

Global Arrays User's Manual

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This manual is intended for use with release 3.0 of Global Arrays

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ABOUT THIS MANUAL

The online version of this manual is available at

<http://www.emsl.pnl.gov:2080/docs/global/user.html>

Additional information about the Global Arrays can be found at

<http://www.emsl.pnl.gov:2080/docs/global>, and

<http://www.emsl.pnl.gov:2080/docs/global/Capi.html> for C documentation, and

<http://www.emsl.pnl.gov:2080/docs/global/Gaapi.html> for Fortran documentation.

Most of the undelined words (primarily function names) correspond to hyperlinks in the HTML version of this document on the web.

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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 it was stored in the shared memory. Details of the data distribution, addressing, and communication are encapsulated in the array objects. The information on the actual data distribution and locality can be obtained and taken advantage of whenever data locality is important.

The primary target architecture for which GA was developed are massively-parallel distributed memory or scalable shared memory systems. GA divides logically shared data structures into local and remote portions and it recognizes variable data transfer costs required to access the data. A "local" portion of the shared memory is assumed to be faster to access and the remainder ("remote" portion) is considered slower to access. GA is implemented as a library with C and Fortran-77 bindings. Therefore, explicit library calls are required to use GA model in a parallel program. GA was designed to complement rather than substitute the message-passing model, and it allows 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.

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 the 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 location. At least one global array has to be created before data transfer operations can be used. These 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 require a polling operation used in some other tools to assure communication progress.

A programmer in the GA program has 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 array index interface rather than addresses of shared data. Unlike systems based on global address space that support remote memory (*put/get*) operations, GA does not require user to specify the target process(es) where the referenced shared data resides. 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

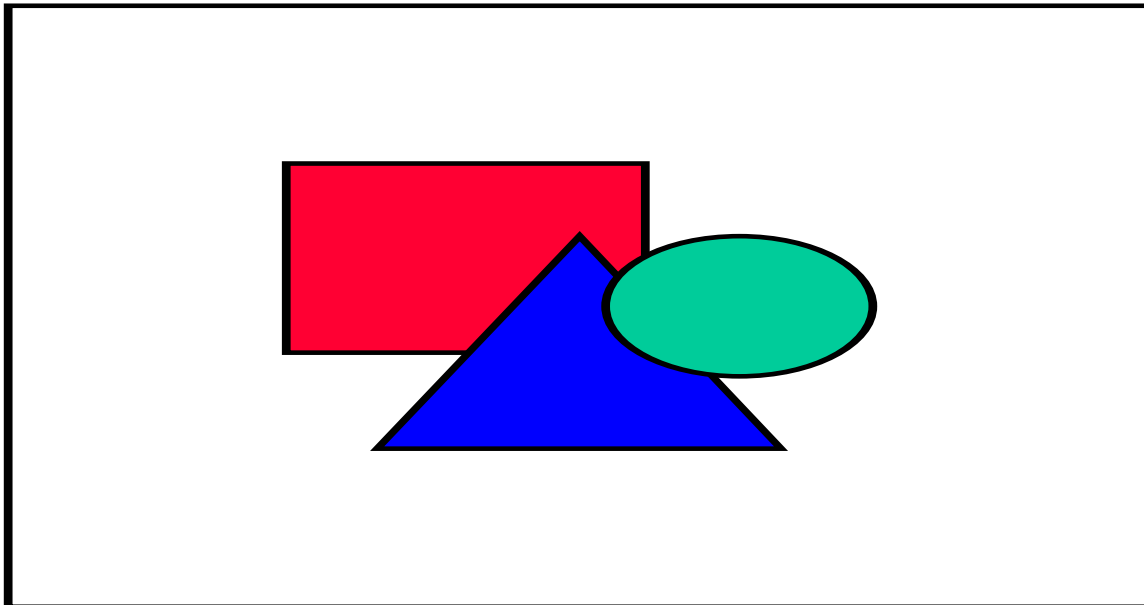
processes. If necessary, the programmer is always able to inquire:

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

The GA toolkit supports three data types: integer, double precision, and double complex. 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 GA model of computations is based on an 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. However, 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 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 *locks*, *barrier*, and *fence* operations available in the library.

1.4 Application Guidelines

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

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 for out-of-core array-based algorithms (GA + DRA)

Usability Considerations

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

When not to use GA:

Algorithmic Considerations

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

Usability Considerations

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

2. Writing, Building and Running GA Programs

2.1 Platform and Library Dependencies

2.1.1 Supported Platforms

- IBM SP, CRAY T3E/J90, SGI Origin, Fujitsu VX/VPP
- Cluster of workstations: Solaris, IRIX, AIX, HP/UX, Digital/True64 Unix, Linux
- 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 current (3.0) version because we do not have access to these systems. We recommend using GA 2.4 on these platforms.

Because of limited interest in heterogenous computing from the GA users, the Global Array library still does not support heterogenous platforms. This capability can be added if required.

2.1.2 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:

- with TCGMSG
- with MPI and TCGMSG emulation library: TCGMSG-MPI, that implements functionality of TCGMSG using MPI. In this mode, message-passing library is initialized using TCGMSG *PBEGIN(F)* call which internally references *MPI_Initialize*. To enable this mode, define environmental variable *USE_MPI*.
- directly with MPI. In this mode, GA program should contain MPI initialization calls instead *PBEGIN(F)*.

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
- use *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 is that GA makefile 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, this could cause the package to build incorrectly (test programs fail or do not compile).

On Windows NTs, the current version of GA was tested with WMPI, and NT implementation derived from MPICH in Portugal.

2.1.3 Dependencies on other software

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

- [MA \(Memory Allocator\)](#), a library for management 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 (an included with GA subset 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 PEIGS library; (Please contact [George Fann <gi_fann@pnl.gov>](mailto:gi_fann@pnl.gov) about PEIGS)
- SCALAPACK, PBLAS, 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 `-DGA_TRACE` define flag should be specified for C and Fortran compilers.

2.2 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'`.

