UPC Overview

http://upc.lbl.gov

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What’s Wrong with MPI Everywhere

• We can run 1 MPI process per core (“flat MPI”)
  – This works now on dual and quad-core machines
  – It will work on 12-24 core machines like Hopper as well

• What are the problems?
  – Latency: some copying required by semantics
  – Memory utilization: partitioning data for separate address space requires some replication
    • How big is your per core subgrid? At 10x10x10, over 1/2 of the points are surface points, probably replicated
    • Weak scaling: success model for the “cluster era,” will not be for the many core era -- not enough memory per core
  – Heterogeneity: MPI per CUDA thread-block?

• Approaches
  – MPI + X, where X is OpenMP, Pthreads, OpenCL, TBB,…
  – A PGAS language like UPC, Co-Array Fortran, Chapel or Titanium
PGAS Languages

- **Global address space**: thread may directly read/write remote data
  - Hides the distinction between shared/distributed memory
- **Partitioned**: data is designated as local or global
  - Does not hide this: critical for locality and scaling

- **UPC, CAF, Titanium**: Static parallelism (1 thread per proc)
  - Does not virtualize processors
- **X10, Chapel and Fortress**: PGAS, but not static (dynamic threads)
UPC Outline

1. Background
2. UPC Execution Model
3. Basic Memory Model: Shared vs. Private Scalars
4. Synchronization
5. Collectives
6. Data and Pointers
7. Dynamic Memory Management
8. Performance
9. Beyond UPC
Context

• Most parallel programs are written using either:
  – Message passing with a SPMD model (MPI)
    • Scales easily on clusters
  – Shared memory with threads in OpenMP, Threads
    • In practice, requires shared memory hardware
• Partitioned Global Address Space (PGAS) Languages take the best of both:
  – Global address space like threads (programmability)
  – SPMD parallelism like most MPI programs (performance)
  – Local/global distinction, i.e., layout matters (performance)
History of UPC

• Initial Tech. Report from IDA in collaboration with LLNL and UCB in May 1999 (led by IDA).
  – UCB version based on Split-C
    – based on course project, motivated by Active Messages
  – IDA based on AC:
    – think about “GUPS” or histogram; “just do it” programs

• UPC Consortium controls the language spec:
  – **UPC is a community effort, well beyond UCB/LBNL**
    – ARSC, CSC, Cray Inc., Etnus, GMU, HP, IDA CCS, Intrepid, LBNL, LLNL, MTU, NSA, SGI, Sun, UCB, U. Florida, DOD
  – Design goals: high performance, expressive, consistent with C goals, …, portable

• Several compilers, both commercial and open source:
  – Cray, HP, IBM, Berkeley, gcc-upc (Intrepid)
UPC Execution Model
UPC Execution Model

- A number of threads working independently in a SPMD fashion
  - Number of threads specified at compile-time or run-time; available as program variable THREADS
  - MYTHREAD specifies thread index (0 .. THREADS - 1)
  - upc_barrier is a global synchronization: all wait
  - There is a form of parallel loop that we will see later

- There are two compilation modes
  - Static Threads mode:
    - THREADS is specified at compile time by the user
    - The program may use THREADS as a compile-time constant
  - Dynamic threads mode:
    - Compiled code may be run with varying numbers of threads
Hello World in UPC

- Any legal C program is also a legal UPC program
- If you compile and run it as UPC with P threads, it will run P copies of the program.
- Using this fact, plus the identifiers from the previous slides, we can parallel hello world:

```c
#include <upc.h>    /* needed for UPC extensions */
#include <stdio.h>

main() {
    printf("Thread %d of %d: hello UPC world\n", MYTHREAD, THREADS);
}
```
Example: Monte Carlo Pi Calculation

- Estimate Pi by throwing darts at a unit square
- Calculate percentage that fall in the unit circle
  - Area of square = $r^2 = 1$
  - Area of circle quadrant = $\frac{1}{4} \pi r^2 = \pi/4$
- Randomly throw darts at x,y positions
- If $x^2 + y^2 < 1$, then point is inside circle
- Compute ratio:
  - # points inside / # points total
  - $\pi = 4 \times \text{ratio}$
Pi in UPC

