An Ecosystem for the New HPC: Heterogeneous Parallel Computing

Wu FENG

Dept. of Computer Science and Dept. of Electrical & Computer Engineering Virginia Bioinformatics Institute





Japanese 'Computnik' Earth Simulator Shatters U.S. Supercomputer Hegemony

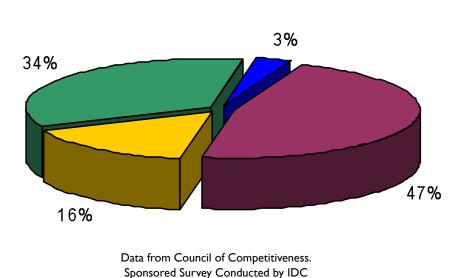
Tokyo 20 April 2002 The Japanese Earth Simulator is online and producing results that alarm the USA, that considered itself as being leading in supercomputing technology. With over 35 Tflop/s, it five times outperforms the Asci White supercomputer that is leading the current TOP500 list. No doubt that position is for the Earth Simulator, not only for the next list, but probably even for





Importance of High-Performance Computing (HPC)

Competitive Risk From Not Having Access to HPC



■ Could exist and compete

■ Could not exist as a business

□ Could not compete on quality & testing issues

Could not compete on time to market & cost







A Chinese scientific research center has built the

fastest supercomputer ever made, replacing the

United States as maker of the swiftest machine,

Computnik 2.0?



The Second Coming of Computnik? Computnik 2.0?

RECOMMEND

TWITTER

LINKEDIN

- No ... "only" 43% faster than the previous #1 supercomputer, but
 - → \$20M cheaper than the previous #1 supercomputer
 - → 42% less power consumption
- The Second Coming of the "Beowulf Cluster" for HPC
 - The further commoditization of HPC





Vision

Commoditizing personal supercomputing for the masses





2.5 x 10¹⁵ floating-pt ops per sec = 2.5 petaflops (Linpack benchmark)

iPad2: 1.5 x 10⁹ flops = 1.5 gigaflops 1.5 gigaflops/iPad2 * 9.3M iPad2 (Q2 2011) = 14 petaflops (Linpack benchmark extrapolated)

- A software ecosystem
 - ... for supporting heterogeneous parallel computing
 - ... by exploiting intra-node parallelism
 - ... to commoditize personal supercomputing for the masses





CPU Core Counts ...

- Doubling every 18-24 months
 - 2006: 2 cores
 - Examples: AMD Athlon 64 X2, Intel Core Duo
 - 2010: 8-12 cores
 - Examples: AMD Magny Cours, Intel Nehalem EX
- Penetrating all markets ...
 - Desktops
 - Laptops: Most in this room are multicore
 - Tablets: Apple iPad 2, HP TX1000, Sony S2
 - Cell Phones: LG Optimus 2X, Motorola Droid X2

A world of ubiquitous parallelism ...

... how to extract performance ... and then scale out





Paying For Performance

- "The free lunch is over..." †
 - Programmers can no longer expect substantial increases in singlethreaded performance.
 - The burden falls on developers to exploit parallel hardware for performance gains.
- How do we lower the cost of concurrency?

† H. Sutter, "The Free Lunch Is Over: A Fundamental Turn Toward Concurrency in Software," Dr. Dobb's Journal, 30(3), March 2005. (Updated August 2009.)

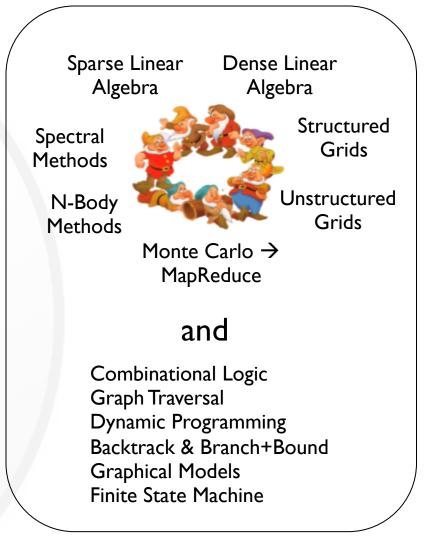




The Berkeley View †

- Traditional Approach
 - Applications that target existing hardware and programming models
- Berkeley Approach
 - Hardware design that keeps future applications in mind
 - Basis for future applications?
 13 computational dwarfs

A computational dwarf is a pattern of communication & computation that is common across a set of applications.



† Asanovic, K., et al. *The Landscape of Parallel Computing Research: A View from Berkeley*. Tech. Rep. UCB/EECS-2006-183, University of California, Berkeley, Dec. 2006.





Project Goal

An Ecosystem for Heterogeneous Parallel Computing

- Deliver personalized supercomputing to the masses
 - Heterogeneity of hardware devices for a "cluster on a chip" plus ...
 - Enabling software that tunes the parameters of the hardware devices with respect to performance, power, and programmability

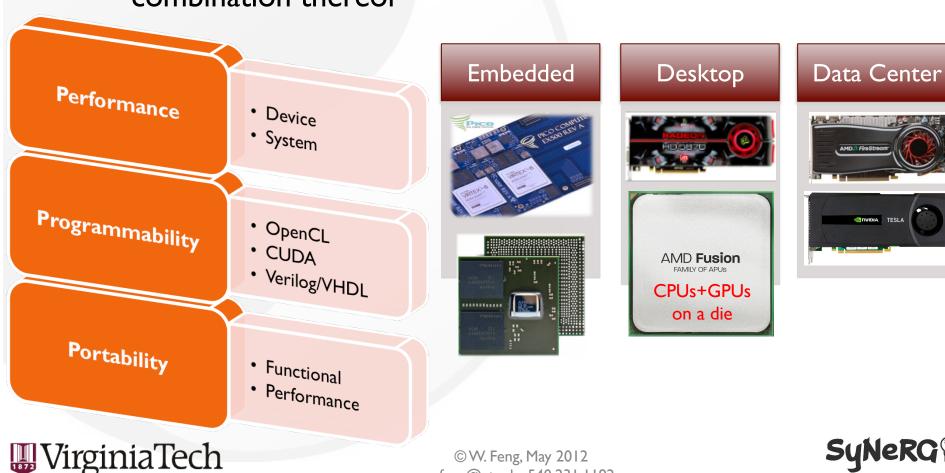
via a benchmark suite of computational dwarfs and apps





Multi-Dimensional Understanding of 3 P's

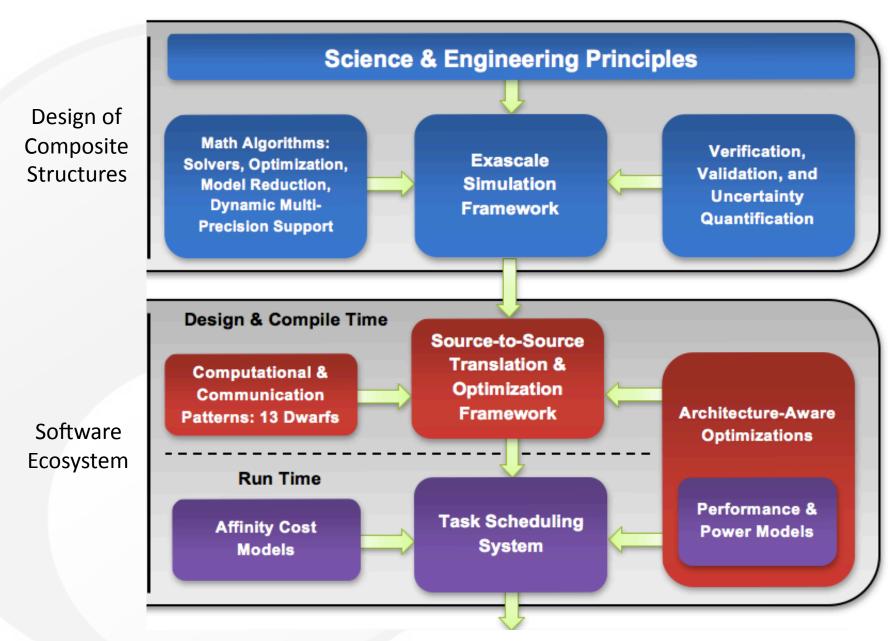
 A multi-dimensional understanding of how to optimize <u>performance</u>, <u>programmability</u>, <u>portability</u> or some combination thereof



