. Only one set of mutexes can exist at a time. Mutexes can be created and destroyed as many times as needed. Mutexes are numbered: 0, ..., number-1.

The function

```
\textcolor{blue}{Fortran}~logical~function~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.

\textcolor{blue}{C}~~~~~~~int~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_c

\textcolor{blue}{C++}~~~~~int~GA::GAServices::destroyMutexes()
```

destroys the set of mutexes created with ga_create_mutexes.

Both *ga_create_mutexes* and *ga_destroy_mutexes* are collective operations.

The functions

```
\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

~~~~~~~~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#ga_unlock}{ga\_{}u

\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_

~~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_unlock}{GA\_{}unlo

\textcolor{blue}{C++}~~~~~void~GA::GAServices::lock(int~mutex)~

~~~~~~~~void~GA::GAServices::unlock(int~mutex)
```

lock and unlock a mutex object identified by the mutex number, respectively. It is a fatal error for a process to attempt to lock a mutex which has already been locked by this process, or unlock a mutex which has not been locked by this process.

Example 1:

Use one mutex and the lock mechanism to enter the critical section.

```
status~=~ga\_create\_mutexes(1)~

if(.not.status)~then~
```

```
~~~call~ga\_error('ga\_create\_mutexes~failed~',0)~

endif~

call~ga\_lock(0)

~~~...~do~something~in~the~critical~section~

call~ga\_put(g\_a,~...)~

~~~...

call~ga\_unlock(0)~

if(.not.ga\_destroy\_mutexes())~then~

~~~call~ga\_error('mutex~not~destroyed',0)~
```

5.2 Fence

Fence blocks the calling process until all the data transfers corresponding to the Global Array operations initiated by this process complete. The typical scenario that it is being used is

```
1.~~Initialize~the~fence~

2.~~...~

~~~~~~~~Global~array~operations~

~~~~...~

3.~~Fence
```

This would guarantee the operations between step 1 and 3 are complete.

The function

```
\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_

\textcolor{blue}{C++}~~~~~void~GA::GAServices::initFence()
```

Initializes tracing of completion status of data movement operations.

The function

```
\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

\textcolor{blue}{C}\textcolor{blue}{\underbar{~}}~~~~~~void~\href{http://www.emsl.pnl.gov/do

\textcolor{blue}{C++}~~~~~void~GA::GAServices::fence()
```

blocks the calling process until all the data transfers corresponding to GA operations called after *ga_init_fence* complete.

ga_fence must be called after *ga_init_fence*. A barrier, *ga_sync*, assures completion of all data transfers and implicitly cancels outstanding ga_init_fence. *ga_init_fence* and *ga_fence* must be used in pairs, multiple calls to *ga_fence* require the same number of corresponding *ga_init_fence* calls. *ga_init_fence/ga_fence* pairs can be nested.

Example 1:

Since *ga_put* might return before the data reaches the final destination *ga_init_fence* and *ga_fence* allow the process to wait until the data is actually moved:

```
call~ga\_init\_fence()~

call~ga\_put(g\_a,~...)~

call~ga\_fence()
```

Example 2:

ga_fence works for multiple GA operations.

```
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 data movements initiated by two calls to `ga_put` and one `ga_scatter` complete.

5.3 Sync

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 function is

```
\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

\textcolor{blue}{C}~~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_

\textcolor{blue}{C++}~~~~~~void~GA::GAServices::sync()
```

Sync should be inserted as necessary. With many sync calls, the application performance would suffer.

Chapter 6

Collective Array Operations

Global Arrays provide functions for collective array operations, targeting both whole arrays and patches (portions of global arrays). Collective operations require all the processes to make the call. In the underlying implementation, each process deals with its local data. These functions include:

- basic array operations,
- linear algebra operations, and
- interfaces to third party software packages.

6.1 Basic Array Operations

Global Arrays provide several mechanisms to manipulate contents of the arrays. One can set all the elements in an array/patch to a specific value, or as a special case set to zero. Since GA does not explicitly initialize newly created arrays, these calls are useful for initialization of an array/patch. (To fill the array with different values for each element, one can choose the one sided operation putor each process can initialize its local portion of an array/patch like ordinary local memory). One can also scale the array/patch by a certain factor, or copy the contents of one array/patch to another.

6.1.1 Whole Arrays

These functions apply to the entire array.

The function

```
\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_

\textcolor{blue}{C++}~~~~~void~GA::GlobalArray::zero()
```

sets all the elements in the array to zero.

To assign a single value to all the elements in an array, use the function

```
\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_

\textcolor{blue}{C++}~~~~~void~GA::GlobalArray::fill(void~{*}val)
```

It sets all the elements in the array to the value *val*. The *val* must have the same data type as that of the array.

The function

```
\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_

\textcolor{blue}{C++}~~~~~void~GA::GlobalArray::scale(void~{*}val)
```

scales all the elements in the array by factor *val*. Again the val must be the same data type as that of the array itself.

The above three functions are dealing with one global array, to set values or change all the elements together. The following functions are for copying data between two arrays.

The function

```
\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_

\textcolor{blue}{C++}~~~~~void~GA::GlobalArray::copy

~~~~~~~~~~~~~(const~GA::GlobalArray~{*}~g\_a)
```

copies the contents of one array to another. The arrays must be of the same data type and have the same number of elements.

For global arrays containing ghost cells, the ghost cell data can be filled in with the corresponding data from neighboring processors using the command

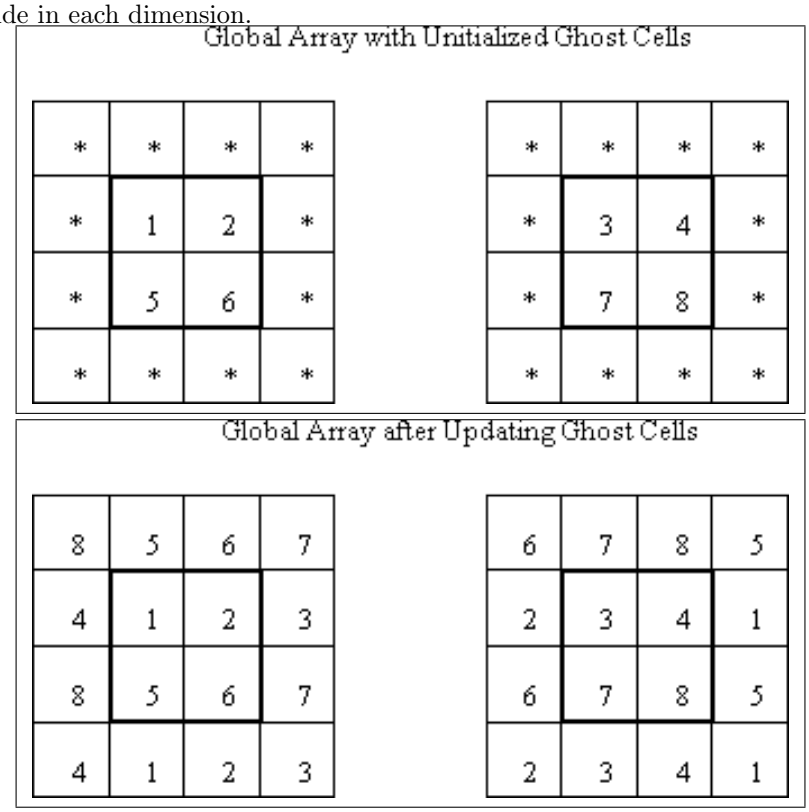
```
\textcolor{blue}{n-d~Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.ht

\textcolor{blue}{C~}~~~~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\

\textcolor{blue}{C++}~~~~~~~~~void~GA::GlobalArray::

~~~~~~~~~~~~~~~~~~copy(const~GA::GlobalArray~{*}~g\_a)
```

\textcolor{blue}{n-d~Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.ht

\textcolor{blue}{C}~~~~~~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\

\textcolor{blue}{C++}~~~~~~~~~~void~GA::GlobalArray::updateGhosts()~

This operation updates the ghost cell data by assuming periodic, or wrap-around, boundary conditions similar to those described for the `nga_periodic_get` operations described above. The wrap-around conditions are always applied, it is up to the individual application to decide whether or not the data in the ghost cells should be used. The update operation is illustrated below for a simple 4x2 global array distributed across two processors. The ghost cells are one element wide in each dimension.



\textcolor{blue}{n-d~Fortran}~logical~function~\href{http://www.emsl.pnl.gov/docs/global/ga_

~~~~~~~~~~~~~~~~~~~~~~~~dimension,~idir,~flag)~

\textcolor{blue}{C}~~~~~~~~~~~~int~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#

~~~~~~~~~~~~~~~~~~~~~~~~dimension,~int~idir,~int~cflag)~

```
\textcolor{blue}{C++}~~~~~~~~~int~GA::GlobalArray::updateGhostsDir

~~~~~~~~~~~~~~~~~~~~~~(int~dimension,~int~idir,~int~cflag)~
```

This function can be used to update the ghost cells along individual directions.

It is designed for algorithms that can overlap updates with computation. The variable dimension indicates which coordinate direction is to be updated (e.g. dimension = 1 would correspond to the y axis in a two or three dimensional system), the variable idir can take the values +/-1 and indicates whether the side that is to be updated lies in the positive or negative direction, and cflag indicates whether or not the corners on the side being updated are to be included in the update. The following calls would be equivalent to a call to `GA_Update_ghosts` for a 2-dimensional system:

```
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);
```

The variable *cflag* is set equal to 1 (or non-zero) in the first two calls so that the corner ghost cells are update, it is set equal to 0 in the second two calls to avoid redundant updates of the corners. Note that updating the ghosts cells using several independent calls to the `nga_update_ghost_dir` functions is generally not as efficient as using `GA_Update_ghosts` unless the individual calls can be effectively overlapped with computation. This is a collective operation.

6.1.2 Patches

GA provides a set of operations on segments of the global arrays, namely patch operations. These functions are more general, in a sense they can apply to the entire array(s). As a matter of fact, many of the Global Array collective operations are based on the patch operations, for instance, the `GA_Printis` only a special case of `NGA_Print_patch`, called by setting the bounds of the patch to the entire global array. There are two interfaces for Fortran, one for two dimensional and the other for n-dimensional (one to seven). The (n-dimensional) interface can surely handle the two dimensional case as well. It is available for backward compatibility purposes. The functions dealing with n-dimensional patches use the "`nga`"prefix and those dealing with two dimensional patches start with the "`ga`" prefix.

The function

```
\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#
```

```
\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_

\textcolor{blue}{C++}~~~~~void~GA::GlobalArray::zeroPatch(int~lo{[}{]}~int~hi{[}{]})
```

is similar to *ga_ zero*, except that instead of applying to entire array, it sets only the region defined by *lo* and *hi* to zero.

One can assign a single value to all the elements in a patch with the function:

```
\textcolor{green}{n-D}\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/doc

\textcolor{green}{2-D}\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/doc

~~~~~~~~~~~~~~~~~~jlo,~jhi,~val)~

\textcolor{blue}{C}~~~~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#

~~~~~~~~~~~~~~~~~~int~hi{[}{]},~void~{*}val)~

\textcolor{blue}{C++}~~~~~~~~void~GA::GlobalArray::fillPatch(int~lo{[}{]}~

~~~~~~~~~~~~~~~~~~int~hi{[}{]},~void~{*}val)
```

The `lo` and `hi` defines the patch and the `val` is the value to set.

The function

```
\textcolor{green}{n-D}\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/doc

\textcolor{green}{2-D}\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/doc

~~~~~~~~~~~~~~~~~~jhi,~val)~

\textcolor{blue}{C}~~~~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#

~~~~~~~~~~~~~~~~~~hi{[}{]},~void~{*}val)~

\textcolor{blue}{C++}~~~~~~~~void~GA::GlobalArray::scalePatch(int~lo{[}{]}~

~~~~~~~~~~~~~~~~~~int~hi{[}{]},~void~{*}val)
```

scales the patch defined by `lo` and `hi` by the factor `val`.

The copy patch operation is one of the fundamental and frequently used functions. The function

```
\textcolor{green}{n-D}\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/doc

~~~~~~~~~~~~~~~~~~~~~~ahi,~g\_b,~blo,~bhi)~

\textcolor{green}{2-D}\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/doc
```

```
~~~~~~~~~~~~~~~~~~~~~~aihi,~ajlo,~ajhi,~g\_b,~bilo,~bihi,~

~~~~~~~~~~~~~~~~~~~~~~bjlo,~bjhi)~

\textcolor{blue}{C~}~~~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#

~~~~~~~~~~~~~~~~~~~~~~int~alo{[}{]},~int~ahi{[}{]},~int~g\_b,~

~~~~~~~~~~~~~~~~~~~~~~int~blo{[}{]},~int~bhi{[}{]})~

\textcolor{blue}{C++}~~~~~~~~voidGA::GlobalArray::copyPatch(char~trans,~

~~~~~~~~~~~~~~~~~~~~~~const~GA::GlobalArray{*}~g\_a,~int~alo{[}{]},~

~~~~~~~~~~~~~~~~~~~~~~int~ahi{[}{]},~int~blo{[}{]},~int~bhi{[}{]})
```

copies one patch defined by `alo` and `ahi` in one global array `g_ato` another patch defined by `blo` and `bhi` in another global array `g_b`. The current implementation requires that the source patch and destination patch must be on different global arrays. They must also be the same data type. The patches may be of different shapes, but the number of elements must be the same. During the process of copying, the transpose operation can be performed by specifying trans.

Example: Assume that there two 8x6 Global Arrays, `g_a` and `g_b`,distributed on three processes. The operation of `nag_copy_patch`(Fortran notation), from

```
g\_a:~alo~=~\{2,~2\},~ahi~=~\{4,~5\}
```

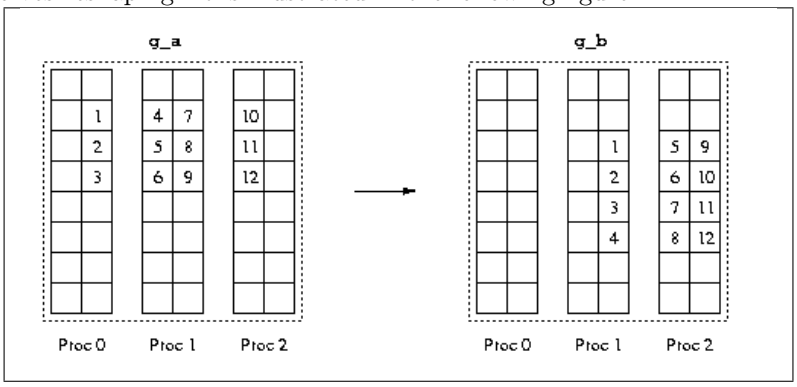
to

```
g\_b:~blo~=~\{3,~4\},~bhi~=~\{6,~6\}
```

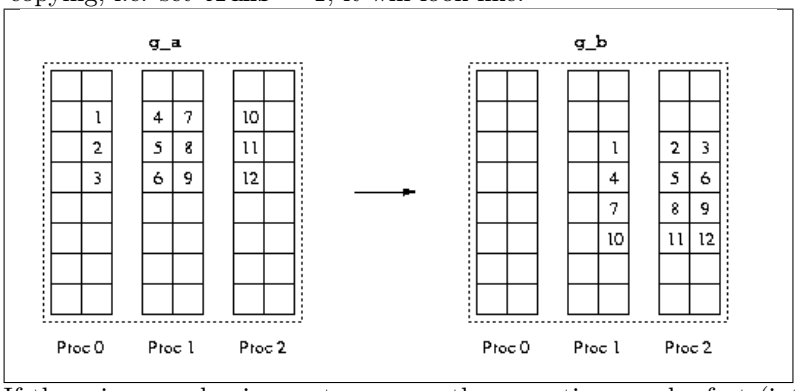
and

```
trans~=~0
```

involves reshaping. It is illustrated in the following figure.



One step further, if one also want to perform the transpose operation during the copying, i.e. set `trans = 1`, it will look like:



If there is no reshaping or transpose, the operation can be fast (internally calling `nga_put`). Otherwise, it would be slow (internally calling `nga_scatter`, where extra time is spent on preparing the indices). Also note that extra memory is required to hold the indices if the operation involves reshaping or transpose.

6.2 Linear Algebra

Global arrays provide three linear algebra operations: addition, multiplication, and dot product. There are two sets of functions, one for the whole array and the other for the patches.

6.2.1 Whole Arrays

The function

```
\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_

~~~~~~~~void~{*}beta,int~g\_b,~int~g\_c)~

\textcolor{blue}{C++}~void~GA::GlobalArray::add(void~{*}alpha,~~

~~~~~~~~const~GA::GlobalArray{*}~g\_a,~

~~~~~~~~void~{*}beta,~const~GA::GlobalArray{*}~g\_b)
```

adds two arrays, `g_a` and `g_b`, and saves the results to `g_c`. The two source arrays can be scaled by certain factors. This operation requires the two source arrays have the same number of elements and the same data types, but the arrays can have different shapes or distributions. `g_c` can also be `g_a` or `g_b`. It is encouraged to use this function when the two source arrays are identical

in distributions and shapes, because of its efficiency. It would be less efficient if the two source arrays are different in distributions or shapes.

