PGAS Applications
What, Where and Why?

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What is PGAS? Partitioned Global Address Space

- Global Address Space: Directly access remote memory
- Partitioned: Programmer controls data layout for scalability
PGAS Languages and Libraries

- **Language mechanisms for distributed arrays**
  
  - (CoArray) Fortran
    
    ```fortran
    REAL:: X(2,3)[*]
    X(1,2) .... X(1,3)[5]
    ```

  - UPC
    
    ```c
    shared double X[100]; or double X[THREADS*6];
    X[] .... X[MYTHREAD]
    ```

  - Chapel
    
    ```chapel
    const ProblemSpace= {1..m}
    dmapped Block(boundingBox={1..m});
    var X: [ProblemSpace] real;
    ```

  - UPC++
    
    ```cpp
    upcxx::shared_array<Type> X;
    X.init(128); or X.init(128,4)
    X [upcxx:ranks()] ... X[6]
    ```

Many others...
Programming Data Analytics vs Simulation

**Simulation: More Regular**
- Divide up domain in pieces
- Compute one piece
- Send/Receive data from others

**Analytics: More Irregular**
- Global Address Space Programming
  - Each start computing
  - Grab whatever / whenever

**Message Passing Programming**
- MPI, and many libraries

**Global Address Space Programming**
- UPC, UPC++, CAF, X10, Chapel, Shmem, GA
Many UPC programs avoid the UPC style arrays in favor of directories of objects

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
Example: Hash Table in PGAS

- <key, value> pairs, stored in some bucket based on hash(key)
- One-sided communication; never having to say “receive”
- Allows for Terabyte-Petabyte size data sets vs ~1 TB in shared memory
Other Programming Model Variations

• What can you do remotely?
  – Read, Write, Lock
  – Atomics (compare-and-swap, fetch-and-add)
  – Invoke functions
  – Signal processes to wake up (task graphs)

• What type of parallelism is there
  – Data parallel (single threaded semantics, e.g., A = B + C)
    • Collective communication
  – Single Program Multiple Data (SPDM): if (MYTHREAD == 0)...
  – Hierarchical SPMD (teams): if (MYTEAM....)...
  – Fork-join: fork / async
  – Task graph (events)
Where is PGAS programming used?

1. Asynchronous fine-grained reads/write/atomics
De novo Genome Assembly

• DNA sequence consists of 4 bases: A/C/G/T
• Read: short fragment of DNA
• De novo assembly: Construct a genome (chromosomes) from a collection of reads
For complex metagenomes (soil) most of the reads cannot be assembled
De novo Genome Assembly a la Meraculous

Input: Reads that may contain errors

1. Chop reads into k-mers, process k-mers to exclude errors
   - Bloom filter (statistical)
   - Intensive I/O
   - High memory footprint

2. Construct & traverse de Bruijn graph of k-mers, generate contigs
   - Huge graph as a hash table
   - Irregular accesses
   - Injection limited

3. Leverage read information to link contigs and generate scaffolds.
   - Multiple hash tables
   - High memory requirements
   - Intensive computation
   - Intensive I/O

Georganas, Buluc, Chapman, Oliker, Rokhsar, Yelick, [Aluru,Egan,Hofmeyr] in SC14, IPDPS15, SC15
Application Challenge: Random Access to Large Data

- Parallel DFS (from randomly selected K-mers) to compute contigs
- Some tricky synchronization to deal with conflicts

- Hash tables used in all phases
  - Different use cases, different implementations
- No a priori locality: that is the problem you’re trying to solve
Distributed Hash Tables in PGAS

- Remote Atomics, Dynamic Aggregation, Software Caching
- 13x Faster than another HPC/MPI code (Ray) on 960 cores

Evangelos Georganas, Aydin Buluç, Jarrod Chapman, Steven Hofmeyr, Chaitanya Aluru, Rob Egan, Lenny Oliker, Dan Rokhsar, and Kathy Yelick. **HipMer: An Extreme-Scale De Novo Genome Assembler, SC’15**
Comparison to other Assemblers

Runtime on Assemblers

- **Meraculous**: 140 hours
- **SGA**: 4 minutes
- **ABySS 960 Contig only**: Equal core counts (960 Edison)
- **Ray 960**
- **HipMer 960**
- **HipMer 20K**
Science Impact: HipMer is transformative

• Human genome (3Gbp) “de novo” assembled:
  – Meraculous: 48 hours
  – HipMer: 4 minutes (720x speedup relative to Meraculous)

• Wheat genome (17 Gbp) “de novo” assembled (2014):
  – Meraculous (did not run):
  – HipMer: 39 minutes; 15K cores (first all-in-one assembly)

• Pine genome (20 Gbp) “de novo” assembled (2014):
  – Masurca: 3 months; 1 TB RAM

• Wetland metagenome (1.25 Tbp) analysis (2015):
  – Meraculous (projected): 15 TB of memory
  – HipMER: Strong scaling to over 100K cores (contig gen only)

Makes unsolvable problems solvable!

