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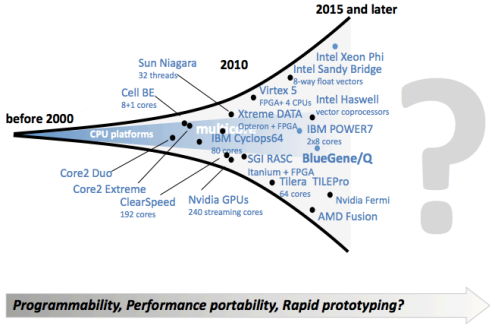
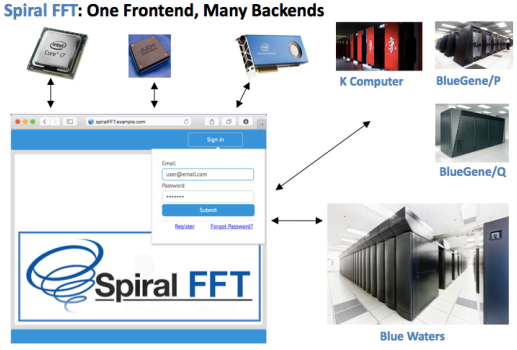
Spiral FFT

The ~~(Future)~~ Present is Parallel and Heterogeneous



Programmability, Performance portability, Rapid prototyping?

Spiral FFT: One Frontend, Many Backends

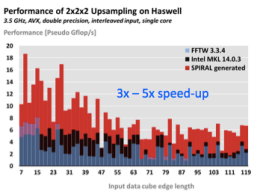


This research is part of the Blue Waters sustained-petascale computing project, which is supported by the National Science Foundation (awards OCI-0725070 and ACI-1238993) and the state of Illinois. Blue Waters is a joint effort of the University of Illinois at Urbana-Champaign and its National Center for Supercomputing Applications.

Performance

Spiral FFT: Performance, Driven by Machine/Project

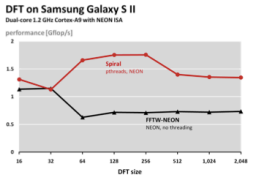
- **2006 Gordon Bell Prize (Peak Performance Award):** "Large-Scale Electronic Structure Calculations of High-Z Metals on the BlueGene/L Platform" [1].
- **2010 HPC Challenge Class II Award (Most Productive System):** "Automatic Generation of the HPC Challenge's Global FFT Benchmark for BlueGene/P" [2].



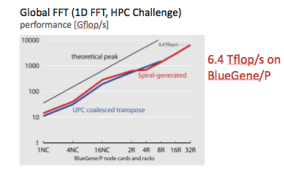
ONETEP = Order-*N* Electronic Total Energy Package [3]

T. Popovici, et. al., **"Generating Optimized Fourier Interpolation Routines for Density Functional Theory Using SPIRAL,"** 29th International Parallel & Distributed Processing Symposium (IPDPS), 2015, *to appear.*

[1] F. Gygi, F. Franchetti, et. al., in Proceedings of Supercomputing, 2006.
[2] G. Almási, F. Franchetti, et. al., "2010 IBM HPC Challenge Class II Submission"
[3] P. D. Haynes, et. al., **"ONETEP: linear-scaling density-functional theory with plane waves,"** Psi-k Newsletter 72, 78-91 (2005)



Samsung I9100 Galaxy S II
Dual-core ARM at 1.2GHz with NEON ISA

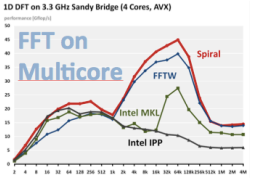


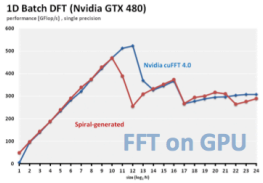
6.4 Tflop/s on BlueGene/P

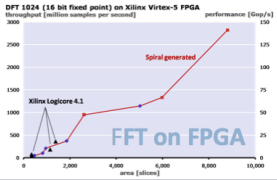
BlueGene/P at Argonne National Laboratory
128k cores (quad-core CPUs) at 850 MHz