Matrix multiplication operates on two matrices, therefore the array must be two dimensional. The function

```
\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

~~~~~~~~~~~~~~alpha,~g\_a,~g\_b,~beta,~g\_c~)~

\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_

~~~~~~~~~~~~~~int~k,~double~alpha,~int~g\_a,~int~g\_b,~

~~~~~~~~~~~~~~double~beta,~int~g\_c~)~

\textcolor{blue}{C++}~~~~~void~GA::GlobalArray::dgemm(char~ta,~char~tb,~

~~~~~~~~~~~~~~int~m,~int~n,~int~k,~double~alpha,~

~~~~~~~~~~~~~~const~GA::GlobalArray{*}~g\_a,~const~GA::GlobalArray{*}~

~~~~~~~~~~~~~~g\_b,~double~beta)
```

Performs one of the matrix-matrix operations:

*C := alpha*op(A)*op(B) + beta*C,*

where op(X) is one of

op(X) = X or op(X) = X',

alpha and beta are scalars, and *A, B,* and *C* are matrices, with *op(A)* an *m* by *k* matrix, *op(B)* a *k* by *n* matrix and *C* an *m* by *n* matrix.

On entry, transa specifies the form of *op(A)* to be used in the matrix multiplication as follows:

ta = 'N' or *'n', op(A) = A.*

ta = 'T' or *'t', op(A) = A'.*

The function

```
Fortran~integer~function~ga\_idot(g\_a,~g\_b)~

~~~~~~~~double~precision~function~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#ga_

~~~~~~~~double~complex~function~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#ga_zd

C~~~~~~~long~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_dot}{GA\_{}Idot}(i

~~~~~~~~double~G\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_dot}{GA\_{}Ddot

~~~~~~~~DoubleComplex~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_dot}{GA\_
```

```
C++~~~~~long~GA::GlobalArray::idot

~~~~~~~~~~~~~~~~~(const~GA::GlobalArray{*}~g\_a)~

~~~~~~~~double~GA::GlobalArray::ddot

~~~~~~~~~~~~~~~~~(const~GA::GlobalArray{*}~g\_a)~

~~~~~~~~DoubleComplex~GA::GlobalArray::zdot

~~~~~~~~~~~~~~~~~(const~GA::GlobalArray{*}~g\_a)
```

computes the element-wise dot product of two arrays. It is available as three separate functions, corresponding to *integer*, *double precision* and *double complex* data types.

The following functions apply to the 2-dimensional whole arrays only. There are no corresponding functions for patch operations.

The function

```
\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_

\textcolor{blue}{C++}~~~~~void~GA::GlobalArray::symmetrize()
```

symmetrizes matrix A represented with handle `g_a`:*A = .5 * (A+A')*.

The function

```
\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_

\textcolor{blue}{C++}~~~~~void~GA::GlobalArray::transpose

~~~~~~~~~~~~~(const~GA::GlobalArray{*}~g\_a)
```

transposes a matrix: B = A'.

6.2.2 Patches

The functions

```
\textcolor{green}{n-D}\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/doc

~~~~~~~~~~~~~~~~~~~~~~alo,~ahi,~beta,~g\_b,~blo,~

~~~~~~~~~~~~~~~~~~~~~~bhi,~g\_c,~clo,~chi)~
```

```
\textcolor{green}{2-D}\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/doc

~~~~~~~~~~~~~~~~~~~~~~ailo,~aihi,~ajlo,~ajhi,~

~~~~~~~~~~~~~~~~~~~~~~beta,~g\_b,~bilo,~bihi,~bjlo,~

~~~~~~~~~~~~~~~~~~~~~~bjhi,~g\_c,~cilo,~cihi,~cjlo,~cjhi)~

\textcolor{blue}{C}~~~~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#

~~~~~~~~~~~~~~~~~~~~~~alo{[}{]},~int~ahi{[}{]},~void~{*}beta,~

~~~~~~~~~~~~~~~~~~~~~~int~g\_b,~int~blo{[}{]},~int~bhi{[}{]},~

~~~~~~~~~~~~~~~~~~~~~~int~g\_c,~int~clo{[}{]},~int~chi{[}{]})~

\textcolor{blue}{C++}~~~~~~~~void~GA::GlobalArray::addPatch(void~{*}alpha,~

~~~~~~~~~~~~~~~~~~~~~~const~GA::GlobalArray{*}~g\_a,~

~~~~~~~~~~~~~~~~~~~~~~int~alo{[}{]},~int~ahi{[}{]},~void~{*}beta,~

~~~~~~~~~~~~~~~~~~~~~~const~GA::GlobalArray{*}~g\_b,~int~blo{[}{]},~

~~~~~~~~~~~~~~~~~~~~~~int~bhi{[}{]},~int~clo{[}{]},~int~chi{[}{]})~
```

add element-wise two patches and save the results into another patch. Even though it supports the addition of two patches with different distributions or different shapes (the number of elements must be the same), the operation can be expensive, because there can be extra copies which effect memory consumption. The two source patches can be scaled by a factor for the addition. The function is smart enough to detect the case that the patches are exactly the same but the global arrays are different in shapes. It handles the case as if for the arrays were identically distributed, thus the performance will not suffer.

The matrix multiplication is the only operation on array patches that is restricted to the two dimensional domain, because of its nature. It works for *double* and *double complex* data types. The prototype is

```
\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

~~~~~~~~~~~~~~~~~~~alpha,~beta,~g\_a,~ailo,~aihi,~

~~~~~~~~~~~~~~~~~~~ajlo,~ajhi,~g\_b,~bilo,~bihi,~bjlo,~

~~~~~~~~~~~~~~~~~~~bjhi,~g\_c,~cilo,~cihi,~cjlo,~cjhi)~

\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_
```

```
~~~~~~~~~~~~~~~~~~void{*}~alpha,~void~{*}beta,~int~g\_a,~

~~~~~~~~~~~~~~~~~~int~ailo,~int~aihi,~int~ajlo,~int~ajhi,~

~~~~~~~~~~~~~~~~~~int~g\_b,~int~bilo,~int~bihi,~int~bjlo,~

~~~~~~~~~~~~~~~~~~int~bjhi,~int~g\_c,~int~cilo,~int~cihi,~

~~~~~~~~~~~~~~~~~~int~cjlo,~int~cjhi)~

\textcolor{blue}{C++}~~~~~void~GA::GlobalArray::matmulPatch(char~{*}transa,

~~~~~~~~~~~~~~~~~~char{*}~transb,~void{*}~alpha,~void~{*}beta,~

~~~~~~~~~~~~~~~~~~const~GlobalArray~{*}~g\_a,~int~ailo,~

~~~~~~~~~~~~~~~~~~int~aihi,~int~ajlo,~int~ajhi,~const~

~~~~~~~~~~~~~~~~~~GlobalArray~{*}~g\_b,~int~bilo,~int~bihi,~

~~~~~~~~~~~~~~~~~~int~bjlo,~int~bjhi,~int~cilo,~int~cihi,~

~~~~~~~~~~~~~~~~~~int~cjlo,~int~cjhi)
```

It performs

```
C{[}cilo:cihi,cjlo:cjhi{]}~:=~alpha{*}~AA{[}ailo:aihi,ajlo:ajhi{]}~{*}

~~~~~BB{[}bilo:bihi,bjlo:bjhi{]}~)~+~beta{*}C{[}cilo:cihi,cjlo:cjhi{]}
```

where *AA = op(A), BB = op(B),* and *op(X)* is one of
op(X) = X or op(X) = X',
Valid values for transpose argument: *'n', 'N', 't', 'T'.*

The dot operation computes the element-wise dot product of two (possibly transposed) patches. It is implemented as three separate functions, corresponding to integer, double precision and double complex data types. They are

```
\textcolor{green}{n-D}\textcolor{blue}{Fortran}~integer~function~nga\_idot\_patch(g\_a,~ta,~

~~~~~~~~~~~~~~~~~alo,~ahi,~g\_b,~tb,~blo,~bhi)~

~~~~~~~~~~~double~precision~functionn~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\

~~~~~~~~~~~~~~~~(g\_a,~ta,~alo,~ahi,~g\_b,~tb,~blo,~bhi)~

~~~~~~~~~~~double~complex~functionn~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#g
```

```
~~~~~~~~~~~~~~~~~(g\_a,~ta,~alo,~ahi,~g\_b,~tb,~blo,~bhi)


\textcolor{green}{2-D}\textcolor{blue}{Fortran}~integer~function~ga\_idot\_patch(g\_a,~ta,~a
~~~~~~~~~~~~~~~~~ajlo,~ailo,~g\_b,~tb,~bilo,~bihi,~bjlo,~bjhi)~
~~~~~~~~~~~double~precision~function~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#
~~~~~~~~~~~~~~~~~ailo,~aihi,~ajlo,~ailo,~g\_b,~tb,~bilo,~bihi,~
~~~~~~~~~~~~~~~~~bjlo,~bjhi)~
~~~~~~~~~~~double~complex~function~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#ga
~~~~~~~~~~~~~~~~~aihi,~ajlo,~ailo,~g\_b,~tb,~bilo,~bihi,~bjlo,~bjhi)


\textcolor{blue}{C}~~~~~~~~~~Integer~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.htm
~~~~~~~~~~~~~~~~~int~ahi{[}{]},~int~g\_b,~char{*}~tb,~int~blo{[}{]},~
~~~~~~~~~~~~~~~~~int~bhi{[}{]})~
~~~~~~~~~~~double~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_dot_patch}{NO
~~~~~~~~~~~~~~~~~int~ahi{[}{]},~int~g\_b,~char{*}~tb,~int~blo{[}{]},~
~~~~~~~~~~~~~~~~~int~bhi{[}{]})~
~~~~~~~~~~~DoubleComplex~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_dot_pa
~~~~~~~~~~~~~~~~~int~alo{[}{]},~int~ahi{[}{]},~int~g\_b,~char{*}~tb,~
~~~~~~~~~~~~~~~~~int~blo{[}{]},~int~bhi{[}{]})


\textcolor{blue}{C++~}~~~~~~~IntegerGA::GlobalArray::idotPatch(const~GA::GlobalArray{*}
~~~~~~~~~~~~~~~~~g\_a,~char{*}~ta,~int~alo{[}{]},~int~ahi{[}{]},~char{*}~
~~~~~~~~~~~~~~~~~tb,~int~blo{[}{]},~int~bhi{[}{]})~
```

```
~~~~~~~~~~~double~GA::GlobalArray::ddotPatch(const~GA::GlobalArray{*}

~~~~~~~~~~~~~~~~~g\_a,~char{*}~ta,~int~alo{[}{]},~int~ahi{[}{]},~char{*}~tb,~

~~~~~~~~~~~~~~~~int~blo{[}{]},~int~bhi{[}{]})~

~~~~~~~~~~~DoubleComplex~GA::GlobalArray::zdotPatch

~~~~~~~~~~~~~~~~~(const~GA::GlobalArray{*}~g\_a,~char{*}~ta,~int~alo{[}{]},~

~~~~~~~~~~~~~~~~~int~ahi{[}{]},~char{*}~tb,~int~blo{[}{]},~int~bhi{[}{]})
```

The patches should be of the same data types and have the same number of elements. Like the array addition, if the source patches have different distributions/shapes, or it requires transpose, the operation would be less efficient, because there could be extra copies and/or memory consumption.

6.2.3 Element-wise operations

These operations work on individual array elements rather than arrays as matrices in the sense of linear algebra operations. For example multiplication of elements stored in arrays is a completely different operation than matrix multiplication.

```
\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

\textcolor{blue}{C}~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_a

\textcolor{blue}{C++}~~~~void~GA::GlobalArray::absValue(int~g\_a)
```

Take element-wise absolute value of the array.

```
\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_

\textcolor{blue}{C++}~~~~~void~GA::GlobalArray::absValuePatch

~~~~~~~~~~~~~(int~lo{[}{]},~int~hi{[}{]})
```

Take element-wise absolute value of the patch.

```
\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_

\textcolor{blue}{C++}~~~~~void~GA::GlobalArray::addConstant(void{*}~alpha)
```

Add the contant pointed by alpha to each element of the array.

```
\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_

~~~~~~~~~~~~~int~hi{[}{]},~void{*}alpha)~

\textcolor{blue}{C++}~~~~~void~GA::GlobalArray::addConstantPatch(void{*}~alpha)
```

Add the contant pointed by alpha to each element of the patch.

```
\textcolor{blue}{Fortran~}subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_

\textcolor{blue}{C++}~~~~~void~GA::GlobalArray::recip()
```

Take element-wise reciprocal of the array.

```
\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_

\textcolor{blue}{C++~}~~~~void~GA::GlobalArray::recipPatch(int~lo{[}{]},~int~hi{[}{]})
```

Take element-wise reciprocal of the patch.

```
\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_

\textcolor{blue}{C++}~~~~~void~GA::GlobalArray::elemMultiply(const~

~~~~~~~~~~~~~~~~~GA::GlobalArray~{*}~g\_a,~

~~~~~~~~~~~~~~~~~const~GA::GlobalArray~{*}~g\_b)
```

Computes the element-wise product of the two arrays which must be of the same types and same number of elements. For two-dimensional arrays,

c(i, j) = a(i,j)*b(i,j)

The result (c) may replace one of the input arrays (a/b).

```
\textcolor{blue}{Fortra}n~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

~~~~~~~~~~~~~~~ahi,~g\_b,~blo,~bhi,~g\_c,~clo,chi)~

\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_
```

```
~~~~~~~~~~~~~~~int~ahi{[}{]},~int~g\_b,~int~blo{[}{]},~int~bhi{[}{]},

~~~~~~~~~~~~~~~int~g\_c,~int~clo{[}{]},~int~chi{[}{]})~

\textcolor{blue}{C++~}~~~~void~GA::GlobalArray::elemMultiplyPatch

~~~~~~~~~~~~~~~(~const~GA::GlobalArray~{*}~g\_a,~int~alo{[}{]},~

~~~~~~~~~~~~~~~int~ahi{[}{]},~const~GA::GlobalArray~{*}~g\_b,~

~~~~~~~~~~~~~~~int~blo{[}{]},~int~bhi{[}{]},~int~clo{[}{]},~int~chi{[}{]})
```

Computes the element-wise product of the two patches which must be of the same types and same number of elements. For two-dimensional arrays,

c(i, j) = a(i,j)*b(i,j)

The result (c) may replace one of the input arrays (a/b).

```
\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_

~~~~~~~~~~~~~~~~~~~~~~g\_b,~Integer~g\_c)

\textcolor{blue}{C++}~~~~~void~GA::GlobalArray::elemDivide(const~GA::GlobalArray~{*}~

~~~~~~~~~~~~~~~~~~~~~~g\_a,~const~GA::GlobalArray~{*}~g\_b)
```

Computes the element-wise quotient of the two arrays which must be of the same types and same number of elements. For two-dimensional arrays,

c(i, j) = a(i,j)/b(i,j)

The result (c) may replace one of the input arrays (a/b). If one of the elements of array g_b is zero, the quotient for the element of g_c will be set to GA_NEGATIVE_INFINITY.

```
\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

~~~~~~~~~~~~~~~~~~ahi,~g\_b,~blo,~bhi,~g\_c,~clo,~chi)~

\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_

~~~~~~~~~~~~~~~~~~int~ahi{[}{]},~int~g\_b,~int~blo{[}{]},~int~bhi{[}{]},~

~~~~~~~~~~~~~~~~~~int~g\_c,~int~clo{[}{]},~int~chi{[}{]})~

\textcolor{blue}{C++}~~~~~void~GA::GlobalArray::elemDividePatch(~const~

~~~~~~~~~~~~~~~~~~GA::GlobalArray~{*}~g\_a,~int~alo{[}{]},~
```

```
~~~~~~~~~~~~~~~~~~int~ahi{[}{]},~const~GA::GlobalArray~{*}~g\_b,~

~~~~~~~~~~~~~~~~~~int~blo{[}{]},~int~bhi{[}{]},~int~clo{[}{]},~int~chi{[}{]})
```

Computes the element-wise quotient of the two patches which must be of the same types and same number of elements. For two-dimensional arrays,
c(i, j) = a(i,j)/b(i,j)
The result (c) may replace one of the input arrays (a/b).

```
\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_

~~~~~~~~~~~~~~~~~~Integer~g\_c)

\textcolor{blue}{C++}~~~~~void~GA::GlobalArray::elemMaximum(const~GA::GlobalArray~

~~~~~~~~~~~~~~~~~~{*}~g\_a,~const~GA::GlobalArray~{*}~g\_b)
```

Computes the element-wise maximum of the two arrays which must be of the same types and same number of elements. For two dimensional arrays,
c(i, j) = max{a(i,j), b(i,j)}
The result (c) may replace one of the input arrays (a/b).

```
\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

~~~~~~~~~~~~~~~~~~ahi,~g\_b,~blo,~bhi,~g\_c,~clo,~chi)~

\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_

~~~~~~~~~~~~~~~~~~int~ahi{[}{]},~int~g\_b,~int~blo{[}{]},~int~bhi{[}{]},~

~~~~~~~~~~~~~~~~~~int~g\_c,~int~clo{[}{]},~int~chi{[}{]})

\textcolor{blue}{C++}~~~~~void~GA::GlobalArray::elemMaximumPatch(const~

~~~~~~~~~~~~~~~~~~GA::GlobalArray~{*}~g\_a,~int~alo{[}{]},~int~ahi{[}{]},~

~~~~~~~~~~~~~~~~~~const~GA::GlobalArray~{*}~g\_b,~int~blo{[}{]},~

~~~~~~~~~~~~~~~~~~int~bhi{[}{]},~int~clo{[}{]},~int~chi{[}{]})
```

Computes the element-wise maximum of the two patches which must be of the same types and same number of elements. For two-dimensional of noncomplex arrays,
c(i, j) = max{a(i,j), b(i,j)}

If the data type is complex, then c(i, j).real = max{ |a(i,j)|, |b(i,j)|} while c(i,j).image = 0.

