A Productive Framework for Generating High Performance, Portable, Scalable Applications for Heterogeneous computing

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4,224 Kepler GPUs in Blue Waters

- NAMD
 - 100 million atom benchmark with Langevin dynamics and PME once every 4 steps, from launch to finish, all I/O included
 - 768 nodes, Kepler+Interlagos is 3.9X faster over Interlagos-only
 - 768 nodes, XK7 is 1.8X XE6
- Chroma
 - Lattice QCD parameters: grid size of 48³ x 512 running at the physical values of the quark masses
 - 768 nodes, Kepler+Interlagos is 4.9X faster over Interlagos-only
 - 768 nodes, XK7 is 2.4X XE6
- QMCPACK
 - Full run Graphite 4x4x1 (256 electrons), QMC followed by VMC
 - 700 nodes, Kepler+Interlagos is 4.9X faster over Interlagos-only
 - 700 nodes, XK7 is 2.7X XE6

Two Current Challenges

- At scale use of GPUs
 - Communication costs dominate beyond 2048 nodes
 - E.g., NAMD Limited by PME
 - Insufficient computation work
- Programming Efforts

 This talk

Blue Waters K7 Nodes NAMD Strong Scaling – 100M Atoms





Writing efficient parallel code is complicated. Tools can provide focused help or broad help

Planning how to execute an algorithm Implementing the plan



Levels of GPU Programming Languages

Prototype & in development

X10, Chapel, Nesl, Delite, Par4all, Triolet...

Implementation manages GPU threading and synchronization invisibly to user

Next generation OpenACC, C++AMP, Thrust, Bolt

Simplifies data movement, kernel details and kernel launch Same GPU execution model (but less boilerplate)

Current generation

CUDA, OpenCL, DirectCompute



IWCSE 2013

Where should the smarts be for Parallelization and Optimization?

- General-purpose language + parallelizing compiler
 - Requires a very intelligent compiler
 - Limited success outside of regular, static array algorithms
- Domain-specific language + domain-specific compiler
 - Simplify compiler's job with language restrictions and extensions
 - Requires customizing a compiler for each domain
- Parallel meta-library + general-purpose compiler
 - Library embodies parallelization decisions
 - Uses a general-purpose compiler infrastructure
 - Extensible—just add library functions
 - Historically, library is the area with the most success in parallel computing



Triolet – Composable Library-Driven Parallelization

- EDSL-style library: build, then interpret program packages
- Allows library to collect multiple parallel operations and create an optimized arrangement
 - Lazy evaluation and aggressive inlining
 - Loop fusion to reduce communication and memory traffic
 - Array partitioning to reduce communication overhead
 - Library source-guided parallelism optimization of sequential, shared-memory, and/or distributed algorithms
- Loop-building decisions use information that is often known at compile time
 - By adding typing to Python



Example: Correlation Code





Triolet Compiler Intermediate Representation

- List comprehension and par build a package containing
 - 1. Desired parallelism
 - 2. Input data structures
 - 3. Loop body
 - for each loop level
- Loop structure and parallelism annotations are statically known



Triolet Meta-Library

- Compiler inlines histogram
- histogram has code paths for handling different loop structures
- Loop structure is known, so compiler can remove unused code paths

```
correlation xs ys =
  case TdxNest HintPar
                (arraySlice xs)
                 (λx. IdxFlat HintSeq
                               (arraySlice ys)
                               (\lambda y. f x y)
  of IdxNest parhint input body.
       case parhint
       of HintSeq. code for sequential nested histogram
           HintPar. parReduce input
                                (\lambda chunk.
                                    seqHistogram 100 body chunk)
     IdxFlat parhint input body. code for flat histogram
```

Example: Correlation Code

- Result is an outer loop specialized for this application
- Process continues for inner loop





Cluster-Parallel Performance and Scalability

- Triolet delivers large speedup over sequential C
- On par with manually parallelized C for computation-bound code (left)
- Beats similar highlevel interfaces on communicationintensive code (right)





Chris Rodriues Rodrigues, et al, PPoPP 2014

Tangram

- A parallel algorithm framework for solving linear recurrence problems
 - Scan, tridiagonal matrix solvers, bidiagonal matrix solvers, recursive filters, …
 - Many specialized algorithms in literature
- Linear Recurrence very important for converting sequential algorithms into parallel algorithms



Tangrams Linear Optimizations

- Library operations to simplify application tiling and communication
 - Auto-tuning for each target architecture
- Unified Tiling Space
 - Simple interface for register tiling, scratchpad tiling, and cache tiling
 - Automatic thread fusion as enabler
- Communication Optimization
 - Choice/hybrid of three major types of algorithms
 - Computation vs. communication tradeoff



Linear Recurrence Algorithms and Communication



Brent-Kung Circuit

Kogge-Stone Circuit

Group Structured



Tangram Initial Results



Prefix scan on Fermi (C2050)

14

12

10 samples

8

6

4

1-32bit

second)

рег

οf

Throughput (billions

1867





Prefix scan on Kepler(Titan)



Tridiagonal solver on both GPUs

Next Steps

- Triolet released as an open source project
 - Develop additional Triolet library functions and their implementations for important application domains
 - Develop Triolet library functions for GPU clusters
- Publish and release Tangram
 - Current tridiagonal solver in CUSPARSE is from UIUC based on the Tangram work
 - Integration with Triolet



THANK YOU!

