SINGLE-SIDED PGAS COMMUNICATIONS LIBRARIES

Basic usage of OpenSHMEM

Outline

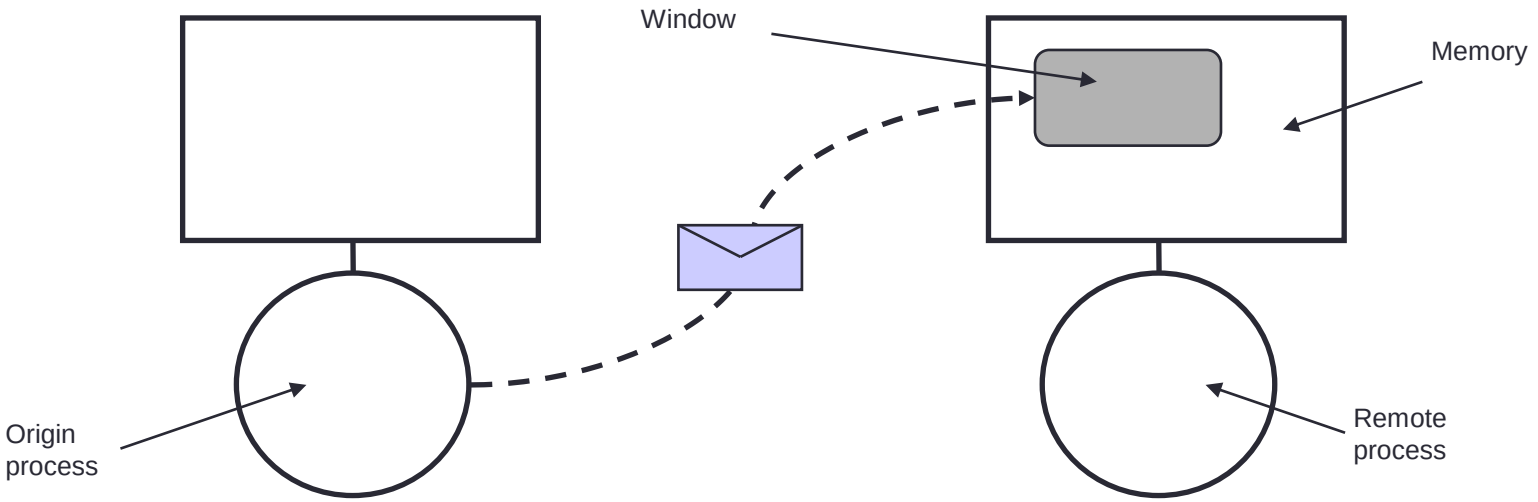
- Concept and Motivation
- Remote Read and Write
- Synchronisation
- Implementations
  - OpenSHMEM
- Summary

Philosophy of the talks

- In general, we will
  - describe a concept (e.g. synchronisation) that is relevant in general for PGAS models
  - explain how this is implemented specifically in OpenSHMEM
- Why?
  - writing correct PGAS programs can be hard
  - experiences from MPI or OpenMP can be misleading
- Recommended approach
  - **don't** think "how can I write this in OpenSHMEM"
  - **do** think "how can I write this using a PGAS approach"
  - **do** think "what issues (e.g. synchronisation) should be addressed"
  - **then** implement (e.g. in OpenSHMEM)

Single-Sided Model

- Remote memory can be read or written directly using library calls



- Remote process does not actively participate
  - No matching receive (or send) needs to be performed
  - Synchronisation is now a major issue
  - May be difficult to calculate remote addresses

Motivation

- Why extend the basic message-passing model?
- Hardware
  - Many MPPs support *R*emote *M*emory *A*ccess (RMA) in hardware
  - This is the fundamental model for SMP systems
  - Many users have started to use RMA calls for efficiency
    - Has lead to the development of non-portable parallel applications
- Software
  - Many algorithms naturally single-sided
    - e.g., sparse matrix-vector
  - Matching send/receive pairs requires extra programming
  - Even worse if communication structure changes
    - e.g., adaptive decomposition