The GA program should look like:

- When GA runs with MPI

Fortran	C
<code>call mpi_init(..)</code>	<code>MPI_Init(..)</code> ! start MPI
<code>call ga_initialize()</code>	<code>GA_Initialize()</code> ! start global arrays
<code>status = ma_init(..)</code>	<code>MA_Init(..)</code> ! start memory allocator
 <code>.... do work</code>	 <code>.... do work</code>
<code>call ga_terminate()</code>	<code>GA_Terminate()</code> ! tidy up global arrays
<code>call mpi_finalize()</code>	<code>MPI_Finalize()</code> ! tidy up MPI
<code>stop</code>	<code>! exit program</code>

- When GA runs with TCGMSG or TCGMSG-MPI

Fortran	C	
<code>call pbeginf()</code>	<code>PBEGIN_(..)</code>	<code>! start TCGMSG</code>
<code>call ga_initialize()</code>	<code>GA_Initialize()</code>	<code>! start global arrays</code>
<code>status = ma_init(..)</code>	<code>MA_Init(..)</code>	<code>! start memory allocator</code>
 <code>.... do work</code>	 <code>.... do work</code>	
 <code>call ga_terminate()</code>	 <code>GA_Terminate()</code>	 <code>! tidy up global arrays</code>
<code>call pend()</code>	<code>PEND_()</code>	<code>! tidy up tcgmsg</code>
<code>stop</code>		<code>! exit program</code>

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 [3.3.1](#) for the details and information on more advanced usage of MA in GA programs.

2.3 Building GA Programs

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
- Makefile.h: definitions & include symbols
- MakeFiles.h: files to be compiled depending on the TARGET machine
- Makelib.h: specification of libraries to be linked with when test programs are built

User needs to specify TARGET in the GNUmakefile or on the command line when calling make. The library and test programs should be built by calling make in the current directory. The appropriate value of VERSION will be determined automatically.

Valid TARGET is one of:

SUN, SOLARIS, FUJITSU, SGI, SGI_N32, SGITFP, DECOSF, IBM, LAPI,
CRAY-T3D, CRAY-T3E, HPUX, CONVEX-SPP, LINUX on Unix systems.

or

WIN32, CYGNUS on Windows NT.

2.3.1 Unix Environment

To build the GA with 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
```

Additionally, if the TCGMSG-MPI library is not needed, the make/environmental variable MSG_COMMS should be defined as MSG_COMMS = MPI.

Interface routines to ScaLAPACK are only available with MPI, and of course with ScaLAPACK. The user is required to define environment variables *USE_SCALAPACK*, and location of ScaLAPACK & Co. libraries in variable *SCALAPACK*.

Example: using csh/tcsh

```
setenv USE_SCALAPACK y
setenv SCALAPACK '-L/msrc/proj/scalapack/LIB/rs6000
                -lscalapack -lpblas -l tools -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.

To build the library, type
make or gmake

To build an application based on GA, 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/global/Makefile.h to make sure that Fortran and C compiler flags are consistent with flags use to compile your application. This may be critical when Fortran compiler flags are used to change default length of integer datatype.

2.3.2 Windows NT

To build GA on Windows NT, one needs to have an MS Power Fortran 4 or DEC Visual Fortran 5 or 6 and MS Visual C 4, 5, or 6. When commercial Windows compilers are not available, one can choose to use CYGNUS. Set the TARGET environment variable to CYGNUS, and build it as any other Unix box.

First of all, one needs to set environment variables (same as in Unix environment). GA needs to know where find 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:\Wmpi\Include
set MPI_LIB as d:\Wmpi\Console
```

Make sure that the dynamic link libraries required by the particular implementation of MPI is 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 `g\global\testing` directory:

```
nmake test.exe
```

Current GA works on a single PC only using shared memory and NT threads with separate address spaces. HPVM package offers GA in the NT cluster environment.

Ga could be built on Windows 95. 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 NT makefiles.

2.3.3 Writing and building new GA programs

For small programs contained in a single file, the most convenient approach is to put your file into `g/global/testing` directory. The existing GNU make suffix rules would build an executable with ".x" suffix from the C or Fortran source files. Windows *nmake* is not as powerful as GNU make - you would need to modify the NT makefile.

This approach obviously is not preferred for large packages developed with GA. In that case you need to incorporate in your makefile:

- GA/MA/... include directory, `g/include`, where all public header files are copied in the process of building GA
- add references to `libglobal.a/global.lib`, `libma.a/ma.lib` in `g/lib/$(TARGET)` and message-passing libraries
- follow compilation flags for the GA test programs in GNU and Windows makefiles

2.4 Running GA Programs

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

- On MPP, such as Cray T3E, or IBM SP
Use appropriate system command to specify the number of processors, load and run the programs.

Example: to run on four processors on the Cray T3E, use

```
mpprun -n 4 app.x
```

- On shared memory system and (network of) workstations (including linux cluster)
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 SGI workstation, use

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

If the `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 file, make it: `make app.x.p`). This file can be edited to specify how many processors and tasks to use, how to load the executables. Make sure that the 'parallel' is accessible (you might copy it into your 'bin' directory). Now ready to go, type:

```
parallel app.x
```

- On Microsoft NT, there is not 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.exe
```

3. Initialization and Termination

For the historical reasons (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, and the later can definitely handle two dimensional arrays as well. The supported data types are *integer*, *double precision*, *double complex*. Global Arrays provides 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.

The 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 systems - all dynamically allocated local memory comes from MA. We will describe details of memory allocation later in this section.

3.1 Message Passing

The first version 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 GA authors (Robert Harrison) had developed before. In 1995, GA added support for MPI. At present time, GA distribution still includes the TCGMSG library for backward compatibility purposes, and because it is small, fast to compile, and provides a minimal message-passing support required by the GA programs to run. The user can enable the MPI-compatible version of GA by defining `USE_MPI` environment variable before compiling the GA toolkit. On systems where vendors provide MPI with interoperable C and Fortran interfaces, there is no advantage in compiling or using TCGMSG.

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 GA library and terminated after 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, `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 `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 memory 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 is completed.