- Independent estimates of pi:

```c
main(int argc, char **argv) {
    int i, hits, trials = 0;
    double pi;

    if (argc != 2) trials = 1000000;
    else trials = atoi(argv[1]);

    srand(MYTHREAD*17);

    for (i=0; i < trials; i++) hits += hit();
    pi = 4.0*hits/trials;
    printf("PI estimated to %f.\n", pi);
}
```

Each thread gets its own copy of these variables

Each thread can use input arguments

Initialize random in math library

Each thread calls “hit” separately
Helper Code for Pi in UPC

• Required includes:
  
  ```
  #include <stdio.h>
  #include <math.h>
  #include <upc.h>
  ```

• Function to throw dart and calculate where it hits:
  
  ```
  int hit()
  {
      int const rand_max = 0xFFFFFFFF;
      double x = ((double) rand()) / RAND_MAX;
      double y = ((double) rand()) / RAND_MAX;
      if ((x*x + y*y) <= 1.0) {
          return(1);
      } else {
          return(0);
      }
  }
  ```
Shared vs. Private Variables
Private vs. Shared Variables in UPC

- Normal C variables and objects are allocated in the private memory space for each thread.
- Shared variables are allocated only once, with thread 0
  ```c
  shared int ours;  // use sparingly: performance
  int mine;
  ```
- Shared variables may not have dynamic lifetime: may not occur in a in a function definition, except as static. Why?
Pi in UPC: Shared Memory Style

- Parallel computing of pi, but with a bug

```c
shared int hits;
main(int argc, char **argv) {
    int i, my_trials = 0;
    int trials = atoi(argv[1]);
    my_trials = (trials + THREADS - 1)/THREADS;
    srand(MYTHREAD*17);
    for (i=0; i < my_trials; i++)
        hits += hit();
    upc_barrier;
    if (MYTHREAD == 0) {
        printf("PI estimated to %f.", 4.0*hits/trials);
    }
}
```

shared variable to record hits
divide work up evenly
accumulate hits

What is the problem with this program?
Shared Arrays Are Cyclic By Default

- Shared scalars always live in thread 0
- Shared arrays are spread over the threads
- Shared array elements are spread across the threads

```c
shared int x[THREADS]  /* 1 element per thread */
shared int y[3][THREADS]  /* 3 elements per thread */
shared int z[3][3]  /* 2 or 3 elements per thread */
```

- In the pictures below, assume THREADS = 4
- Red els have affinity to thread 0

```
x
```
```
y
```
```
z
```

Think of linearized C array, then map in round-robin
As a 2D array, y is logically blocked by columns
z is not
Pi in UPC: Shared Array Version

• Alternative fix to the race condition
• Have each thread update a separate counter:
  – But do it in a shared array
  – Have one thread compute sum

```c
shared int all_hits [THREADS];
main(int argc, char **argv) {
  ... declarations an initialization code omitted
  for (i=0; i < my_trials; i++)
    all_hits[MYTHREAD] += hit();
  upc_barrier;
  if (MYTHREAD == 0) {
    for (i=0; i < THREADS; i++)
      hits += all_hits[i];
    printf("PI estimated to \%f.\n", 4.0*hits/trials);
  }
}
```

all_hits is shared by all processors, just as hits was

update element with local affinity
UPC Synchronization
UPC Global Synchronization

- UPC has two basic forms of barriers:
  - Barrier: block until all other threads arrive
    upc_barrier
  - Split-phase barriers
    upc_notify; this thread is ready for barrier
do computation unrelated to barrier
    upc_wait; wait for others to be ready
- Optional labels allow for debugging
  #define MERGE_BARRIER 12
  if (MYTHREAD%2 == 0) {
    ... 
    upc_barrier MERGE_BARRIER;
  } else {
    ... 
    upc_barrier MERGE_BARRIER;
  }
Synchronization - Locks

- Locks in UPC are represented by an opaque type:
  
  ```c
  upc_lock_t
  ```

- Locks must be allocated before use:
  
  ```c
  upc_lock_t *upc_all_lock_alloc(void);
  ```
  allocates 1 lock, pointer to all threads
  
  ```c
  upc_lock_t *upc_global_lock_alloc(void);
  ```
  allocates 1 lock, pointer to one thread

- To use a lock:
  
  ```c
  void upc_lock(upc_lock_t *l)
  void upc_unlock(upc_lock_t *l)
  ```
  use at start and end of critical region