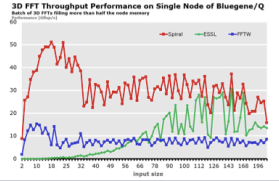
F. Gygi, E. W. Draeger, M. Schulz, B. R. de Supinski, J. A. Gunnels, V. Austel, J. C. Sexton, F. Franchetti, S. Kral, C. W. Ueberhuber, J. Lorenz, "Large-Scale Electronic Structure Calculations of High-Z Metals on the BlueGene/L Platform," In Proceedings of Supercomputing, 2006. *2006 Gordon Bell Prize (Peak Performance Award).*

G. Almási, B. Dalton, L. L. Hu, F. Franchetti, Y. Liu, A. Sidelnik, T. Spelce, I. G. Tănase, E. Tiotto, Y. Voronenko, X. Xue, "2010 IBM HPC Challenge Class II Submission," *2010 HPC Challenge Class II Award (Most Productive System).*



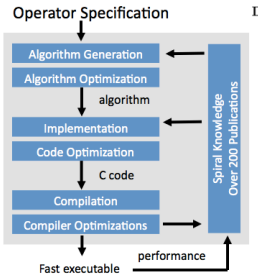






Project

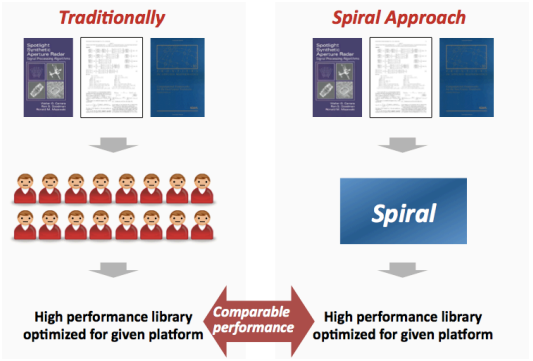
Spiral FFT: Automated Optimization/Implementation



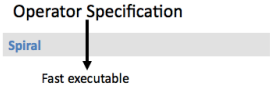
$$\mathrm{DFT}_4 = (\mathrm{DFT}_2 \otimes \mathrm{I}_2)\mathrm{T}^4_2(\mathrm{I}_2 \otimes \mathrm{DFT}_2)\,\mathrm{L}^4_2$$

Spiral-Synthesized code in Intel IPP 6 and 7

- Generated: 3984 C functions (signal processing) = 1M lines of code
- Full parallelism support
- Computer-generated code: Faster than what was achievable by hand



Spiral FFT: Capabilities and Blue Waters



- Multithreading (Multicore) $\mathrm{I}_p \otimes_{\parallel} A_{\mu n}$, $\mathrm{L}^{mn}_m \otimes \mathrm{I}_\mu$
- Vector SIMD (SSE, VMX/Altivec,...) $A \otimes \mathrm{I}_\nu$, $\underbrace{\mathrm{L}^{\nu^2}_\nu}_{\text{isa}}$, $\underbrace{\mathrm{L}^{\nu^2}_\nu}_{\text{isa}}$, $\underbrace{\mathrm{L}^{\nu^2}_\nu}_{\text{isa}}$
- Message Passing (Clusters, MPP) $\mathrm{I}_p \otimes_{\parallel} A_m$, $\underbrace{\mathrm{L}^{p^2}_p \otimes \mathrm{I}_{m/p^2}}_{\text{all-to-all}}$
- Streaming/multibuffering (Cell) $\mathrm{I}_n \otimes_2 A_{\mu m}$, $\mathrm{L}^{mn}_m \otimes \mathrm{I}_\mu$
- Graphics Processors (GPUs) $\prod_{i=0}^{n-1} A_i$, $A_m \otimes \mathrm{I}_w$, $P_n \otimes Q_w$

Spiral FFT on Blue Waters: Machine + Project driven...