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 it was local memory. All the data in shared memory is directly visible to every process that attached to that segment. On shared memory systems and clusters of SMP (symmetric 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 used in serial mode GA uses local memory to store data in global arrays.

All 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
- provides 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 for the MA offers. Because MA is used implicitly by GA, it has to be initialized before a first global array is allocated. `MA_init` function requires user to specify memory for *heap* and *stack*. 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 the their sum at any given time.

3.2.1 How to determine what values of MA stack and heap size should be?

The answer to this question depends on the run-time environment of the program including availability of shared memory. A part of GA initialization involves initialization of the ARMCI run-time library. ARMCI dynamically determines if the program can or should use shared memory based on the architecture type and the 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 is. This decision is made at run-time. GA reports the information about the type of memory used with `ga_uses_ma()`. This function returns false when shared memory is used and true when MA is used.

Based on this information the programmer who cares about 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 should not be probably less than 4MB. The stack space is only used when a GA operation 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:

```
C      void GA\_Initialize\(\)
Fortran  subroutine ga\_initialize\(\)
```

and

```
C      void GA\_Initialize\_ltd\(size\_t limit\)
Fortran  subroutine ga\_initialize\_ltd\(limit\)
```

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

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 limit is set, GA would not allocate more memory in global arrays that would exceed the specified value - the user calls to allocate new arrays that would simply fail (return false). There are two ways to set the limit:

- at initialization time by calling `ga_initialize_ltd`, or
- after initialization by calling the function


```

C      void GA\_Set\_memory\_limit(size_t limit)
Fortran  subroutine ga\_set\_memory\_limit(limit)

```

It is encouraged that the user choose the first option, even though the user can initialize 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 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 GA program is to call the function

```

C      void GA\_Terminate()
Fortran  subroutine ga\_terminate()

```

The programmer can also abort a running program

am, for example as part of handling a programmatically detected error condition by calling the function

```

C      void GA\_Error(char *message, int code)
Fortran  subroutine ga\_error(message, code)

```

3.5 Creating arrays

There are two ways to create new arrays:

1. from scratch, for regular distribution, use the function

```

C      int NGA\_Create(int type, int ndim, int dims[],
                    char *array_name, int chunk[])
n-d Fortran  logical function nga\_create(type, ndim, dims,
                    array_name, chunk, g_a)
2-d Fortran  logical function ga\_create(type, dim1, dim2,
                    array_name, chunk, g_a)

```

Or for irregular distribution, use the function

```

C          int NGA_Create_irreg(int type, int ndim, int dims[],
                                char *array_name, int map[], int block[])
n-d Fortran logical function nga_create_irreg(type, ndim,
                                                dims, array_name, map, nblock, g_a)
2-d Fortran logical function ga_create_irreg(type, dim1, dim2,
                                                array_name, map1, nblock1, map2, nblock2, g_a)

```

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

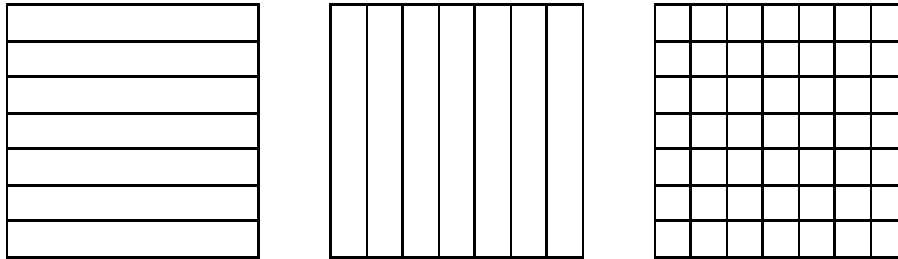
```

C          int GA_Duplicate(int g_a, char *array_name)
Fortran    logical function ga_duplicate(g_a, g_b, array_name)

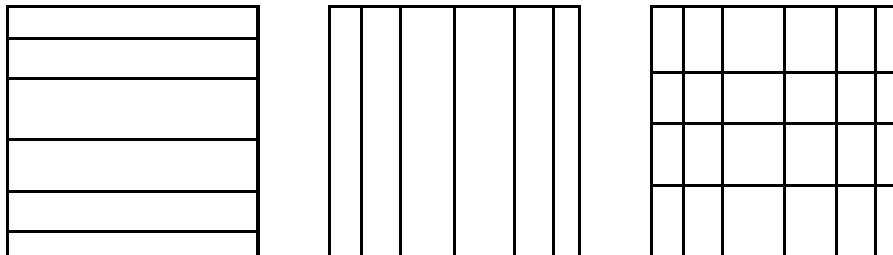
```

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

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



With the irregular distribution, the programmer specifies distribution points for every dimension. The library creates an array with the overall distribution that is a Cartesian product of distributions for each dimension.



If array cannot be created, for example due to the memory shortages or enforced memory consumption limit, these calls return *false*. Otherwise an integer handle is returned. This handle represents a global array object. 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 . It is not necessary to keep track of this type of data in the application.

3.6 Destroying arrays

Global arrays can be destroyed by calling the function

```
C          void GA\_Destroy(int g_a)
Fortran    subroutine ga\_destroy(g_a)
```

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 user calls `ga_terminate` as well.

4. One-sided Operations

Global Arrays provide one-sided communications that allow one process to specify all communication parameters, both for the sending side and for the receiving side. In such a case, each process can compute what data it needs to access or update at other processes. However, processes may not know which data in their own memory need to be accessed or updated by remote processes, and may not even know the identity of these processes. Thus, the transfer parameters are all available only on one side.

The one-sided operations that global arrays provide can be summarized into three categories:

<i>Remote blockwise write/read:</i>	<code>ga_put/ga_get</code>
<i>Remote atomic update:</i>	<code>ga_acc/ga_read_inc</code>
<i>Remote elementwise write/read:</i>	<code>ga_scatter/ga_gather</code>

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 the cooperation from the process(es) that own the data. The semantics of these operations does not require the user to specify which remote process or processes own the accessed portion of a global array. The data is simply accessed like it were in a shared memory.