Invent the Future

wfeng@vt.edu, 540.231.1192

synergy.cs.vt.edu



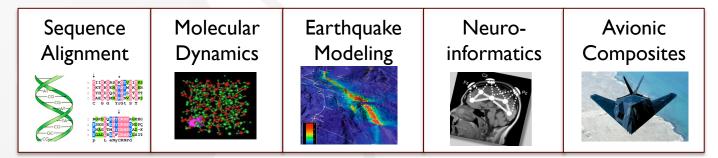


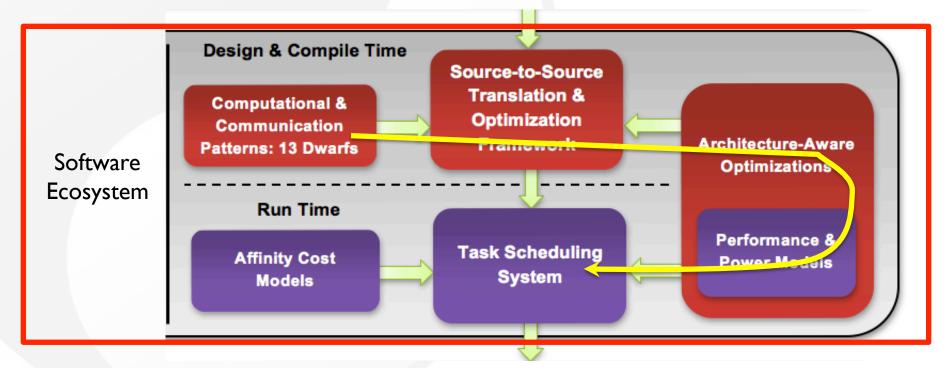




An Ecosystem for Heterogeneous Parallel Computing

Applications



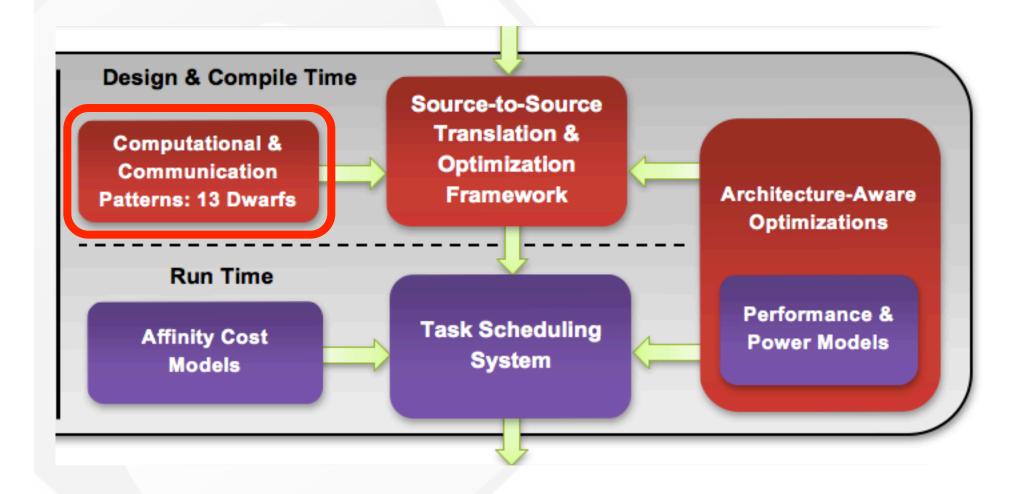




Heterogeneous Parallel Computing (HPC) Platform



Roadmap

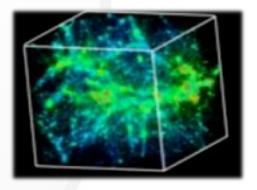




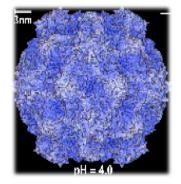


Example of a Computational Dwarf: N-Body

- Computational Dwarf: Pattern of computation & communication
 ... that is common across a set of applications
- N-Body problems are studied in
 - Cosmology, particle physics, biology, and engineering
- All have similar structures
- An N-Body benchmark can provide meaningful insight to people in all these fields
- Optimizations may be generally applicable as well



RoadRunner Universe: Astrophysics



GEM: Molecular Modeling

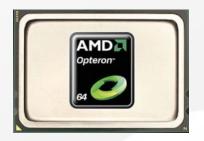




First Instantiation: OpenCL & the 13 Dwarfs

Goal

- Provide common algorithmic methods, i.e., dwarfs, in a language that is "write once, run anywhere" (CPU, GPU, or even FPGA), i.e., OpenCL











 Part of a larger umbrella project (2008-2012) funded by the NSF Center for High-Performance Reconfigurable Computing (CHREC)























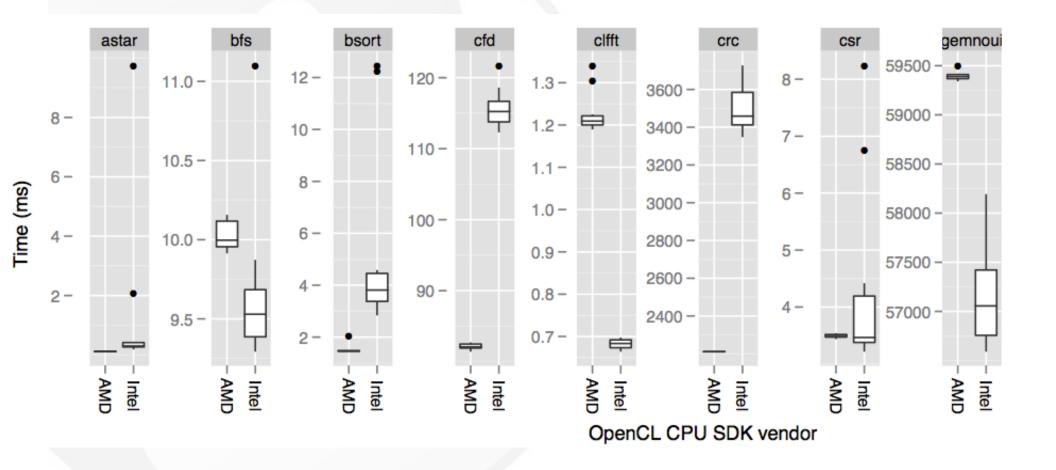
Status of OpenCL and the 13 Dwarfs

Dwarf	Done	In progress
Dense linear algebra	LU Decomposition	
Sparse linear algebra	Matrix Multiplication	
Spectral methods	FFT	
N-Body methods	GEM	
Structured grids	SRAD	
Unstructured grids	CFD Solver	
MapReduce		StreamMR
Combinational logic	CRC	
Graph traversal	Breadth-First Search	
Dynamic programming	Needleman-Wunsch	
Backtrack and Branch-and-Bound		N-Queens, Traveling Salesman
Graphical models	Hidden Markov Model	
Finite state machines	Temporal Data Mining	





Execution Time (ms) of Dwarfs with SDKs







The Future is Fusion

Experimental Set-Up: Machines and Workload

Platform	AMD Zacate APU	AMD Radeon HD 5870	AMD Radeon HD 5450
Stream Processors	80	1600	80
Compute Units	2	20	2
Memory Bus Type	NA	GDDR5	DDR3
Device Memory	192 MB	1024 MB	512 MB
Local Memory	32 KB	32 KB	32 KB
Max. Workgroup Size	256 Threads	256 Threads	128 Threads
Core Clock Frequency	492 MHz	850 MHz	675 MHz
Peak FLOPS	80 GFlops/s	2720 GFlops/s	104 GFlops/s
Host:		_	
Processor	AMD Engg. Sample @1.6 GHz	Intel Xeon E5405 @2.0 GHz	Intel Celeron 430 @1.8 GHz
System Memory	2 GB (NA)	2 GB DDR2	2 GB DDR2
Cache	L1: 32K, L2: 512K	L1: 32K, L2: 6M	L1: 32K, L2: 512K
Kernel	Ubuntu 2.6.35.22	Ubuntu 2.6.28.19	Ubuntu 2.6.32.24

