Productivity and Performance of the HPC Challenge Benchmarks with the XcalableMP PGAS Language

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Overview of XcalableMP (XMP)

  - The same **directives** are used in XMP/C and XMP/Fortran
  - **Coarray syntax** is available in XMP/C and XMP/Fortran

### XMP/C

```c
int array[16];
#pragma xmp nodes p(4)
#pragma xmp template t(0:15)
#pragma xmp distribute t(block) onto p
#pragma xmp align array[i] with t(i)

main(){
    ...
    #pragma xmp loop on t(i)
    for(i = 0; i < 16; i++){
        array[i] = func(i);
    }
}
```

### XMP/Fortran

```fortran
integer array(16);
!$xmp nodes p(4)
!$xmp template t(1:16)
!$xmp distribute t(block) onto p
!$xmp align array(i) with t(i)

program main
    ...
    !$xmp loop on t(i)
    do i=1,16
        array(i) = func(i)
    done
end program
```
Overview of XcalableMP (XMP)

  - The same **directives** are used in XMP/C and XMP/Fortran
  - **Coarray syntax** is available in XMP/C and XMP/Fortran

XMP/C

```c
int b[10][*];

if(me == 1){
    b[0:5][2] = b[0:5]; // Put
}
```

XMP/Fortran

```fortran
integer b(10)[*]

if(me == 1) then
    b(1:5)[2] = b(1:5)  // Put
end if
```

XMP/Fortran is upward compatible with the Fortran2008
Objective

- Examine effectiveness of designs of the XMP PGAS language for improved **productivity** and **performance** of HPC systems
  - Evaluate the productivity and the performance of XMP through implementations of the HPC Challenge (HPCC) Benchmarks
  - Use 32,768 compute nodes at a maximum on the K computers (which consists of 88,128 compute nodes)

ranked 1st in the Top500 on June, 2011
Agenda

1. Introduce XMP features
   - Global-view memory model with XMP directives
   - Local-view memory model with coarray syntax
   - Designs of XMP for HPC applications

2. Explain implementations of the HPCC Benchmarks and evaluate their productivity and performance

3. Discuss experimental results

4. Summarize our presentation
XMP Global-view model (1/3)

- The directives specify a data distribution among nodes

```c
int array[16];
#pragma xmp nodes p(4)
#pragma xmp template t(0:15)
#pragma xmp distribute t(block) on p
#pragma xmp align array[i] with t(i)
```

Distributed Array
Loop directive is to parallelize loop statement

```c
#pragma xmp loop on t(i)
for(i=2;i<=10;i++){...}
```

```
int array[16];
#pragma xmp nodes p(4)
#pragma xmp template t(0:15)
#pragma xmp distribute t(block) on p
#pragma xmp align array[i] with t(i)
```
XMP Global-view model (3/3)

- Data communication directives: broadcast, reduction, gmove

- gmove directive
  - Transfer data while keeping the global image by using "array section notation"

```c
#pragma xmp gmove
a[2:4] = b[3:4];
```

```
Node 1

<table>
<thead>
<tr>
<th>0</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
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Node 2

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<th>4</th>
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Node 3

<table>
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<th>4</th>
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Node 4

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<tr>
<th>0</th>
<th>1</th>
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<th>3</th>
<th>4</th>
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</tbody>
</table>
```
XMP Local-view model

- Support coarray syntax in XMP/C and XMP/Fortran
  - XMP/Fortran is upward compatible with the Fortran 2008
  - XMP/C also uses array section notation in coarray syntax

```c
int b[10]:[*];  // Declare

: if(me == 1)
a[0:3] = b[4:3]:[2];  // Get
```

The node 1 gets b[4:3] in the node 2

It is easy to express one-sided communication for local data (Put/Get). Can mix XMP global-view directives with coarray-syntax.
Designs of XMP for HPC applications

- PGAS programming language must have both **high productivity** and **high performance**
  - The productivity of HPC applications consists of **programming cost**, **educational cost**, **porting cost**, and **tuning cost**
- Designs of XMP for HPC applications (1/3)
  - Easy writing of various parallel applications **programming cost ↓**
  - [Global-view] Enable parallelization of an original sequential code using minimal modification with simple directives
  - [Local-view] Easy to express one-sided comm. with coarray-syntax
  - Easy learning **educational cost ↓**
  - Extension of C and Fortran
Designs of XMP for HPC applications

- Design of XMP for HPC applications (2/3)
  - Numerical libraries (BLAS etc.) & MPI library can be invoked from XMP program \(<\text{porting}\downarrow, \text{tuning cost}\downarrow, \text{performance}\uparrow>\)

```c
int array[16];
#pragma xmp nodes p(4)
#pragma xmp template t(0:15)
#pragma xmp distribute t(block) onto p
#pragma xmp align array[i] with t(i)
main(){
  ...
  cblas_dgemm(.., &array[k], ...);
}
```

This is a code example where a **global array** is used in BLAS library. A pointer of a global array indicates a local pointer on the node to which it is distributed.