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

```
C      void NGA\_Put(int g_a, int lo[], int hi[], void *buf, int ld[])
n-D Fortran  subroutine nga\_put(g_a, lo, hi, buf, ld)
2-D Fortran  subroutine ga\_put(g_a, ilo, ihi, jlo, jhi, buf, 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 user, which means the user doesn't have to worry where the region defined by `lo` and `hi` is located. It can be in the memory of one or many remote processes, or owned by local process, or even mixed (part of it belongs to a 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.

```
C      void NGA\_Get(int g_a, int lo[], int hi[], void *buf, int ld[])
n-D Fortran  subroutine nga\_get(g_a, lo, hi, buf, ld)
2-D Fortran  subroutine ga\_get(g_a, ilo, ihi, jlo, jhi, buf, ld)
```

Similar to *put*, `lo` and `hi` specify where the data should come from in the global array, and `ld` specify 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 `ga_get` operation transferring data from the (11:15,1:5) section of 2-dimensional 15 x10 global array into local buffer 5 x10 array we have: (in Fortran notation)

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



4.2 Accumulate/Read_inc

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 than replacing the data there. *Accumulate* and *read_inc* perform **atomic** remote update to a patch 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 local array with data in the global array section, which is

```
C          void NGA\_Acc(int g_a, int lo[], int hi[], void *buf,
                        int ld[],void *alpha)
n-D Fortran subroutine nga\_acc(g_a, lo, hi, buf, ld, alpha)
2-D Fortran subroutine ga\_acc(g_a,ilo,ihi,jlo,jhi,buf,ld, 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. It performs (in C notation)

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

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

```
C          void NGA\_Read\_inc(int g_a, int subscript[], long inc)
n-D Fortran subroutine nga\_read\_inc(g_a, subscript, inc)
2-D Fortran subroutine ga\_read\_inc(g_a, i, j, inc)
```

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

a(subscripts) += 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 owns the referenced elements in the global array.

Scatter puts array elements into a global array, which is

```

C      void NGA\_Scatter(int g_a, void *v, int *subarray[], int n)
n-D Fortran  subroutine nga\_scatter(g_a, v, subarray, n)
2-D Fortran  subroutine ga\_scatter(g_a, v, i, j, n)

```

It performs (in C notation)

```

for(k=0; k<= n; k++) {
    a[subArray[k][0]][subArray[k][1]][subArray[k][2]]... = v[k];
}

```

Example: Scatter the 5 elements into a 10x10 global array

Element 1	v[0] = 5	subarray[0][0] = 2	subarray[0][1] = 3
Element 2	v[1] = 3	subarray[1][0] = 3	subarray[1][1] = 4
Element 3	v[0] = 8	subarray[0][0] = 8	subarray[0][1] = 5
Element 4	v[1] = 7	subarray[1][0] = 3	subarray[1][1] = 7
Element 5	v[0] = 2	subarray[0][0] = 6	subarray[0][1] = 3

After the scatter operation, the five elements would be scattered into the global array as shown in the following figure.

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

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

```

C          void NGA\_Gather(int g_a, void *v, int *subarray[], int n)
n-D Fortran subroutine nga\_gather(g_a, v, subarray, n)
2-D Fortran subroutine ga\_gather(g_a, v, i, j, n)

```

It performs (in C notation)

```

for(k=0; k<= n; k++){
    v[k] = a[subArray[k][0]][subArray[k][1]][subArray[k][2]]...;
}

```

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 completed. Sync operation is collective.

5.1 Lock and Mutex

Lock works together with mutex. It is a simple synchronization mechanism used to protect 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

```
C          int GA\_Create\_mutexes(int number)
Fortran    logical function ga\_create\_mutexes(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

```
C          int GA\_Destroy\_mutexes()
Fortran    logical function ga\_destroy\_mutexes()
```

destroys the set of mutexes created with `ga_create_mutexes`.

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

The functions

```
C          void GA\_lock(int mutex)
           void GA\_unlock(int mutex)
Fortran    subroutine ga\_lock(int mutex)
           subroutine ga\_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.

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 the 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

```
C          void GA\_Init\_fence\(\)  
Fortran    subroutine ga\_init\_fence\(\)
```

Initializes tracing of completion status of data movement operations.

The function

```
C          void GA\_Fence\(\)  
Fortran    subroutine ga\_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 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

```
C      void GA\_Sync()  
Fortran subroutine ga\_sync()
```

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

6. Collective Array Operations

Global Arrays provide functions for collective array operations, targeting both the 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 initialize explicitly 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 *put* or 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

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

sets all the elements in the array to zero.

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

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

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

```
C          void GA_Copy(int g_a, int g_b)
Fortran  subroutine ga_copy(g_a, g_b)
```

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

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_Print` is 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

```
C          void NGA_Zero_patch(int g_a, int lo[] int hi[])
Fortran  subroutine nga_zero_patch(g_a, alo, ahi)
```

is similar to `ga_zero`, except that instead of applying to entire array, it sets 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:

```
C          void NGA_Fill_patch(int g_a, int lo[] int hi[], void *val)
n-D Fortran  subroutine nga_fill_patch(g_a, lo, hi, val)
2-D Fortran  subroutine ga_fill_patch(g_a, ilo, ihi, jlo, jhi, val)
```

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

The function

```
C          void NGA_Scale_patch(int g_a, int lo[] int hi[], void *val)
n-D Fortran  subroutine nga_scale_patch(g_a, lo, hi, val)
2-D Fortran  subroutine ga_scale_patch(g_a, ilo, ihi, jlo, jhi, 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

```
C          void NGA_Copy_patch(char trans, int g_a, int alo[],
                                int ahi[], int g_b, int blo[], int bhi[])
n-D Fortran  subroutine nga_copy_patch(trans, g_a, alo, ahi,
                                g_b, blo, bhi)
2-D Fortran  subroutine ga_copy_patch(trans, g_a, ailo, aihi, ajlo,
                                ajhi, g_b, bilo, bihi, bjlo, bjhi)
```

copies one patch defined by `alo` and `ahi` in one global array `g_a` to 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 on different global arrays. They must be the same data type. The patches may be of different shapes though, 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}`