OpenCL and the 13 Dwarfs

Sparse Linear Algebra: SpMV

N-body: Molecular Modeling

Spectral: FFT

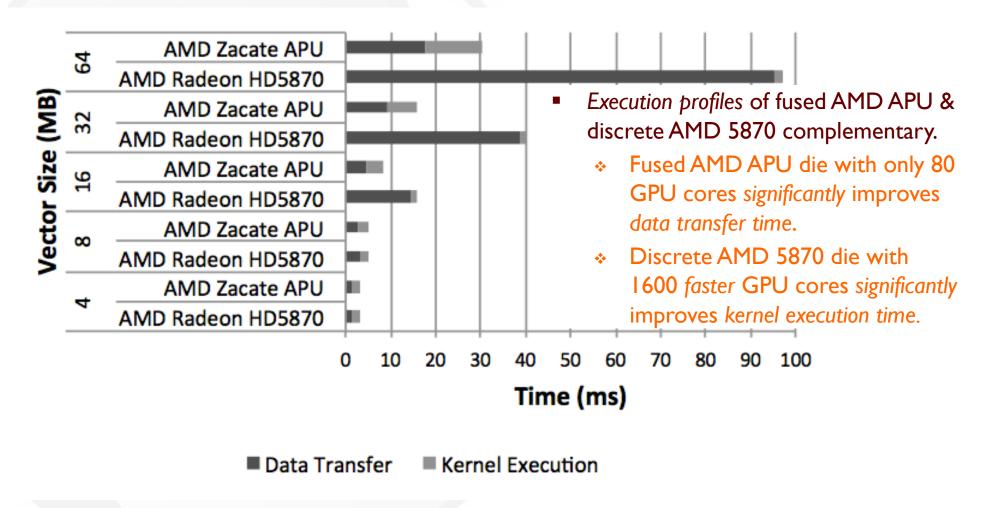
M. Daga, A. Aji, W. Feng, "On the Efficacy of a Fused CPU+GPU Processor for Parallel Computing," Symposium on Application Accelerators in High Performance Computing, Jul. 2011.

Dense Linear Algebra: Scan and Reduce (SHOC @ ORNL)





Performance: Reduction (Dense Linear Algebra)







System Power

AMD Fusion APU

At idle: 12 watts

At load: 17 watts(Spectral Method: FFT)

At load: 20 watts(N-body: Molecular Modeling)

AMD Radeon HD 5870
 Machine w/ 2-GHz Intel
 Xeon E5405

- At idle: 188 watts

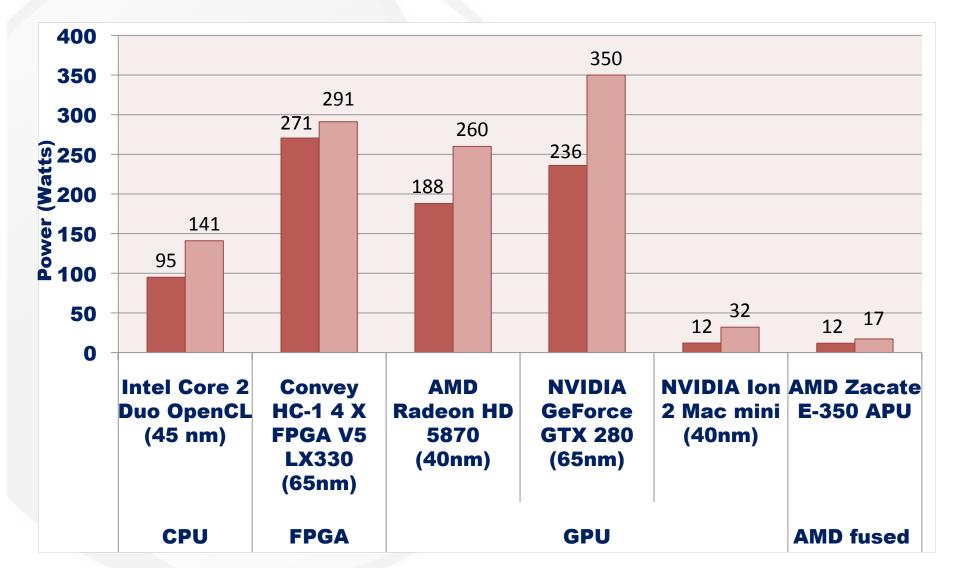
- At load: 260 watts







Total System Power: Idle vs. At Load (w/ FFT)







Status of OpenCL & the 13 Dwarfs

2009 - 2011

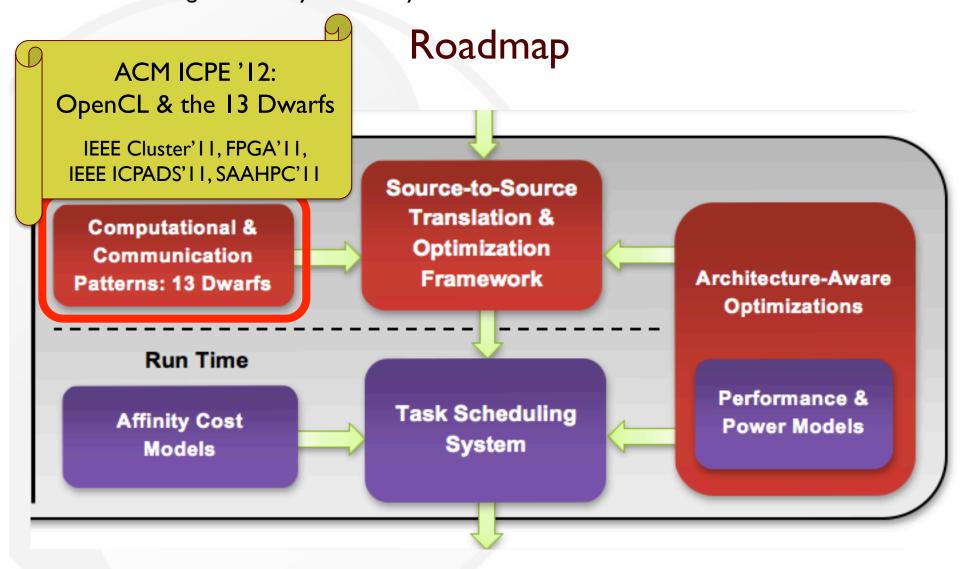
Dwarf	Done	
Dense linear algebra	LU Decomposition	
Sparse linear algebra	Matrix Multiplication	
Spectral methods	FFT	
N-Body methods	GEM	
Structured grids	SRAD	
Unstructured grids	CFD solver	
MapReduce		
Combinational logic	CRC	
Graph traversal	Breadth-First Search (BFS)	
Dynamic programming	Needleman-Wunsch	
Backtrack and Branch-and-Bound		
Graphical models	Hidden Markov Model	
Finite state machines	Temporal Data Mining	