The result (c) may replace one of the input arrays (a/b).

```
\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_

\textcolor{blue}{C++~}~~~~void~GA::GlobalArray::elemMinimum(const~GA::GlobalArray~{*}

~~~~~~~~~~~~~~~~~g\_a,~const~GA::GlobalArray~{*}~g\_b)
```

Computes the element-wise minimum of the two arrays which must be of the same types and same number of elements. For two dimensional arrays,

c(i, j) = min{a(i,j), b(i,j)}

The result (c) may replace one of the input arrays (a/b).

```
\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

~~~~~~~~~~~~~~~~~~g\_b,~blo,~bhi,~g\_c,~clo,~chi)~

\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_

~~~~~~~~~~~~~~~~~~int~ahi{[}{]},~int~g\_b,~int~blo{[}{]},~int~bhi{[}{]},~

~~~~~~~~~~~~~~~~~~int~g\_c,~int~clo{[}{]},~int~chi{[}{]})

\textcolor{blue}{C++}~~~~~void~GA::GlobalArray::elemMinimumPatch~~

~~~~~~~~~~~~~~~~~~(const~GA::GlobalArray~{*}~g\_a,~int~alo{[}{]},~

~~~~~~~~~~~~~~~~~~int~ahi{[}{]},~const~GA::GlobalArray~{*}~g\_b,~

~~~~~~~~~~~~~~~~~~int~blo{[}{]},~int~bhi{[}{]},~int~clo{[}{]},~int~chi{[}{]})
```

Computes the element-wise minimum of the two patches which must be of the same types and same number of elements. For two-dimensional of noncomplex arrays,

c(i, j) = min{a(i,j), b(i,j)}

If the data type is complex, then

c(i, j).real = min{ |a(i,j)|, |b(i,j)|} while c(i,j).image = 0.

The result (c) may replace one of the input arrays (a/b).

```
\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_

\textcolor{blue}{C++}~~~~~void~GA::GlobalArray::shiftDiagonal(void~{*}c)
```

Adds this constant to the diagonal elements of the matrix.

```
\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_

\textcolor{blue}{C++}~~~~~void~GA::GlobalArray::setDiagonal~

~~~~~~~~~~~~~(const~GA::GlobalArray~{*}~g\_v)
```

Sets the diagonal elements of this matrix g_a with the elements of the vector g_v.

```
Fortran~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#ga_zero_diagonal}{

C~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_zero_diagonal}{GA\

C++~~~~~void~GA::GlobalArray::zeroDiagonal()
```

Sets the diagonal elements of this matrix g_a with zeros.

```
\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_

\textcolor{blue}{C++}~~~~~void~GA::GlobalArray::addDiagonal(const~

~~~~~~~~~~~~~~~~~~~GA::GlobalArray~{*}~g\_v)
```

Adds the elements of the vector g_v to the diagonal of this matrix g_a.

```
\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_

\textcolor{blue}{C++~}~~~~void~GA::GlobalArray::getDiagonal

~~~~~~~~~~~~~~~~~~~(const~GA::GlobalArray~{*}~g\_v)
```

Inserts the diagonal elements of this matrix g_a into the vector g_v.

```
\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_

\textcolor{blue}{C++}~~~~~void~GA::GlobalArray::scaleRows

~~~~~~~~~~~~~~~~~~~(const~GA::GlobalArray~{*}~g\_v)
```

Scales the rows of this matrix g_a using the vector g_v.

\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_

\textcolor{blue}{C++}~~~~~void~GA::GlobalArray::scaleCols

~~~~~~~~~~~~~~~~~~~~(const~GA::GlobalArray~{*}~g_v)

Scales the columns of this matrix g_a using the vector g_v.

\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_

\textcolor{blue}{C++}~~~~~void~GA::GlobalArray::norm1(double~{*}nm)

Computes the 1-norm of the matrix or vector g_a.

\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_

\textcolor{blue}{C++}~~~~~void~GA::GlobalArray::normInfinity(double~{*}nm)

Computes the 1-norm of the matrix or vector g_a.

\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_

\textcolor{blue}{C++}~~~~~void~GA::GlobalArray::median(const~GA::GlobalArray~

~~~~~~~~~~~~~~~~~~~~{*}~g_a,~const~GA::GlobalArray~

~~~~~~~~~~~~~~~~~~~~{*}~g_b,~const~GA::GlobalArray~{*}~g_c)

Computes the componentwise Median of three arrays `g_a`, `g_b`, and `g_c`, and stores the result in this array `g_m`. The result (m) may replace one of the input arrays (a/b/c).

\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

~~~~~~~~~~~~~~~~~~~~blo,~bhi,~g_c,~clo,~chi,~g_m,mlo,~mhi)~

\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_

~~~~~~~~~~~~~~~~~~~~int~g_b,~int~blo{[}{]},~int~bhi{[}{]},~int~g_c,~

~~~~~~~~~~~~~~~~~~~~int~clo{[}{]},~int~chi{[}{]},~int~g_m,~int~mlo{[}{]},

```
~~~~~~~~~~~~~~~~~~~~int~mhi{[}{]})~

\textcolor{blue}{C++}~~~~~void~GA::GlobalArray::medianPatch(const~GA::GlobalArray

~~~~~~~~~~~~~~~~~~~~{*}~g\_a,~int~alo{[}{]},~int~ahi{[}{]},~const~

~~~~~~~~~~~~~~~~~~~~GA::GlobalArray~{*}~g\_b,~int~blo{[}{]},~int~bhi{[}{]},~

~~~~~~~~~~~~~~~~~~~~const~GA::GlobalArray~{*}~g\_c,~int~clo{[}{]},~

~~~~~~~~~~~~~~~~~~~~int~chi{[}{]},~int~mlo{[}{]},int~mhi{[}{]})
```

Computes the componentwise Median of three patches g_a, g_b, and g_c, and stores the result in this patch g_m. The result (m) may replace one of the input patches (a/b/c).

```
\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_

\textcolor{blue}{C++~}~~~~void~GA::GlobalArray::stepMax(const~

~~~~~~~~~~~~~~~~~~~~GA::GlobalArray~{*}g\_a,~double~{*}step)
```

Calculates the largest multiple of a vector g_b that can be added to this vector g_a while keeping each element of this vector nonnegative.

```
\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_

~~~~~~~~~~~~~~~~~~~~int~g\_xxuu,~double~{*}step2)

\textcolor{blue}{C++}~~~~~void~GA::GlobalArray::stepMax2(const~GA::GlobalArray~{*}g\_vv,~

~~~~~~~~~~~~~~~~~~~~const~GA::GlobalArray~{*}g\_xxll,~

~~~~~~~~~~~~~~~~~~~~const~GA::GlobalArray~{*}g\_xxuu,~double~{*}step2)
```

Calculates the largest step size that should be used in a projected bound line search.

```
\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

~~~~~~~~~~~~~~~~~~~~bhi,~step)~

\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_
```

```
~~~~~~~~~~~~~~~~~~~~int~g\_b,~int~{*}blo,~int~{*}bhi,~double~{*}step)

\textcolor{blue}{C++}~~~~~void~GA::GlobalArray::stepMaxPatch(int~{*}alo,~

~~~~~~~~~~~~~~~~~~~~int~{*}ahi,~const~GA::GlobalArray~{*}~

~~~~~~~~~~~~~~~~~~~~g\_b,~int~{*}blo,~int~{*}bhi,~double~{*}step)
```

Calculates the largest multiple of a vector g_b that can be added to this vector g_a while keeping each element of this vector nonnegative.

```
\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

~~~~~~~~~~~~~~~~~~~~g\_vv,vvlo,~vvhi,~g\_xxll,~xxlllo,~xxllhi,~

~~~~~~~~~~~~~~~~~~~~g\_xxuu,~xxuulo,~xxuuhi,~step2)~

\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_

~~~~~~~~~~~~~~~~~~~~int~{*}xxhi,

~~~~~~~~~~~~~~~~~~~~int~g\_vv,~int~{*}vvlo,~int~{*}vvhi,~int~g\_xxll,~

~~~~~~~~~~~~~~~~~~~~int~{*}xxlllo,~int~{*}xxllhi,~int~g\_xxuu,~

~~~~~~~~~~~~~~~~~~~~int~{*}xxuulo,~int~{*}xxuuhi,~double~{*}step2)~

\textcolor{blue}{C++}~~~~~void~GA::GlobalArray::stepMax2Patch(int~{*}xxlo,~int~{*}xxhi,

~~~~~~~~~~~~~~~~~~~~const~GA::GlobalArray~{*}~g\_vv,~int~{*}vvlo,~

~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~int~{*}vvhi,~

~~~~~~~~~~~~~~~~~~~~const~GA::GlobalArray~{*}~g\_xxll,~

~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~int~{*}xxlllo,~int~{*}xxllhi,~

~~~~~~~~~~~~~~~~~~~~const~GA::GlobalArray~{*}~g\_xxuu,~int~{*}xxuulo,~

~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~int~{*}xxuuhi,~double~{*}step2)
```

Calculates the largest step size that should be used in a projected bound line search.

6.3 Interfaces to Third Party Software Packages

There are many existing software packages designed for solving engineering problems. They are specialized in one or two problem domains, such as solving linear systems, eigen-vectors, and differential equations, etc. Global Arrays provide interfaces to several of these packages.

6.3.1 Scalapack

Scalapack is a well known software library for linear algebra computations on distributed memory computers. Global Arrays uses this library to solve systems of linear equations and also to invert matrices.

The function

```
\textcolor{blue}{Fortran}~integer~function~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.

\textcolor{blue}{C}~~~~~~~int~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_s

\textcolor{blue}{C++}~~~~~int~GA::GlobalArray::solve(const~GA::GlobalArray~{*}~g\_a)
```

solves a system of linear equations *A * X = B*. It first will call the Cholesky factorization routine and, if successful, will solve the system with the Cholesky solver. If Cholesky is not able to factorizeA, then it will call the LU factorization routine and will solve the system with forward/backward substitution. On exit *B* will contain the solution *X*.

The function

```
\textcolor{blue}{Fortran}~integer~function~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.

\textcolor{blue}{C}~~~~~~~int~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_l

\textcolor{blue}{C++}~~~~~int~GA::GlobalArray::lltSolve(const~GA::GlobalArray~{*}~g\_a)
```

also solves a system of linear equations *A * X = B*, using the Cholesky factorization of an *NxN* double precision symmetric positive definite matrix *A* (handle `g_a`). On successful exit *B* will contain the solution *X*.

The function

```
\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_

\textcolor{blue}{C++}~~~~~void~GA::GlobalArray::luSolve(char~trans,~const~

~~~~~~~~~~~~~~~~~GA::GlobalArray~{*}~g\_a)
```

solves the system of linear equations *op(A)X = B* based on the LU factorization. *op(A) = A or A'* depending on the parameter `trans`. Matrix *A* is a general real

matrix. Matrix B contains possibly multiple *rhs* vectors. The array associated with the handle `g_b` is overwritten by the solution matrix X.

The function

```
\textcolor{blue}{Fortran}~integer~function~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.

\textcolor{blue}{C}~~~~~~~int~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_s

\textcolor{blue}{C++}~~~~~int~GA::GlobalArray::spdInvert()
```

computes the inverse of a double precision matrix using the Cholesky factorization of a NxN double precision symmetric positive definite matrix A stored in the global array represented by `g_a`. On successful exit, A will contain the inverse.

6.3.2 PeIGS

The PeIGS library contains subroutines for solving standard and generalized real symmetric eigensystems. All eigenvalues and eigenvectors can be computed. The library is implemented using a message-passing model and is portable across many platforms. For more information and availability send a message to fangi@ornl.gov. Global Arrays use this library to solve eigenvalue problems.

The function

```
\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_

\textcolor{blue}{C++}~~~~~void~GA::GlobalArray::diag~(const~GA::GlobalArray{*}g\_s,~

~~~~~~~~~~~~~~~~~~~const~GA::GlobalArray{*}~g\_v,~void~{*}eval)
```

solves the generalized eigenvalue problem returning all eigenvectors and values in ascending order. The input matrices are not overwritten or destroyed.

The function

```
\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_

~~~~~~~~~~~~~~~~~~~int~g\_v,void~{*}eval)~

\textcolor{blue}{C++}~~~~~void~GA::GlobalArray::diagReuse~(int~control,~const

~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~GA::GlobalArray{*}~g\_s,~~~~~

~~~~~~~~~~~~~~~~~~~const~GA::GlobalArray{*}g\_v,~void~{*}eval)
```

solves the generalized eigen-value problem returning all eigenvectors and values in ascending order. Recommended for REPEATED calls if `g_s` is unchanged.

The function

```
\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_

\textcolor{blue}{C++}~~~~~void~GA::GlobalArray::diagStd(~const~GA::GlobalArray{*}~

~~~~~~~~~~~~~~~~~~~g\_v,~void~{*}eval)
```

solves the standard (non-generalized) eigenvalue problem returning all eigenvectors and values in the ascending order. The input matrix is neither overwritten nor destroyed.

6.3.3 Interoperability with Others

Global Arrays are interoperable with several other libraries, but do not provide direct interfaces for them. For example, one can make calls to and link with these libraries:

PETSc (the Portable, Extensible Toolkit for Scientific Computation) is developed by Argonne National Laboratory. PETSc is a suite of data structures and routines for the scalable (parallel) solution of scientific applications modeled by partial differential equations. It employs the MPI standard for all message-passing communication, and is written in a data-structure-neutral manner to enable easy reuse and flexibility. Here are the instructionsfor using PETSc with GA.

CUMULVS(Collaborative User Migration User Library for Visualization and Steering) is developed by the Oak Ridge National Laboratory. CUMULVS is a software framework that enables programmers to incorporate fault-tolerance, interactive visualization and computational steering into existing parallel programs. Here are theinstructions for using CUMULVS with GA.

6.4 Synchronization Control in Collective Operations

GA collective array operations are implemented by exploiting locality information to minimize or even completely avoid interprocessor communication or data copying. Before each processor accesses its own portion of the GA data we must assure that the data is in a consistent state. That means that there are no outstanding communication operations targeting that given global array portion pending while the data owner is accessing it. To accomplish that the GA collective array operations have implicit synchronization points: at the beginning and at the end of the operation. However, in many cases when collective array operations are called back-to-back or if the user does an explicit sync just

before a collective array operation, some of the internal synchronization points could be merged or even removed if user can guarantee that the global array data is in the consistent state. The library offers a call for the user to eliminate the redundant synchronization points based on his/her knowledge of the application.

