

Coarrays in the Context of XcalableMP

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Abstract Coarray features has been implemented into the Omni XcalableMP compiler with a source-to-source translator and layered runtime libraries. Three memory allocation methods for coarrays were implemented for communication libraries GASNet, MPI-3 and Fujitsu's native interface. For the coarray PUT/GET communication, algorithms using DMA (zero-copy) and buffering were introduced. The important techniques for achieving high performance were the non-blocking PUT communication implemented in the runtime library and the optimization for the GET communication in the translator. Using the ping-pong benchmark and the modified version, the fundamental performance was evaluated and analyzed. The MPI version of the Himeno benchmark is ported to coarray version and modified for fully using the non-blocking PUT. As the result of the evaluation, non-blocking coarray version clearly outperformed the original and non-blocking MPI versions.

1 Introduction

XcalableMP (XMP) [1] has complementary programming models of global-view and local-view. The former is a directive-base language extension to the base language Fortran and C, and the latter adopts the coarray features defined in Fortran 2008 [2] and a part of the ones in Fortran 2018 [3]. The purpose of the coarray features as the local-view part of XMP is 1) writing the application programs that is difficult for the global-view programming and 2) writing such important parts of the program that is critical for the performance with easier programming model than the MPI message

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passing. Therefore, the coarray features in XMP must be naturally merged into the global-view XMP language and must perform with high performance comparable to MPI.

The Omni XMP compiler is an open-source implementation developed at RIKEN and the University of Tsukuba [4]. Its kernel is a source-to-source compiler that converts an XMP program into a Fortran program by calling a runtime library. The coarray translator has been implemented into the Omni XMP compiler. Since the images is mapped one-to-one to XMP nodes, each image was implemented as a process, and the definition and reference to coarrays were implemented as the inter-node one-sided communications.

This chapter describes the techniques in the coarray compiler and the runtime library with some evaluation compared with the MPI message passing. In the rest of this chapter, Section 2 introduces the requirements from the coarray features, Section 3 describes the implementation to solve the requirements, and Section 4 evaluates the performance and the productivity of coarray programs. After related work is shown in Section 5, Section 6 concludes this chapter.

2 Requirements from Language Specifications

XMP Fortran language specification [1] supports a major part of coarray features defined in Fortran 2008 standard [2], and intrinsic procedures `CO_SUM`, `CO_MAX`, `CO_MIN` and `CO_BROADCAST` defined in Fortran 2018 standard [3] were supported. And also XMP C language specification extended to support coarray features.

This section introduces the coarray features and what is required to the compiler in order to implement the coarray features.

2.1 Images Mapped to XMP Nodes

In the Fortran standard, an **image** is defined as a instance of a program. Each image executes the same program and has its own data individually. Each image has a different image index k . While the Fortran standard itself does not specify where each image is executed, XMP specifies that images are mapped to executing nodes on a one-to-one basis. Therefore, image k is always executed on executing node k , where $1 \leq k \leq n$ and n is the number of images and also the number of the executing nodes. Since each MPI rank number of `MPI_COMM_WORLD` (0-origin) is always mapped to an XMP node number in order, image k is corresponding to rank $(k - 1)$.

Note that the executing nodes can be a subset of the entire (initial) node set. For example, two distinct node sets can execute two coarray subprograms concurrently. The first executing images at the start of the program is the entire images. Coarray features are compatible to the ones of the Fortran standard unless the `TASK` and `END`

TASK directives are used. If the execution encounters a TASK directive specified with a subset of nodes, the corresponding subset of the images will be the executing images for the task region. The current number of images and my image number, which are given by inquire functions `num_images` and `this_image`, also match with the executing images, and the SYNC_IMAGES statement synchronizes among the executing images. When the execution encounters the END TASK directive corresponding to the TASK directive, the set of executing image is reinstated.

Requirement to the implementation. The runtime library should manage the executing image set and the current image index in stack in order to reinstate them at the exit point of the task.

2.2 Allocation of Coarrays

A **coarray** or a coarray variable is a variable that can be referred from the other images. A coarray with the ALLOCATABLE attribute is called an **allocatable coarray**, otherwise called a non-allocatable coarray. A non-allocatable coarray may not be a pointer and must have an explicit shape and the SAVE attribute. In order to help intuitive understanding, we call a non-allocatable coarray as a **static coarray**. The lifetime of a static coarray is throughout execution of the program on all images even if the coarray is declared in a procedure called with a subset of images.

On the other hand, an allocatable coarray is allocated with the ALLOCATE statement and freed either explicitly with the DEALLOCATE statement or implicitly at the end of the scope in which the ALLOCATE statement is executed (**automatic deallocation**).

Static coarrays can be declared as scalar or array variables as follows:

```
real(8), save :: a(100,100)[*]
type(user_defined_type), save :: s[2,2,*]
```

The square bracket notation in the declaration distinguishes coarray variables from the others (non-coarrays). It declares the virtual shape of the images and the last dimension must be deferred (as '*').

Allocatable coarrays can be declared as follows:

```
real(8), allocatable :: b(:,,:)[:]
type(user_defined_type), allocatable :: t[:,:,:]
```

A notable constraint is that at any synchronization point in program execution, coarrays must have the same dimensions (sizes of all axes) between all images (**sym-metric memory allocation**). Therefore, an static coarray must have the same shape between all images during the program execution, and an allocatable coarray must be allocated and deallocated collectively at the same time with the same dimensions between the executing images. Thanks to the syn-metric memory allocation rule, all executing images can have the same symmetrical memory layout, which makes it possible to calculate the address of the remote coarray with no prior inter-image communication.

Requirement to the implementation. Static coarrays must be allocated and made accessible remotely before the execution of the user program, and made inaccessible remotely and be freed after the execution of the user program. In contrast, allocatable coarrays must be allocated and made accessible remotely when the ALLOCATE statement is encountered, and made inaccessible remotely and be freed when the DEALLOCATE statement or the exit point of the scope that the corresponding ALLOCATE statement is encountered is encountered.

2.3 Communication

Coarray features in XMP include three types of communications between images, i.e., reference and definition to remote coarrays, collective communications (intrinsic subroutines CO_SUM, CO_MAX, CO_MIN and CO_BROADCAST), and atomic operations (ATOMIC_DEFINE and ATOMIC_REF). Collective communications and atomic operations are similar to the ones in MPI library. Communication for reference and definition to remote coarrays are characteristic for coarray features.

PUT communication is caused by an assignment statement with a **coindexed variable** as the left-hand side expression, e.g.,

$$a(i,j)[k] = \alpha * b(i,j) + c(i,j)$$

This statement is to cause the PUT communication to the array element $a(i,j)$ on image k with the value of the left-hand side. Using Fortran array assignment statement, array-to-array PUT communication can be written easily. E.g., the following statement causes $M \times N$ -element PUT communication.

$$a(1:M,1:N)[k] = \alpha * b(1:M,1:N) + c(1:M,1:N)$$

GET communication is caused by referencing the **coindexed object**, which is represented by a coarray variable with cosubscripts enclosed by square brackets, e.g., $s[1,2]$ and $a(i,j)[k]$, where s and a are scalar and two-dimensional array coarrays, respectively. A coindexed object can appear almost in any expressions including array expressions.

