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

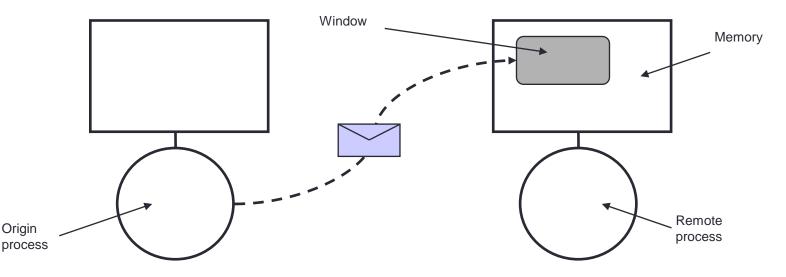
- In general, we will
 - describe a concept (e.g. synchronisation) that is relevant in general for PGAS models
 - explain how this is implemented specifically in OpenSHMEM
- Why?
 - writing correct PGAS programs can be hard
 - experiences from MPI or OpenMP can be misleading
- Recommended approach
 - 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 Remote Memory Access (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



7



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
- GET is a remote read

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

- 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



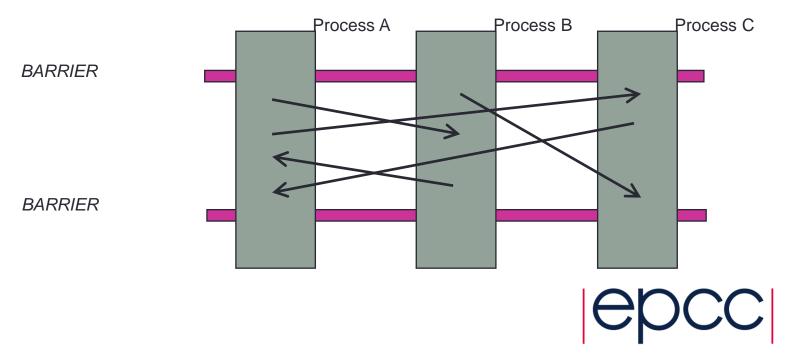


1) Collective

- Simplest form of synchronisation
- Pair of barriers encloses sequence of RMA operations

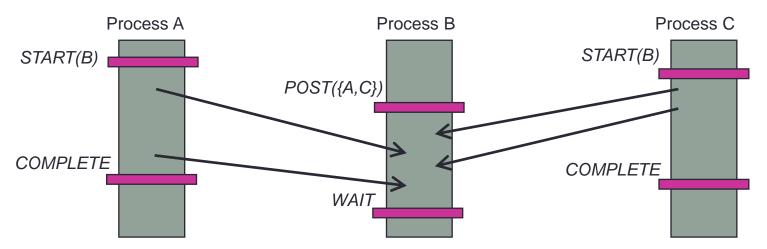
16

- 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



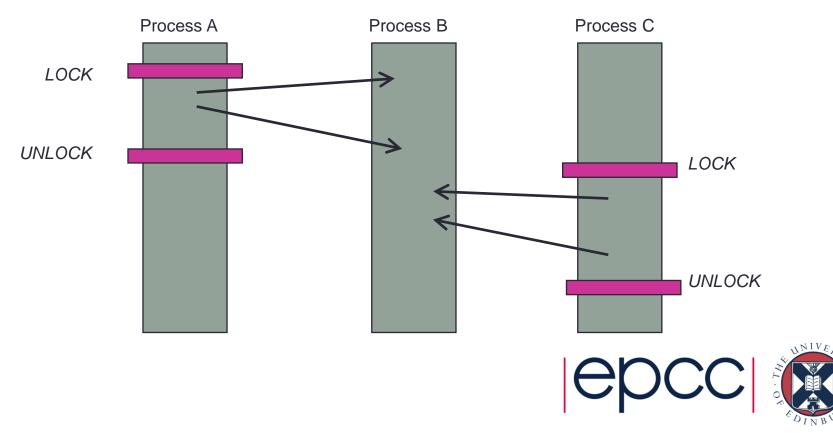
- More complicated model
 - Closer to message-passing than previous collective approach
 - But can be more efficient and flexible





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., implemenation 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: <u>http://www.gaspi.de/en/</u>
 - 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: Low-level Applications Programming Interface (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



26

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?





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