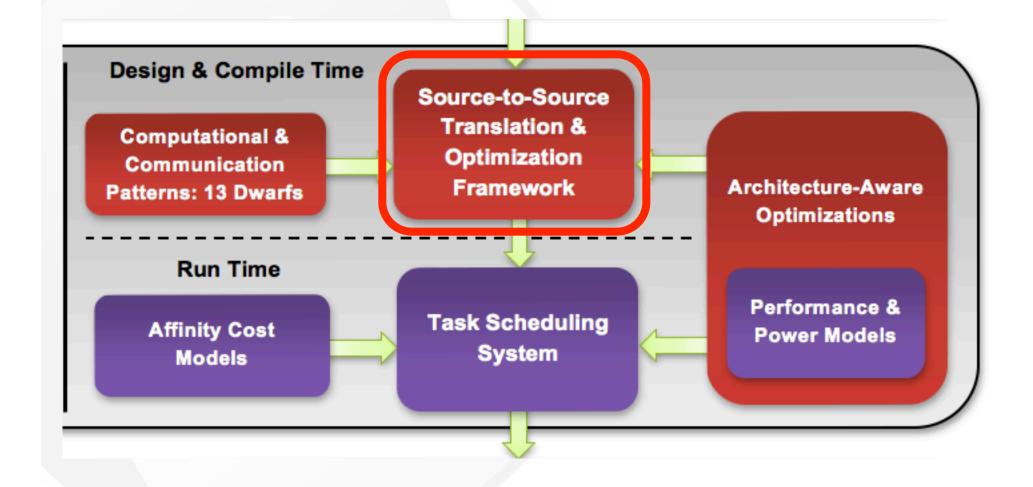
Performance, Programmability, Portability







Roadmap



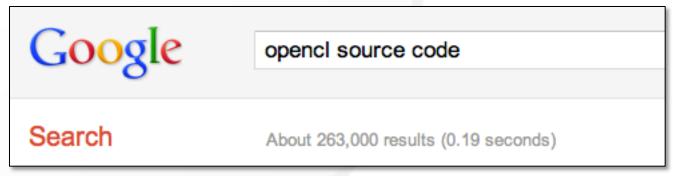




Prevalence



First public release February 2007



First public release December 2008

Search Date: 2011-09-14





CUDA-Accelerated Applications

GOVERNMENT & DEFENSE

Ikena: Imagery Analysis and Video Forensics Signal Processing Library: GPU VSIPL IDL and MATLAB® Acceleration: GPULib GIS: Manifold

MOLECULAR DYNAMICS, COMPUTATIONAL **CHEMISTRY**

OpenMM library for molecular dynamics on GPUs GROMACS using OpenMM NAMD molecular dynamics VMD visualization of molecular dynamics **HOOMD** molecular dynamics Acellera: ACEMD bio-molecular dynamics package BigDFT: DFT (Density functional theory) electronic structure OpenGeoSolutions: Spectral decomposition and inversion **MDGPU** GPUGrid.net

LIFE SCIENCES, BIO-INFORMATICS

GPU HMMER DNA Sequence alignment: MUMmerGPU LISSOM: model of human neocortex using CUDA Silicon Informatics: AutoDock

ELECTRODYNAMICS AND ELECTROMAGNETIC

Acceleware: FDTD Solver Acceleware: EM Solutions Remcom XStream FDTD SPEAG Semcad X

CST Microwave Studio Quantum electrodynamics library GPMAD: Particle beam dynamics simulator

MEDICAL IMAGING, CT, MRI

RealityServer GPULib:IDL acceleration Acceleware: Imaging Solutions Digisens: SnapCT tomographic reconstruction software Techniscan: Whole Breast Ultrasound Imaging System

OIL & GAS

Acceleware: Kirchoff and Reverse Time Migration SeismicCity: 3D seismic imaging for prestack depth migration Mercury Computer systems: 3D data visualization ffA: 3D Seismic processing software Headwave: Prestack data processing

FINANCIAL COMPUTING AND OPTIONS **PRICING**

SciComp: derivatives pricing Hanweck: options pricing Exegy: Risk Analysis Agumin: 3D Visualization of market data Level 3 Finance OnEye (Australia): Accelerated Trading Solutions Arbitragis Trading

MATLAB, LABVIEW, MATHEMATICA, R

CUDA Acceleration for MATLAB Accelereves: lacket[™] engine for MATLAB GPULib: mathematical functions for IDL and MATLAB Integrating Simulink with CUDA using S-functions Enabling GPU Computing in the R Statistical Environment Mathematica plug-in for CUDA National Instruments LabView for NVIDIA GPUs

ELECTRONIC DESIGN AUTOMATION

Agilent EESof: ADS SPICE simulator Synopsys: Sentaraus TCAD Gauda: Optical proximity correction (OPC)

WEATHER AND OCEAN MODELING

CUDA-accelerated WRF code

VIDEO, IMAGING, AND VISION APPLICATIONS

Axxon Intellect Enterprise Video Surveillance Software Pflow CUDA Plugin for Autodesk 3ds Max RUINS Shatter CUDA Plug-in for Maya Bullet 3D Multi-Physics Library with CUDA Support **CUDA Voxel Rendering Engine** Furryball: Direct3D GPU Rendering Plugin for Maya

See: http://www.nvidia.com/object/cuda app tesla.html





CU2CL:

CUDA-to-OpenCL Source-to-Source Translator†

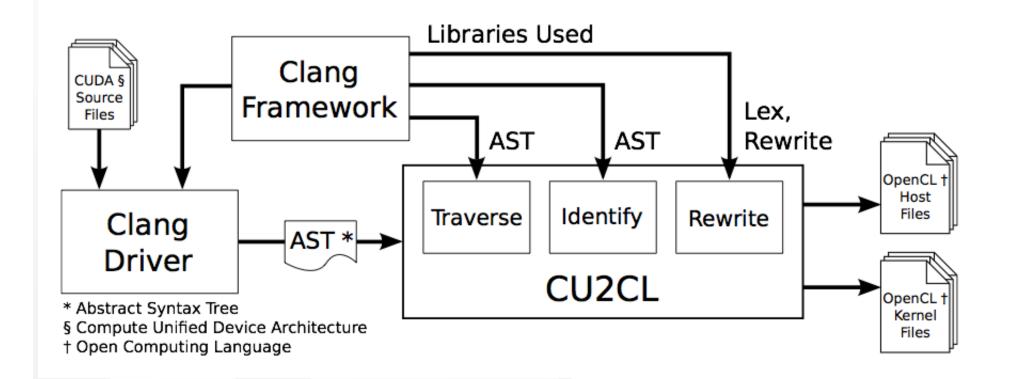
- Implemented as a Clang plug-in to leverage its productionquality compiler framework and target LLVM bytecode.
- Covers primary CUDA constructs found in CUDA C and CUDA run-time API.
- Performs as well as codes manually ported from CUDA to OpenCL.
- Others: OpenCL-to-CUDA and OpenMP-to-OpenCL

† "CU2CL: A CUDA-to-OpenCL Translator for Multi- and Many-core Architectures," 17th IEEE Int'l Conf. on Parallel & Distributed Systems (ICPADS), Dec. 2011.





CU2CL Translation and Performance



 Automatically translated OpenCL codes (via CU2CL) yield similar execution times to manually translated OpenCL codes





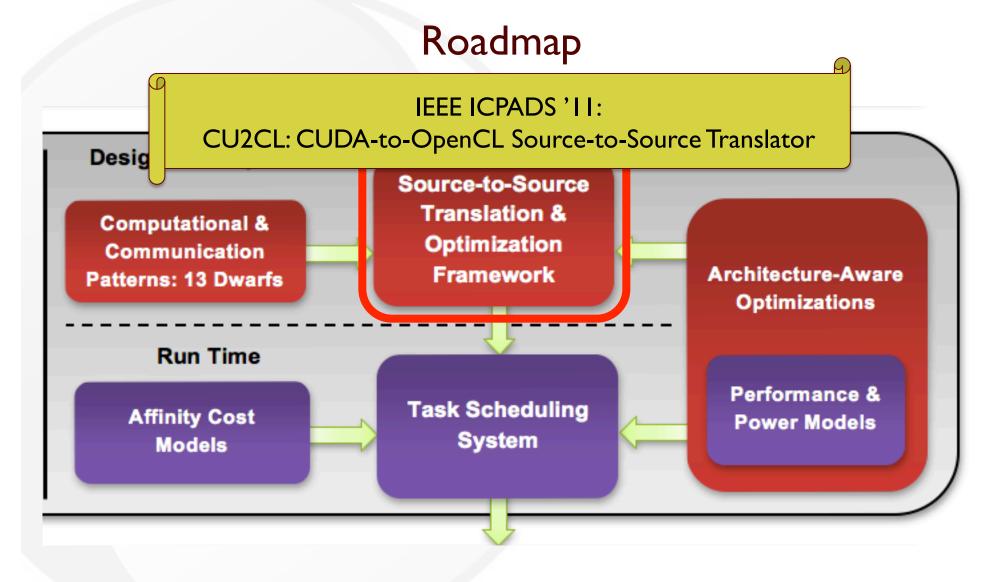
CU2CL Coverage

Source	Application	Lines	Changed	Percentage
CUDA SDK	BlackScholes	347	4	98.85
	matrixMul	351	2	99.43
	scalarProd	171	4	97.66
	vectorAdd	147	0	100.00
Rodinia	Back Propagation	313	5	98.40
	Hotspot	328	7	97.87
	Needleman-Wunsch	418	0	100.00
	SRAD	541	0	100.00
Virginia Tech	GEM: n-body molecular	2,511	5	99.80