Requirement to the implementation. To implement definition/reference to coindexed variable/object, PUT/GET one-sided communication is suitable to be used. To avoid costly processing such as remote procedure call, RDMA (Remote Direct Memory Access)-based implementation is desirable. On PUT/GET communication for large data, redundant multiple memory copies should carefully be avoided for all software layers, the communication library, the runtime, the Fortran library, and the object.

2.4 Synchronization

The access order of coarrays between images is explicitly controlled by the programmer using the **image control statement**, such as `SYNC ALL` and `SYNC IMAGES` statements. It allows the compiler system to make PUT/GET communication asynchronous. The sequence of execution between the image control statements is called as a **segment**. An asynchronous communication must be completed by the end of the segment.

While, inside each image, the compiler must maintain data dependency as before even if it contains coarray communications. It suppress the **non-blocking communication**, which postpones waiting for communication completion. In order to keep data dependency among the definitions and references to the same coarray in the same segment, the non-blocking communication should be restricted. The example bellow in which the same remote coarray is accessed some times inside the same segment.

```

1      if (this_image()==1) then
2          a[2]=
3          =a[2]
4          a[2]=
5          a[2]=
6      endif

```

Between lines 2 and 3, the completion wait for PUT communication is necessary to avoid referencing data that is not defined completely. Similarly, between lines 3 and 4, the completion wait for GET communication is necessary to avoid referencing data that is getting updated. However, between lines 4 and 5, the completion wait is not necessary. The issue of race condition on image 2 cannot be avoid by the completion wait on image 1 in general and avoiding it is the matter of the programmer.

Requirement to the implementation. Unless the same remote data is accessed from the same segment, completion of non-blocking completion is can be delayed until the end of the segment. Because the data received by the GET communication is usually referenced soon, non-blocking GET communication is hard to be used. So if GET communication is always on blocking, only the flow dependency (between lines 2 and 3) should be care of.

2.5 Subarrays and Data Contiguity

Except dummy argument, an array is fully **contiguous** across the dimensions. A subarray of the array can be fully or partially contiguous or non-contiguous. For example, if an array is declared with the shape `a(1:M, 1:N)`, the whole array (referenced as `a` or `a(:, :)` or `a(1:M, 1:N)`) is fully contiguous and a subarray `a(2:5, 3)` is partially contiguous. We defined a term **contiguous length** as the length how long the data is partially contiguous. For example, the contiguous lengths of `a(2, 3)` and `a(2:5, 3)` are 1 and 4 respectively. `a(1:M, 1:3)` is two-dimensionally contiguous

and has contiguous length $2 \times M$. $a(1:M-1, 1:3)$ is one-dimensionally contiguous and has contiguous length $(M - 1)$.

Requirement to the implementation. For high-performance communication, it is important to find the contiguous length across the dimensions. Because, thousands of bytes of contiguous data is needed to be comparable to the communication latency in general, and only the first dimension of the array is not always long enough.

2.6 Coarray C Language Specifications

XMP language specification extends C language to support coarray features. Array notations such as subarray and array assignment statement is adopted into C language. In XMP/C, a coarray is a data object but is not a pointer. A coarray is either 1) of basic type, 2) a structure whose any component is not a pointer, or 3) an array of 1 or 2 or 3.

XMP/C also has static and allocatable coarrays. Coarray variables declared directly in the file and declared with the `static` attribute are static. Coarray variables can be allocated with intrinsic functions.

3 Implementation

3.1 Omni XMP Compiler Framework

The CAF translator was added into the Omni XMP compiler [4] as shown in Figure 1. The Omni XMP compiler is a source-to-source translator that converts XMP programs into the base language (Fortran or C). The component ‘coarray translator’ is located in front of the XMP translator to solve coarray features previously. The output of the decompiler is a standard Fortran/C program that may include calls to the XMP runtime library.

The following procedures are generated in advance or in the coarray translator to initialize static coarray variables prior to the execution of the user program:

- The built-in main program calls subroutine `xmpf_traverse_init`, the entry procedure of initialization subroutines, before executing the user main program.
- Subroutine `xmpf_traverse_init` is generated by the coarray translator to call initialization subroutines corresponding to all user-defined procedures.
- Each initialization subroutine `xmpf_init_foo` is generated from user-defined procedure `foo` by the coarray translator. It initializes all static coarrays declared in `foo`.

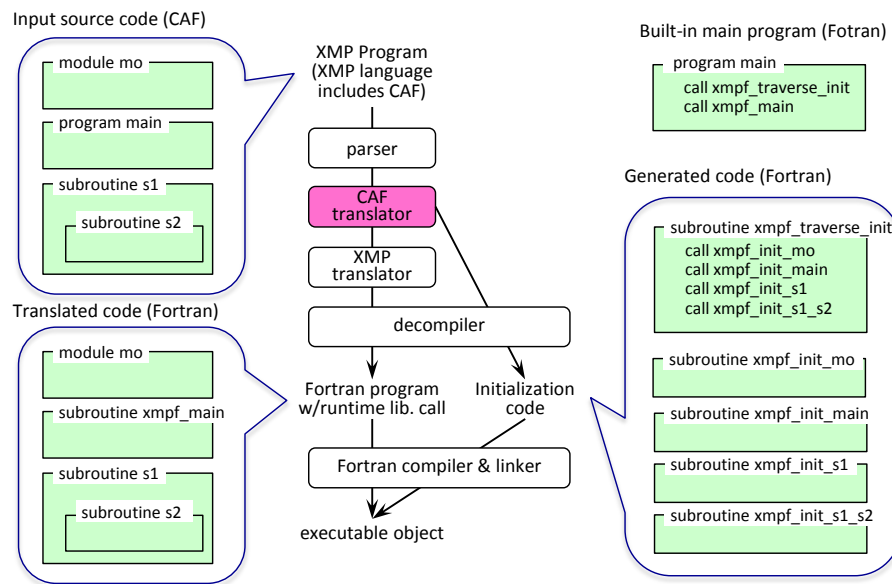


Fig. 1 XMP compiler and an example of coarray program compilation
CAF translator → coarray translator

3.2 Allocation and Registration

To be accessed using the underlying communication library, the allocated coarray data must be registered to the library. The registration contains all actions to allow the data to be accessed from the other nodes, including pin-down memory, acquirement of the global address, and sharing information among all nodes.

3.2.1 Three methods of memory management

The coarray translator and the runtime library implements three methods of memory management.

- The **Runtime Sharing (RS) Method** allocates and registers a large memory for all static and dynamic coarrays at the initialization phase. The registered memory is shared by all static and allocatable coarrays.
- The **Runtime Allocation (RA) Method** allocates and registers a large memory for all static coarrays at the initialization phase. And it allocates and registers each allocatable coarray at runtime.