History (official)

- Cray SHMEM (MP-SHMEM, LC-SHMEM)
  - Cray first introduced SHMEM in 1993 for its Cray T3D systems.
  - Cray SHMEM was also used in other models: T3E, PVP and XT
- SGI SHMEM (SGI-SHMEM)
  - Cray Research merged with Silicon Graphics (SGI) February 1996.
  - SHMEM incorporated into SGI's Message Passing Toolkit (MPT)
- Quadrics SHMEM (Q-SHMEM)
  - an optimised API for the Quadrics QsNet interconnect in 2001
- First OpenSHMEM standard in 2012

History (unofficial)

- SHMEM library developed for Cray T3D in 1993
  - basis of Cray MPI libary as developed by EPCC
  - many users called the SHMEM library directly for performance
  - very hard to use correctly (e.g. manual cache coherency!)
- Continued on Cray T3E
  - easier to use as cache coherency is automatic
  - possibility of smaller latencies than (EPCC-optimised) Cray T3E MPI
- Maintained afterwards mainly for porting existing codes
  - eg from important US customers such as ORNL
  - although performance on SGI NUMA machines presumably good
- OpenSHMEM an important standardisation process
  - originally rather messy in places
  - recent version 1.2 much cleaner

OpenSHMEM Terminology

- PE
  - a Processing Element (i.e. process), numbered as 0, 1, 2, …, N-1
- origin
  - Process that performs the call
- remote_pe
  - Process on which memory is accessed
- source
  - Array which the data is copied from
- target
  - Array which the data is copied to

Puts and Gets

- Key routines
- PUT is a remote write
- GET is a remote read

Puts and Gets

- Key routines

How do we know it is safe to overwrite **`target`**?

- PUT is a remote write
  - generically: **`put(target,source,len,remote_pe)`**
  - write **`len`** elements from **`source`** on origin to **`target`** on **`remote_pe`**
  - returns *before* data has arrived at target

How do we know **`source`** is ready to be accessed?

- GET is a remote read
  - generically : **`get(target,source,len,remote_pe)`**
  - …but data is transferred in the opposite direction
  - read **`len`** elements from **`source`** on **`remote_pe`** to **`target`** on origin
  - returns *after* data has arrived at target

Making Data Available for RMA

- For safety, only allow RMA access to certain data
  - Under the control of the user
- Such data must be explicitly *published* in some way
- All data on the **`remote_pe`** must be published
  - i.e., the source of a get or the destination of a put
- Data on the origin PE may not need to be published
  - can access as standard arrays
  - e.g., the target of a get or the source of a put

Remote Addresses

- In general, each process has its own local memory
- Even in SPMD, each instance of a particular variable on different processors may have a different address
  - not all processes may even declare a particular array at runtime
- It is possible for processors to access remote memory by
  - Ensuring all variable instances have the same relative address
  - Registering variables as available for RMA
  - Registering windows of memory as available for RMA
- OpenSHMEM takes the first approach

Symmetric Memory

- Consider **`put(target,source,len,remote_pe)`**
  - all parameters provided by the origin PE
  - but **`target`** is to be interpreted at the **`remote_pe`**

- Solution
  - ensure address of **`target`** is the same on every PE
  - not possible for data allocated on the stack or dynamically (e.g. via malloc)
  - in OpenSHMEM it must be allocated in *symmetric memory*

- Symmetric objects
  - Fortran: any data that is saved
  - C/C++: global/static data
  - or call special versions of malloc (see next talk)