- Locks can be freed when not in use
  
  ```c
  void upc_lock_free(upc_lock_t *ptr);
  ```
Pi in UPC: Shared Memory Style

- Parallel computing of pi, without the bug

```c
shared int hits;
main(int argc, char **argv) {
    int i, my_hits, my_trials = 0;
    upc_lock_t *hit_lock = upc_all_lock_alloc();
    int trials = atoi(argv[1]);
    my_trials = (trials + THREADS - 1)/THREADS;
    srand(MYTHREAD*17);
    for (i=0; i < my_trials; i++)
        my_hits += hit();
    upc_lock(hit_lock);
    hits += my_hits;
    upc_unlock(hit_lock);
    upc_barrier;
    if (MYTHREAD == 0)
        printf("PI: \%f\n", 4.0*hits/trials);
}
```

- create a lock
- accumulate hits locally
- accumulate across threads
Recap: Private vs. Shared Variables in UPC

- We saw several kinds of variables in the pi example
  - Private scalars (*my_hits*)
  - Shared scalars (*hits*)
  - Shared arrays (*all_hits*)
  - Shared locks (*hit_lock*)

<table>
<thead>
<tr>
<th>Global address space</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
</tr>
<tr>
<td>Thread$_0$</td>
</tr>
<tr>
<td>my_hits:</td>
</tr>
<tr>
<td>hit_lock:</td>
</tr>
<tr>
<td>all_hits[0]:</td>
</tr>
<tr>
<td>Thread$_1$</td>
</tr>
<tr>
<td>my_hits:</td>
</tr>
<tr>
<td>all_hits[1]:</td>
</tr>
<tr>
<td>Thread$_n$</td>
</tr>
<tr>
<td>my_hits:</td>
</tr>
<tr>
<td>all_hits[n]:</td>
</tr>
</tbody>
</table>

where: 

$n=Threads-1$

**Shared**

**Private**
UPC Collectives
UPC Collectives in General

• The UPC collectives interface is in the language spec:
  – http://upc.lbl.gov/docs/user/upc_spec_1.2.pdf
• It contains typical functions:
  – Data movement: broadcast, scatter, gather, …
  – Computational: reduce, prefix, …
• Interface has synchronization modes:
  – Avoid over-synchronizing (barrier before/after is simplest semantics, but may be unnecessary)
  – Data being collected may be read/written by any thread simultaneously
• Simple interface for collecting scalar values (int, double,…)
  – Berkeley UPC value-based collectives
  – Works with any compiler
  – http://upc.lbl.gov/docs/user/README-collectivev.txt
Pi in UPC: Data Parallel Style

- The previous version of Pi works, but is not scalable:
  - On a large # of threads, the locked region will be a bottleneck
- Use a reduction for better scalability

```c
#include <bupc_collectivev.h>

#include <bupc_collectivev.h>

// shared int hits;

main(int argc, char **argv) {
...
for (i=0; i < my_trials; i++)
    my_hits += hit();

my_hits = // type, input, thread, op
    bupc_allv_reduce(int, my_hits, 0, UPC_ADD);

// upc_barrier;
if (MYTHREAD == 0)
    printf("PI: %f", 4.0*my_hits/trials);
}
```

Berkeley collectives
no shared variables

barrier implied by collective
UPC (Value-Based) Collectives in General

• General arguments:
  – rootthread is the thread ID for the root (e.g., the source of a broadcast)
  – All 'value' arguments indicate an l-value (i.e., a variable or array element, not a literal or an arbitrary expression)
  – All 'TYPE' arguments should the scalar type of collective operation
  – upc_op_t is one of: UPC_ADD, UPC_MULT, UPC_AND, UPC_OR, UPC_XOR, UPC_LOGAND, UPC_LOGOR, UPC_MIN, UPC_MAX

• Computational Collectives
  – TYPE bupc_allv_reduce(TYPE, TYPE value, int rootthread, upc_op_t reductionop)
  – TYPE bupc_allv_reduce_all(TYPE, TYPE value, upc_op_t reductionop)
  – TYPE bupc_allv_prefix_reduce(TYPE, TYPE value, upc_op_t reductionop)