- The **Compiler Allocation (CA) Method** allocates all coarray objects by the Fortran system (at compile time or at runtime) and the address is passed to the runtime library to be registered.

For the RS and RA methods, because the allocated memory address is determined in the runtime library, the object code must accept the address allocated inside the runtime system as an address of a real Fortran variable. To make this connection, it was necessary to use the Cray pointer, which is not in the Fortran standard. In the case of the CA method, the runtime library accepts the address allocated in the Fortran system, and registers to the communication library.

3.2.2 Initial Allocation for Static Coarrays

Static coarrays are allocated and registered in the initialization subroutines `xmpf_init_foo`.

On the RS and RA methods, static coarrays are initialized before the execution of the user program, as follows.

- In the first pass, all sizes of static (non-allocatable) coarrays are summed. The size of each static coarray is evaluated from the lower and upper bounds specified in the dimension declaration statement of each coarray. The lower and upper bound expressions, possibly including binary and unary operations, reference to name of constants, and basic intrinsic functions such as min/max and sum, are evaluated by constant folding techniques. Since the size of the structure that contains allocatable or pointer components differs depending on for the target compiler, the coarray translator get the necessary parameters to calculate the size of structures at the build time.
- Then, the total size of static coarrays is allocated and the address and the size is registered to the underlying communication library.
- In the second pass, the addresses of the all coarrays are calculated to share the registered data. Due to the language specification, sizes of the same coarray are the same among all images (nodes). So the offset from the base address of the registered data for each coarray can be the same among all images.

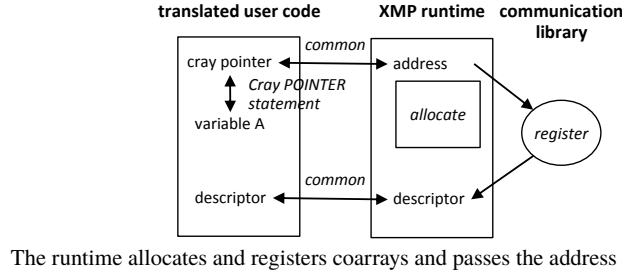
In the RS method, allocatable coarrays are also shared the registered memory. The total size of the memory to be registered should be specified with an environment variable by the user. While in the RA method, the total size is fully calculated by the runtime library and no information is required to the user because allocatable coarrays will be dynamically allocated on the other memories.

On the CA method, the Fortran processor allocates each coarray and then the runtime library registers the address. Each static coarray is converted into a common (external) variable to share between the user-defined procedure (say *foo*) and its initialization procedure (`xmpf_init_foo`). The data is statically allocated by the Fortran system similarly to the usual common variable. the address is registered in the initialization procedure via the runtime library.

3.2.3 Runtime Allocation for Allocatable Coarrays

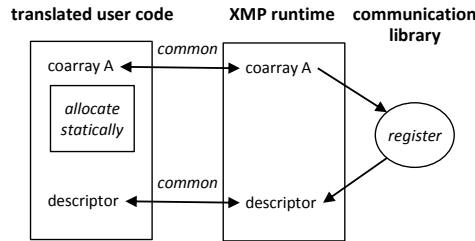
For the RS method, the runtime library has a memory management system for cutting out and retrieving memory for each allocation and deallocation of coarrays.

Figure 2 illustrates the memory allocation and registration for allocatable coarrays on the RA and CA methods.



The runtime allocates and registers coarrays and passes the address to the user code.

(a) RA method



The user code allocates coarrays and causes the runtime to register with the address.

(b) CA method

Fig. 2 Memory allocation for coarrays in RA and CA methods

These methods are properly used by the underlying communication library. On GASNet, only the RS method is adopted because its allocation function can be used only once in the program. On MPI-3, the CA method is not suitable because frequent allocation and deallocation of coarrays cause expensive creation and freeing MPI windows. Over FJ-RDMA, the RS method has no advantage over the other methods. Since the allocated address is used for registration to FJ-RDMA, no advantage was found for managing memory outside of the Fortran system. The unusual connection through the Cray pointer causes the degrade of the Fortran compiler optimization.

3.3 PUT/GET Communication

To avoid disturbing the execution on the remote image, PUT and GET communications are implemented always using Remote Direct Memory Access (RDMA) provided by the communication library (except coarrays with pointer/allocatable structure components). In contrast, local data access is selective between using Direct Memory Access (DMA) or using a local buffer. For the buffer scheme, one of four algorithms will be chosen.

3.3.1 Determining the possibility of DMA

Coarray variables must be registered when allocated to be the target of RDMA communication. In contrast, since the local data, which is the source of PUT or the destination of GET, was not registered or not linked to registered information, it could not to be the target of DMA communication. It had to be communicated via the registered buffer.

When the local data is an entire or a part of coarray, the coarray must be registered and efficient DMA-RDMA communication can be made. Since the analysis at compile time is limited, we had implemented the detector in the runtime library using binary-tree search as follows.

1. When a chunk of coarray data is registered to the communication library, runtime library adds the set of the local address and the size into a sorted table called `SortedChunkTable`. The sort key is the local base address of the data.
2. When a chunk of coarray data is deregistered from the communication library, runtime library deletes the record in `SortedChunkTable`.
3. When a PUT or GET runtime library is called corresponding to a reference/definition to a coindexed object/variable, the local address is searched in `SortedChunkTable` with binary search. The local data is already registered if $addr_i \leq addr < addr_i + size_i$ for any i , where $addr$ is the said local address and $addr_i$ and $size_i$ are the i -th address and size in `SortedChunkTable`, respectively.

If the communication data is large, the cost of procedure 3 is relatively small enough and it is worth to be used. If the data is small, buffering algorithm as shown in Section 3.3.2 may be better.

3.3.2 Buffering Communication Methods

For the buffer scheme, one of four algorithms will be chosen depending on three parameters, the size of the local buffer B and the local and remote contiguous lengths N_L and N_R . B should be large enough to ignore communication latency overhead and we use about 400 kilo-bites in default. Unlike the case of MPI message passing, coarray PUT/GET communication requires only one local buffer for any numbers of other images. N_L and N_R can be evaluated at runtime. The Fortran syntax

guarantees that N_L is a multiple of N_R or N_R is a multiple of N_L . An algorithm to get the contiguous length is shown in the paper [5].

Table 1 summarizes our algorithm for PUT/GET communication for five cases. The unit size is the chunk length of the PUT/GET communication. Case 0 shows the algorithm using RDMA-DMA PUT/GET communication and Cases 1 through 4 shows the algorithms using RDMA and local-buffering. Due to its strict condition, the DMA scheme is rarely used. And it is not always faster than the buffering scheme cases 2 and 3 because of the difference of the unit sizes. The merit of cases 2 and 3 is that the unit size is extended to a multiple of N_L by gathering number of short contiguous data in the buffer, or by scattering from the buffer into number of short contiguous data.