Data Allocation

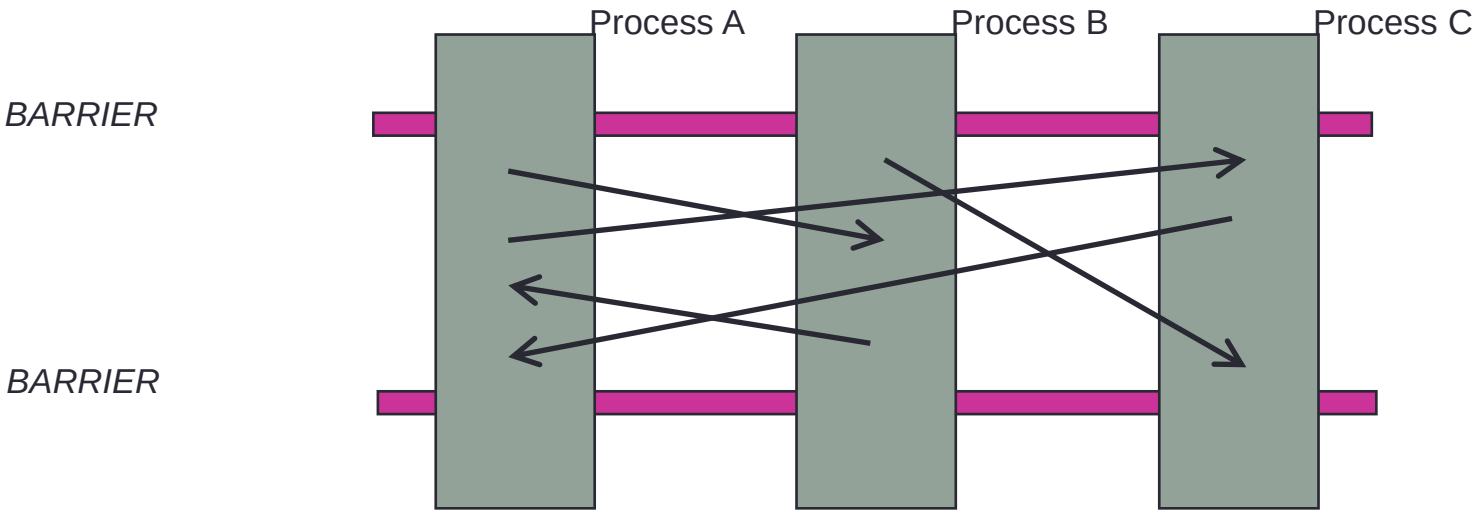
```
! Fortran
subroutine fred
  real :: x(4,4)         ! not symmetric
  real, save :: x(4,4)   ! symmetric
  …
end subroutine fred

// C
float x[4][4];           // symmetric

void fred()
{
  float x[4][4];         // not symmetric
  …
}
```

Synchronisation is critical for RMA

- Various different approaches exist
  - Collective synchronisation across all processors
  - Pairwise synchronisation
  - Locks
- Flexibility needed for different algorithms/applications
  - Differing performance costs
- Synchronisation issues can become very complicated
  - RMA libraries can have subtle synchronisation requirements
  - EPCC taught (correct) use of SHMEM for the T3D/T3E
    - but saw many codes that worked in practice, but were technically incorrect!
- Ease-of-use sacrificed for performance