Georganas, Buluc, Chapman, Oliker, Rokhsar, Yelick, [Aluru,Egan,Hofmeyr] in SC14, IPDPS15, SC15
UPC++: PGAS with “Mixins” (Teams and Asyncs)

- UPC++ uses templates (no compiler needed)
  
  ```
  shared_var<int> s;
  global_ptr<LLNode> g;
  shared_array<int> sa(8);
  ```

- Default execution model is SPMD, but

- Remote methods, async
  
  ```
  async(place) (Function f, T1 arg1,...);
  wait();   // other side does poll();
  ```

- Research in teams for hierarchical algorithms and machines
  
  ```
  teamsplit (team) { ... }
  ```

- Use these for “domain-specific” runtime systems
Where is PGAS programming used?

1. Asynchronous fine-grained reads/write/atomics (aggregation and software caching when possible)
2. Strided irregular updates (adds) to distributed matrix
Application Challenge: Data Fusion

- “Fusing” observational data into simulation
- Interoperates with MPI/Fortran/ScalAPACK

Distributed Matrix Construction
- Remote asyncs with user-controlled resource management
- Divide threads into injectors / updaters
- 6x faster than MPI 3.0 on 1K XE6 nodes

Scott French, Yili Zheng, Barbara Romanowicz, Katherine Yelick; "Parallel Hessian Assembly for Seismic Waveform Inversion Using Global Updates", IPDPS 2015
Application Challenge: Data Fusion

Strong Scaling (NERSC Edison)

Relative Parallel Efficiency (%) vs Cores

- 1.1e5 x 1.1e5 (45 GB)
- 2.2e5 x 2.2e5 (180 GB)
- 8.2e5 x 8.2e5 (2.5 TB)

Scott French, Yili Zheng, Barbara Romanowicz, Katherine Yelick; "Parallel Hessian Assembly for Seismic Waveform Inversion Using Global Updates", IPDPS 2015
Science Impact: Whole-Mantle Seismic Model

- First-ever whole-mantle seismic model from numerical waveform tomography
- Finding: Most volcanic hotspots are linked to two spots on the boundary between the metal core and rocky mantle 1,800 miles below Earth's surface.

Scott French, Barbara Romanowicz, "Broad plumes rooted at the base of the Earth’s mantle beneath major hotspots", Nature, 2015
Multidimensional Arrays in UPC++

- UPC++ arrays have a rich set of operations
  - translate
  - restrict
  - slice (n dim to n-1)
  - transpose

- Create new views of the data in original array
- Example: ghost cell exchange in AMR

```cpp
ndarray<double, 3, global> gridB = bArrays[i, j, k];
...
gridA.async_copy(gridB.shrink(1));
```
Where is PGAS programming used?

1. Asynchronous fine-grained reads/write/atomics (aggregation and software caching when possible)
2. Strided irregular updates (adds) to distributed matrix
3. Dynamic work stealing
Application Challenge: Dynamic Load Balancing

- **Hartree Fock example (e.g., in NWChem which is already PGAS)**
  - Inherent load imbalance
- **UPC++ version**
  - Dynamic work stealing and fast atomic operations enhanced load balance
  - Transpose an irregularly blocked matrix

![Local Array](image)

David Ozog (CSGF Fellow), A. Kamil, Y. Zheng, P. Hargrove, J. Hammond, A. Malony, W. de Jong, K. Yelick
Hartree Fock Code

Improved Scalability

Strong Scaling of UPC++ HF on NERSC Edison
Compared to (highly optimized) GTFock with Global Arrays

David Ozog (CSGF Fellow), A. Kamil, Y. Zheng, P. Hargrove, J. Hammond, A. Malony, W. de Jong, K. Yelick
Towards NWChem in UPC++

- New Global Arrays Toolkit over GASNet
  - Over 20% faster on Infiniband
- More scalable aggregate FFTs than FFTW

Goal of making this ready for production use (Bert de Jong)