Table 1 Summary of the PUT/GET algorithm related to N_L , N_R and B

scheme	case	condition	unit size
DMA		Local data is registered.	$\min(N_L, N_R)$
buffering	1	$N_R \leq B, N_R \leq N_L$	N_R
	2	$N_L < N_R \leq B$	N_R
	3	$N_L < B < N_R$	multiple of N_L ($\leq B$)
	4	$B < N_R, B \leq N_L$	B (or less than B at last)

scheme	case	PUT action for each unit	GET action for each unit
DMA		put once	get once
buffering	1	buffer once and put once	get once and unbuffer once
	2	buffer for each N_L , and put once	get once, and unbuffer for each N_L
	3	buffer for each N_L , and put once	get once, and unbuffer for each N_L
	4	buffer once and put once	get once and unbuffer once

3.3.3 Non-blocking PUT communication

For higher performance, the PUT communication should be in non-blocking and the completion wait should be delayed to the end of the segment. It seems a very rare case that writing and reading the same remote data from the same image in the same segment, as described in Section 2.4. However, it is difficult to detect with low cost. Because the subscripts and image indices are often variable expressions, the compiler rarely select non-blocking and usually generates safe but slow code. We do not have reasonable solution for this issue.

In the current implementation, the user selects blocking or non-blocking for PUT communication at runtime with the environment variable.

3.3.4 Optimization of GET communication

A reference to an array coindexed object is converted to a call of a runtime library function that returns a Fortran array value. For example, array assignment statement:

```
b(j1:j2) = a(i1:i2)[k]
```

is converted to:

```
b(j1:j2) = xmpf_coarray_get_generic(dp_a,k,a(i1:i2))
```

by the coarray translator, where `dp_a` is the descriptor of coarray `a`. The issue is the result of the library function is an array value, which causes several numbers of memory copies. As a countermeasure, we optimized specific but common case by the translator. If a coindexed object is only the right-hand side of an array assignment statement, the entire assignment statement can be converted into one library call. The example above satisfies the condition, so it can be converted again as follows:

```
call xmpf_coarray_getsub_generic(dp_a,k,a(i1:i2),b(j1:j2))
```

In this runtime library subroutine, the variable `b(j1:j2)` is expected to be the local target of GET communication instead of the local buffer that would be generated by the Fortran runtime.

3.4 Runtime Libraries

The layer of the runtime libraries are shown in Figure 3. One of three communication libraries is selected at the build time of the Omni compiler. The coarray runtime consists of layered three libraries. The **Fortran wrapper** mediates the arguments and the result value of the translated user program (written in Fortran) and ULR (written in C). The **upper-layer runtime (ULR) library** performs the algorithms described above in this section. The **lower-layer runtime (LLR) library** abstracts the difference between the communication libraries except the memory management of coarray data.

3.4.1 Fortran wrapper

Each set of Fortran wrapper procedures has a generic name and dozens of the corresponding specific names. For example, the object code contains a call to a function with the generic name “`xmpf_coarray_get_generic`”. If the data is two-dimensional array of 16-byte complex type, the Fortran compiler selects the corresponding specific name “`xmpf_coarray_get2d_z16`” at compile time, and generates the object code with calling a ULR function by the specific name.

The Fortran wrapper accepts Fortran array notations as the arguments and the result variable, and converts them into some structures which can be handled in the

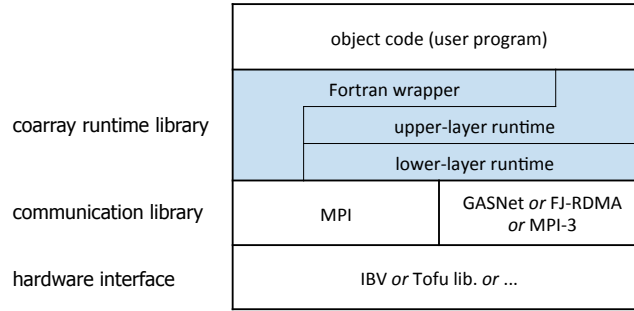


Fig. 3 Software stack for coarray features

runtime library written in C. It also converts a C pointer to a Fortran pointer with the shape, using the Cray pointer.

The Fortran wrapper calls ULR procedures basically and directly MPI library functions for collective communications.

3.4.2 Upper-layer runtime library (ULR)

The major role of ULR is performing the algorithms for coarray data allocation/registration (Section 3.2) and PUT/GET communications (Section 3.3). Additionally for atomic communications caused by intrinsic subroutines `ATOMIC_DEFINE` and `ATOMIC_REF`, ULR calls the corresponding function of LLR after address calculation.

3.4.3 Lower-layer runtime library (LLR)

LLR basically abstracts the difference between the communication libraries. The only exception is about allocation and registration of coarray data. Major functions are shown below.

- Functions to allocate and register coarray variables, and functions to register coarray variables that are already allocated. They are alternatively used in the RS and RA methods and in the CA method. Corresponding to each, a set of functions to deregister and deallocate and a set of functions to deregister are provided.
- Fundamental functions for RDMA-DMA GET communication and DMA-RDMA PUT communication. It is assumed that both remote and local data are previously registered. Blocking and non-blocking can be switched.

- Functions corresponding to image control statements, atomic subroutines, and inquire functions.

LLR also has the features for multi-dimensional data developed for the C implementation, which are not used in the Fortran implementation because it is solved in ULR.

3.4.4 Communication libraries

MPI-3 can be selected for all platform on which MPI-3 is implemented. Coarrays are registered and deregistered at the start and end point of the MPI window. Coarrays are performed one-sided communication by `MPI_Put` and `MPI_Get`, and synchronized by `MPI_Win_fence`. Implementation on MPI incurs certain costs for dynamic allocation of coarrays and waiting for communication completion.

GASNet can be selected for more advanced implementation over InfiniBand. Since allocation and registration of are inseparable and can be done only once on GASNet, the implementation allocates and registers a pool of memory whose size should be large enough to contain all static and allocatable coarrays. The XMP runtime should allocate and deallocate coarrays not using the Fortran library but using the memory manager made for the pool.

FJ-RDMA can be selected for the implementation over Tofu interconnect of the K computer and Fujitsu PRIMEHPC FX series supercomputers. Basically, each coarray is allocated by the Fortran library and registered the address with the FJ-RDMA interface `FJMPI_Rdma_reg_mem`. And it is deregistered with `FJMPI_Rdma_dereg_mem` before deallocated (freed) by the Fortran library. One-sided communication is performed with `FJMPI_Rdma_put` and `FJMPI_Rdma_get`.

4 Evaluation

We evaluated the Omni XMP coarray compiler on the environments shown in Table 2.

4.1 Fundamental Performance

Using EPCC Fortran Coarray micro-benchmark [6], we evaluated ping-pong performance of PUT and GET communications compared with `MPI_Send/Recv`. The codes are shortly shown in Table 3.