The function

```
\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_

\textcolor{blue}{C++}~~~~~void~GA::GlobalArray::maskSync(int~prior\_sync\_mask,

~~~~~~~~~~~~~~~~~int~post\_sync\_mask)
```

This operation should be used with a lot of care and only when the application code has been debugged and the user wishes to tune its performance. Making a call to this function with prior_sync_mask parameter set to false disables the synchronization done at the beginning of first collective array operation called after a call to this function. Similarly, making a call to this function by setting the post_sync_mask parameter to false disables the synchronization done at the ending of the first collective array operation called after a call to this function.

Chapter 7

Utility Operations

Global Arrays includes some utility functions to provide process, data locality, information, check the memory availability, etc. There are also several handy functions that print array distribution information, or summarize array usage information.

7.1 Locality Information

For a given global array element, or a given patch, sometimes it is necessary to find out who owns this element or patch. The function

```
\textcolor{green}{n-D}\textcolor{blue}{Fortran}~logical~function~\href{http://www.emsl.pnl.g

\textcolor{green}{2-D}\textcolor{blue}{Fortran}~logical~function~\href{http://www.emsl.pnl.g

\textcolor{blue}{C}~~~~~~~~~~int~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#g

\textcolor{blue}{C++}~~~~~~~~int~GA::GlobalArray::locate(int~subscript{[}{]})
```

tells who (process id) owns the elements defined by the array subscripts.

The function

```
\textcolor{green}{n-D}\textcolor{blue}{Fortran}~logical~function~\href{http://www.emsl.pnl.g

~~~~~~~~~~~~~~~~~~hi,~map,proclist,~np)~

\textcolor{green}{2-D}\textcolor{blue}{Fortran}~logical~function~\href{http://www.emsl.pnl.g

~~~~~~~~~~~~~~~~~~jlo,jhi,~map,~np)~

\textcolor{blue}{C}~~~~~~~~~~int~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#g

~~~~~~~~~~~~~~~~~~int~hi{[}{]},int~{*}map{[}{]},~int~procs{[}{]})~
```

```
\textcolor{blue}{C++}~~~~~~~~int~GA::GlobalArray::locateRegion(int~lo{[}{]},~

~~~~~~~~~~~~~~~~~~~int~hi{[}{]},int~{*}map{[}{]},~int~procs{[}{]})
```

returns a list of GA process IDs that 'own' the patch.

The Global Arrays support an abstraction of a distributed array object. This 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:

1. find the distribution of an array, which part of the data the calling process own
2. access the data
3. operate on the date: read/write
4. release the access to the data

The function

```
n-D\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.htm

2-D\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.htm

\textcolor{blue}{C}~~~~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#

~~~~~~~~~~~~~~~~~~~int~hi{[}{]})

\textcolor{blue}{C++}~~~~~~~~void~GA::GlobalArray::distribution(int~iproc,~

~~~~~~~~~~~~~~~~~~~int~lo{[}{]},~int~hi{[}{]})
```

finds out the range of the global array `g_a` that process `iproc` owns and `iproc` can be any valid process ID.

The function

```
\textcolor{green}{n-D}\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/doc

\textcolor{green}{2-D}\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/doc

\textcolor{blue}{C}~~~~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#

~~~~~~~~~~~~~~~~~~~void~{*}ptr,~int~ld{[}{]})~

\textcolor{blue}{C++~}~~~~~~~void~GA::GlobalArray::access(int~lo{[}{]},~int~hi{[}{]},~

~~~~~~~~~~~~~~~~~~~void~{*}ptr,~int~ld{[}{]})
```

provides access to local data in the specified patch of the array owned by the calling process. The C interface gives the pointer to the patch. The Fortran interface gives the patch address as the index (distance) from the reference address (the appropriate MA base addressing array).

The function

```
\textcolor{green}{n-D}\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/doc

\textcolor{green}{2-D}\textcolor{blue}{Fortran~}subroutine~\href{http://www.emsl.pnl.gov/doc

\textcolor{blue}{C}~~~~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#

\textcolor{blue}{C++~}~~~~~~~void~GA::GlobalArray::release(lo{[}{]},~int~hi{[}{]})
```

and

```
\textcolor{green}{n-D}\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/doc

\textcolor{green}{2-D}\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/doc

\textcolor{blue}{C}~~~~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#

\textcolor{blue}{C++~}~~~~~~~void~GA::GlobalArray::releaseUpdate(int~lo{[}{]},~int~hi{[}{]})
```

releases access to a global array. The former set is used when the data was read only and the latter set is used when the data was accessed for writing.

Global Arrays also provide a function to compare distributions of two arrays. It is

```
\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_

\textcolor{blue}{C++}~~~~~void~GA::GlobalArray::compareDistr(const~

~~~~~~~~~~~~~~~~~~GA::GlobalArray~{*}~g\_a)
```

The only method currently available for accessing the ghost cell data for global arrays that have ghost cell data is to use the `nga_access_ghosts` funtion. This function is similar to the `nga_access` function already described, except that it returns an index (pointer) to the origin of the locally held patch of global array data. This local patch includes the ghost cells so the index (pointer) will be pointing to a ghost cell. The `nga_access_ghosts` function also returns the physical dimensions of the local data patch, which includes the additional ghost cells, so it is possible to access both the visible data of the global array and the ghost cells using this information. The `nga_access_ghosts` functions have the format

```
\textcolor{blue}{n-d~Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.ht

\textcolor{blue}{C}~~~~~~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\

~~~~~~~~~~~~~~~~~~void~{*}ptr,~int~ld{[}{]}){~

\textcolor{blue}{C++~}~~~~~~~~void~GA::GlobalArray::accessGhosts(int~dims{[}{]},

~~~~~~~~~~~~~~~~~~void~{*}ptr,~int~ld{[}{]}){~
```

The array `dims` comes back with the dimensions of the local data patch, including the ghost cells, for each dimension of the global array, `ptr` is an index (pointer) identifying the beginning of the local data patch, and `ld` is any array of leading dimensions `fpr` the local data patch, which also includes the ghost cells. The array `ld` is actually redundant since the information in `ld` is also contained in `dims`, but is included to maintain continuity with other GA functions.

7.1.1 Process Information

When developing a program, one needs to use charateristics of its parallel environment: process ID, how many processes are working together and what their IDs are, and what the topology of processes look like. To answer these questions, the following functions can be used.

The function

```
\textcolor{blue}{Fortran}~integer~function~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.

\textcolor{blue}{C}~~~~~~~int~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_n

\textcolor{blue}{C++~}~~~~int~GA::GAServices::nodeid()
```

returns the GA process ID of the current process, and the function

```
\textcolor{blue}{Fortran}~integer~function~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.

\textcolor{blue}{C}~~~~~~~int~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_n

\textcolor{blue}{C++~}~~~~int~GA::GAServices::nodes()
```

tells the number of computing processes.

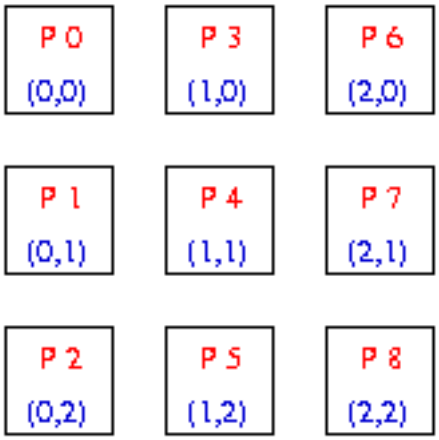
The function

```
\textcolor{blue}{Fortran~}subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_

~~~~~~~~~~~~~~~~~~int~coordinates)
```

```
\textcolor{blue}{C++~}~~~~void~GA::GlobalArray::procTopology(int~proc,~

~~~~~~~~~~~~~~~~~~int~coordinates)
```

determines the coordinates of the specified processor in the virtual processor grid corresponding to the distribution of array g_a.

Example: A global array is distributed on 9 processors. The processors are numbered from 0 to 8 as shown in the following figure. If one wants to find out the coordinates of processor 7 in the virtual processor grid, by calling the fuction `ga_proc_topology`, the coordinates of (`2,1`) will be returned.



7.1.2 Cluster Information

The following functions can be used to obtain information like number of nodes that the program is running on, node ID of the process, and other cluster information as discussed below:

The function

```
\textcolor{blue}{Fortran}~integer~function~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.

\textcolor{blue}{C}~~~~~~~int~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_c

\textcolor{blue}{C++}~~~~~int~GA::GAServices::clusterNnodes()
```

returns the total number of nodes that the program is running on. On SMP architectures, this will be less than or equal to the total number of processors.

The function

```
\textcolor{blue}{Fortran}~integer~function~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.

\textcolor{blue}{C}~~~~~~~int~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_c
```

```
\textcolor{blue}{C++}~~~~~int~GA::GAServices::clusterNodeid()
```

returns the node ID of the process. On SMP architectures with more than one processor per node, several processes may return the same node id.

The function

```
\textcolor{blue}{Fortran}~integer~function~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.

\textcolor{blue}{C}~~~~~~~int~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_c

\textcolor{blue}{C++~~~~}~int~GA::GAServices::clusterNprocs(int~inode)
```

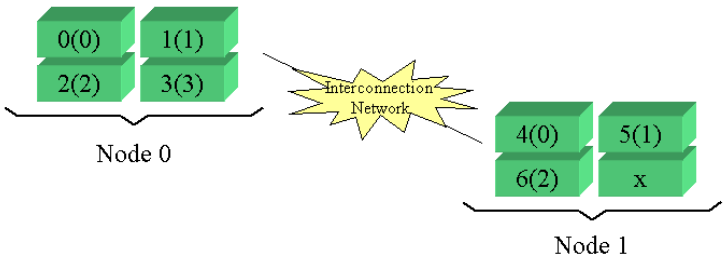
returns the number of processors available on node inode.

The function

```
\textcolor{blue}{Fortran}~integer~function~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.

\textcolor{blue}{C}~~~~~~~int~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_c

\textcolor{blue}{C++}~~~~~int~GA::GAServices::clusterProcid(int~inode,~int~iproc)
```

returns the processor id associated with node inode and the local processor id iproc. If node inode has N processors, then the value of iproc lies between 0 and N-1.

Example: 2 nodes with 4 processors each. Say, there are 7 processes created. Assume 4 processes on node 0 and 3 processes on node 1. In this case: number of nodes=2, node id is either 0 or 1 (for example, nodeid of process 2 is 0), number of processes in node 0 is 4 and node 1 is 3. The global rank of each process is shown in the figure and also the local rank (rank of the process within the node.i.e., `cluster_procid`) is shown in the parenthesis.



7.2 Memory Availability

Even though the memory management does not have to be performed directly by the user, Global Arrays provide functions to verify the memory availability. Global Arrays provide the following information:

1. How much memory has been used by the allocated global arrays.
2. How much memory is left for allocation of new the global arrays.
3. Whether the memory in global arrays comes from the Memory Allocator (MA).
4. Is there any limitation for the memory usage by the Global Arrays.

The function

```
\textcolor{blue}{Fortran~}integer~function~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.

\textcolor{blue}{C}~~~~~~~size\_t~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#

\textcolor{blue}{C++~}~~~~size\_t~GA::GAServices::inquireMemory()
```

answers the first question. It returns the amount of memory (in bytes) used in the allocated global arrays on the calling processor.

The function

```
\textcolor{blue}{Fortran}~integer~function~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.

\textcolor{blue}{C}~~~~~~~size\_t~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#

\textcolor{blue}{C++}~~~~~size\_t~GA::GAServices::memoryAvailable()
```

answers the second question. It returns the amount of memory (in bytes) left for allocation of new global arrays on the calling processor.

Memory Allocator (MA) is a library of routines that comprises a dynamic memory allocator for use by C, Fortran, or mixed-language applications. Fortran-77 applications require such a library because the language does not support dynamic memory allocation. C (and Fortran-90) applications can benefit from using MA instead of the ordinary malloc() and free() routines because of the extra features MA provides. The function

```
\textcolor{blue}{Fortran}~logical~function~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.

\textcolor{blue}{C}~~~~~~~int~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_u

\textcolor{blue}{C++}~~~~~int~GA::GAServices::usesMA()
```

tells whether the memory in Global Arrays comes from the Memory Allocator (MA) or not.

The function

```
\textcolor{blue}{Fortran}~logical~function~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.

\textcolor{blue}{C}~~~~~~~int~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_m

\textcolor{blue}{C++}~~~~~int~GA::GAServices::memoryLimited()
```

Indicates if a limit is set on memory usage in Global Arrays on the calling processor.

7.3 Message-Passing Wrappers to Reduce/Broadcast Operations

Global Arrays provide convenient operations for broadcast/reduce regardless of the message-passing library the process is running with.

The function

```
\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_

\textcolor{blue}{C++}~~~~~void~GA::GAServices::brdcst(void~{*}buf,~int~lenbuf,~int~root)
```

broadcasts from process root to all other processes a message buffer of length lenbuf.

The functions

```
\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

~~~~~~~~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#ga_igop}{ga\_{}dgo

\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_

~~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_dgop}{GA\_{}Dgop}(

\textcolor{blue}{C++}~~~~~void~GA::GAServices::igop(long~x{[}{]},~int~n,~char~{*}op)~

~~~~~~~~void~GA::GAServices::dgop(double~x{[}{]},~int~n,~char~{*}op)
```

'sum' elements of *X(1:N)* (a vector present on each process) across all nodes using the communicative operator `op`, The result is broadcasted to all nodes. Supported operations include

```
\textbf{+,~{*},~Max,~min,~Absmax,~absmin}
```

The integer version also includes the `bitwise OR` operation.

These operations unlike `ga_sync`, do not include embedded `ga_gence` operations.

7.4 Others

There are some other useful functions in Global Arrays. One group is about inquiring the array attributes. Another group is about printing the array or part of the array.

7.4.1 Inquire

A global array is represented by a handle. Given a handle, one can get the array information, such as the array name, memory used, array data type, and array dimension information, with the help of the following functions.

The functions

```
\textcolor{green}{n-D}~\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/do

\textcolor{green}{2-D}~\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/do

\textcolor{blue}{C}~~~~~~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\

~~~~~~~~~~~~~~~~~~~~{*}ndim,~int~dims{[}{]})~

\textcolor{blue}{C++}~~~~~~~~~~void~GA::GlobalArray::inquire(int~{*}type,~int~

~~~~~~~~~~~~~~~~~~~~{*}ndim,~int~dims{[}{]})
```

return the data type of the array, and also the dimensions of the array.

The function

```
\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

\textcolor{blue}{C}~~~~~~~~char{*}~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#

\textcolor{blue}{C++}~~~~~~char{*}~GA::GlobalArray::inquireName()
```

finds out the name of the array.

One can also inquire the memory being used with `ga_inquire_memory` (discussed above).

7.4.2 Print

Global arrays provide functions to print

1. content of the global array
2. content of a patch of global array
3. the status of array operations
4. a summary of allocated arrays

The function

```
\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

\textcolor{blue}{C}~~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_

\textcolor{blue}{C++}~~~~~void~GA::GlobalArray::print()
```

prints the entire array to the standard output. The output is formatted.

A utility function is provided to print data in the patch, which is

```
\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_

~~~~~~~~~~~~~~~~~~~int~hi{[}{]},~int~pretty)~

\textcolor{blue}{C++}~~~~~void~GA::GlobalArray::printPatch(int~lo{[}{]},~

~~~~~~~~~~~~~~~~~~~int~hi{[}{]},~int~pretty)
```

One can either specify a formatted output (set `pretty` to one) where the output is formatted and rows/ columns are labeled, or (set `pretty` to zero) just dump all the elements of this patch to the standard output without any formatting.

The function

```
\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_

\textcolor{blue}{C++}~~~~~void~GA::GAServices::printStats()
```

prints the global statistics information about array operations for the calling process, including

- number of calls to the GA create/duplicate, destroy, get, put, scatter, gather, and read_and_inc operations
- total amount of data moved in the GA primitive operations
- amount of data moved in GA primitive operations to logically remote locations
- maximum memory consumption in global arrays, the "high-water mark"

The function

```
\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

\textcolor{blue}{C~}~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_

\textcolor{blue}{C}~~~~~~~void~GA::GlobalArray::printDistribution()
```

prints the global array distribution. It shows mapping array data to the processes.

The function

```
\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

\textcolor{blue}{C~}~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_

\textcolor{blue}{C++}~~~~~void~GA::GAServices::summarize(int~verbose)
```

prints info about allocated arrays. verbose can be either one or zero.