• Data movement collectives
  – TYPE bupc_allv_broadcast(TYPE, TYPE value, int rootthread)
  – TYPE bupc_allv_scatter(TYPE, int rootthread, TYPE *rootsrcarray)
  – TYPE *bupc_allv_gather(TYPE, TYPE value, int rootthread, TYPE *rootdestarray)
    • Gather a 'value' (which has type TYPE) from each thread to 'rootthread', and place them (in order by source thread) into the local array 'rootdestarray' on 'rootthread'.
  – TYPE *bupc_allv_gather_all(TYPE, TYPE value, TYPE *destarray)
  – TYPE bupc_allv_permute(TYPE, TYPE value, int tothreadid)
    • Perform a permutation of 'value's across all threads. Each thread passes a value and a unique thread identifier to receive it - each thread returns the value it receives.
Full UPC Collectives

- Value-based collectives pass in and return scalar values
- But sometimes you want to collect over arrays
- When can a collective argument begin executing?
  
  • Arguments with affinity to thread $i$ are ready when thread $i$ calls the function; results with affinity to thread $i$ are ready when thread $i$ returns.
  
  • This is appealing but it is incorrect: In a broadcast, thread 1 does not know when thread 0 is ready.
UPC Collective: Sync Flags

• In full UPC Collectives, blocks of data may be collected
• A extra argument of each collective function is the sync mode of type upc_flag_t.
• Values of sync mode are formed by or-ing together a constant of the form UPC_IN_XSYNC and a constant of the form UPC_OUT_YSYNC, where \( X \) and \( Y \) may be NO, MY, or ALL.
• If sync_mode is (UPC IN_XSYNC | UPC OUT YSYNC), then if \( X \) is:
  – NO the collective function may begin to read or write data when the first thread has entered the collective function call,
  – MY the collective function may begin to read or write only data which has affinity to threads that have entered the collective function call, and
  – ALL the collective function may begin to read or write data only after all threads have entered the collective function call
• and if \( Y \) is
  – NO the collective function may read and write data until the last thread has returned from the collective function call,
  – MY the collective function call may return in a thread only after all reads and writes of data with affinity to the thread are complete, and
  – ALL the collective function call may return only after all reads and writes of data are complete.
Work Distribution Using \texttt{upc\_forall}
Example: Vector Addition

- Questions about parallel vector additions:
  - How to layout data (here it is cyclic)
  - Which processor does what (here it is “owner computes”)

```c
/* vadd.c */
#include <upc_relaxed.h>
#define N 100*THREADS

shared int v1[N], v2[N], sum[N];
void main() {
    int i;
    for(i=0; i<N; i++)
        if (MYTHREAD == i%THREADS)
          sum[i]=v1[i]+v2[i];
}
```
Work Sharing with upc forall()

• The idiom in the previous slide is very common
  – Loop over all; work on those owned by this proc
• UPC adds a special type of loop
  upc forall(init; test; loop; affinity)
    statement;
• Programmer indicates the iterations are independent
  – Undefined if there are dependencies across threads
• Affinity expression indicates which iterations to run on each thread. It may have one of two types:
  – Integer: affinity%THREADS is MYTHREAD
  – Pointer: upc_threadof(affinity) is MYTHREAD
• Syntactic sugar for loop on previous slide
  – Some compilers may do better than this, e.g.,
    for(i=MYTHREAD; i<N; i+=THREADS)
  – Rather than having all threads iterate N times:
    for(i=0; i<N; i++) if (MYTHREAD == i%THREADS)
Vector Addition with upc_forall

- The `vadd` example can be rewritten as follows
  - Equivalent code could use “&sum[i]” for affinity
  - The code would be correct but slow if the affinity expression were `i+1` rather than `i`.

```c
#define N 100*THREADS

shared int v1[N], v2[N], sum[N];

void main() {
    int i;
    upc_forall(i=0; i<N; i++; i)
        sum[i]=v1[i]+v2[i];
}
```

The cyclic data distribution may perform poorly on some machines.
Distributed Arrays in UPC
Blocked Layouts in UPC

• If this code were doing nearest neighbor averaging (3pt stencil) the cyclic layout would be the worst possible layout.
• Instead, want a blocked layout
• Vector addition example can be rewritten as follows using a blocked layout

```c
#define N 100*THREADS
    shared int [*] v1[N], v2[N], sum[N];

void main() {
    int i;
    upc_forall(i=0; i<N; i++; &sum[i])
        sum[i]=v1[i]+v2[i];
}
```