Performance, Programmability, Portability

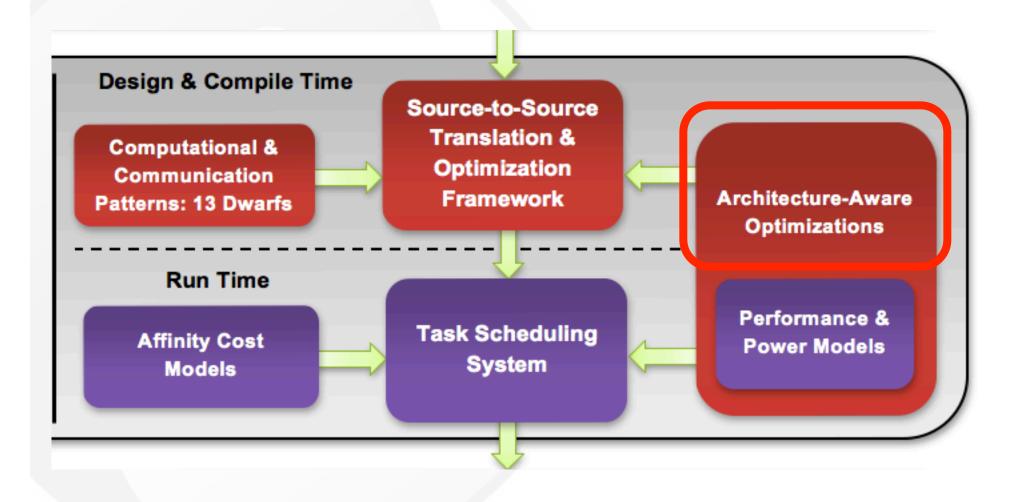






Performance, Programmability, Portability

Roadmap

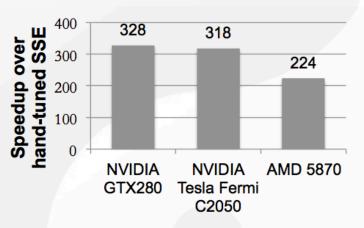


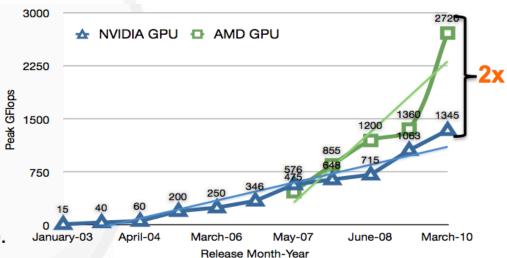




Computational Units Not Created Equal

- "AMD CPU ≠ Intel CPU" and "AMD GPU ≠ NVIDIA GPU"
- Initial performance of a CUDA-optimized N-body dwarf



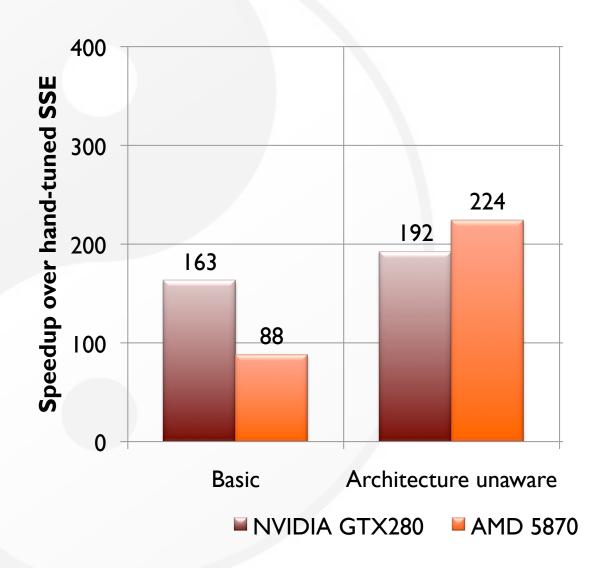


Performance of a Molecular Modeling App.





Basic & Architecture-Unaware Execution







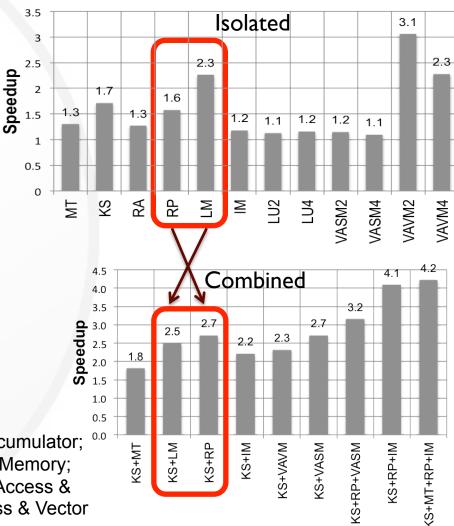
Architecture-Aware Optimization

(N-body Code for Molecular Modeling)

- Optimization techniques on AMD GPUs
 - Removing conditions → kernel splitting
 - Local staging
 - Using vector types
 - Using image memory
- Speedup over basic OpenCL GPU implementation
 - Isolated optimizations
 - Combined optimizations

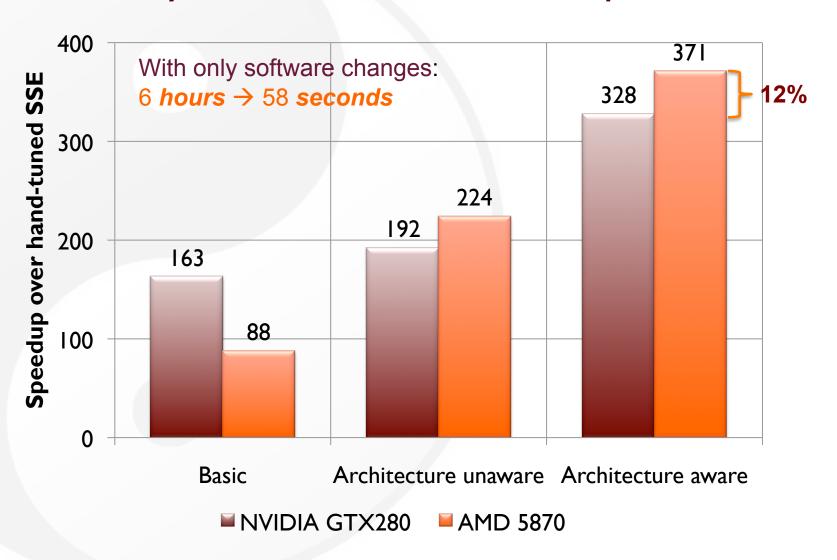
MT: Max Threads; KS: Kernel Splitting; RA: Register Accumulator; RP: Register Preloading; LM: Local Memory; IM: Image Memory; LU{2,4}: Loop Unrolling{2x,4x}; VASM{2,4}: Vectorized Access & Scalar Math{float2, float4}; VAVM{2,4}: Vectorized Access & Vector Math{float2, float4}