E. Hoffman (GAGA), H. Simhadri (FFTs)
Where is PGAS programming used?

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4. Hierarchical algorithms / one programming model
UPC++ Communication Speeds up AMR

- **Adaptive Mesh Refinement on Block-Structured Meshes**
  - Used in ice sheet modeling, climate, subsurface (fracking), astrophysics, accelerator modeling and many more

![Graph showing FillBoundary Test on 2048 Cori Cores]

**Hierarchical UPC++ (distributed / shared style)**
- UPC++ plus UPC++ is 2x faster than MPI plus OpenMP
- MPI + MPI also does well
Reducing Metadata Overhead in AMR

- Reducing the metadata size

  phase I: Reduce the size of the grid class
  phase II: Split the grid class into grid_local and grid_remote

- Distribute the grid hierarchy data structure using UPC
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5. Task Graph Scheduling (UPC++)
• Sparse matrix factorization (Cholesky)
• Novel fan in/out algorithm programmed in UPC++

Mathias Jacqueline, Esmond Ng, Yili Zheng, Kathy Yelick
Dynamic scheduling outperforms other

The combination of algorithm and implementation (in UPC++) outperforms the competition

Mathias Jacqueline, Esmond Ng, Yili Zheng, Kathy Yelick
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5. Task Graph Scheduling (UPC++)
6. Dynamic runtimes (CHARM++, Legion, HPX)
HPX Asynchronous Runtime Performs on Manycore

LibGeoDecomp - Weak Scaling - Distributed
(Host Cores)

<table>
<thead>
<tr>
<th>Cores</th>
<th>0</th>
<th>3K</th>
<th>6K</th>
<th>9K</th>
<th>13K</th>
<th>16K</th>
</tr>
</thead>
<tbody>
<tr>
<td>GFLOPS</td>
<td>0</td>
<td>10</td>
<td>20</td>
<td>30</td>
<td>40</td>
<td>50</td>
</tr>
</tbody>
</table>

Credit: Harmut Kaiser, LSU and HPX team
Legion Programming Model & Runtime

- **Dynamic task-based**
  - Data-centric – tasks specify what data they access and how they use them (read-only, read-write, exclusive, etc.)
  - Separates task implementation from hardware mapping decisions
  - Latency tolerant

- **Declarative specification of task graph in Legion**
  - Serial program
  - Read/Write effects on regions of data structures
  - Determine maximum parallelism

- **Port of S3D complete**

Legion team from Stanford, ExaCT Co-Design Center
Why is PGAS used? (Besides Application Characteristics)
One-Sided Communication is Closer to Hardware

- **One-sided communication (put/get) is what hardware does**
  - Even underneath send/receive
  - Information on where to put the date is in the message
  - Decouples synchronization from transfer

- **Two-sided message passing (e.g., send/receive in MPI)**
  - Requires matching with remote side to “find” the address to write data
  - Couples data transfer with synchronization (often, but not always what you want)

**Exascale should offer programmers / vendors a lightweight option**
• For communication-intensive problems, the gap is substantial
  – Problems with small messages
  – Bisection bandwidth problems (global FFTs)
Overhead for Messaging

- Overhead (processor busy time) gets worse on “exascale” cores
- Having a low overhead option is increasingly important

<table>
<thead>
<tr>
<th>Avg cycles per call (to do nothing) On Intel Ivybridge</th>
<th>Off Node</th>
<th>On-Node</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>iSend()</strong></td>
<td>3,692 cycles</td>
<td>1,262 cycles</td>
</tr>
<tr>
<td><strong>iRecv()</strong></td>
<td>1,154 cycles</td>
<td>1,924 cycles</td>
</tr>
</tbody>
</table>

**Diagram: Overhead for Messaging**

- **isend (off)** and **irecv (off)** have minimal overhead.
- **isend (on)** and **irecv (on)** exhibit increased overhead.
- **Graph labels**:
  - x-axis: Software Overhead (Nanoseconds)
  - y-axis: Nanoseconds
  - Colors:
    - 2.9 GHz x86
    - 1 GHz x86 (model)
    - 1 GHz 3-SIMT (model)

Computer Architecture Group (CAL)
Summary

- Successful PGAS applications are mostly asynchronous

1. Asynchronous fine-grained reads/write/atomics (aggregation and software caching when possible)
2. Dynamic work stealing
3. Strided irregular updates (adds) to distributed matrix
4. Hierarchical algorithms / one programming model
5. Task Graph Scheduling (UPC++)
6. Dynamic runtimes (CHARM++, Legion, HPX)

- Exascale architecture trends