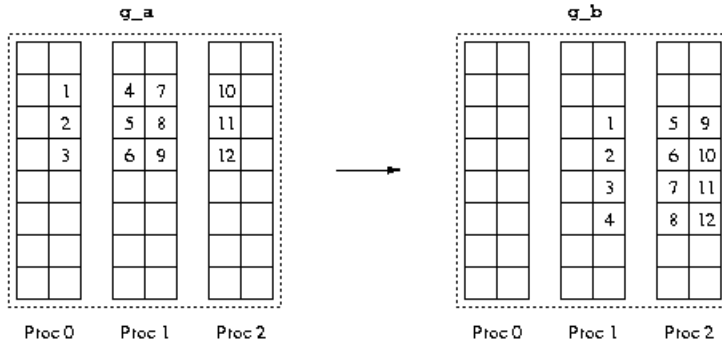
to

`g_b: blo = {3, 4}, bhi = {6, 6}`

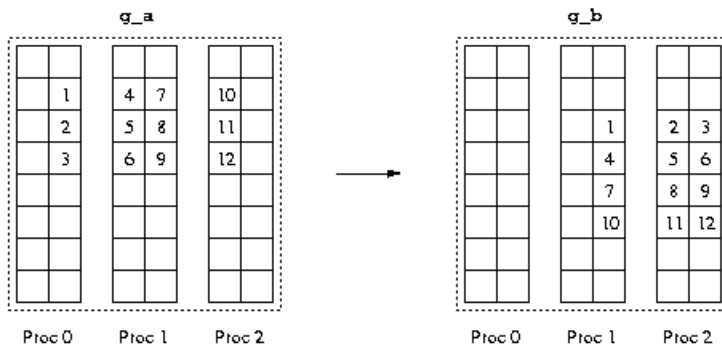
and

`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`, 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

```
C    void GA\_Add(void *alpha, int g_a, void *beta, int g_b, int g_c)
Fortran subroutine ga\_add(alpha, g_a, beta, g_b, g_c)
```

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. 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

```
C        void GA\_Dgemm(char ta, char tb, int m, int n, int k,
                      double alpha, int g_a, int g_b,
                      double beta, int g_c )
Fortran subroutine ga\_dgemm(transa, transb, m, n, k,
                          alpha, g_a, g_b, beta, g_c )
```

Performs one of the matrix-matrix operations:

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

where $op(X)$ is one of

$$op(X) = X \text{ or } op(X) = X',$$

α and β 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

```
C        long      GA\_Idot(int g_a, int g_b)
         double     GA\_Ddot(int g_a, int g_b)
         DoubleComplex GA\_Zdot(int g_a, int g_b)
Fortran integer      function ga\_idot(g_a, g_b)
         double precision function ga\_ddot(g_a, g_b)
         double complex  function ga\_zdot(g_a, g_b)
```

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

```
C          void GA\_Symmetrize(int g_a)
Fortran subroutine ga\_symmetrize(g_a)
```

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

The function

```
C          void GA\_Transpose(int g_a, int g_b)
Fortran subroutine ga\_transpose(g_a, g_b)
```

transposes a matrix: $B = A'$.

6.2.2 Patches

The functions

```
C          void NGA\_Add\_patch(void *alpha, int g_a, int alo[],
                           int ahi[], void *beta, int g_b, int blo[],
                           int bhi[], int g_c, int clo[], int chi[])
n-D Fortran subroutine nga\_add\_patch(alpha, g_a, alo, ahi,
                                   beta, g_b, blo, bhi,
                                   g_c, clo, chi)
2-D Fortran subroutine ga\_add\_patch(alpha, g_a, ailo, aihi, ajlo,
                                   ajhi, beta, g_b, bilo, bihi, bjlo,
                                   bjhi, g_c, cilo, cihi, cjlo, cjhi)
```

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 and 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 like for the arrays were identically distributed, thus the performance would 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

```
C          void GA\_Matmul\_patch(char *transa, char* transb,
                              void* alpha, void* beta,
                              int g_a, int ailo, int aihi, int ajlo, int ajhi,
                              int g_b, int bilo, int bihi, int bjlo, int bjhi,
                              int g_c, int cilo, int cihi, int cjlo, int cjhi)
Fortran subroutine ga\_matmul\_patch(transa, transb, alpha, beta,
                                   g_a, ailo, aihi, ajlo, ajhi,
                                   g_b, bilo, bihi, bjlo, bjhi,
                                   g_c, cilo, cihi, cjlo, 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

$$op(X) = X \text{ or } op(X) = X',$$

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

```

C      Integer NGA\_Idot\_patch(int g_a, char* ta, int alo[],
                                int ahi[], int g_b, char* tb, int blo[], int bhi[])
      double NGA\_Ddot\_patch(int g_a, char* ta, int alo[],
                             int ahi[], int g_b, char* tb, int blo[], int bhi[])
      DoubleComplex NGA\_Zdot\_patch(int g_a, char* ta, int alo[],
                                   int ahi[], int g_b, char* tb, int blo[], int bhi[])
n-D Fortran integer function nga_idot_patch(g_a, ta, alo, ahi,
                                             g_b, tb, blo, bhi)
      double precision function nga\_ddot\_patch(g_a, ta, alo, ahi,
                                             g_b, tb, blo, bhi)
      double complex function nga\_zdot\_patch(g_a, ta, alo, ahi,
                                             g_b, tb, blo, bhi)
2-D Fortran integer function ga_idot_patch(g_a, ta, ailo, aihi,
                                             ajlo, ahilo, g_b, tb, biloo, bihi, bjlo, bjhi)
      double precision function ga\_ddot\_patch(g_a, ta, ailo, aihi,
                                             ajlo, ahilo, g_b, tb, biloo, bihi, bjlo, bjhi)
      double complex function ga\_zdot\_patch(g_a, ta, ailo, aihi,
                                             ajlo, ahilo, g_b, tb, biloo, bihi, bjlo, bjhi)

```

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 a extra copies and/or memory consumption.

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 solving the 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 the invert matrices.

The function