XMP inquiry functions obtain local memory information from a global array. For example, `xmp_array_lead_dim()` obtains a local leading dimension of a global array.
Designs of XMP for HPC applications

- Design of XMP for HPC applications (3/3)
  
  - "OpenMP-safe", except for comm. directives <performance↑>
  
  - Programmer can use **OpenMP directives** in XMP

**XMP/C**

```c
int array[16];
#pragma xmp nodes p(4)
#pragma xmp template t(0:15)
#pragma xmp distribute t(block) onto p
#pragma xmp align array[i] with t(i)

main(){
  ...
  #pragma xmp loop on t(i)
  #pragma omp parallel for
  for(i = 0; i < 16; i++){
    array[i] = func(i);
  }
}
```

**XMP/Fortran**

```fortran
integer array(16);
!$xmp nodes p(4)
!$xmp template t(1:16)
!$xmp distribute t(block) onto p
!$xmp align array(i) with t(i)

program main
  ...
  !$xmp loop on t(i)
  !$omp parallel do
do i=1,16
    array(i) = func(i)
done
end program
```
Agenda

1. Introduce XMP features
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HPC Challenge (HPCC) Benchmarks

- The HPCC Benchmarks are a set of benchmarks to evaluate multiple attributes on an HPC system.
- The HPCC Benchmarks are also used at HPCC Award Competition at Supercomputer Conference.
  - In Class 1, only the performance of an HPC system is evaluated.
  - In Class 2, the productivity and performance of a programming language are evaluated.
    - RandomAccess
    - High Performance Linpack (HPL)
    - Fast Fourier Transform (FFT)
    - STREAM

- based on hpcc-1.4 written in C + Fortran + MPI which is released by the HPCC community (http://icl.cs.utk.edu/hpcc/software/)
- weak scaling
Evaluation

- Omni XMP Compiler version 0.7-alpha
  - Reference Implementation
  - Optimized for the K computer
    - "./configure --target=Kcomputer-linux-gnu"
    - To use high-speed one-sided communication on the K computer, the coarray syntax is translated into calling the extended RDMA
  - This Compiler will be released in Nov. 2013
Environment

<table>
<thead>
<tr>
<th></th>
<th>The K computer</th>
<th>HA-PACS</th>
</tr>
</thead>
<tbody>
<tr>
<td>CPU</td>
<td>SPARC64 VIIIfx 2.0GHz 8Cores, 128GFlops</td>
<td>Xeon E5-2670 2.6GHz x2 8Cores x2, 332.8GFlops</td>
</tr>
<tr>
<td>Memory</td>
<td>DDR3 SDRAM 16GB 64GB/s/Socket</td>
<td>DDR3 SDRAM 128GB 51.4GB/s/Socket</td>
</tr>
<tr>
<td>Network</td>
<td>Torus fusion six-dimensional mesh/torus network, 5GB/s</td>
<td>Infiniband QDRx2rails Fat-tree network, 4GB/s</td>
</tr>
</tbody>
</table>

HA-PACS has GPUs as an accelerator. But we used only CPU.

To measure the performance, we used 32,768 nodes at a maximum of the K computer and 64 nodes at a maximum of HA-PACS.
RandomAccess

- The RandomAccess benchmark measures the performance of random integer updates of memory via interconnect
  - Each process randomly updates table of other processes
  - It is suitable to use coarray syntax
  - To reduce communication times, our algorithm is iterated over sets of CHUNK updates on each node
    - Our algorithm is almost the same as the hpcc-1.4 RandomAccess
RandomAccess

Source lines of code (SLOC) is 258, written in XMP/C

```c
u64Int recv[MAXLOGPROCS][RCHUNK+1]:[*];

for(...){
    ...
    send[isend][0] = nsend; // set "number of transfer elements"
    recv[j][0:nsend+1]:[send_target] = send[isend][0:nsend+1];
    #pragma xmp sync_memory
    #pragma xmp post(p(send_target), 0)
    ...
    #pragma xmp wait(p(recv_target))
    #pragma xmp sync_memory
    nrecv = recv[j-1][0];
    sort_data(&recv[j-1][1], nrecv, ..);
    ...
}
```
The modified hpcc-1.4 RandomAccess, for which the functions updating the table are specifically optimized for the K computer.