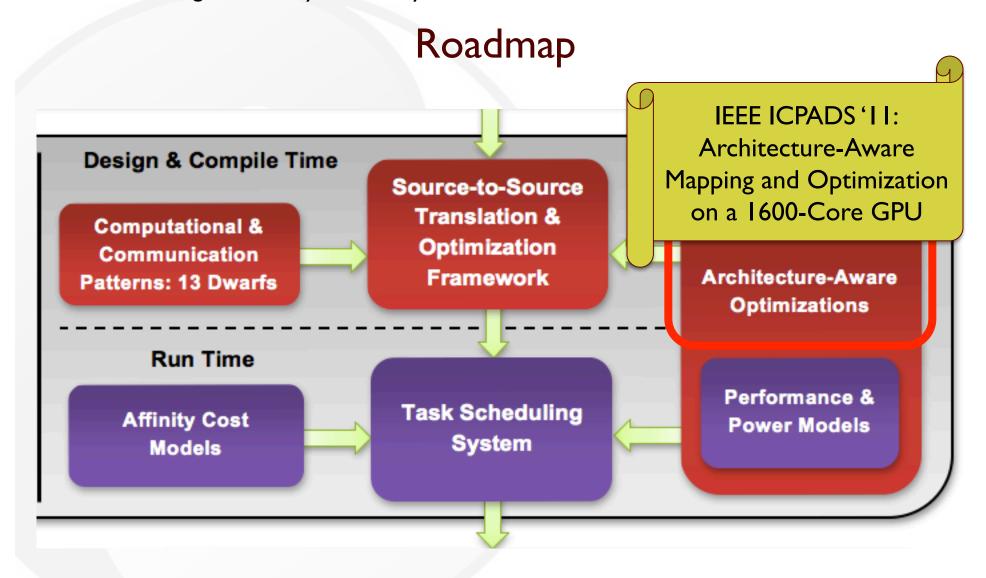
Summary: Architecture-Aware Optimization





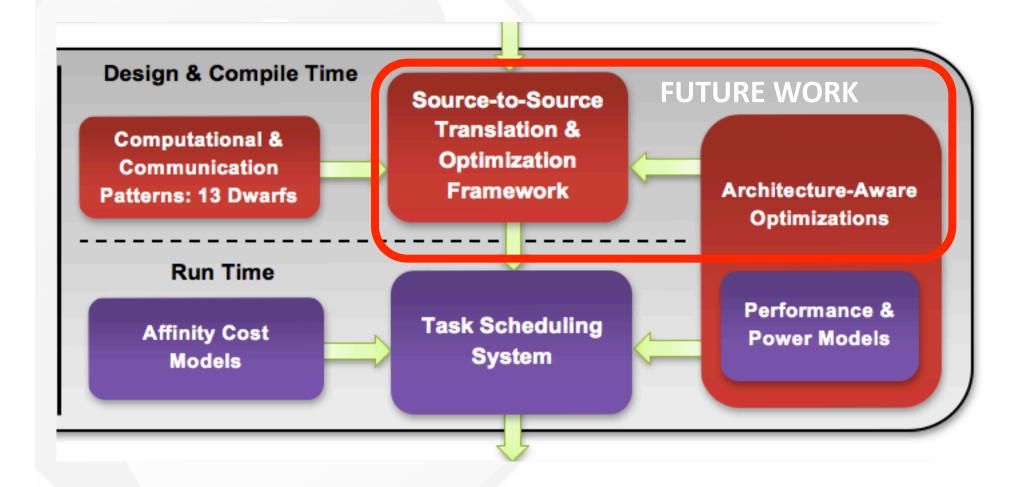


Performance, Programmability, Portability





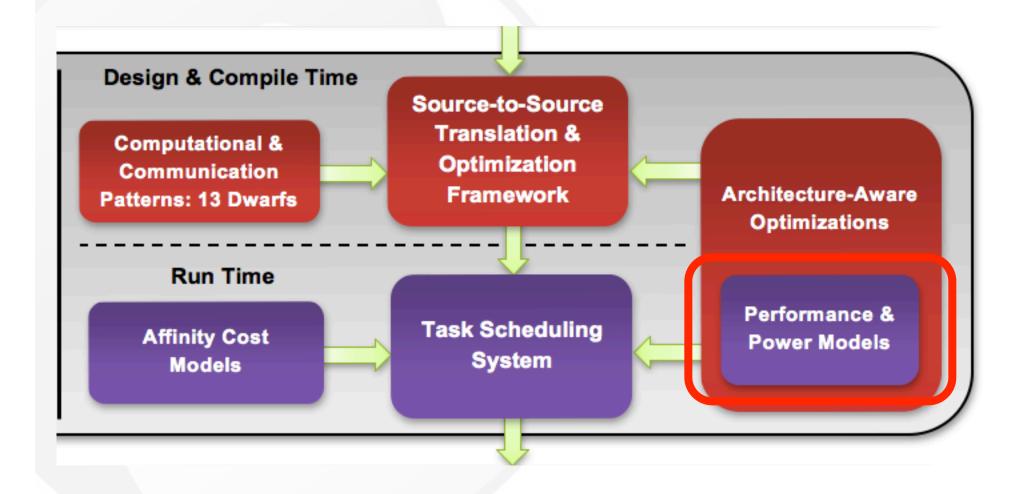








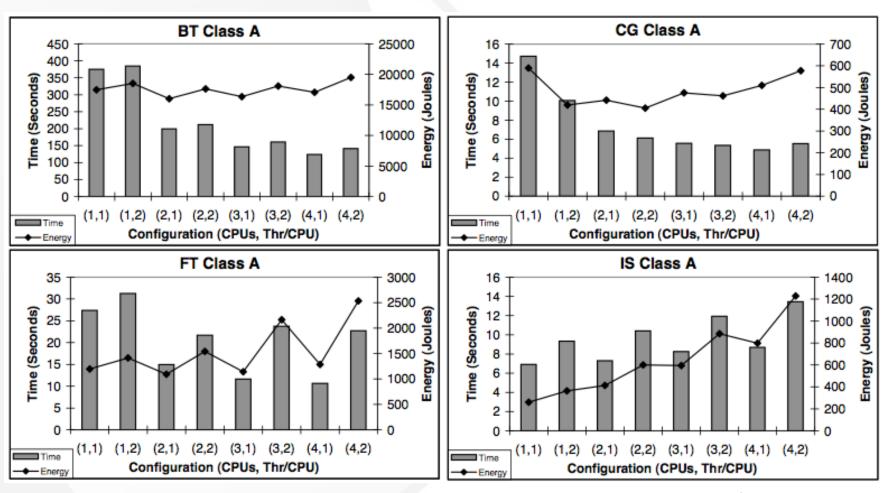
Performance, Programmability, Portability







Need for Performance & Power Modeling









Performance & Power Modeling

Goals

- Robust framework
- Very high accuracy (Target: < 5% prediction error)
- Identification of portable predictors for performance and power
- Multi-dimensional characterization
 - Performance → sequential, intra-node parallel, inter-node parallel
 - Power → component level, node level, cluster level





Problem Formulation:

LP-Based Energy-Optimal DVFS Schedule

- Definitions
 - A DVFS system exports $n \{ (f_i, P_i) \}$ settings.
 - T_i : total execution time of a program running at setting i
- Given a program with deadline D, find a DVS schedule $(t_1^*, ..., t_n^*)$ such that
 - If the program is executed for t_i seconds at setting i, the total energy usage E is minimized, the deadline D is met, and the required work is completed.

$$\min E = \sum_{i} P_i \cdot t_i$$

subject to

$$\sum_{i} t_{i} \le D$$
$$\sum_{i} t_{i} / T_{i} = 1$$
$$t_{i} \ge 0$$





Single-Coefficient β Performance Model

Our Formulation

- Define the relative performance slowdown δ as

$$T(f) / T(f_{MAX}) - I$$

 Re-formulate two-coefficient model as a single-coefficient model:

$$\frac{T(f)}{T(f_{max})} = \beta \cdot \frac{f_{max}}{f} + (1 - \beta)$$

with

$$\beta = \frac{W_{cpu}}{W_{cpu} + T_{mem} \cdot f_{max}}$$

- The coefficient β is computed at run-time using a regression method on the past MIPS rates reported from the built-in PMU.