```

C      int GA\_Solve(int g_a, int g_b)
Fortran integer function ga\_solve(g_a, g_b)

```

solves a system of linear equations $A * X = B$. It first will call the Cholesky factorization routine

and, if successfully, will solve the system with the Cholesky solver. If Cholesky will be not be able to factorize A , 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

```
C          int GA\_Llt\_solve(int g_a, int g_b)
Fortran    integer function ga\_llt\_solve(g_a, g_b)
```

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

The function

```
C          void GA\_Lu\_solve(char trans, int g_a, int g_b)
Fortran    subroutine ga\_lu\_solve(trans, g_a, g_b)
```

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

```
C          int GA\_Spd\_invert(int g_a)
Fortran    integer function ga\_spd\_invert(g_a)
```

computes the inverse of a double precision matrix using the Cholesky factorization of a $N \times N$ 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 message-passing model and is portable across many platforms. For more information and availability send a message to gi_fann@pnl.gov. Global Arrays use this library to solve eigenvalue problems.

The function

```
C          void GA\_Diag(int g_a, int g_s, int g_v, void *eval)
Fortran    subroutine ga\_diag(g_a, g_s, g_v, eval)
```

solves the generalized eigen-value problem returning all eigen-vectors and values in ascending order. The input matrices are not overwritten or destroyed.

The function

```
C          void GA\_Diag\_reuse(int control, int g_a, int g_s,
                             int g_v, void *eval)
Fortran    subroutine ga\_diag\_reuse(control, g_a, g_s, g_v, eval)
```

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

The function

```
C          void GA\_Diag\_std(int g_a, int g_v, void *eval)
Fortran    subroutine ga\_diag\_std(g_a, g_v, 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 the [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. The [instruction of using PETSc with GA](#) is in Appendix 1.

[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. The [instruction of using CUMULVS with GA](#) is at Appendix 2.

7. Utility Operations

Global arrays provide some utility functions to get the local process/data information, check the memory availability, etc. There are also several handy functions that print array distribution, 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

```
C          int NGA\_Locate(int g_a, int subscript[])
n-D Fortran logical function nga\_locate(g_a, subscript, owner)
2-D Fortran logical function ga\_locate(g_a, i, j, owner)
```

tells who (process id) owns the elements defined by the array subscripts.

The function

```
C          int NGA\_Locate\_region(int g_a, int lo[], int hi[],
                                int *map[], int procs[])
n-D Fortran logical function nga\_locate\_region(g_a, lo, hi, map,
                                                proclist, np)
2-D Fortran logical function ga\_locate\_region(g_a, ilo, ihi, jlo,
                                                jhi, map, np)
```

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:

- find the distribution of an array, which part of data the calling process owns
- access the data
- operate on the data: read/write
- release the access of data

The function

```
C          void NGA\_Distribute(int g_a, int iproc, int lo[], int hi[])
n-D Fortran subroutine nga\_distribute(g_a, iproc, lo, hi)
2-D Fortran subroutine ga\_distribute(g_a, iproc, ilo, ihi, jlo, jhi)
```

finds out the range of the global array g_a that process iproc owns. This can be any valid process ID.

The function

```
C void NGA\_Access(int g_a, int lo[], int hi[], void *ptr, int ld[])
n-D Fortran subroutine nga\_access(g_a, lo, hi, index, ld)
2-D Fortran subroutine ga\_access(g_a, ilo, ihi, jlo, jhi, index, 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

```
C          void NGA\_Release(int g_a, lo[], int hi[])
n-D Fortran subroutine nga\_release(g_a, lo, hi)
2-D Fortran subroutine ga\_release(g_a, ilo, ihi, jlo, jhi)
```

and

```
C          void NGA\_Release\_update(int g_a, int lo[], int hi[])
n-D Fortran subroutine nga\_release\_update(g_a, lo, hi)
2-D Fortran subroutine ga\_release\_update(g_a, ilo, ihi, jlo, jhi)
```

releases access to a global array. The former set is used when the data was read only, and the later set is used when the data was accessed for writing.

Global Arrays also provide a function to compare distributions of two arrays. It is

```
C          void NGA\_Compare\_distr(int g_a, int g_b)
Fortran    subroutine ga\_compare\_distr(g_a, g_b)
```

7.1.1 Process Information

When developing a program, one needs to use the characteristics 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

```
C          int GA\_Nodeid()
Fortran    integer function ga\_nodeid()
```

returns the GA process ID of current process, and the function

```
C          int GA\_Nnodes()
Fortran    integer function ga\_nnodes()
```

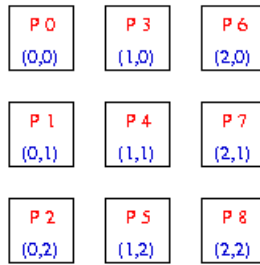
tells the number of computing processes.

The function

```
C          void NGA\_Proc\_topology(int g_a, int proc, int coordinates)
Fortran    subroutine ga\_proc\_topology(ga, proc, prow, pcol)
```

determines the coordinates of the specified processor in the virtual processor grid corresponding to the distribution of array `g_a`.

Example: An 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.



7.2 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:

- How much memory has been used by the allocated global arrays.
- How much memory is left for allocation of new global arrays.
- Whether the memory in global arrays comes from the [Memory Allocator \(MA\)](#).
- Is there any limitation for the memory usage by the Global Arrays.

The function

```
C          size_t GA\_Inquire\_memory\(\)
Fortran   integer function ga\_inquire\_memory\(\)
```

answers the first question. It returns the amount of memory (in bytes) used in the allocated global arrays on the calling processor.

The function

```
C          size_t GA\_Memory\_avail\(\)
Fortran   integer function ga\_memory\_avail\(\)
```

answers the second question. it returns 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

```
C          int GA\_Uses\_ma\(\)
Fortran   logical function ga\_uses\_ma\(\)
```

tells whether the memory in Global Arrays comes from the Memory Allocator (MA) or not.

The function

```
C          int GA\_Memory\_limited\(\)
Fortran   logical function ga\_memory\_limited\(\)
```

Indicates if 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 that program is running with.

The function

```
C          void GA\_Brdcst(void *buf, int lenbuf, int root)
Fortran    subroutine ga\_brdcst(type, buf, lenbuf, root)
```

broadcasts from process root to all other processes a message of length lenbuf.

The functions

```
C          void GA\_Igop(long x[], int n, char *op)
           void GA\_Dgop(double x[], int n, char *op)
Fortran    subroutine ga\_igop(type, x, n, op)
           subroutine ga\_dgop(type, x, n, 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

+, *, Max, min, Absmax, absmin

The integer version also include the **bitwise OR** operation.