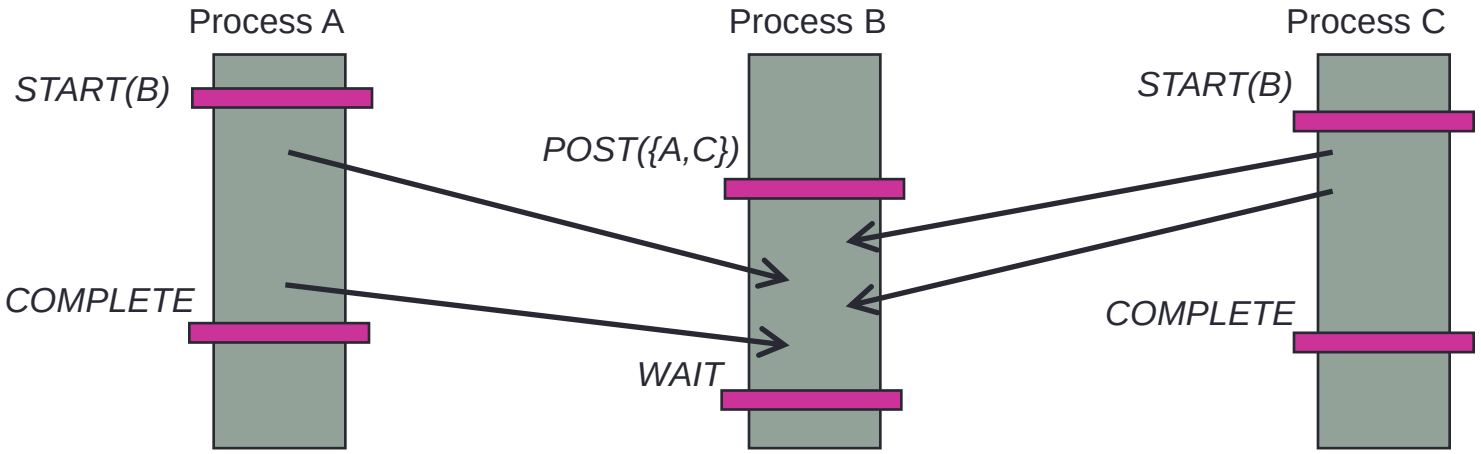
1) Collective

- Simplest form of synchronisation
- Pair of barriers encloses sequence of RMA operations
  - 2nd call only returns when all communications are complete
  - Useful when communications pattern is not known
  - Simple and robust programming model



2) Pairwise Model

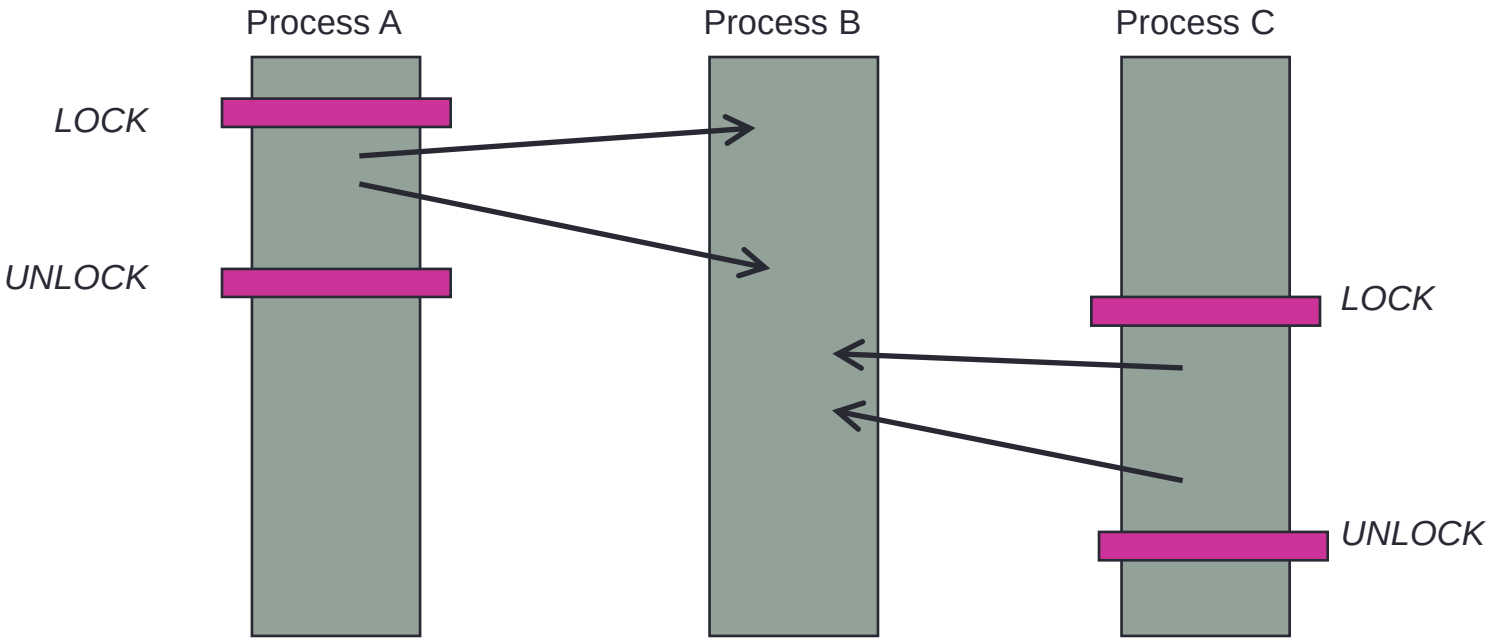
- Useful when comms pattern is known in advance
- Implemented via library routines and/or flag variables