• If this code were doing nearest neighbor averaging (3pt stencil) the cyclic layout would be the worst possible layout.
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• Vector addition example can be rewritten as follows using a blocked layout

```c
#define N 100*THREADS
    shared int [*] v1[N], v2[N], sum[N];

void main() {
    int i;
    upc_forall(i=0; i<N; i++; &sum[i])
        sum[i]=v1[i]+v2[i];
}
```
Layouts in General

- All non-array objects have affinity with thread zero.
- Array layouts are controlled by layout specifiers:
  - Empty (cyclic layout)
  - [*] (blocked layout)
  - [0] or [] (indefinite layout, all on 1 thread)
  - [b] or [b1][b2]...[bn] = [b1*b2*...*bn] (fixed block size)
- The affinity of an array element is defined in terms of:
  - block size, a compile-time constant
  - and THREADS.
- Element i has affinity with thread
  \[
  \left(\frac{i}{\text{block\_size}}\right) \mod \text{THREADS}
  \]
- In 2D and higher, linearize the elements as in a C representation, and then use above mapping
Pointers to Shared vs. Arrays

- In the C tradition, array can be accessed through pointers.
- Here is the vector addition example using pointers:

```c
#define N 100*THREADS
shared int v1[N], v2[N], sum[N];
void main() {
    int i;
    shared int *p1, *p2;
    p1=v1; p2=v2;
    for (i=0; i<N; i++, p1++, p2++)
        if (i %THREADS= = MYTHREAD)
            sum[i]= *p1 + *p2;
}
```
UPC Pointers

Where does the pointer point?

<table>
<thead>
<tr>
<th></th>
<th>Local</th>
<th>Shared</th>
</tr>
</thead>
<tbody>
<tr>
<td>Private</td>
<td>p1</td>
<td>p2</td>
</tr>
<tr>
<td>Shared</td>
<td>p3</td>
<td>p4</td>
</tr>
</tbody>
</table>

Where does the pointer reside?

- `int *p1;` /* private pointer to local memory */
- `shared int *p2;` /* private pointer to shared space */
- `int *shared p3;` /* shared pointer to local memory */
- `shared int *shared p4;` /* shared pointer to shared space */

Shared to local memory (p3) is not recommended.
int *p1; /* private pointer to local memory */
shared int *p2; /* private pointer to shared space */
int *shared p3; /* shared pointer to local memory */
shared int *shared p4; /* shared pointer to shared space */

Pointers to shared often require more storage and are more costly to dereference; they may refer to local or remote memory.
Dynamic Memory Allocation in UPC

- Dynamic memory allocation of shared memory is available in UPC
- Functions can be collective or not
  - A collective function has to be called by every thread and will return the same value to all of them
Global Memory Allocation

```c
shared void *upc_global_alloc(size_t nbblocks, size_t nbytes);

   nbblocks : number of blocks
   nbytes   : block size

• Non-collective: called by one thread
• The calling thread allocates a contiguous memory space in the shared space with the shape:

  shared [nbytes] char[nblocks * nbytes]

shared void *upc_all_alloc(size_t nbblocks, size_t nbytes);

• The same result, but must be called by all threads together
• All the threads will get the same pointer

void upc_free(shared void *ptr);
• Non-collective function; frees the dynamically allocated shared memory pointed to by ptr
```
Distributed Arrays Directory Style

- Many UPC programs avoid the UPC style arrays in factor of directories of objects

```c
typedef shared [] double *sdblptr;
shared sdblptr directory[THREADS];
directory[i]=upc_alloc(local_size*sizeof(double));
```

- These are also more general:
  - Multidimensional, unevenly distributed
  - Ghost regions around blocks
Performance of UPC
PGAS Languages have Performance Advantages

Strategy for acceptance of a new language
- Make it run faster than anything else

Keys to high performance
- Parallelism:
  - Scaling the number of processors
- Maximize single node performance
  - Generate friendly code or use tuned libraries (BLAS, FFTW, etc.)
- Avoid (unnecessary) communication cost
  - Latency, bandwidth, overhead
  - Berkeley UPC and Titanium use GASNet communication layer
- Avoid unnecessary delays due to dependencies
  - Load balance; Pipeline algorithmic dependencies
One-Sided vs Two-Sided