163GUPS in 16,384 nodes (131,072 CPU Cores)

- GUPS (Giga UPdates per Second)
- flat-MPI (8 Process/Node)
- Good Performance !!
High Performance Linpack (HPL)

- HPL measures the floating point rate of execution to solve a dense system of linear equations using LU factorization
  - In our implementation, the coefficient matrix is distributed in block-cyclic manner like hpcc-1.4 HPL
  - This distribution is useful to perform good load balance
- BLAS Library is used

```c
double A[N][N];
#pragma xmp nodes p(4,2)
#pragma xmp template t(0:N-1, 0:N-1)
#pragma xmp distribute t(cyclic(NB), \  
cyclic(NB)) onto p
#pragma xmp align A[i][j] with t(j,i)
```
Panel Broadcast by using \texttt{gmove} directive

```c
double A_L[N][NB];
#pragma xmp align L[i][*] with t(*,i)
#pragma xmp gmove
L[k:len][0:NB] = A[k:len][j:NB];
```

SLOC is \textbf{288}, written in XMP/C
Performance of HPL

- 8 Threads/Process on 1 node
  - 543 TFlops in 8,192 nodes (65,536 CPU Cores), 53% of the theoretical peak
- 100 GFlops in 1 node, 8 CPU Cores, 78% of the theoretical peak

In spite of weak scaling, the parallel efficiency is not very good.
Fast Fourier Transform (FFT)

- FFT measures the floating point rate of execution for double-precision complex one-dimensional Discrete Fourier Transform
- We parallelized only a subroutine “PZFFT1D0”, which is the main kernel of the hpcc-1.4 FFT
Fast Fourier Transform (FFT)

- Matrix transposition is implemented by using `gmove` directive.

The SLOC of PZFFT1D0 is 65, written in XMP/Fortran + OpenMP.

```fortran
!$XMP distribute tx(block) onto p
!$XMP distribute ty(block) onto p
!$XMP align A(*,i) with ty(i)
!$XMP align A_WORK(i,*) with tx(i)
!$XMP align B(*,i) with tx(i)

!$XMP gmove
A_WORK(:, :) = A(:, :) ! all-to-all

!$XMP loop on tx(I)
!$OMP parallel do
DO 60 I=1,NX
   DO 70 J=1,NY
      B(J,I)=A_WORK(I,J)
   60 CONTINUE
70 CONTINUE
```

1. Node 2 transfers data to node 1 with packing it.
2. Node 1 copies `A_WORK()` to `B()` by using XMP and OpenMP directives.
Performance of FFT

- 8 Thread/process on 1 node

- 24 TFlops in 32,768 nodes (262,144 CPU Cores)

- 50% of performance of the hpcc-1.4 FFT
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Comparison with hpcc-1.4 (MPI)

- **Productivity**
  - RandomAccess : SLOC : 938 -> 258
    - coarray is a more convenient to express communications
  - HPL : SLOC : 8,800 -> 288
  - PZFFT1D0 of FFT : SLOC : 101 -> 65
    - XMP global view enables programmers to develop parallel applications easily

- **Performance**
  - RandomAccess : Good!
  - HPL and FFT : The performances of XMP implementations are worse than those of hpcc-1.4
Discussion (2/3)

- Overhead of **gmove directive**

- [HPL] **Gmove directive** is a blocking operation. Communication and computation are not overlapped.

  ```c
  #pragma xmp gmove
  A_L[k:len][0:NB] = A[k:len][j:NB];
  ```

- [FFT] In **gmove directive**, data pack/unpack operation is not executed with thread-parallelization

  ```c
  !$XMP gmove
  A_WORK(:, :) = A(:, :)
  ```
Discussion (3/3)

- To improve performance
  - non-blocking gmove operation
  - data pack/unpack with threaded-parallelization in gmove

- Improving the performance of the gmove is important. **But, ...**
  - While level of abstraction of the gmove is very high, the performance of the gmove remains unclarity
    - Gmove improves the productivity, but may become worse the performance
  - If the performance of the gmove has a problem, we recommend that programmer will be able to rewrite the communication with coarray-syntax or MPI library

```c
#pragma xmp gmove async(async-id)
A_L[k:len][0:NB] = A[k:len][j:NB];
```

(overlapped computation)
```c
#pragma xmp wait_async async(async-id)
```
Summary

- Examine the effectiveness of designs of XMP for improved the productivity and the performance of a HPC system
  - Global-view model and Local-view model
  - Can use Numerical Library with XMP inquiry functions
- Evaluate the productivity and the performance through implementations of HPCC Benchmarks on the K computer
  - Good productivity and performance in 32,768 nodes at a maximum
    - But the gmove directive has scope to continue to improve
- Future work
  - Support non-blocking operation and thread-parallelization
  - Retry to evaluate their performances for next HPCC Award at SC13