- More complicated model
  - Closer to message-passing than previous collective approach
  - But can be more efficient and flexible

3) Locks

- Remote process neither synchronises nor communicates
- Origin process locks data on remote process
  - Exclusive locks ensure sequential access



Synchronisation

- Must consider appropriate synchronisation for all RMA operations
- Results often only guaranteed to be available *after* a synchronisation point
  - Some communications could actually be delayed until this point
  - May even happen out of order!
- E.g., implementation on a machine ***without*** native RMA
  - Issue non-blocking MPI sends for the puts
  - Wait for them all to complete at the synchronisation point
  - Inefficient, but at least allows RMA to be implemented

Implementations

- OpenSHMEM
  - Portable standard
- GASPI: http://www.gaspi.de/en/
  - e.g. as implemented in GPI-2
- MPI-2: Single-sided communication is part of the MPI-2 standard
  - recently revised in MPI 3 to take advantage of local shared memoy
- BSP: Bulk Synchronous Parallel
- LAPI: *L*ow-level *A*pplications *P*rogramming *I*nterface (IBM)
- SHMEM: SHared MEMory (Cray/SGI)
- Languages
  - Universal Parallel C (UPC), Fortran Coarrays

OpenSHMEM PUT

- **`shmem_[funcname]_put(target,source,len,remote_pe)`**
  - Writes **`len`** elements of contiguous data from address **`source`** on the origin PE to address **`target`** on **`remote_pe`**
  - **`target`** must be the address of a *symmetric data object*

- Fortran
  - **`[funcname]`** can be: INTEGER, REAL, DOUBLE, COMPLEX, LOGICAL or CHARACTER
  - e.g. **`CALL SHMEM_REAL_PUT(x, y, 1, 5)`**
- C
  - **`[funcname]`** can be: int, float, double, short, long, longlong or longdouble
  - e.g. **`shmem_float_put(&x, &y, 1, 5)`**

Other Routines

- Alternative functions for single elements (i.e. len = 1) in C only
  - `shmem_[type]_p(type *target, type source, int remote_pe)`
  - `e.g. shmem_float_p(&x, y, 5)`
- Alternative functions which count in terms of memory
  - `shmem_putX(target,source,len,remote_pe)`
- Fortran
  - `[PUTX]` can be PUTMEM, PUT4, PUT8, PUT32, PUT64, PUT128
  - PUTMEM, PUT4, PUT8 count in multiples of 1, 4 and 8 bytes
  - PUT32, PUT64, PUT128 count in 32, 64 and 128 bits
- C
  - `[PUTX]` can be PUTMEM, PUT32, PUT64, PUT128
  - multiples of bytes (8 bits), 32, 64 and 128 bits

OpenSHMEM GET

- **`CALL SHMEM_[funcname]_GET(target,source,len,remote_pe)`**
  - Reads **`len`** elements of contiguous data from address **`source`** on **`remote_pe`** to address **`target`** on origin PE
  - **`[funcname]`** can be: INTEGER, DOUBLE, COMPLEX, LOGICAL, REAL or CHARACTER
  - **`source`** must be the address of a *symmetric data object*
- Similar range of routines as for PUT
  - **`SHMEM_GET32, SHMEM_INTEGER_GET,`** …
- Similar interfaces for C routines
  - e.g., **`void shmem_int_get(int *target, const int *source, size_t nelems, int remote_pe);`**

Support Routines (Fortran)