- A one-sided put/get message can be handled directly by a network interface with RDMA support
  - Avoid interrupting the CPU or storing data from CPU (preposts)
- A two-sided messages needs to be matched with a receive to identify memory address to put data
  - Offloaded to Network Interface in networks like Quadrics
  - Need to download match tables to interface (from host)
  - Ordering requirements on messages can also hinder bandwidth
Ping Pong Latency

- UPC
- MPI - Large Pages
- MPI - Regular Pages

Time (us)
PingPong Bandwidths
GASNet: Portability and High-Performance

GASNet excels at mid-range sizes: important for overlap

Joint work with UPC Group

2/7/11

Cray XE Training
Communication Strategies for 3D FFT

• Three approaches:
  • **Chunk:**
    • Wait for 2nd dim FFTs to finish
    • Minimize # messages
  • **Slab:**
    • Wait for chunk of rows destined for 1 proc to finish
    • Overlap with computation
  • **Pencil:**
    • Send each row as it completes
    • Maximize overlap and
    • Match natural layout

Joint work with Chris Bell, Rajesh Nishtala, Dan Bonachea
FFT Performance on BlueGene/P

- PGAS implementations consistently outperform MPI
- Leveraging communication/computation overlap yields best performance
  - More collectives in flight and more communication leads to better performance
  - At 32k cores, overlap algorithms yield 17% improvement in overall application time
- Numbers are getting close to HPC record
  - Future work to try to beat the record

HPC Challenge Peak as of July 09 is ~4.5 Tflops on 128k Cores

![Graph showing FFT performance with various lines representing different methods and cores]
NAS FT Variants Performance Summary

Slab is always best for MPI; small message cost too high

Pencil is always best for UPC; more overlap

Joint work with Chris Bell, Rajesh Nishtala, Dan Bonachea

.5 Tflops
Case Study: LU Factorization

- Direct methods have complicated dependencies
  - Especially with pivoting (unpredictable communication)
  - Especially for sparse matrices (dependence graph with holes)
- LU Factorization in UPC
  - Use overlap ideas and multithreading to mask latency
  - Multithreaded: UPC threads + user threads + threaded BLAS
    - Panel factorization: Including pivoting
    - Update to a block of U
    - Trailing submatrix updates
- Status:
  - Dense LU done: HPL-compliant
  - Sparse version underway
UPC HPL Performance

• Comparison to ScaLAPACK on an Altix, a 2 x 4 process grid
  - ScaLAPACK (block size 64) 25.25 GFlop/s (tried several block sizes)
  - UPC LU (block size 256) - 33.60 GFlop/s, (block size 64) - 26.47 GFlop/s
• n = 32000 on a 4x4 process grid
  - ScaLAPACK - 43.34 GFlop/s (block size = 64)
  - UPC - 70.26 Gflop/s (block size = 200)

• MPI HPL numbers from HPCC database
• Large scaling:
  • 2.2 TFlops on 512p,
  • 4.4 TFlops on 1024p (Thunder)

Joint work with Parry Husbands
Application Work in PGAS

• Network simulator in UPC (Steve Hofmeyr, LBNL)
• Rea-space multigrid (RMG) quantum mechanics (Shirley Moore, UTK)
• Landscape analysis, i.e., “Contributing Area Estimation” in UPC (Brian Kazian, UCB)
• GTS Shifter in CAF (Preissl, Wichmann, Long, Shalf, Ethier, Koniges, LBNL, Cray, PPPL)
Summary

• UPC designed to be consistent with C
  – Some low level details, such as memory layout are exposed
  – Ability to use pointers and arrays interchangeably
• Designed for high performance
  – Memory consistency explicit
  – Small implementation
• Berkeley compiler (used for next homework)
  http://upc.lbl.gov
• Language specification and other documents
  http://upc.gwu.edu
PGAS Languages for Manycore

- PGAS memory are a good fit to machines with explicitly managed memory (local store)
  - Global address space implemented as DMA reads/writes
  - New “vertical” partition of memory needed for on/off chip, e.g., upc_offchip_alloc
  - Non-blocking features of UPC put/get are useful
- SPMD execution model needs to be adapted to heterogeneity