Corresponding to the codes in Table 3, Figure 4 shows how data and messages are exchanged between two images or processes. In coarray PUT (a) and GET (b), inter-image synchronization is necessary for each end of phases to make the passive image active and to make the active image passive. While, in MPI message-passing (c) and (d), such synchronization is not necessary because both processes are always

Table 2 Specs of the computers and evaluation environment

	RIKEN RCCS The K computer	RIKEN RCCS HOKUSAI GreatWare Fujitsu PRIMEHPC FX100	CCS, University of Tsukuba HA-PACS/TCA
CPU	SPARK64™VIIIfx, 2GHz, 128 Gflop/s, 8-core, 1CPU/node	SPARK64™XIIfx, 1.975GHz, 1CPU/node, 4-SIMD × 32-core	E5-2680 v2 (Ivy Bridge), 10- core, 224Gflop/s, 2CPU/node
memory	16GB/node, bandwidth 64GB/s	32GB/node, bandwidth 480GB/s	128GB/node, 119.4GB/s
inter- connect	Tofu	Tofu2, 12.5GB/s × 2	InfiniBand FDR, 7GB/s
coarray	Omni XscalableMP 1.3.1	Omni XscalableMP 1.3.1	Omni XscalableMP 1.3.1
Fortran	Fujitsu Fortran 2.0.0	Fujitsu Fortran 2.0.0	Intel Fortran 16.0.4
MPI	Fujitsu MPI 2.0.0	Fujitsu MPI 2.0.0	Intel MPI 5.1.3
comm. layer	Tofu library	Tofu library	GASNet 1.24.2 (IBV-conduit, built with Intel compilers)

Table 3 pingpong-code.pdf

	PUT version	GET version	MPI version
ping phase	if (me == 1) then x(1:n)[2] = x(1:n) sync images(2) else if (me == 2) then sync images(1) end if	if (me == 1) then sync images(1) else if (me == 2) then x(1:n) = x(1:n)[1] sync images(1) end if	if (id == 0) then call MPI_Send(x, n, ... 1, ...) else if (id == 1) then call MPI_Recv(x, n, ... 0, ...) end if
pong phase	if (me == 1) then sync images(2) else if (me == 2) then x(1:n)[1] = x(1:n) sync images(1) end if	if (me == 1) then x(1:n) = x(1:n)[2] sync images(2) else if (me == 2) then sync images(1) end if	if (id == 0) then call MPI_Recv(x, n, ... 1, ...) else if (id == 1) then call MPI_Send(x, n, ... 0, ...) end if

me is the image index. id is the MPI rank number.

active. On the other hand, MPI message-passing has its own overhead that coarray PUT/GET does not have. Because the eager protocol (c) does not use RDMA, the receiver must copy the received data in the local buffer to the target. The larger the data, the greater the overhead cost. In the rendezvous protocol (d), negotiations including remote address notification are required prior to the communication. The overhead cost is not negligible when the data is small.

The result of the comparison between coarray PUT/GET and MPI message passing is shown in Figure 5. As the underlying communication libraries, FJ-RDMA and MPI-3 are used on FX100 and GASNet and MPI-3 are used on HA-PACS. GET(a) and GET(b) are using the code without and with the optimization described in Section 3.3.4, respectively. Bandwidth is the communication data size per elapsed time, and latency is half of the ping-pong elapsed time. The difference between GET(a)

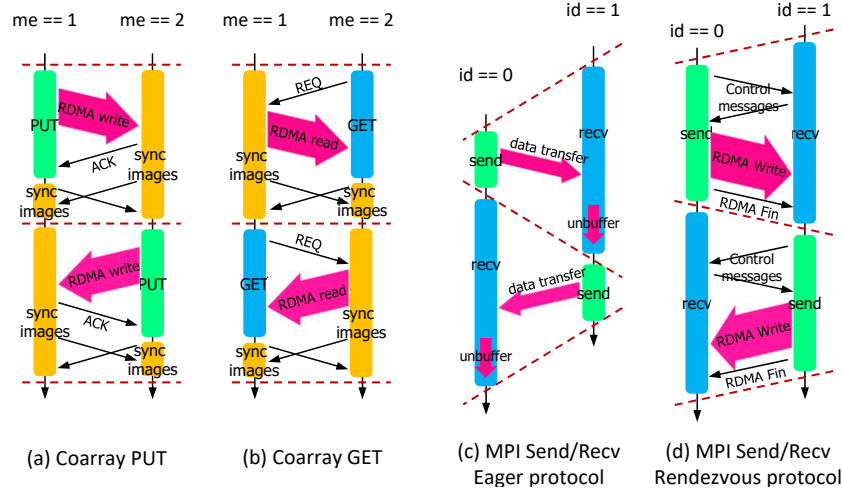


Fig. 4 pingpong-fig.pdf

and (b) is the compile-time optimization level of the coarray translator described in Section 3.3.4.

As the result, the following was found about coarray PUT/GET communication.

Bandwidth Coarray PUT and GET are slightly outperforms MPI rendezvous communication for large data on FJ-RDMA and MPI-3. On FJ-RDMA/FX100 (a), the bandwidth of PUT and GET(b) are respectively +0.1% to +18% and -0.4% to +9.3% higher than MPI rendezvous in the rendezvous range of 32k through 32M bytes. Also on MPI-3/HA-PACS, respectively +0.3% to +0.8% and +0.1% to +1.3% higher in the rendezvous range of 512k through 32M bytes.

It was confirmed from the runtime log that zero-copy communication was performed both in PUT and GET(b) by selecting DMA scheme described in Section 3.3.1.

However, on GASNet/HA-PACS (c), PUT and GET(b) has only about 60% bandwidth for large data than MPI rendezvous. It is presumed that data copy was caused internally.

Latency On FJ-RDMA (a) and MPI-3 (b) and (d), PUT and GET(b) have larger (worse) latency than MPI eager communication, in the range of $\leq 16\text{kB}$ on FX100 and $\leq 256\text{kB}$ on HA-PACS.

Coarray on GASNet (c) behaves differently than other cases on (a), (b) and (d). Though the latency is larger than the one of MPI for all data sizes, the difference is smaller than the other cases. At data size 8B, the latency of PUT is $2.93\mu\text{s}$ and 2.1 times larger than the one of MPI while $5.73\mu\text{s}$ and 3.7 times larger on the case of MPI-3 (d).