These operations unlike ga_sync, do not include embedded ga_fence 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 following functions.

The functions

```
C          void NGA\_Inquire(int g_a, int *type, int *ndim, int dims[])
n-D Fortran subroutine nga\_inquire(g_a, type, ndim, dims)
2-D Fortran subroutine ga\_inquire(g_a, type, dim1, dim2)
```

return the data type of the array, and also the dimensions of the array.

The function

```
C          char* GA\_Inquire\_name(int g_a)
Fortran    subroutine nga\_inquire\_name(g_a, array_name)
```

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

- content of the global array
- content of a patch of global array
- the status of array operations
- a summary of allocated arrays

The function

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

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

```
C          void NGA_Print_patch(int g_a, int lo[], int hi[], int pretty)
Fortran    subroutine nga_print_patch(g_a, lo, hi, pretty)
```

One can either specify a formatted output (set `pretty` to one): 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

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

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

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

prints the global array distribution. It shows mapping array data to the processes.

The function

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

prints info about allocated arrays

7.4.3 Miscellaneous

The function

```
C          void GA\_Check\_handle(int g_a, char *string)
Fortran    subroutine ga\_check\_handle(g_a, string)
```

checks if the global array handle `g_a` represents a valid array.

Appendix 1: *Instructions of using PETSc with GA*

Inter-operability of Global Arrays with PETSc

[PETSc\(the Portable, Extensible Toolkit for Scientific Computation\)](#) was developed by the [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.

The following summarizes the inter-operability status of Global Arrays and PETSc:

Inter-operability

Global Arrays toolkit is inter-operable with PETSc. In a application using Global Arrays, the PETSc solvers can be called to solve PDEs that require solving large-scale, sparse nonlinear systems of equations. The primary issue is how to convert the data structures of Global Arrays to those of PETSc before calling the PETSc solvers, and how to convert the data structures of PETSc back to Global Arrays after calling the PETSc solvers. PETSc provides enough mechanisms to deal with this issue. For vector operations, there are `VecCreateMPI()`, `VecSetValues()`, `VecGetArrsy()`, `VecRestoreArray()`, etc.. Same functions exist for matrix operation.

The packages used in the testing are:

- Global Arrays Version 3.0
- PETSc Version 2.0.24

Instructions of using PETSc in a Global Arrays application

[PETSc online documentation](#) is a well maintained site for PETSc resources. Examples can be accessed both online or from the package itself.

A typical scenario to use PETSc in a Global Arrays application is that there is a global array x which represents the approximate solution initialized with some initial values. It needs to call one of the PETSc solvers to solve the problem, and restore the results back to x .

Here is the instructions for implementing an example $Ax = b$, where A is the matrix defining linear system, b is the right hand side, and x is the approximate solution and an global array.

- Initialize PETSC (`PetscInitialize()`)
- Convert the global array x to the PETSc format
 - Create a PETSc Vector `pets_x` (`VecCreateMPI()`)
 - Get the range of `pets_x` resides in the local process(or) (`VecGetOwnershipRange()`)
 - Get access to the local portion of `pets_x` (`VecGetArray()`)
 - Get the corresponding data block (the range of `pets_x` in local process(or)) in the global array x (`ga_get()`)
 - Put the data block to `pets_x` (`VecRestoreArray()`)
- Create the linear solver and set various options

- Solve the linear system
- Write the solution back to Global Array.
 - Get access to the local portion of `pets_x` (`VecGetArray()`)
 - Put the local portion of solution back to global array `x` (`ga_put()`)
 - Close the access to the local portion of `pets_x` (`VecRestoreArray()`)

There are detailed instructions for setting up environment variables on different platforms, coming with the PETSc package. For example, users on Cray T3E at NERSC only need to the load the petsc module: insert

```
module load petsc
```

into the `.login` file.

Discussion

Data conversion between the Global Arrays and PETSc is the key issue for the inter-operability. PETSc provides several ways to create Vectors and Matrices and set values to them. We found that the most efficient way to connect the Global Arrays and PETSc is to use the `GetArray` and `RestoreArray` mechanism. `GetArray` and `RestoreArray` are not intended to set values though, they open a window to access and update the local Vector/Matrix of PETSc. Global Arrays provide the one-sided operations, `get` and `put`, which are perfect match for PETSc's `GetArray` and `RestoreArray` mechanism. The array segment of Global Arrays can be sent to or received from PETSc in block fashion, instead of updating element by element.

Here is how it works:

From Global Arrays to PETSc

- Access the local portion of PETSc Vector/Matrix
- Use `ga_get()` to get the corresponding section of Global Array
- Close the access to (also update) the local portion of PETSc Vector/Matrix

From PETSc to Global Arrays

- Access the local portion of PETSc Vector/Matrix
- Use `ga_put()` to put the PETSc data the corresponding section of Global Array
- Close the access to the local portion of PETSc Vector/Matrix

Appendix 2: *Instructions of using CUMULVS with GA*

Inter-operability of Global Arrays with CUMULVS

[CUMULVS \(Collaborative User Migration User Library for Visualization and Steering\)](#) is developed by the [Oak Ridge National Laboratory](#). It is a software framework that enables programmers to incorporate fault-tolerance, interactive visualization and computational steering into existing parallel programs.