7.4.3 Miscellaneous

The function

```
\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

\textcolor{blue}{C~~}~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_

\textcolor{blue}{C++}~~~~~void~GA::GlobalArray::checkHandle(char~{*}string)
```

checks if the global array handle `g_a` represents a valid array. The `string` is the message to be printed when the handle is invalid.

Chapter 8

GA++: C++ Bindings for Global Arrays

8.1 Overview

GA++ provides a C++ interface to global arrays (GA) libraries. The doxygen documentation of GA++ is located here: http://www.emsl.pnl.gov/docs/global/ga++/index.html. The GA C++ bindings are a layer built directly on top of the GA C bindings. GA++ provides new names for the C bindings of GA functions (For example, GA_Add_patch() is renamed as addPatch()).

8.2 GA++ Classes

All GA classes (GAServices, GlobalArray) are declared within the scope of GA namespace.

Namespace issue: Although namespace is part of the ANSI C++ standard, not all C++ compilers support namespaces (A non-instantiable GA class is provided for implementations using compilers without namespace). **Note**: define the variable _GA_USENAMESPACE_ as 0 in ga++.h if your compiler does not support namespaces.

```
namespace~GA~\{

~~~~~~class~GAServices;~

~~~~~~class~GlobalArray;~

\};
```

The current implementation has no derived classes (no (virtual) inheritance), templates, or exception handling. Eventually, more object oriented functionali-

ties will be added, and standard library facilities will be used without affecting the performance.

8.3 Initialization and Termination:

GA namespace has the following static functions for initialization and termination of Global Arrays.

GA::Initialize(): Initialize Global Arrays, allocates and initializes internal data structures in Global Arrays. This is a collective operation.

GA::Terminate(): Delete all active arrays and destroy internal data structures. This is a collective operation.

namespace GA { _GA_STATIC_ void Initialize(int argc, char *argv[], size_t limit = 0); _GA_STATIC_ void Initialize(int argc, char *argv[], unsigned long heapSize, unsigned long stackSize, int type, size_t limit = 0); _GA_STATIC_ void Terminate(); };

Example:

#include <iostream.h> #include "ga++.h"

int main(int argc, char **argv) { GA::Initialize(argc, argv, 0); cout << "Hello World\n"; GA::Terminate(); }

8.4 GAServices

GAServices class has member functions that does all the global operations (non-array operations) like Process Information (number of processes, process id, ..), Inter-process Synchronization (sync, lock, broadcast, reduce,..), etc,.

SERVICES Object: GA namespace has a global "SERVICES" object (of type "GAServices"), which can be used to invoke the non-array operations. To call the functions (for example, sync()), we invoke them on this SERVICES object (for example, GA::SERVICES.sync()). As this object is in the global address space, the functions can be invoked from anywhere inside the program (provided the ga++.h is included in that file/program).

8.5 Global Array

GlobalArray class has member functions that perform:

* Array operations * One-sided (get/put), * Collective array operations, * Utility operations, etc,.

Chapter 9

Mirrored Arrays

9.1 Overview

Mirrored arrays use a hybrid approach to replicate data across cluster nodes and distribute data within each node. It uses shared memory for caching latency sensitive distributed data structures on Symmetric Multi-Processor nodes of clusters connected with commodity networks as illustrated in Figure 9.1. The user is responsible for managing consistency of the data cached within the mirrored arrays. Instead of applying mirroring to all distributed arrays, the user can decide, depending on the nature of the algorithm and the communication requirements (number and size of messages), which arrays can or should use mirroring and which should be left fully distributed and accessed without the shared memory cache.

This hybrid approach is particularly useful for problems where it is important to solve a moderate sized problem many times, such as an ab initio molecular dynamics simulation of a moderate size molecule. A single calculation of the energy and forces that can be run in a few minutes may be suitable for a geometry optimization, where a few tens of calculations are required, but is still too long for a molecular dynamics trajectory, which can require tens of thousands of separate evaluations. For these problems, it is still important to push scalability to the point where single energy and force calculations can be performed on the order of seconds. Similar concerns exist for problems involving Monte Carlo sampling or sensitivity analysis where it is important to run calculations quickly so that many samples can be taken.

Mirrored arrays differ from traditional replicated data schemes in two ways. First, mirrored arrays can be used in conjunction with distributed data and there are simple operations that support conversion back and forth from mirrored to distributed arrays. This allows developers maximum flexibility in incorporating mirrored arrays into their algorithms. Second, mirrored arrays are distributed within an SMP node (see the above figure). For systems with a large number of processors per node, e.g., 32 in the current generation IBM SP, this can result

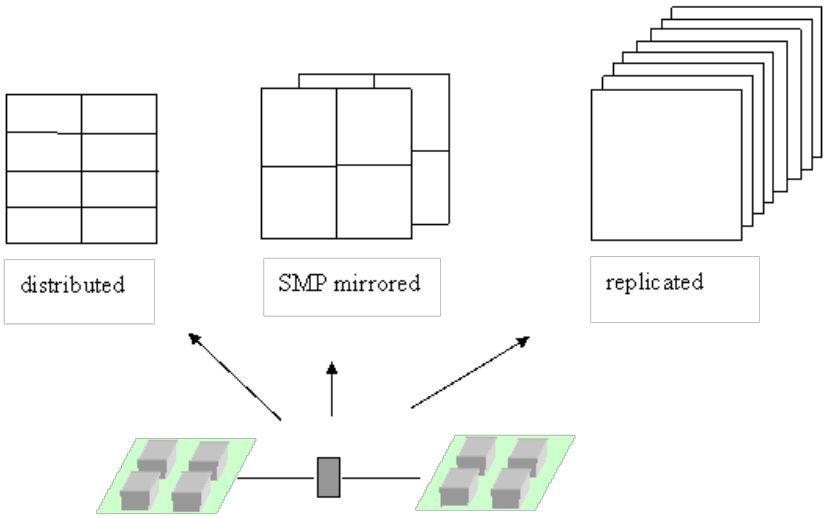


Figure 9.1: Example of a two-dimensional array fully distributed, SMP mirrored, and replicated on two 4-way SMP cluster nodes.

in significant distribution of the data. Even for systems with only 2 nodes per processor, this will result in an immediate savings of 50% over a conventional replicated data scheme.

The disadvantage of using mirrored arrays is that problems are limited in size by what can fit onto a single SMP node. This can be partially offset by the fact that almost all array operations can be supported on both mirrored and distributed arrays, so that it is easy to develop code that can switch between using mirrored arrays and conventional distributed arrays, depending on problem size and the number of available processors.

9.2 Mirrored Array Operations

Fortran~integer~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#GA_PGROUP_GET_MIRROR}

C~~~~~~~int~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#GA_PGROUP_GET_MIRROR}{

C++~~~~~int~GA::GAServices::pgroupGetMirror()

This function returns a handle to the mirrored processor list, which can then be used to create a mirrored global array using one of the NGA_Create_*_config calls.

Fortran~integer~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#GA_MERGE_MIRRORED}{ga

C~~~~~~~int~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#GA_MERGE_MIRRORED}{GA\

```
C++~~~~~int~GA::GlobalArray::mergeMirrored()
```

This subroutine merges mirrored arrays by adding the contents of each array across nodes. The result is that the each mirrored copy of the array represented by g_a is the sum of the individual arrays before the merge operation. After the merge, all mirrored arrays are equal. This is a collective operation.

```
Fortran~integer~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#GA_MERGE_DISTR_PATCH}

~~~~~~~~~~~~~~~~g\_b,~blo,~bhi)~

C~~~~~~~int~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#GA_MERGE_DISTR_PATCH}{

~~~~~~~~~~~~~~~~int~ahi{[}{]},~int~g\_b,~int~blo{[}{]},~int~bhi{[}{]})~

C++~~~~~int~GA::GlobalArray::mergeDistrPatch(int~alo{[}{]},~

~~~~~~~~~~~~~~~~int~ahi{[}{]},~int~g\_b,~int~blo{[}{]},~int~bhi{[}{]})
```

This function merges all copies of a patch of a mirrored array (g_a) into a patch in a distributed array (g_b). This is same as GA_merge_mirrored, except, this function is operated on a patch rather than the whole array. This is a collective operation.

```
Fortran~integer~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#ga_is_mirrored}{ga\_{

C~~~~~~~int~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#ga_is_mirrored}{GA\_{}

C++~~~~~int~GA::GlobalArray::isMirrored()
```

This subroutine checks if the array is mirrored array or not. Returns 1 if it is a mirrored array, else it returns 0. This is a local operation.

Chapter 10

Processor Groups

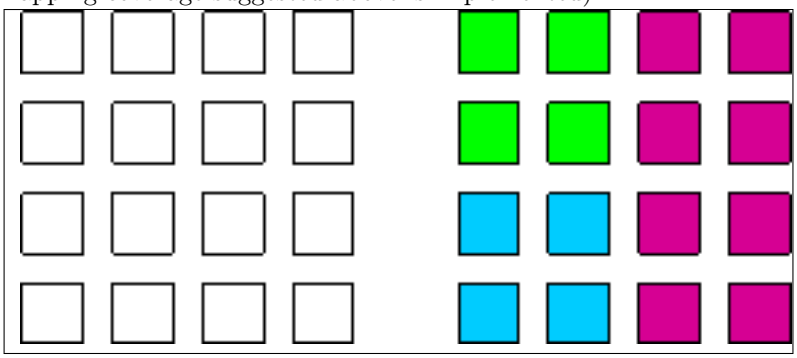
10.1 Overview

The Global Arrays toolkit has recently been extended to support global arrays defined on processor groups. The processor groups in GA programs follow the MPI approach. The MPI processor groups can be used in GA programs. However, since the MPI standard does not support fault tolerance, GA provides a set of APIs for process group managment which offers some opportunities for supporting environments with hardware faults.

In general, processor groups allow the programmer to subdivide the domain containing the complete set of processors ("the world group") into subsets of processors that can act more or less independently of one another. Global arrays that are created on processor groups are only distributed amongst the processors in the group and not on all processors in the system. Collective operations executed on specific groups are also restricted to processors in the group and do not require any action from processors outside the group. A simple example is a synchronization operation. If the synchronization operation is executed on a group that is a subgroup of the world group, then only those processors in the subgroup are blocked until completion of the synchronization operation. Processors outside the subgroup can continue their operations without interruption.

The Global Arrays toolkit contains a collection of library calls that can be used to explicitly create groups, assign specific groups to global arrays, and execute global operations on groups. There is also a mechanism for setting the "default" group for the calculation. This is a powerful way of converting large amounts of parallel code that has already been written using the Global Arrays library to run as a subroutine on a processor group. Normally, the default group for a parallel calculation is the world group, but a call is available that can be used to change the default group to something else. This call must be executed by all processors in the subgroup. Furthermore, although it is not required, it is probably a very good idea to make sure that the default groups for all processors in the system (i.e., all processors contained in the original world group) represent

a complete non-overlapping covering of the original world group (see figure). Once the default group has been set, all operations are implicitly assumed to occur on the default processor group unless explicitly stated otherwise. Global Arrays are only created on the default processor group and global operations, such as synchronizations, broadcasts, and other operations, are restricted to the default group. Inquiry functions, such as the number of nodes and the node ID, return values relative to the default processor group. Thus, a call to the ga_nodeid function will return a value of 0 for each processor designated as the zero processor within each default group. The number of processors returning 0 will be equal to the number of default groups (assuming the complete non-overlapping coverage suggested above is implemented).



Original set of 16 processors decomposed into 3 non-overlapping groups.

At present there are not many function calls that support operations between groups. The only calls that can be used to copy data from one group to another are the `nga_copy` and `nga_copy_patch` calls. These can be used to copy global arrays between two groups, provided that one group is completely contained in the other (this will always be the case if one of the groups is the world group). These commands will work correctly as long as they are executed only by processors contained in the smaller group. The `nga_put` and `nga_get` commands can also be used to communicate between Global Arrays on different groups (using an intermediate buffer), provided that the two groups share at least one processor (again, this will always be the case if one group is the world group).

The new functions included in the Global Arrays library are described below.

10.2 Creating New Groups

```
\textcolor{blue}{Fortran}~integer~function~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.

\textcolor{blue}{C}~~~~~~~int~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#GA_P
```

This call can be used to create a processor group of size `size` containing the processors in the array `list`. This call must be executed on all processors in the group. It returns an integer handle (for the processors group) that can be used to reference the processor group in other library calls.

Assigning groups:

\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#GA_

This call can be used to assign the processor group `p_handle` to a global array handle `g_a` that has been previously created using the `ga_create_handle` call. The processor group associated with a global array can also be set by creating the global array with one of the `nga_create_XXX_config` calls.

10.3 Setting the Default Group

\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#GA_

This call can be used to set the default group to something besides the world group. This call must be made on all processors contained in the group represented by `p_handle`. Once the default group has been set, all operations are restricted to the default group unless explicitly stated otherwise.

10.4 Inquiry functions

\textcolor{blue}{Fortran}~integer~function~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.

\textcolor{blue}{C}~~~~~~~int~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#GA_P

\textcolor{blue}{Fortran}~integer~function~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.

\textcolor{blue}{C}~~~~~~~int~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#GA_P

These functions can be used to access information about the group. The `ga_pgroup_nnodes` function returns the number of processors in the group specified by the handle `p_handle`, `ga_pgroup_nodeid` returns the local node ID of the processor within the group.

\textcolor{blue}{Fortran}~integer~function~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.

\textcolor{blue}{C}~~~~~~~int~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#GA_P

\textcolor{blue}{Fortran}~integer~function~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.

\textcolor{blue}{C}~~~~~~~int~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#GA_P

\textcolor{blue}{Fortran}~integer~function~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.

\textcolor{blue}{C}~~~~~~~int~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#GA_P

These functions can be used to get the handles for some standard groups at any point in the program. This is particularly useful for gaining access to the world group if the default group has been reset to a subgroup and also for gaining access to the handle for the mirror group (see section on mirrored arrays). Note that the mirror group is actually a group defined on the complete set of processors.

10.5 Collective operations on groups

\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#GA_PGP

\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

~~~~~~~~~~~~~~~~~~buf,lenbuf,root)

\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#GA_PGP

~~~~~~~~~~~~~~~~~~{*}buf,~root)

\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

~~~~~~~~~~~~~~~~~~buf,~lenbuf,~op)

\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

~~~~~~~~~~~~~~~~~~buf,~lenbuf,~op)

\textcolor{blue}{Fortran}~subroutine~\href{http://www.emsl.pnl.gov/docs/global/ga_ops.html\#

~~~~~~~~~~~~~~~~~~buf,~lenbuf,~op)

\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#GA_

~~~~~~~~~~~~~~~~~~{*}buf,~int~lenbuf,~char~{*}op)

\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#GA_

~~~~~~~~~~~~~~~~~~{*}buf,~int~lenbuf,~char~{*}op)

\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#GA_
~~~~~~~~~~~~~~~~~~

```
~~~~~~~~~~~~~~~~~~~{*}buf,~int~lenbuf,~char~{*}op)

\textcolor{blue}{C}~~~~~~~void~\href{http://www.emsl.pnl.gov/docs/global/c_nga_ops.html\#GA_

~~~~~~~~~~~~~~~~~~~{*}buf,~int~lenbuf,~char~{*}op)
```

These operations are all identical to the standard global operations, the only difference is that they have an extra argument that takes a group handle. The action of these calls is restricted to the set of processors contained in the group represented by `p_handle`. All processors in the group must call these subroutines.

Chapter 11

Sparse Data Operations

The Global Arrays Toolkit contains several subroutines designed to support operations on sparse data sets. Most sparse data objects, such as sparse matrices, are generally described using a collection of 1-dimensional arrays, so the operations discussed below are primarily focused on 1D Global Arrays. The discussion of sparse data operations will begin by describing the sparse data subroutines and then will show how they can be used by describing an algorithm for doing a sparse matrix-dense vector multiply.