Effect of GET optimization For all ranges of all cases, GET(a) has smaller bandwidth and larger latency than GET(b). On FJ-RDMA (a), the bandwidth is 1.41

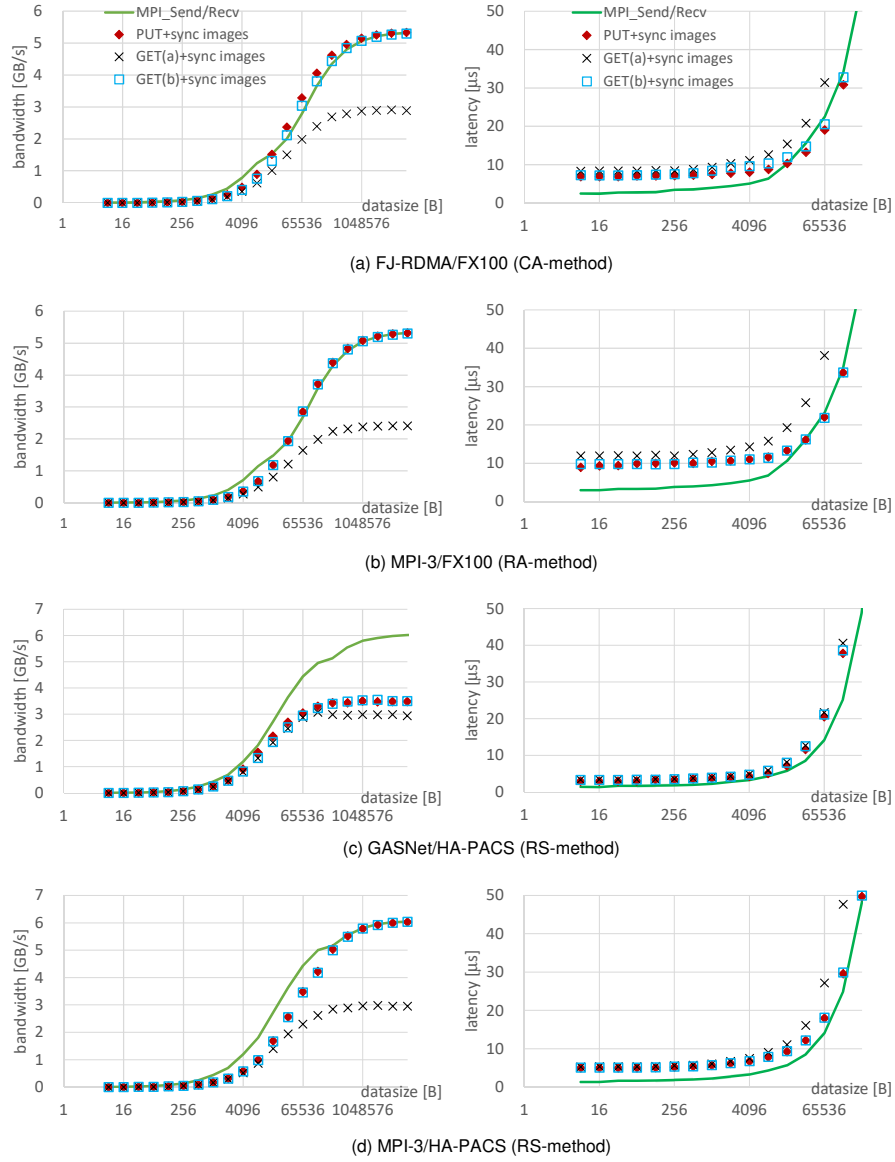


Fig. 5 Ping-pong performance on Fujitsu PRIMEHPC FX100 and HA-PACS/TCA

to 1.85 times improved in the range of 32kB to 32MB by changing the object code of GET(a) to (b). We found GET(a) caused two extra memory copies; one is performing the array assignment by the Fortran library and the other is the copy from the communication buffer to the result variable of the array function `xmpf_coarray_get_generic`. The optimization described in Section 3.3.4 has eliminated these two data copies.

The issue is the large latency of coarray PUT/GET communication. In the next subsection, it is discussed how it should be solved by the compiler and the programming.

4.2 Non-blocking Communication

For latency hiding, asynchronous and non-blocking features can be expected on coarray PUT communication. The principle is shown in Figure 6.

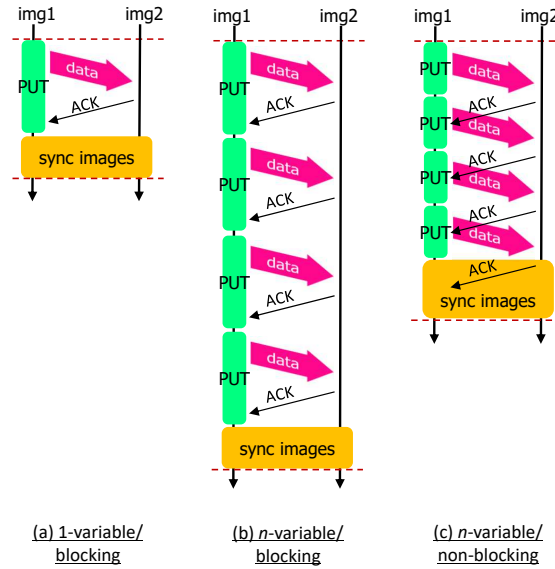


Fig. 6 Blocking and non-blocking PUT communications

Figure 6 (a) illustrates the half pattern of the ping-pong PUT communication. Coarray one-sided communication is basically asynchronous unless synchronization

is explicitly specified. Therefore, multiple communications without synchronization between them, as shown in (b), is closer to actual applications. In addition, it can be optimized using non-blocking communication as shown in (c). Blocking and non-blocking communications can be switched with the runtime environment variable in the current implementation of the Omni compiler. In MPI message passing, non-blocking communication can be written with `MPI_Isend`, `MPI_Irecv` and `MPI_Wait`.

Figure 7 compares blocking/non-blocking coarray PUT and MPI message passing communications. Two original graphs are the same as the ones of Figure 5 (a). Other four graphs display the result of 8-variable ping-pong program, which repeats the ping phase sending eight individual variables from one to the other in order and the pong phase doing similarly in the opposite direction. Each block size indicates the size of variables and latency includes the time for eight variables.

The following was found from the results:

- Non-blocking PUT significantly improves the latency of PUT communication. It is 4.63 times faster than blocking PUT on average from 8B to 8kB. Compared to the original PUT, it performs 8 times the communication in just 2.11 times longer on average from 8B to 8kB. Hiding completion wait behind communication (Figure 6 (c)) greatly improves the performance.
- Reduction of synchronization (Figure 6 (b)) itself does not improve the performance. Compared to the original blocking PUT, 8-variable blocking PUT has 9.5 to 10.1 times larger latency for 8 times larger data.
- Unless data size exceeds about 8kB, the latency of non-blocking PUT is not depend on the amount of data. The graph of non-blocking PUT is very flat within $\pm 4\%$ over the range from 8B to 4kB.
- MPI eager communication has no effect with non-blocking for latency hiding. Eager protocol including receiver's unbuffering process seems not suitable for non-buffering.
- Non-blocking coarray PUT outperforms MPI eager message-passing except for very fine grain data. Latency of 8-variable non-blocking PUT is -9% to 54% and 18% to 61% compared to 8-variable blocking and non-blocking MPI eager, respectively. Only at two plots of 8B and 16B, non-blocking PUT is 4% and 9% slower than blocking MPI. Otherwise, it is faster than MPI eager, and the more block size, the larger difference of the latencies.