The following summarizes the interoperability status of Global Arrays and CUMULVS:

Inter-operability

Global Array is inter-operable with CUMULVS's computational steering capability. In a application using Global Arrays, steering parameters can be defined for a CUMULVS front-end viewer and manipulated by the viewer during the lifetime of execution. The packages used in the testing are:

- Global Arrays Version 3.0
- CUMULVS Version 1.0

The Global Arrays can be configured to work with one of several communication libraries. The one we used was based on MPI. The CUMULVS is based on PVM (Version 3.3.11 or later).

Instructions for using CUMULVS in a Global Arrays application

[CUMULVS User's Guide](#) provides instructions of how to use CUMULVS, and the definitions of library functions. Examples that come with the CUMULVS package serves a good starting point, which give the user some insight of what to do, even though they are written in PVM. Here is what quoted from the CUMULVS User's Guide:

A typical statement sequence that a programmer would follow is

```
Initialize CUMULVS data structures (stv_init())
Define data decomposition (stv_decompDefine())
Define data field with a previously defined decomposition (stv_fieldDefine())
Define steering parameters (stv_paramDefine())

Start main iterative loop
    <usual calculation
    nchanged = stv_sendToFE()
    <program response to nchanged steered parameters
End of main iterative loop
```

Before doing anything, the STV_ROOT environment variable should be set, either in \$HOME/.cshrc or equivalent shell startup file. The value of \$STV_ROOT should be the directory where the CUMULVS is, as in:

```
setenv STV_ROOT /home/me/CUMULVS
```

The applications should include the header files of

`fpvm3.h` (Fortran) or `pvm3.h` (C)
`fstv.h` (Fortran) or `stv.h` (C)

Compile the application and link it with either `libfstv.a` or `libstv.a`, depending on whether the application is written in Fortran or C.

Next, start the pvm daemon and run the application.

Start the viewer to manipulate the steering parameters.

Discussion

CUMULVS is fairly easy to use in a Global Arrays application. We successfully testing the inter-operability of Global Arrays with CUMULVS's computational steering capacity. The capacity of CUMULVS's visualization needs further investigation.

Appendix 3: *List of GA functions*

ga_acc.....	16, 17	GA_Init_fence.....	21
ga_access.....	31	ga_initialize.....	12, 13
ga_add.....	26	GA_Initialize.....	12
GA_Add.....	26	ga_initialize_ltd.....	12
ga_add_patch.....	27	GA_Initialize_ltd.....	12
ga_brdcst.....	34	ga_inquire.....	33, 34
GA_Brdcst.....	34	ga_inquire_memory.....	33, 35
ga_check_handle.....	36	GA_Inquire_memory.....	33
GA_Check_handle.....	36	GA_Inquire_name.....	34
ga_compare_distr.....	32	ga_llt_solve.....	29
ga_copy.....	24	GA_Llt_solve.....	29
GA_Copy.....	24	ga_locate.....	31
ga_copy_patch.....	24	ga_locate_region.....	31
ga_create.....	13	ga_lock.....	20
ga_create_irreg.....	14	GA_lock.....	20
ga_create_mutexes.....	20	ga_lu_solve.....	29
GA_Create_mutexes.....	20	GA_Lu_solve.....	29
ga_ddot_patch.....	28	ga_matmul_patch.....	27
ga_destroy.....	15, 20	GA_Matmul_patch.....	27
GA_Destroy.....	15	ga_memory_avail.....	33
ga_destroy_mutexes.....	20	GA_Memory_avail.....	33
GA_Destroy_mutexes.....	20	ga_memory_limited.....	33
ga_dgemm.....	26	GA_Memory_limited.....	33
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ga_dgop.....	34	GA_Nnodes.....	32
GA_Dgop.....	34	ga_nodeid.....	10, 32
ga_diag.....	29	GA_Nodeid.....	32
GA_Diag.....	29	ga_print.....	35
ga_diag_reuse.....	30	GA_Print.....	35
GA_Diag_reuse.....	30	ga_print_distribution.....	35
ga_diag_std.....	30	GA_Print_distribution.....	35
GA_Diag_std.....	30	ga_print_stats.....	35
ga_distribute.....	31	GA_Print_stats.....	35
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ga_error.....	13	ga_read_inc.....	16, 17
GA_Error.....	13	ga_release.....	32
ga_fence.....	21	ga_release_update.....	32
GA_Fence.....	21	ga_scale.....	23
ga_fill.....	23	GA_Scale.....	23
GA_Fill.....	23	ga_scale_patch.....	24
ga_fill_patch.....	24	ga_scatter.....	16, 18, 21, 22
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ga_get.....	16, 17, 37, 38	GA_Set_memory_limit.....	13
ga_idot_patch.....	28	ga_solve.....	29
ga_igop.....	34	GA_Solve.....	29
GA_Igop.....	34	ga_spd_invert.....	29
ga_init_fence.....	21	GA_Spd_invert.....	29

ga_summarize	35	NGA_Fill_patch.....	24
GA_Summarize	35	nga_gather	19
ga_symmetrize	27	NGA_Gather	19
GA_Symmetrize	27	nga_get	16
ga_sync	11, 21, 22	NGA_Get	16
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ga_terminate	11, 13, 15	NGA_Idot	26
GA_Terminate	13	nga_idot_patch.....	28
ga_transpose	27	NGA_Idot_patch.....	28
GA_Transpose	27	nga_inquire.....	34
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GA_Uses_ma	33	NGA_Locate	31
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ga_zero	23	NGA_Locate_region	31
GA_Zero	23	nga_print_patch.....	35
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NGA_Acc	17	NGA_Proc_topology	32
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NGA_Access	31	NGA_Put	16
nga_add_patch.....	27	nga_read_inc	17
NGA_Add_patch.....	27	NGA_Read_inc	17
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NGA_Copy_patch.....	24	nga_release_update.....	32
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NGA_Ddot	26	nga_zdot.....	26
nga_ddot_patch.....	28	NGA_Zdot.....	26
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nga_distribute.....	31	NGA_Zdot_patch.....	28
NGA_Distribute.....	31	nga_zero_patch.....	24
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