```
Fortran~subroutine~ga\_patch\_enum(g\_a,~lo,~hi,~istart,~istride)~

C~~~~~~~void~GA\_Patch\_enum(int~g\_a,~int~lo,~int~hi,~

~~~~~~~~~~~~~~~~~~~~~~~~~~int~istart,~int~istride)
```

This subroutine enumerates the elements of an array between elements `lo` and `hi` starting with the value istart and incrementing each subsequent value by `istride`. This is a collective operation. Some examples of its use are shown below:

```
call~ga\_patch\_enum(g\_a,~1,~n,~1,~1)~

g\_a:~1~2~3~4~5~6~7~8~9~10~...~n

call~ga\_zero(g\_a)~

call~ga\_patch\_enum(g\_a,~5,~n,~7,~2)~

g\_a:~0~0~0~0~7~9~11~13~15~...

Fortran~subroutine~ga\_scan\_copy(g\_src,~g\_dest,~g\_mask,~lo,~hi)~

C~~~~~~~void~GA\_Scan\_copy(int~g\_src,~int~g\_dest,~int~g\_mask,~
```

```
~~~~~~~~~~~~~~~~~~~~~~~~~int~lo,~int~hi)
```

This subroutine does a segmented scan-copy of values in the source array `g_src` into a destination array `g_dest` with segments defined by values in an integer mask array `g_mask`. The scan-copy operation is only applied to the range between the `lo` and `hi` indices. The resulting destination array will contain segments of consecutive elements with the same value. This is a collective operation. An example is shown below to illustrate the behavior of this operation.

```
call~ga\_scan\_copy(g\_src,~g\_dest,~g\_mask,~1,~n)~

g\_mask:~1~0~0~0~0~1~0~1~0~0~1~0~0~0~1~1~0~

g\_src:~5~8~7~3~2~6~9~7~3~4~8~2~3~6~9~10~7~

g\_dest:~5~5~5~5~5~6~6~7~7~7~8~8~8~8~9~10~10~
```

```
Fortran~subroutine~ga\_scan\_add(g\_src,~g\_dest,~g\_mask,~lo,~hi,~excl)~

C~~~~~~~void~GA\_Scan\_add(int~g\_src,~int~g\_dest,~int~g\_mask,~

~~~~~~~~~~~~~~~~~~~~~~~~int~lo,~int~hi,~int~excl)
```

This operation will add successive elements in a source vector `g_src` and put the results in a destination vector `g_dest`. The addition will restart based on the values of the integer mask vector `g_mask`. The scan is performed within the range defined by the indices `lo` and `hi`. The excl flag determines whether the sum starts with the value in the source vector corresponding to the location of a 1 in the mask vector (`excl=0`) or whether the first value is set equal to 0 (`excl=1`). Some examples of this operation are given below.

```
call~ga\_scan\_add(g\_src,~g\_dest,~g\_mask,~1,~n,~0)~

g\_mask:~1~0~0~0~0~0~1~0~1~0~0~1~0~0~1~1~0~

g\_src:~1~2~3~4~5~6~7~8~9~10~11~12~13~14~15~16~17~

g\_dest:~1~3~6~10~15~21~7~15~9~19~30~12~25~39~15~16~33
```

```
call~ga\_scan\_add(g\_src,~g\_dest,~g\_mask,~1,~n,~1)~

g\_mask:~1~0~0~0~0~0~1~0~1~0~0~1~0~0~1~1~0~
```

```
g\_src:~1~2~3~4~5~6~7~8~9~10~11~12~13~14~15~16~17~

g\_dest:~0~1~3~6~10~15~0~7~0~9~19~0~12~25~0~0~16
```

```
Fortran~subroutine~ga\_pack(g\_src,~g\_dest,~g\_sbit,~lo,~hi,~icount)~

C~~~~~~~void~GA\_Pack(int~g\_src,~int~g\_dest,~

~~~~~~~~~~~~~~~~~~~~~int~g\_sbit,~int~lo,~int~hi,~int~icount)
```

The pack routine is designed to compress the values in the source vector `g_src` into a smaller destination array `g_dest` based on the values in an integer mask array `g_mask`. The values `lo` and `hi` denote the range of elements that should be compressed and `icount` is a variable that on output lists the number of values placed in the compressed array. This is a collective operation. An example of its use is shown below.

```
call~ga\_pack(g\_src,~g\_dest,~g\_mask,~1,~n,~icount)~

g\_mask:~1~0~0~0~0~1~0~1~0~0~1~0~0~0~1~0~0~

g\_src:~1~2~3~4~5~6~7~8~9~10~11~12~13~14~15~16~17~

g\_dest:~1~6~8~11~15~

icount:~5
```

```
Fortran~subroutine~ga\_unpack(g\_src,~g\_dest,~g\_sbit,~lo,~hi,~icount)~

C~~~~~~~void~GA\_Pack(int~g\_src,~int~g\_dest,~int~g\_sbit,~

~~~~~~~~~~~~~~~~~~~~int~lo,~int~hi,~int~icount)
```

The unpack routine is designed to expand the values in the source vector `g_src` into a larger destination array `g_dest` based on the values in an integer mask array `g_mask`. The values `lo` and `hi` denote the range of elements that should be expanded and icount is a variable that on output lists the number of values placed in the uncompressed array. This is a collective operation. An example of its use is shown below.

```
call~ga\_unpack(g\_src,~g\_dest,~g\_mask,~1,~n,~icount)~
```

```
g\_mask:~1~0~0~0~0~1~0~1~0~0~1~0~0~0~1~0~0~

g\_src:~1~6~8~11~15~

g\_dest:~1~0~0~0~0~6~0~8~0~0~11~0~0~0~15~0~0~

icount:~5
```

11.1 Sparse Matrix-Vector Multiply Example:

The utility of these subroutines in actual applications is by no means obvious so to illustrate their use, we describe a simple sparse matrix-vector multiply. The starting point of this calculation is a compressed sparse row (CSR) matrix in which only the non-zero elements are stored. The CSR storage format for an NxN matrix consists of three vectors. The first is a VALUES vector consisting of all the non-zero values contained in the matrix, the second is a J-INDEX vector that contains all the j indices of the values stored in the VALUES vector and the third vector is the I-INDEX vector that contains N+1 entries and contains the offsets in the J-INDEX vector corresponding to each row in the matrix. The last entry in I-INDEX corresponds to the total number of non-zero values in the sparse matrix. The VALUES and J-INDEX vectors should contain the same number of elements. Within each row the values are ordered by increasing values of the j index and then by increasing values of the i index. An example of a sparse matrix and its CSR representation is shown below.

```
~~~~~0~0~1~3~0

~~~~~2~0~0~0~5

~~~~~0~7~0~9~0

~~~~~3~0~4~0~5

~~~~~0~2~0~0~6
```

The CSR representation of this matrix is

```
VALUES:~1~3~2~5~7~9~3~4~5~2~6~

J-INDEX:~3~4~1~5~2~4~1~3~5~2~5~

I-INDEX:~1~3~5~7~10~12
```

Note that each value in I-INDEX corresponds to the location of the first element of the row in J-INDEX. The last element in I-INDEX equals one plust the total number of non-zero elements in the matrix and is a useful number to have available when performing sparse matrix operations. Depending on indexing

conventions, it might be more useful to set the last element equal to the number of non-zero elements.

For a very large sparse matrix, it may be necessary to distribute the CSR representation across multiple processors. This example assumes that the each of the components of the CSR matrix is stored in a 1-dimensional Global Array. To start the calculation, it is first necessary to create the distributed CSR matrix. We assume that it is possible to assign the evaluation of individual rows to individual processors. A simple way of starting is to divide up the number of rows evenly between processors and have each processor evaluate all elements of the rows assigned to it. These can then be stored in a local CSR format. In this case, the I-INDEX vector contains only the number of rows assigned to the processor. In the example shown above, assume that the matrix is divided between three processors and that processes 0 and 1 have two rows each and process 2 has one row. The layout on the three processes looks like

```
Process~0~

VALUES:~1~3~2~5~

J-INDEX:~3~4~1~5~

I-INDEX:~1~3~

INC:~2~2


Process~1~

VALUES:~7~9~3~4~5~

J-INDEX:~2~4~1~3~5~

I-INDEX:~1~3~

INC:~2~3


Process~2~

VALUES:~2~6~

J-INDEX:~2~5~

I-INDEX:~1~
```

```
INC:~2~
```

The local array INC contains the number of non-zero elements in each row. The total number of non-zero elements in the matrix can be found by summing the number of non-zero values on each process. This value can then be used to create distributed VALUES and J-INDEX arrays containing the complete CSR matrix. A distributed I-INDEX array can be constructed from knowledge of the original matrix dimension N. In addition to Global Arrays representing distributed versions of VALUES, J-INDEX, and I-INDEX, an integer Global Array of length N+1 called SBIT is also needed. This array is initialized so that the first element is 1 and the remaining elements are all zero. To create the distributed array I-INDEX a temporary Global Array of length N+1 is created. The following code fragment illustrates the construction of I-INDEX

```
lo~=~imin~+~1~\textcolor{blue}{!~imin~is~lower~index~of~i~values~on~}

\textcolor{blue}{{}~~~~~~~~~~~~~~!~this~processor~}

hi~=~imax~+~1~\textcolor{blue}{!~imax~is~upper~index~of~i~values~on~}

\textcolor{blue}{{}~~~~~~~~~~~~~~!~this~processor~}

if~(me.eq.0)~then~

~~~call~nga\_put(g\_tmp,~one,~one,~one,~one)~

endif~

call~nga\_put(g\_tmp,~lo,~hi,~inc,~one)~

call~ga\_sync~isize~=~n~+~1~

call~ga\_scan\_add(g\_tmp,g\_i\_index,~g\_sbit,~isize,~0)
```

The variable ONE is an integer variable set equal to 1. This code fragment results in a distributed array containing the elements of I-INDEX as described above. Note that the N+1 element in `g_i_index` is equal to one plus the total number of non-zero elements. The SBIT and TMP arrays can now be destroyed as they are no longer needed.

To execute the actual sparse matrix-vector multiply, it is necessary to have a second bit array MASK whose length is equal to the number of non-zero elements in the sparse matrix and which has unit values at the locations corresponding to the start of each row in the CSR and zeros everywhere else. This can be constructed from the I-INDEX array in a fairly straightforward way using the `nga_scatter` routine. The code fragment for constructing this is

```
call~ga\_zero(g\_mask)~
```

```
call~nga\_distribution(g\_i\_index,~me,~lo,~hi)~

call~nga\_access(g\_i\_index,~lo,~hi,~idx,~ld)~

ntot~=~hi~\textendash{}~lo~+~1~if~(me.eq.ga\_nnodes()-1)~then~

ntot~=~ntot~\textendash{}~1~

endif~

do~i~=~1,~ntot~

~~ones(i)~=~1~

end~do~

call~nga\_scatter(g\_mask,~ones,~int\_mb(idx),~ntot)~

call~nga\_release(g\_i\_index,~lo,~hi)
```

This code will create an appropriate mask array with 1's corresponding to the start of each row in the VALUES and J-INDEX arrays. The last element in the I-INDEX array contains the total number of non-zero elements and does not correspond to an offset location, hence the value of NTOT is decreased by 1 for the last processor.

Finally, the remaining task is to copy the values of the j indices and the matrix values from the local arrays into the corresponding Global Arrays. The code fragment for this is

```
call~nga\_get(g\_i\_index,~imin,~imin,~jmin,~one)~

call~nga\_get(g\_i\_index,~imax+1,~imax+1,~jmax,~one)~

jmax~=~jmax~\textendash{}~1~

call~nga\_put(g\_j\_index,~jmin,~jmax,~jvalues,~one)~

call~nga\_put(g\_values,~jmin,~jmax,~values,~one)
```

The value of `jmax` is decreased by 1 since this represents the start of the `imax+1` row. The value for the last row works out correctly since we defined the N+1 element of I-INDEX to equal one plus the total number of non-zero elements in the sparse matrix. At this point the matrix is completely stored in a set of distributed vectors representing a CSR storage format. An additional distributed integer vector representing the bit mask for this matrix has also been created.

Having created a distributed sparse matrix in CSR format, the next step is to construct a sparse matrix-dense vector multiply. This operation is outlined

schematically in Figure 11.1. The original sparse matrix-dense vector multiply is shown in Figure 11.1(a). The first step, shown in Figure 11.1(b) is to express the dense vector as a sparse matrix with the same pattern of non-zero entries as the sparse matrix. Each row in this new matrix represents a copy of the original vector, except that only the values corresponding to the non-zero values of the original matrix are retained. The third step is to multiply the two matrices together element-wise to get a new sparse matrix with the same pattern of non-zero entries as the original sparse matrix. This is shown in Figure 11.1(c). The final step, shown in Figure 11.1(d), is to sum across the rows in the product matrix to get the values of the product vector.

The use of Global Array operations in implementing this operation is described in more detail below. The original dense vector and final product vector are assumed to be located in distributed 1D Global Arrays with handles `g_b` and `g_c`, respectively. The first step in performing the multiply operation is to create a 1D Global Array that is the same size as the original compressed matrix VALUES array and has the same distribution across processors. Denoting the handle of this array as `g_tmp`, it can be filled with the following sequence of operations

```
call~nga\_distribution(g\_j\_index,~me,~lo,~hi)~

call~nga\_access(g\_j\_index,~lo,~hi,~idx,~ld)~

call~nga\_access(g\_tmp,~lo,~hi,~id\_tmp,~ld)~

ld~=~hi~\textendash{}~lo~+~1~

call~nga\_gather(g\_b,~dbl\_mb(id\_tmp),int\_mb(idx),ld)~

call~nga\_release(g\_j\_index,~lo,~hi)~

call~nga\_release(g\_tmp,lo,hi)
```

The first three lines find the location in memory of the local portions of the J-VALUES vector and the `g_tmp` array. These should both correspond to the same values of `lo` and `hi`. The `nga_gather` operation then copies the values of `g_b` in the locations pointed to by the `j` values represented by the index `idx` into the corresponding locations of the local portion of `g_tmp`. The remaining lines release access to the local data. Although this operation can be expressed in only a few lines of code, it is quite complicated in terms of how it manipulates data and may be worth spending some additional time to understand how it works.

The element-wise multiplication of the `g_tmp` and `g_values` arrays can be trivially implemented with a single call to `ga_elem_multiply`(`g_tmp`, `g_values`, `g_tmp`). Similarly, the sum across rows in the `g_tmp` array can be accomplished by calling `ga_scan_add`(`g_tmp`, `g_values`, `g_mask`, `one`, `ntot`, `0`), where `ntot` is the total number of non-zero elements. At this point the values of the product

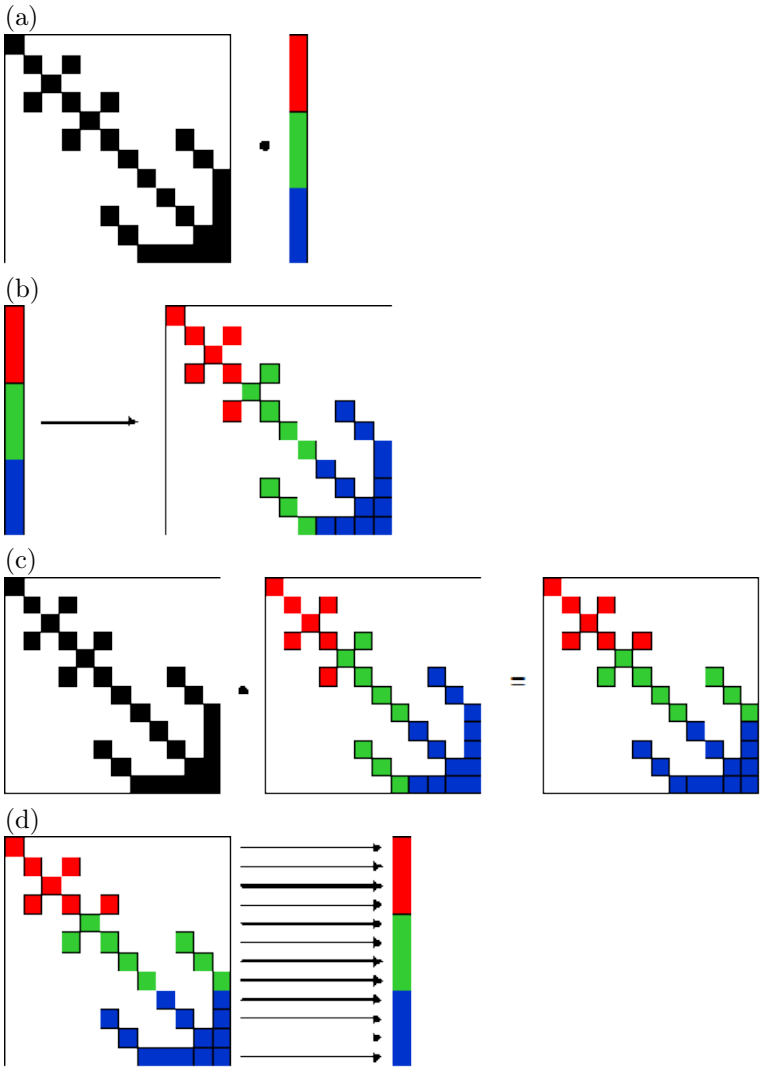


Figure 11.1: Schematic representation of a numerical sparse matrix-dense vector multiply.