- All Fortran programs include the header file 'shmem.fh'

- Initialisation: `CALL SHMEM_INIT()`
  - Initialises the OpenSHMEM library
    - e.g., sets up the symmetric heap, PE numbers, …
    - Must be called before any other library routine is called
- Finalisation: `CALL SHMEM_FINALIZE()`

- Query Routines
  - `SHMEM_MY_PE()`
    - Returns the PE number of the calling PE
  - `SHMEM_N_PES()`
    - Returns the number of processing elements used to run the application

Fortran "Hello World"

```
PROGRAM Hello_World
  IMPLICIT NONE
  INCLUDE 'shmem.fh'

  INTEGER me, npes

  CALL SHMEM_INIT()
  me   = SHMEM_MY_PE()
  npes = SHMEM_N_PES()

  WRITE(*,*) 'I am PE ', me, ' out of ', npes

  CALL SHMEM_FINALIZE()

END PROGRAM Hello_World
```

Support Routines (C)

- All C programs include the header file 'shmem.h'

- Initialisation: **`shmem_init();`**
  - Initialises the OpenSHMEM library
    - e.g., sets up the symmetric heap, PE numbers, …
    - must be called before any other library routine is called
- Finalisation: **`shmem_finalize();`**

- Query Routines
  - **`int shmem_my_pe();`**
    - Returns the PE number of the calling PE
  - **`int shmem_npes();`**
    - Returns the number of processing elements used to run the application

C “Hello World”

```
#include “shmem.h”

int main(void)
{
 int me, npes;

 shmem_init();

 me   = shmem_my_pe();
 npes = shmem_n_pes();

 printf(“I am PE %d out of %d\n”, me, npes);

 shmem_finalize();
}
```

Global Synchronisation

```
CALL SHMEM_BARRIER_ALL()
void shmem_barrier_all();
```

- Suspend execution on the calling PE until all other PEs reach this point of execution path
  - i.e., synchronise all PEs
  - also ensures all outstanding OpenSHMEM puts are complete
- Simplest form of synchronisation
  - perhaps not the most efficient – see later

Communications details

- Vary between PGAS implementations but for OpenSHMEM:
- **`put(target,source,len,remote_pe)`**
  - on return, source is in the network on its way to remote pe
    - source can therefore be safely overwritten at origin pe
    - but is not guaranteed to have arrived at destination
- **`get(target,source,len,remote_pe)`**
  - on return, contents of source written to target on origin pe
    - target can therefore be safely read at origin pe
- So synchronisation is simpler for gets?
  - no!

Using barriers

```
! wait until target is ready to receive
shmem_barrier_all
! write to remote pe
shmem_put(remote, local, ndata, target_pe)
! wait until incoming puts have completed
shmem_barrier_all

! wait until target data is ready to be read
shmem_barrier_all
! read from remote pe
shmem_get(local, remote, ndata, target_pe)
! wait until other pes have read my data
shmem_barrier_all
```

Common mistakes

- Comparison with MPI
  - If you have MPI barriers in your code that you think are required for program correctness then most probably:
    - you are either mistaken (i.e. it will run correctly and faster without barriers)!
    - or you have a bug in your code that just *happens* to disappear when you introduce barriers
  - MPI barriers are **almost never** required for correctness

- For OpenSHMEM
  - If you **do not** have synchronisation before and after puts and gets
    - you probably have an incorrect program – you will need to think **very hard** to ensure that it is correct
    - just because it *happens* to run correctly does not mean it is correct!
  - Synchronisation is **almost always** required both before and after OpenSHMEM puts and gets

Summary

- Single-sided communication is invaluable for certain classes of problem
  - Determined by the algorithm
- Simpler protocol can bring performance benefits
  - But requires thinking about synchronisation, remote addresses,...
- Various single-sided implementations now exist
  - MPI-2: quite general and portable to most platforms
  - OpenSHMEM: more limited functionality but often better performance
- Synchronisation is critical
  - As with all PGAS languages
  - Barriers are simplest OpenSHMEM approach