4.3 Application Program

Himeno benchmark is a part of 2D Poisson's equation solver using the Jacobi iteration method [7]. The MPI version of Himeno benchmark is a strong scaling program

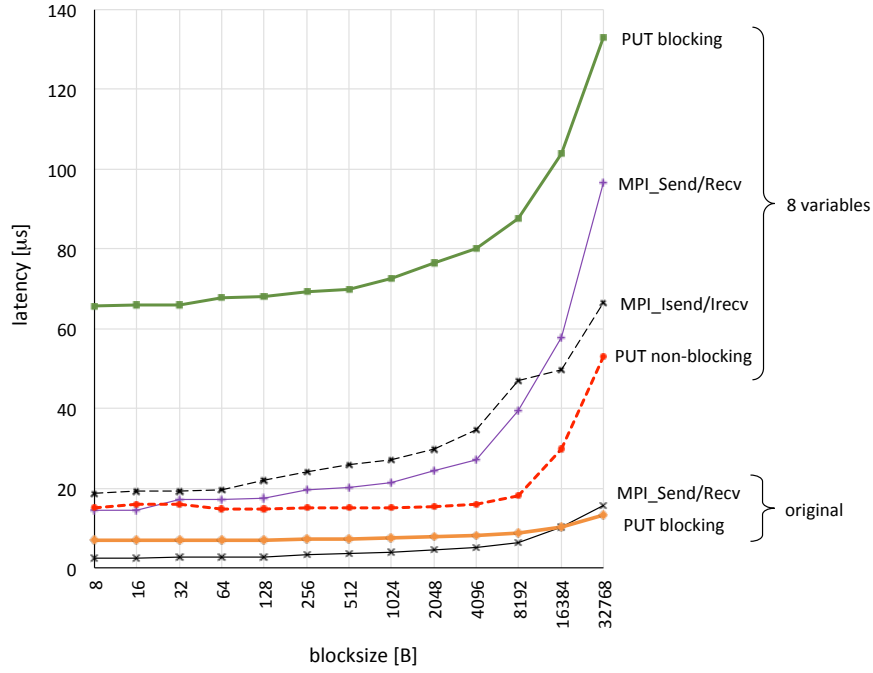


Fig. 7 8-variable ping-pong latency on PRIMEHPC FX100

distributed up to three-dimensional nodes. The K computer shown in Table 2 was used in this evaluation.

4.3.1 Coarray version of Himeno benchmark

For competition, we prepared the following three versions of Himeno programs.

MPI/original The original MPI version of Himeno benchmark was used as a two-dimensionally distributed in the y and z axes. The x axis was automatically SIMD-vectorized by the Fortran compiler. The program executes computation and communication parts repetitively. The communication part consists of two steps, z-axis direction communication, and then y-axis direction communication, as shown in Figure 8 (a). Each communication is written with non-blocking MPI message passing and completion wait at the end of each step.

MPI/non-blocking The 2-step communication was replaced with non-blocking scrambled communication, as shown in Figure 8 (b). With this replacement, the number of communications increases from 4 to 8 per node, but all communications become independent and can be non-blocking.

Coarray PUT/non-blocking The communication pattern is the same as the one of MPI/non-blocking. The data was declared as a coarray and each communication was written with a coarray PUT, i.e., an assignment statement with coindexed variable as the left-hand side. Since the right-hand side of the statement is the reference to the same variable as the left-hand side coarray, the PUT communication was converted to zero-copy DMA-RDMA communication.

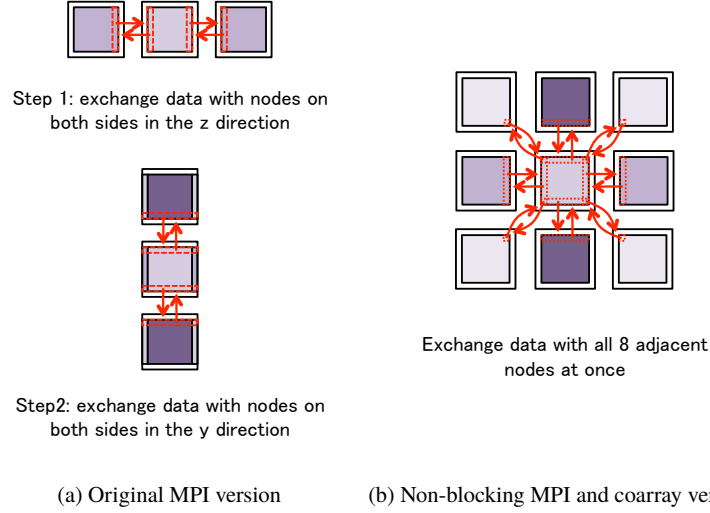


Fig. 8 Two algorithms of stencil communication in Himeno benchmark

4.3.2 Measurement Result

Figure 9 shows the measurement results for Himeno sizes M, L, and XL, executed on 1×1 , 2×2 , 4×4 , \dots , 32×32 nodes on the K computer. The following results were obtained:

- PUT non-blocking was the fastest in 76% of the measurement points of the graph. On 1024 nodes, it is 1.2%, 27% and 42% faster than MPI original for sizes M, L, and XL, respectively.
- As a result of analyzing the contents of elapsed time, it was confirmed that the difference of the performance is caused by the difference in communication time. As shown in (b) and (c), communication times of PUT non-blocking are 56% and 51% of the ones of MPI blocking on 256 nodes, respectively on L and XL sizes.
- MPI non-blocking is not always faster than MPI original. The effect of non-blocking seems to be limited in MPI.

4.3.3 Productivity

Table 4 compares the scale of the source codes. The following features can be found.

- PUT blocking requires less characters for programming than others, especially in subroutines `initcomm` and `initmax`. The MPI programmer must describe Cartesian to represent neighboring nodes in `initcomm`, and must declare MPI vector types to describe the communication pattern in `initmax`. In contrast, the coarray programmer easily represent neighboring images with coindex notation, e.g., `[i, j-1, k]`, and communication patterns with subarray notations, e.g., `p(1:imax, 1:jmax, 1)`.
- Fortran statement of MPI program tends to be longer than coarray's. Because, comparing PUT non-blocking to MPI non-blocking, the number of characters is one third while the number of statements is almost the same. This means that coarray program is more compact than the MPI program for each statement. MPI library functions often require long sequence of arguments.