vector are located at the elements just before the locations indicated by the g_mask array. To get these values back into an ordinary compressed vector, the g_mask vector is shifted to the left by one place, using the following code fragment

```
call~nga\_distribution~(g\_mask,~me,~lo,~hi)~

call~nga\_access(g\_mask,~lo,~hi,~idx,~ld)~

ld~=~hi-lo~

isav~=~int\_mb(idx)~

do~i~=~1,~ld~

~~~int\_mb(idx~+~i~\textendash{}~1)~=~int\_mb(idx~+~i)~

end~do~

if~(lo.eq.1)~then~

~~~ldx~=~isize~

else~

~~~idx~=~lo-1~

endif~call~

nga\_release(g\_mask,~lo,~hi)~

call~ga\_sync~

call~nga\_put(g\_mask,~idx,~idx,~isav,~ld)~

call~g\_sync
```

The results in `g_tmp` can now be packed into the final results vector `g_c` using a single call to `ga_pack`(`t_tmp`, `g_c`, `g_mask`, `one`, `ntot`, `icnt`).

Chapter 12

Restricted Arrays

12.1 Overview

The restricted arrays functionality is designed to provide users with further options for how data is distributed among processors by allowing them to reduce the total number of processors that actually have data and also by allowing users to remap which data blocks go to which processors. There are two calls that allow users to create restricted arrays; both must be used with the new interface for creating arrays. This requires that users must first create an array handle using the `ga_create_handle` call and then apply properties to the handle using different ga_set calls. The two calls that allow users to create restricted arrays are `ga_set_restricted` and `ga_set_restricted_range`. The first call is more general, the second is a convenience call that allows users to create restricted arrays on a contiguous set of processors.

Both calls allow users to restrict the data in a global array to a subset of available processors. The set ga_set_restricted call has two arguments, `nproc`, and an array `list` of size `nproc`. Nproc represents the number of processors that are supposed to contain data and list is an array of the processor IDs that contain data. For the array shown in Figure 12.1, the problem is run on 36 processors but for nproc=4 and list=[8,9,15,21] only the processors shown in the figure will have data. The array will be decomposed assuming that it is distributed amongst only 4 processors so it will be broken up using either a 2x2, 1x4, or 4x1 decomposition. The block that would normally be mapped to process 0 in a 4 processor decomposition will go to process 8, the data that would map to process 1 will go to process 9, etc. This functionality can be used to create global arrays that have data limited to a small set of processors but which are visible to all processors.

The restricted array capability can also be used to alter the default distribution of data. This is ordinarily done in a column major way on the processor grid so that a global array created on 16 processors that has been decomposed into a 4x4 grid of data blocks would have data mapped out as shown in Fig-

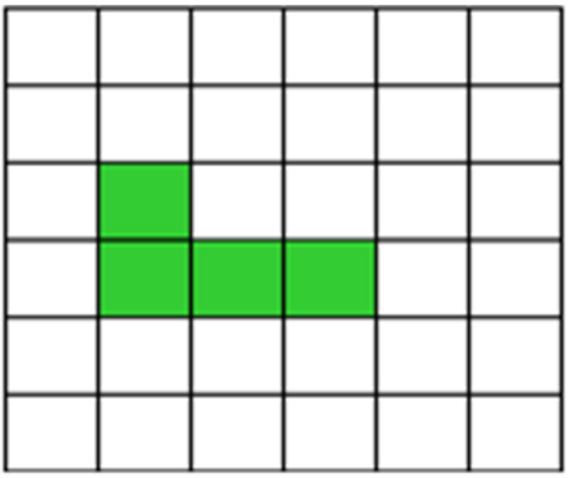


Figure 12.1: A global array distributed on 36 processors. If nproc=4 and list = [8,9,15,21] then only the shaded processor will contain data. The array will be decomposed into 4 blocks.

ure 12.2. The first column of blocks is assigned to processes 0-3, the second to processes 4-7, etc.

Figure 12.3 shows an alternative distribution that could be achieved using restricted arrays and setting the list array to [0,1,4,5,2,3,6,7,8,9,12,13,10,11,14,15]. This distribution might but useful for reducing intranode communication for multiprocessor nodes

12.2 Restricted Arrays Operations

```
\textcolor{blue}{Fortran}~subroutine~ga\_set\_restricted(g\_a,~list,~nproc)~

\textcolor{blue}{C~}~~~~~~void~GA\_Set\_restricted(int~g\_a,~int~list{[}{]},~int~nproc)~

\textcolor{blue}{C++}~~~~~GA::GlobalArray::setRestricted(int~list{[}{]},~int~nproc)~const
```

This subroutine restricts data in the global array `g_a` to only the `nproc` processors listed in the array list. The value of `nproc` must be less than or equal to the number of available processors. If this call is used in conjunction with `ga_set_irreg_distr`, then the decomposition in the `ga_set_irreg_distr` call must be done assuming the number of processors used in the `ga_set_restricted` call. The data that would ordinarily get mapped to process 0 in an `nproc` distribution will get mapped to the processor in `list[0]`, the data that would be mapped to process 1 will get mapped to `list[1]`, etc. This can be used to restructure the data layout in a global array even if the value of `nproc` equals the total number of processors available.

Figure 12.2: Standard data distribution for a global array created on 16 processors and decomposed into a 4x4 grid of data blocks.

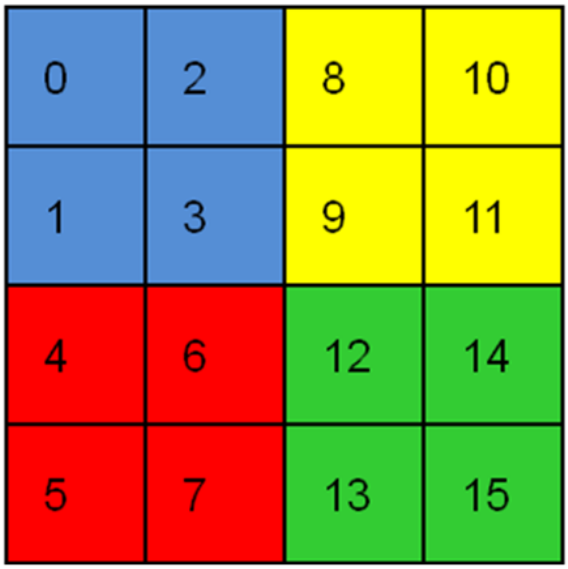


Figure 12.3: An alternative distribution that could be achieved using restricted arrays. An array on 16 processors decomposed into a 4x4 grid of data blocks.

```
\textcolor{blue}{Fortran}~subroutine~ga\_set\_restricted\_range(g\_a,~list,~nproc)~

\textcolor{blue}{C}~~~~~~~void~GA\_Set\_restricted\_range(int~g\_a,~int~lo\_proc,~

~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~int~hi\_proc)~

\textcolor{blue}{C++~}~~~~GA::GlobalArray::setRestrictedRange(int~lo\_proc,~

~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~int~hi\_proc)~const
```

This subroutine restricts data in the global array `g_a` to the processors beginning with `lo_proc` and ending with `hi_proc`. Both `lo_proc` and `hi_proc` must be less than or equal to the total number of processors available minus one (e.g., in the range `[0,N-1]` where N is the total number of processors) and `lo_proc` must be less than or equal to `hi_proc`. If `lo_proc=0` and `hi_proc=N-1` then this command has no effect on the data distribution. This call is equivalent to using the `ga_set_restricted` call where `nprocs = hi_proc-lo_proc+1` and the array `list` contains the processors `[lo_proc, hi_proc]` in consecutive order.

Appendix A

List of C Functions

TODO

Appendix B

List of Fortran Functions

TODO

Appendix C

Global Arrays on Older Systems

Global Arrays supports many computing platforms. This appendix discusses those platforms, including older systems.

The web page `www.emsl.pnl.gov/docs/global/support.html` contains updated information about using GA on different platforms. Please refer to this page frequently for most recent updates and platform information.

C.1 Platform and Library Dependencies

The following platforms are supported by Global Arrays.

C.2 Supported Platforms

- IBM SP, CRAY T3E/J90/SV1, SGI Origin, Fujitsu VX/VPP, Hitachi
- Cluster of workstations: Solaris, IRIX, AIX, HPUX, Digital/Tru64 Unix, Linux, NT
- Standalone uni- or multi-processor workstations or servers
- Standalone uni- or multi-processor Windows NT workstations or servers

Older versions of GA supported some additional (now obsolete) platforms such as: IPSC, KSR, PARAGON, DELTA, CONVEX. They are not supported in the newer (>3.1) versions because we do not have access to these systems. We recommend using GA 2.4 on these platforms.

For most of the platforms, there are two versions available: 32-bit and 64-bit. This table specifies valid TARGET names for various supported platforms.

Platform	32-bit TARGET name	64-bit TARGET name	Remarks
Sun Ultra	SOLARIS	SOLARIS64	64-bit version added in GA 3.1
IBM BlueGene/P		BGP	supported in GA 4.1 and later (Contact your BlueGene sys admin for GA instalation). More info in support page...
IBM BlueGene/L		BGL	added in GA 4.0.2 (Contact your BlueGene sys admin for GA instalation). More info in support page...
Cray XT3/XT4		LINUX64 (or) CATAMOUNT	TARGET based on the OS in compute Nodes (Catamount/Linux). More info and sample settings in support page...
IBM RS/6000	IBM	IBM64	64-bit version added in GA 3.1
IBM SP	LAPI	LAPI64	no support yet for user-space communication in the 64-bit mode by IBM
Compaq/DEC alpha	not available	DECOSF	
HP pa-risc	HPUX	HPUX64	64-bit version added in GA 3.1
Linux (32-bit): x86, ultra, powerpc	LINUX	not available	
Linux (64-bit): ia64 (Itanium), x86_64 (Opteron), ppc64, etc	not available	LINUX64	

Platform	32-bit TARGET name	64-bit TARGET name	Remarks
Linux alpha	not available	LINUX64	64-bit version added in GA 3.1; Compaq compilers rather than GNU required
Cray T3E	not available	CRAY-T3E	
Cray J90	not available	CRAY-YMP	
Cray SV1	not available	CRAY-SV1	
Cray X1	not available	CRAY-SV2	In X1, by default, TARGET is defined by the operating system as cray-sv2
SGI IRIX mips	SGI_N32, SGI	SGIFP	
Hitachi SR8000	HITACHI	not available	
Fujitsu VPP systems	FUJITSU-VPP	FUJITSU-VPP64	64-bit version added in GA 3.
NEC SX series		NEC	
Apple	MACX	MACX64	Running MAC X or higher

To aid development of fully portable applications, in 64-bit mode Fortran integer datatype is 64-bits. It is motivated by 1) the need of applications to use very large data structures and 2) Fortran INTEGER*8 not being fully portable. The 64-bit representation of integer datatype is accomplished by using the appropriate Fortran compiler flag.

Because of limited interest in heterogenous computing among known GA users, the Global Arrays library *still does not support heterogeonous platforms.* This capability can be added if required by new applications.

C.3 Selection of the communication network for ARMCI

Some cluster installations can be equipped with a high performance network which offer instead, or in addition to TCP/IP some special communication protocol, for example GM on Myrinet network. To achieve high performance in Global Arrays, ARMCI must be built to use these protocols in its implementation of one-sided communication. Starting with GA 3.1, this is accomplished by setting an environment variable ARMCI_NETWORK to specify the protocol to be used. In addition, the it might be necessary to provide location for the header files and library path corresponding to location of s/w supporting the appropriate protocol API, see g/armci/config/makecoms.h for details.

Network	Protocol Name	ARMCI_NETWORK Setting	Supported Platforms
Ethernet	TCP/IP	SOCKETS (optional/default)	workstation clusters (32 and 64-bit)
Quadrics/QsNet	Elan3/Shmem	QUADRICS or ELAN3	Linux (alpha,x86,IA64,..), Compaq
Quadrics/QsNet II	Elan4	ELAN4	Linux (32 and 64-bit)
Infiniband	OpenIB	OPENIB	Linux (32 and 64-bit). NOTE: This network is supported in GA versions>=4.1. For more info see the Support page...
Infiniband	VAPI	MELLANOX	Linux (32 and 64-bit)
Myrinet	GM	GM	Linux (x86,ultra,IA64)
Giganet cLAN	VIA	VIA	Linux (32 and 64-bit)
	MPI	MPI-SPAWN	Supported in GA 4.1 or higher. This network setting can be used on any platform that has MPI-2 dynamic process management support. Using this setting is recommended only if your network is not listed above.

Other Platforms: (More settings info for these platforms in theSupport page)

Platforms	Protocol Name	ARMCI_NETWORK Setting
IBM BG/L	BGML	BGMLMPI
Cray XT3/XT4	Shmem Portals	CRAY-SHMEM PORTALS 2.1.3

C.4 Selection of the message-passing library

As explained in Section 3, GA works with either MPI or TCGMSG message-passing libraries. That means that GA applications can use either of these

interfaces. Selection of the message-passing library takes place when GA is built. Since the TCGMSG library is small and compiles fast, it is included with the GA distribution package and built on Unix workstations by default so that the package can be built as fast and as conveniently to the user as possible. There are three possible configurations for running GA with the message-passing libraries:

1. GA with MPI (*recommended*): directly with MPI. In this mode, GA program should contain MPI initialization calls.

2. GA with TCGMSG-MPI (MPI and TCGMSG emulation library): TCGMSG-MPI implements functionality of TCGMSG using MPI. In this mode, the message passing library is initialized using a TCGMSG PBEGIN(F) call which internally references MPI_Initialize. To enable this mode, define the environmental variable USE_MPI.

3. GA with TCGMSG: directly with TCGMSG. In this mode, GA program should contain TCGMSG initialization calls.

For the MPI versions, the optional environmental variables MPI_LIB and MPI_INCLUDE are used to point to the location of the MPI library and include directories if they are not in the standard system location(s). GA programs are started with the mechanism that any other MPI programs use on the given platform.

The recent versions of MPICH (an MPI implementation from ANL/Mississippi State) keep the MPI header files in more than one directory and provide compiler wrappers that implicitly point to the appropriate header files. One can :

- use MPI_INCLUDE by expanding the string with another directory component prefixed with "-I" (you are passing include directory names as a part of compiler flags), or (starting with GA 3.1) separated by comma "," and withot the prefix, OR

- use MPI aware compiler wrappers e.g., mpicc and mpif77 to build GA right out of the box on UNIX workstations:

```
make~FC=mpif77~CC=mpicc~
```

One disadvantage of the second approach it that GA makefile in some circumstances might be not able to determine which compiler (e.g., GNU or PGI) is called underneath by the MPICH compiler wrappers. Since different compilers provide different Fortran/C interface, the package might fail to build. This problem is most likely to occur on non-Linux Unix systems with non-native compilers (e.g., gcc).

On Windows NT, the current version of GA was tested with WMPI, an NT implementation derived from MPICH in Portugal.

C.5 Dependencies on other software

In addition to the message-passing library, GA requires:

- MAMA (Memory Allocator), a library for managment of local memory;
- ARMCI, a one-sided communication library that GA uses as its run-time system;
- BLAS library is required for the eigensolver and ga_dgemm;
- LAPACK library is required for the eigensolver (a subset is included with GA, which is built into *liblinalg.a*);

GA may also depend on other software depending on the functions being used.

- GA eigensolver, ga_diag, is a wrapper for the eigensolver from the PEIGS library; (Please contact George Fannabout PEIGS)
- SCALAPACK, PBBLAS, and BLACS libraries are required for *ga_ lu_ solve, ga_ cholesky, ga_ llt_ solve, ga_ spd_ invert, ga_ solve*. If these libraries are not installed, the named operations will not be available.
- If one would like to generate trace information for GA calls, an additional library *libtrace.a* is required, and the -DGA_TRACE define flag should be specified for C and Fortran compilers.

C.6 Writing GA Programs

C programs that use Global Arrays should include files *'global.h', 'ga.h', 'macdecls.h'*. Fortran programs should include the files *'mafdecls.fh', 'global.fh'*. Fortran source must be preprocessed as a part of compilation.

The GA program should look like:

- When GA runs with MPI

```
\textcolor{blue}{Fortran~}~~~~~~~~~~~~~~~\textcolor{green}{C}

\textcolor{blue}{call~mpi\_init(..)~}~~~\textcolor{green}{MPI\_Init(..)~}~~~!~start~MPI~