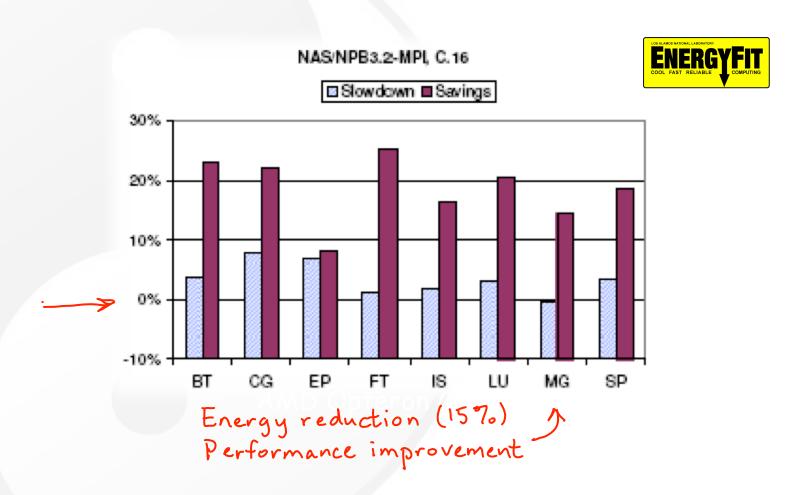
$$\beta = \frac{\sum_i (\frac{f_{max}}{f_i} - 1)(\frac{\texttt{mips}(f_{max})}{\texttt{mips}(f_i)} - 1)}{\sum_i (\frac{f_{max}}{f_i} - 1)^2}$$

C. Hsu and W. Feng.
"A Power-Aware Run-Time
System for High-Performance
Computing," *SC*/05, Nov. 2005.





NAS Parallel on an AMD Opteron Cluster

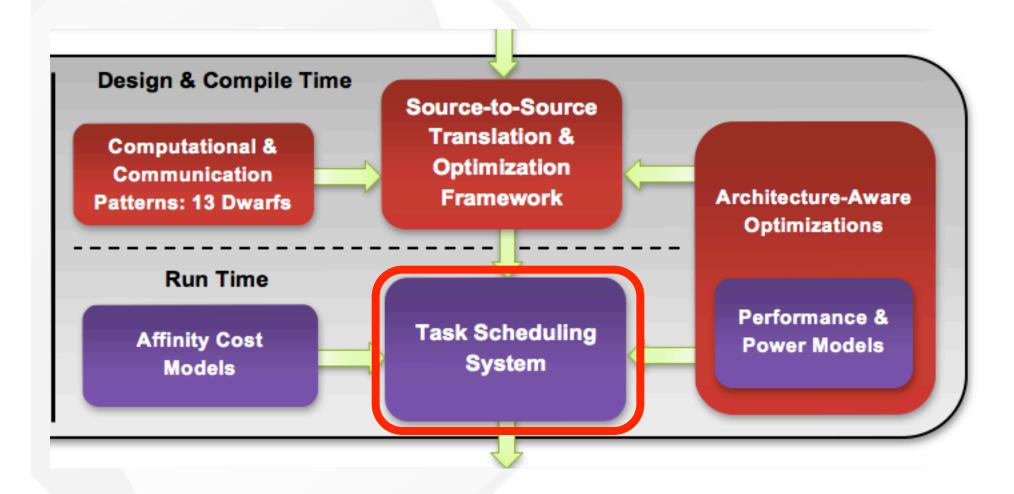


"A Power-Aware Run-Time System for High-Performance Computing," SC/05, Nov. 2005





Performance, Programmability, Portability







What is Heterogeneous Task Scheduling?

- Automatically spreading tasks across heterogeneous compute resources
 - CPUs
 - GPUs
 - APUs
- Specify tasks at a higher level (currently OpenMP extensions)
- Run them across available resources automatically

Goal

- A run-time system that intelligently uses what is available resource-wise and optimize for performance portability
 - Each user should not have to implement this for themselves!





How to Heterogeneous Task Schedule (HTS)

- Accelerated OpenMP offer heterogeneous task scheduling with
 - Programmability
 - Functional portability, given underlying compilers
 - Performance portability
- How?
 - A simple extension to Accelerated OpenMP syntax for programmability
 - Automatically dividing parallel tasks across arbitrary heterogeneous compute resources for functional portability
 - CPUs
 - GPUs
 - APUs
 - Intelligent runtime task scheduling for performance portability





Programmability: Why Accelerated OpenMP?