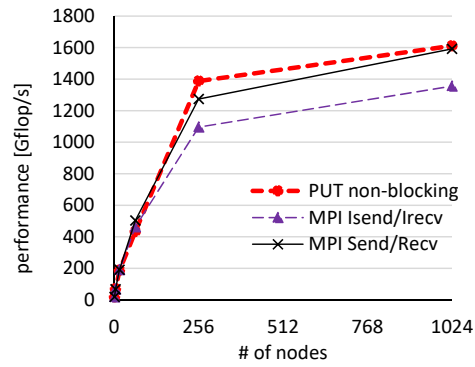
Table 4 Comparison of source code scales for Himeno benchmark

subroutine	MPI original			MPI non-blocking			PUT non-blocking		
	LOC	SOC	chars	LOC	SOC	chars	LOC	SOC	chars
jacobi	50	33	1546	50	32	1546	43	31	1314
initcomm	65	39	1724	80	54	2380	19	19	421
initmax	95	77	2336	115	85	2939	71	71	1584
sendp	152	59	3724	299	91	7617	96	96	2435
others	248	225	5872	250	227	5923	232	231	5276
TOTAL	610	433	15202	794	489	29495	461	448	11030

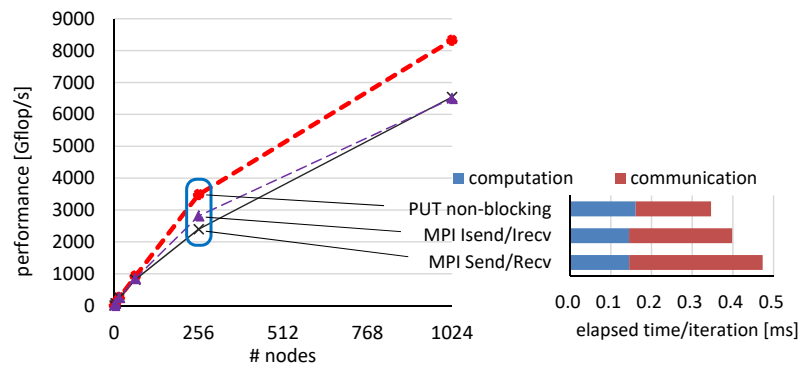
LOC: Number of lines of codes excluding comment and empty lines.
 SOC: Number of Fortran statements, which may span multiple lines.
 chars: Number of characters excluding those in comment lines.

5 Related Work

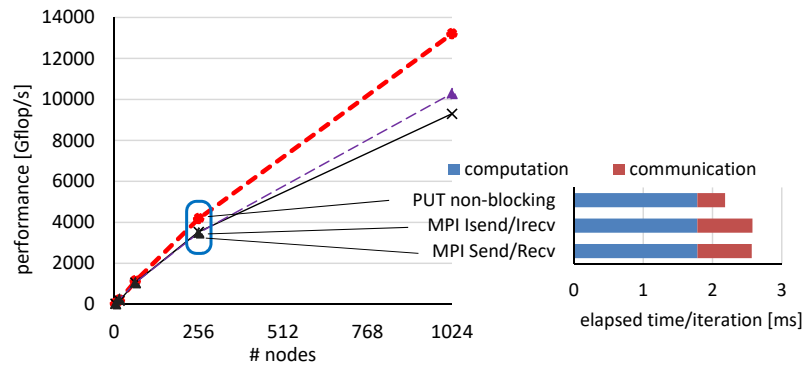
The University of Rice has implemented coarray features with their own extension called CAF2.0 [8]. It is a source-to-source compiler based on the ROSE compiler. GASNet is used as its communication layer. Similarly to our RS and RA methods, they use the Cray pointer to pass the data allocated in C into Fortran. Houston University developed UH-CAF onto the Open64-base OpenUH compiler [9]. It supports coarray features defined in the Fortran 2008 standard. As the communication layer, GASNet and ARMCI can be used selectively. OpenCoarrays is an open-source software project [10]. It is an library which can be used with GNU Fortran (gfortran)



(a) Himeno Size-M (256x128x128)



(b) Himeno Size-L (512x256x256)



(c) Himeno Size-XL (1024x512x512)

Fig. 9 himeno-graph-r2.pdf

V5.1 or later. It supports coarray features specified in Fortran 2008 and a part of Fortran 2018. As the communication layer, MPICH and GASNet can be used selectively. In the vendors, Cray and Intel fully and Fujitsu partially support the coarray features specified in Fortran 2008.

In the latest Fortran standard Fortran 2018, a subset of coarrays is called team. It is similar to the executing images in the term of XMP, but does not affect the parallel execution among images.

While non-blocking PUT communication is effective, non-blocking GET communication is difficult to put into practical use because the acquired data is used immediately. Cray has the directive extension for prefetching remote coarray corresponding to the GET communication.

Coarray C++ is a coarray implementation into C++. The coarray features are implemented with the template library unlike XMP/C based on C language.

6 Conclusion

This chapter described the coarray features in the context of XMP and characteristic implementation of the coarray translator.

For memory allocation and registration, RS, RA and CA methods were implemented corresponding to the communication library GASNet, FJ-RDMA and MPI-3.

For the coarray PUT and GET communications, DMA and four buffering methods were described. The effect of the non-blocking PUT communication was analyzed, and the knowledge is used to make the coarray version Himeno benchmark from the original MPI version. The measurement result on 1024 nodes of the K computer, the coarray version is 27% and 42% faster than the original MPI version, respectively for sizes L and XL. The effect of the optimization of GET communication was also obvious on the ping-pong benchmark on HA-PACS/TCA and Fujitsu PRIMEHPC FX100.

As an evaluation of productivity, the coarray program uses less than half as many characters as MPI message passing program to write the same algorithm of Himeno benchmark.

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References

1. XcalableMP Language Specification, <http://xcalablemp.org/specification.html>
2. John Reid, JKR Associates, UK. Coarrays in the next Fortran Standard. ISO/IEC JTC1/SC22/WG5 N1824, April 21, 2010.
3. ISO/IEC TS 18508:2015, Information technology – Additional Parallel Features in Fortran, Technical Specification, December 1, 2015.
4. Omni Compiler Project. <http://omni-compiler.org>
5. Hidetoshi Iwashita, Masahiro Nakao, Mitsuhsa Sato. 2015. Preliminary Implementation of Coarray Fortran Translator Based on Omni XcalableMP. PGAS2015, Proceedings of 9th International Conference on PGAS Programming Models, pp.70-75, Washington, D.C., USA. September, 2015.
6. EPCC Fortran Coarray micro-benchmark suite.
<https://www.epcc.ed.ac.uk/research/computing/performance-characterisation-and-benchmarking/epcc-co-array-fortran-micro>
7. Himeno Benchmark. <http://accc.riken.jp/en/supercom/himenobmt/>
8. John Mellor-Crummey, Laksono Adhianto, William N. Scherer III, and Guohua Jin. PGAS '09, 3rd Conference on Partitioned Global Address Space Programming Models. Ashburn, VA. October, 2009.
9. Deepak Eachempati, Hyoungh Joon Jun, and Barbara Chapman. An Open-Source Compiler and Runtime Implementation for Coarray Fortran. PGAS '10, 4th Conference on Partitioned Global Address Space Programming Models, No.13. 2010.
10. Alessandro Fanfarillo, Tobias Burnus, Valeria Cardellini, Salvatore Filippone, Dan Nagle, and Damian Rouson. OpenCoarrays: Open-source Transport Layers Supporting Coarray Fortran Compilers, PGAS'14, Proc. of 8th International Conference on Partitioned Global Address Space Programming Models, No. 4. 2014.