\textcolor{blue}{call~ga\_initialize()}~\textcolor{green}{GA\_Initialize()~}!~start~global~a

\textcolor{blue}{status~=~ma\_init(..)}~\textcolor{green}{MA\_Init(..)~}~~~~!~start~memory~a

\textcolor{blue}{....~do~work~~}~~~~~~~\textcolor{green}{....~do~work}

\textcolor{blue}{call~ga\_terminate()}~~\textcolor{green}{GA\_Terminate()~}~!~tidy~up~global

\textcolor{blue}{mpi\_finalize()}~~~~~~~\textcolor{green}{MPI\_Finalize()}~~!~tidy~up~MPI~~
```

```
\textcolor{blue}{stop}~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~!~exit~program
```

- When GA runs with TCGMSG or TCGMSG-MPI

```
\textcolor{blue}{Fortran~C}

\textcolor{blue}{call~pbeginf()~}~~~~~~~~\textcolor{green}{PBEGIN\_(..)~}~~~~!~start~TCGMSG~

\textcolor{blue}{call~ga\_initialize()}~~~\textcolor{green}{GA\_Initialize()}~!~start~global

\textcolor{blue}{status~=~ma\_init(..)}~~~\textcolor{green}{MA\_Init(..)}~~~~~!~start~memory

\textcolor{blue}{....~do~work~}~~~~~~~~~~~\textcolor{green}{....~do~work}

\textcolor{blue}{call~ga\_terminate()}~~~~\textcolor{green}{GA\_Terminate()~}~!~tidy~up~glob

\textcolor{blue}{call~pend()}~~~~~~~~~~~~\textcolor{green}{PEND\_()}~~~~~~~~~!~tidy~up~tcgms

\textcolor{blue}{stop~}~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~!~exit~program~
```

The *ma_init* call looks like :

```
status~=~ma\_init(type,~stack\_size,~heap\_size)
```

and it basically just goes to the OS and gets *stack_size+heap_size* elements of size type. The amount of memory MA allocates need to be sufficient for storing global arrays on some platforms. Please refer to section 3.2 for the details and information on more advanced usage of MA in GA programs.

C.7 Building GA

Use *GNU make* to build the GA library and application programs on Unix and Microsoft nmake on Windows. The structure of the available makefiles are

- GNUmakefile: Unix makefile
- MakeFile: Windows NT makefile
- config/makefile.h: definitions & include symbols

The user must specify TARGET as an environment variable (setenv TARGET TARGET_name) or in the GNUmakefile or on the command line when calling make. For example:
(for IBM/SP platform)

```
setenv~TARGET~LAPI~
```

(or) from the command line,

```
gmake~TARGET=LAPI
```

Valid TARGET_name for various supported platforms can be found in the above table. Valid TARGETs can also be listed by calling make in the top level distribution directory on UNIX family of systems when TARGET is not defined. On Windows, WIN32, CYGNUS and INTERIX (previously known as OpenNT) are supported.

Compiler Settings (optional): For various supported platforms, the default compilers and compiler options are specified in config/makefile.h. One could change the predefined default compilers and compiler flags in GA package either by specifying them on the command line or in the file config/makefile.h. Note: editing config/makefile.h for any platform requires extra care and is intended for intermediate/advanced users.

- CC - name of the C compiler (e.g., gcc, cc, or ccc)
- FC - name of the Fortran compiler (e.g., g77, f90, mpif77 or fort)
- COPT - optimization or debug flags for the C compiler (e.g., -g, -O3)
- FOPT - optimization or debug flags for the Fortran compiler (e.g., -g, -O1)

For example,

```
gmake~FC=f90~CC=cc~FOPT=-O4~COPT=-g
```

Note that GA provides only Fortran-77 interfaces. To use and compile with a Fortran 90 compiler, it has to support a subset of Fortran-77.

C.7.1 Unix Environment

As mentioned in an earlier section, there are three possible configurations for building GA.

1. GA with MPI (recommended): To build GA directly with MPI, the user needs to define environmental variables MPI_LIB and MPI_INCLUDE which should point to the location of the MPI library and include directories. Additionally, the make/environmental variable MSG_COMMS must be defined as MSG_COMMS = MPI. (In csh/tcsh, setenv MSG_COMMS MPI)

2. GA with TCGMSG-MPI: To build GA with the TCGMSG-MPI, user needs to define environmental variables USE_MPI, MPI_LIB and MPI_INCLUDE which should point to the location of the MPI library and include directories.

   Example: using csh/tcsh (assume using MPICH installed in /usr/local on IBM workstation)

```
setenv~USE\_MPI~y~

setenv~MPI\_LOC~/usr/local/mpich~

setenv~MPI\_LIB~\$MPI\_LOC/lib/rs6000/ch\_shmem~

setenv~MPI\_INCLUDE~\$MPI\_LOC/include
```

3. GA with TCGMSG: To build GA directly with TCGMSG, the user must define the environmental variable MSG_COMMS=TCGMSG. Note: When MSG_COMMS=TCGMSG, make sure to unset the environment variable USE_MPI (e.g. unsetenv USE_MPI).

After chosing the configuration, to build the GA library, type

```
make~
```

or

```
gmake
```

If the build is successful, a test program test.x will be created in global/testing directory. Refer to the Section "Running GA programs" on how to run this test.

To build an application based on GA located in g/global/testing, for example, the application's name is app.c (or app.F, app.f), type

```
make~app.x~
```

or

```
gmake~app.x
```

Please refer to compiler flags in file g/config/makefile.h to make sure that Fortran and C compiler flags are consistent with flags uses to compile your application. This may be critical when Fortran compiler flags are used to change the default length of the integer datatype.

Interface to ScaLAPACK GA interface routines to ScaLAPACK are only available, when GA is build with MPI and ScaLAPACK. Before building GA, the user is required to define the environment variables USE_SCALAPACK or USE_SCALAPACK_I8 (for scalapack libraries compiled with 8-byte integers), and the location of ScaLAPACK & Co. libraries in the env variable SCALAPACK.

Example: using csh/tcsh

```
setenv~USE\_SCALAPACK~y~(or)~setenv~USE\_SCALAPACK\_I8~y~

setenv~SCALAPACK~'-L/msrc/proj/scalapack/LIB/rs6000~
```

```
~~~~~~~-lscalapack~-lpblas~-ltools~-lblacsF77cinit~-lblacs'~

setenv~USE\_MPI~y
```

Since there are certain interdependencies between blacs and blacsF77cinit, some system might require specification of -lblacs twice to fix the unresolved external symbols from these libs.

Installing GA C++ Bindings By default, GA C++ bindings are not built. GA++ is built only if GA_C_CORE is defined as follows:

```
setenv~GA\_C\_CORE~y~

cd~GA\_HOME~

make~clean;~make~
```

(This will build GA with C core and C++ binding).

Using GA_C_CORE GA's internal core is implemented using Fortran and C. When GA_C_CORE is set, core Fortran functionalites are replaced by their C counterparts to eliminate the hassle involved in mixing Fortran and C with C++ bindings on certain platforms or for some compilers (like, missing Fortran symols/libraries during the linking phase). NOTE: C and C++ compilers should be from the same family. GA_C_CORE doesnot support mixing C and C++ compilers (e.g.using Intel compiler for C and GNU compiler for C++).

```
make~FC=ifort~CC=icc~CXX=g++~(not~supported~if~GA\_C\_CORE~is~set)~

make~FC=ifort~CC=icc~CXX=icpc~(Intel~compiler~family~-~supported)
```

C.7.2 Windows NT

To buid GA on Windows NT, MS Power Fortran 4 or DEC Visual Fortran 5 or later, and MS Visual C 4 or later are needed. Other compilers might need the default compilation flags modified. When commercial Windows compilers are not available, one can choose to use CYGNUS or INTERIX and build it as any other Unix box using GNU compilers.

First of all, one needs to set environment variables (same as in Unix enviroment). GA needs to know where find the MPI include files and libraries. To do this, select the Environment tab under the Control Panel, then set the variables to point to the location of MPI, for example for WMPI on disk D:

```
set~MPI\_INCLUDE~as~d:\textbackslash{}Wmpi\textbackslash{}Include~

set~MPI\_LIB~as~d:\textbackslash{}Wmpi\textbackslash{}Console
```

Make sure that the dynamic link libraries required by the particular implementation of MPI are copied to the appropriate location for the system DLLs. For WMPI, copy VWMPI.dll to \winnt.

In the top directory do,

```
nmake
```

The GA test.exe program can be built in the g\global\testing directory:

```
nmake~test.exe
```

In addition, the HPVM package from UCSD offers the GA interface in the NT/Myrinet cluster environment.

GA could be built on Windows 95/98. However, due to the DOS shell limitations, the top level NTmakefile will not work. Therefore, each library has to be made separately in its own directory. The environment variables referring to MPI can be hardcoded in the NT makefiles.

C.7.3 Writing and building new GA programs

For small programs contained in a single file, the most convenient approach is to put your program file into the g/global/testing directory. *The existing GNU make suffix rules would build an executable with the ".x" suffix from any C or Fortran source file.* You do not have to modify makefiles in g/global/testing at all. For example, if your program is contained in myfile.c or myfile.F and you place it in that directory, all you need to do to create an executable called myfile.x is to type:

```
make~myfile.x
```

Windows nmake is not as powerful as GNU make - you would need to modify the NT makefile.

This approach obviously is not feasible for large packages that contain multiple source files and directories. In that case you need to provide apropriate definitions in your makefile:

- to header files located in the include directory, g/include, where all public header files are copied in the process of building GA
- add references to libglobal.a (Unix) global.lib (Windows) and libma.a (Unix) ma.lib (Windows) in g/lib/$(TARGET) and for the message-passing libraries
- follow compilation flags for the GA test programs in GNU and Windows makefiles g/config/makefile.h. The recommended approach is to include g/config/makefile.h in your makefile.

Starting with GA 3.1, one could simplify linking of applications by including g/armci/config/makecoms.h and g/armci/config/makemp.h that define all the necessary platform specific libraries that are required by GA. 2.4

C.8 Running GA Programs

Assume the GA program app.x had already been built. To run it,

Running on shared memory systems and clusters*:* (i.e., network of workstations/linux clusters)

If the app.x is built based on MPI, run the program the same way as any other MPI programs.

Example: to run on four processes on clusters, use

```
mpirun~-np~4~app.x
```

Example: If you are using MPICH (or MPICH-like Implementations), and mpirun requires a machinefile or hostfile, then run the GA program same as any other MPI programs. *The only change required is to make sure the hostnames are specified in a consecutive manner in the machinefile.* Not doing this will prevent SMP optimizations and would lead to poor resource utilization.

```
mpirun~-np~4~-machinefile~machines.txt~app.x
```

Contents of machines.txt: (Let us say we have two 2-way SMP nodes (host1 and host2, and correct formats for a 4-processor machinefile is shown in the table below).

Correct	Correct	Incorrect
host1	host2	host1
host1	host2	host2
host2	host1	host1 (This is
host2	host1	wrong, the same
		hosts should be
		specified together)
		host2

If app.x is built based on TCGMSG (not including, Fujitsu, Cray J90, and Windows, because there are no native ports of TCGMSG), to execute the program on Unix workstations/servers, one should use the 'parallel' program (built in tcgmsg/ipcv4.0). After building the application, a file called 'app.x.p' would also be generated (If there is not such a file, make it:

```
make~app.x.p
```

This file can be edited to specify how many processors and tasks to use, and how to load the executables. Make sure that 'parallel' is accessible (you might copy it into your 'bin' directory). To execute, type:

```
parallel~app.x~
```

1. On MPPs, such as Cray XT3/XT4, or IMB SPs, use the appropriate system command to specify the number of processors, load and run the programs. Example:

- to run on IBM SP, run as any other parallel programs (i.e., using *poe*)
- to run on Cray XT3/XT4, use *yod*.

2. On Microsoft NT, there is no support for TCGMSG, which means you can only build your application based on MPI. Run the application program the same way as any other MPI programs. For, WMPI you need to create the .pg file. Example:

```
R:\textbackslash{}nt\textbackslash{}g\textbackslash{}global\textbackslash{}testing>~start~/b
```

C.9 Building Intel Trace Analyzer (VAMPIR) Instrumented Global Arrays

C.9.1 Introduction

The following topics are covered in this section.

- New functions needed for the instrumentation
- Build instructions
- Further information
- Known problems

C.9.2 New Functions Needed for the Instrumentation

- To instrument the GA three C-functions are defined (see g/ga_vt.c):
- vampir_symdef is defined to associate integer identifiers with user defined states and activities. It handles any errors that might occur.
- vampir_begin is defined to register entering a user defined state. It uses a global counter called <vampirtrace_level> to avoid tracing the use of libraries within libraries.
- vampir_end is defined to register leaving a user defined state.

The interfaces of these functions are defined below.

```
void~\textcolor{blue}{vampir\_symdef}~(int~id,~char~{*}state,~char~{*}activity,~

~~~~~~~~~~~~~~~~~~~~char~{*}file,~int~line);~

void~\textcolor{blue}{vampir\_begin}~(int~id,~char~{*}file,~int~line);~

void~\textcolor{blue}{vampir\_end}~(int~id,~char~{*}file,~int~line);
```

In addition to these functions two functions are defined to initialise and finalise MPI when needed. The use of MPI is required because Vampirtrace uses it internally. The functions are

```
void~\textcolor{blue}{vampir\_init}~(int~argc,~char~{*}{*}argv,~char~{*}file,~

~~~~~~~~~~~~~~~~~~int~line);~

void~\textcolor{blue}{vampir\_finalize}~(char~{*}file,~int~line);
```

If the cpp flag -DMPI is provided then these two functions will turn into null functions. In that case the use of MPI within the GAs will ensure that Vampirtrace will be initialised properly.

The values for <file> and <line> are substitute with __FILE__ and __LINE__ macros. On compilation the C-preprocessor replaces these macros with the actual file name and line number. These values are used to generate error messages if needed. These functions are defined in the file g/ga_vt.h.

For each of the instrumented libraries an initialisation routine must be defined that sets the state and activity tables up.

- *tcgmsg*: tcgmsg_vampir_init in g/tcgmsg/tcgmsg_vampir.c. This routine is called from within PBEGINF.
- *tcgmsg-mpi*: tcgmsg_vampir_init in g/tcgmsg-mpi/tcgmsg_vampir.c called from ALT_PBEGIN_ in misc.c.
- *armci*: armci_vampir_init in g/armci/src/armci_vampir.c called from ARMCI_Init in armci.c.
- *global*: ga_vampir_init in g/global/src/ga_vampir.c called from ga_initialize_ and ga_initialize_ltd_ in global.armci.c

C.9.3 Build Instructions

To build GA with Vampir (now called, Intel Trace Analyzer) set the environment variable GA_USE_VAMPIR.

e.g., `setenv GA_USE_VAMPIR y`

to compile the GAs including all the Vampirtrace instrumentation. Further environment variables that are required are

```
LIBVT~:~The~name~of~the~library,~normally~-lVT~which~

~~~~~~~~~~~~~~is~the~default.~

VT\_LIB~:~The~path~to~the~library,~-L<library-path>~

~~~~~~~~~~~~~~e.g.~setenv~VT\_LIB~/usr/local/vampir/lib~
```

```
VT\_INCLUDE:~The~path~to~the~include~file~VT.h,~

~~~~~~~~~~~~-I<include-path>.~e.g.~setenv~VT\_INCLUDE

~~~~~~~~~~~~/usr/local/vampir/include
```

On some platforms it may be necessary to set LIBMPI to -lpmpi to load the MPI profile interfaces that vampirtrace needs.

There are no defaults for VT_PATH and VT_INCLUDE. Beyond this point simply follow the GA make instructions.

Note: that libVT.a should be loaded before mpi or pmpi otherwise the vampirtracing will be ignored.

C.9.4 Further Information

More information on using Intel Trace Analyzer can be found on the Intel website at

http://www.intel.com/software/products/cluster/tanalyzer/

From this location Vampir and Vampirtrace can be downloaded for various platforms including validation licenses if needed.

C.9.5 Known Problems

- Vampirtrace and LAM-MPI clash

In an attempt to produce traces while running with LAM-MPI the program would always abort in MPI_Init due to a segmentation violation. The Pallas website does not mention LAM-MPI at all, but does explicitly state that Vampirtrace does work with MPICH. Indeed the latter has been confirmed in tests. Therefore it is not recommended to use the Vampirtrace instrumentation with LAM-MPI.