Traditional OpenMP

OpenMP Accelerator Directives

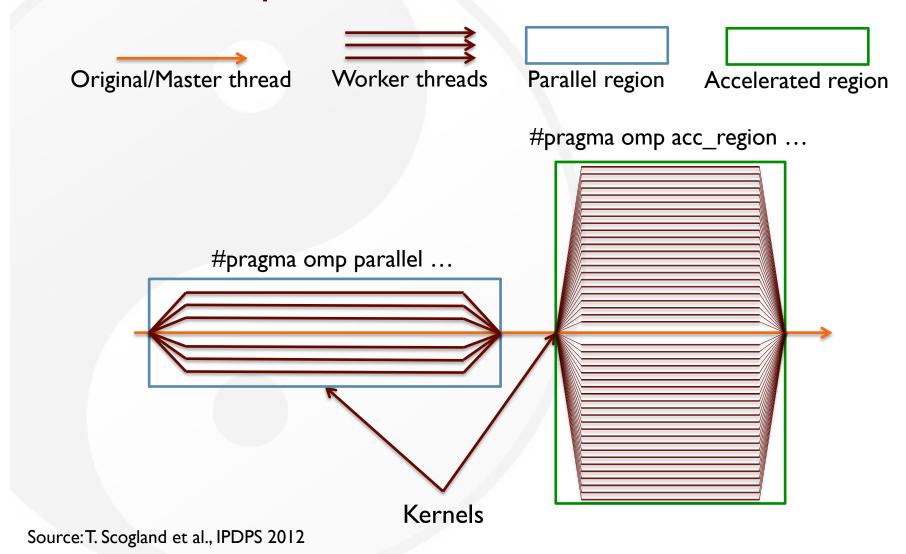
Source: T. Scogland et al., IPDPS 2012

Our Proposed Extension





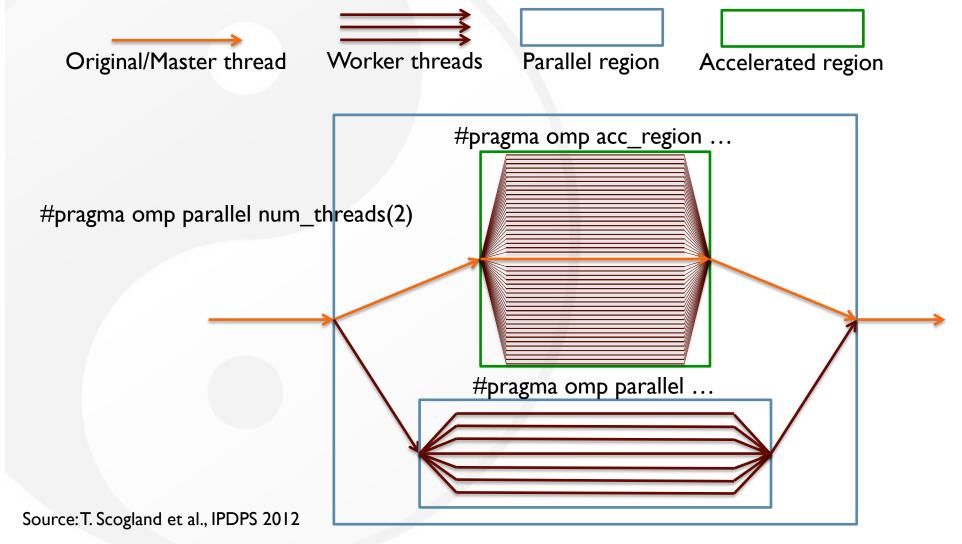
OpenMP Accelerator Behavior







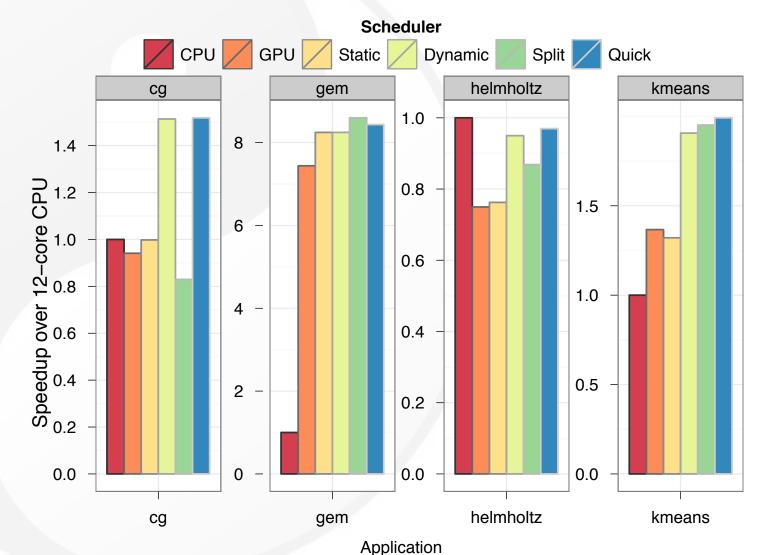
DESIRED OpenMP Accelerator Behavior







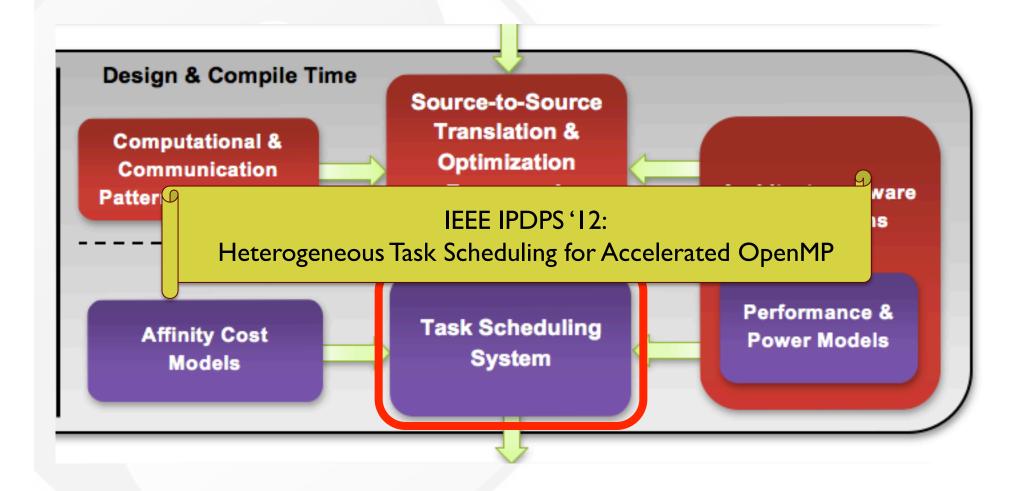
Results Across Schedulers for all Benchmarks





© W. Feng, May 2012 wfeng@vt.edu, 540.231.1192

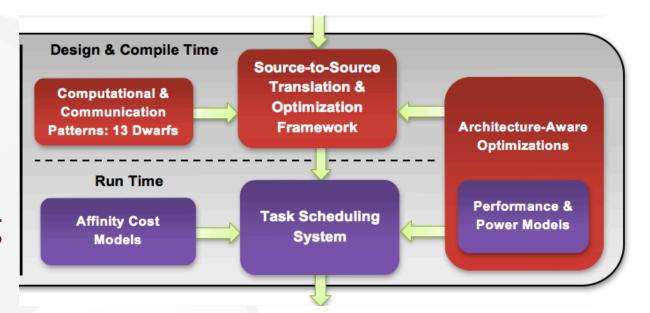








An Ecosystem for the New HPC: Heterogeneous Parallel Computing



Much work still to be done.

- OpenCL and the 13 Dwarfs
- Source-to-Source Translation
- Architecture-Aware Optimization
- Performance & Power Modeling
- Affinity-Based Cost Modeling
- Heterogeneous Task Scheduling

Beta release pending
CU2CL only & no optimization
Only manual optimizations
Preliminary & pre-multicore
Empirical results; modeling in progress
Preliminary with OpenMP





Recent Publications

- M. Daga, T. Scogland, W. Feng, "Architecture-Aware Mapping and Optimization on a 1600-Core GPU," 17th IEEE Int'l Conf. on Parallel & Distributed Systems, Dec. 2011.
- M. Elteir, H. Lin, W. Feng, "StreamMR: An Optimized MapReduce Framework for AMD GPUs," 17th IEEE Int'l Conf. on Parallel & Distributed Systems, Dec. 2011.
- W. Feng, Y. Cao, D. Patnaik, N. Ramakrishnan, "Temporal Data Mining for Neuroscience," GPU Computing Gems, Editor: W. Hwu, Elsevier/Morgan-Kaufmann, Feb. 2011.
- K. Bisset, A. Aji, M. Marathe, W. Feng, "High-Performance Biocomputing for Simulating the Spread of Contagion over Large Contact Networks," BMC Genomics, 2011.
- M. Elteir, H. Lin, W. Feng, "Performance Characterization and Optimization of Atomic Operations on AMD GPUs," IEEE Cluster, Sept. 2011.
- M. Daga, A. Aji, W. Feng, "On the Efficacy of a Fused CPU+GPU Processor for Parallel Computing," Symp. on Application Accelerators in High Performance Computing, Jul. 2011.
- A. Aji, M. Daga, and W. Feng, "Bounding the Effect of Partition Camping in Memory-Bound Kernels," ACM Int'l Conf. on Computing Frontiers, May 2011.
- S. Xiao, H. Lin, and W. Feng, "Accelerating Protein Sequence Search in a Heterogeneous Computing System," 25th Int'l Parallel & Distributed Processing Symp., May 2011.
- W. Feng with cast of many, "Accelerating Electrostatic Surface Potential Calculation with Multi-Scale Approximation on Graphics Processing Units," J. Molecular Graphics and Modeling, Jun. 2010.
- W. Feng and S. Xiao, "To GPU Synchronize or Not GPU Synchronize?" IEEE Int'l Symp. on Circuits and Systems, May-June 2010. wfeng@vt.edu, 540.231.1192

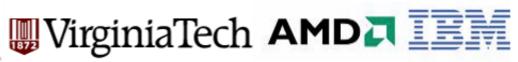
Funding Acknowledgements



























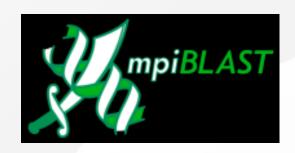
Wu Feng, wfeng@vt.edu, 540-231-1192



http://synergy.cs.vt.edu/



http://www.chrec.org/



http://www.mpiblast.org/



SUPERCOMPUTING in SMALL SPACES

http://sss.cs.vt.edu/



http://www.green500.org/



http://myvice.cs.vt.edu/

"Accelerators 'R US"

http://accel.cs.vt.edu/





An Ecosystem for the New HPC: Heterogeneous Parallel Computing

- Deliver personalized supercomputing to the masses
 - Heterogeneity of hardware devices plus enabling software that tunes for performance (speed & power), programmability, and portability

via a benchmark suite of computational dwarfs and apps

