



Presented by

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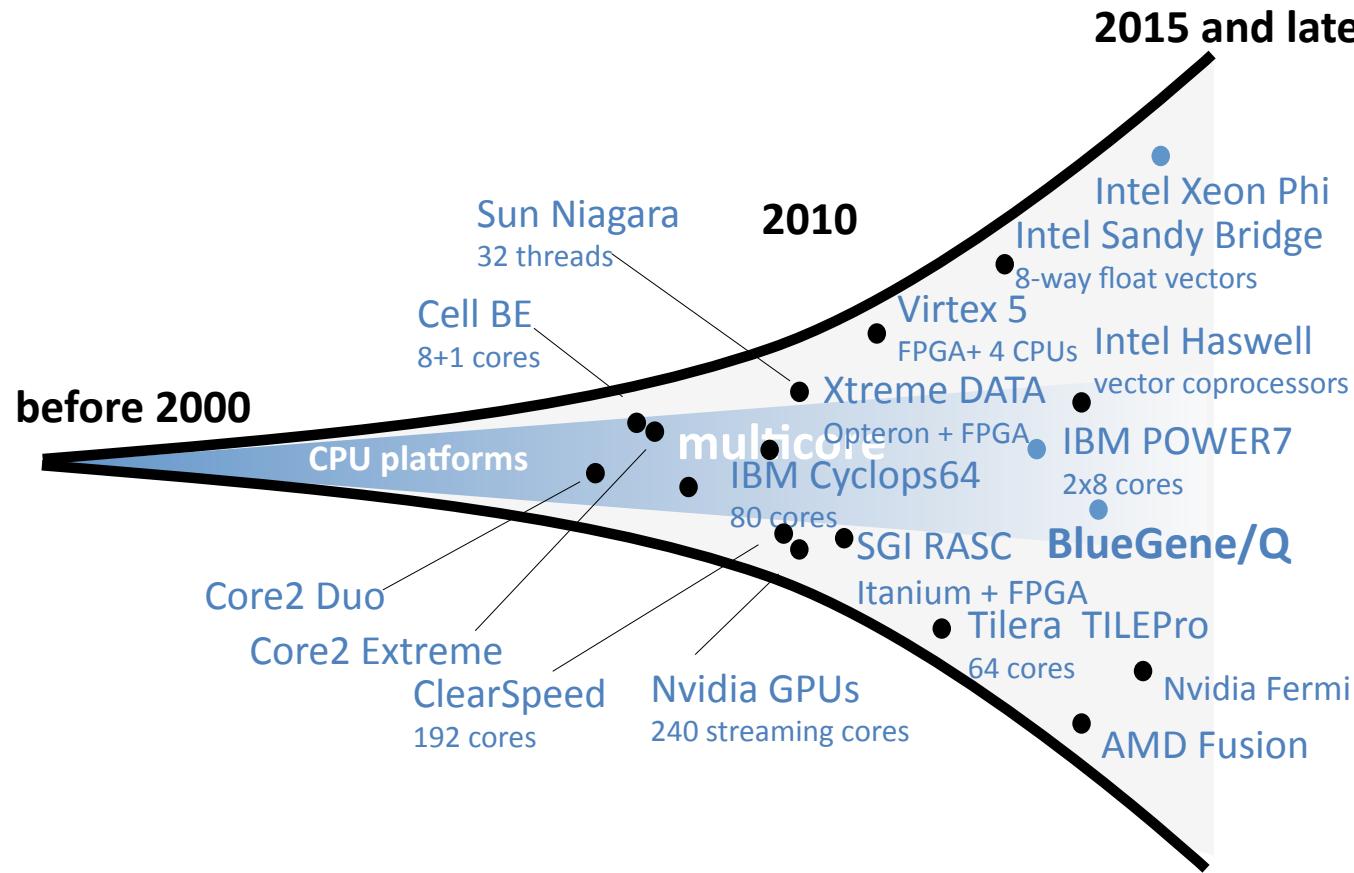
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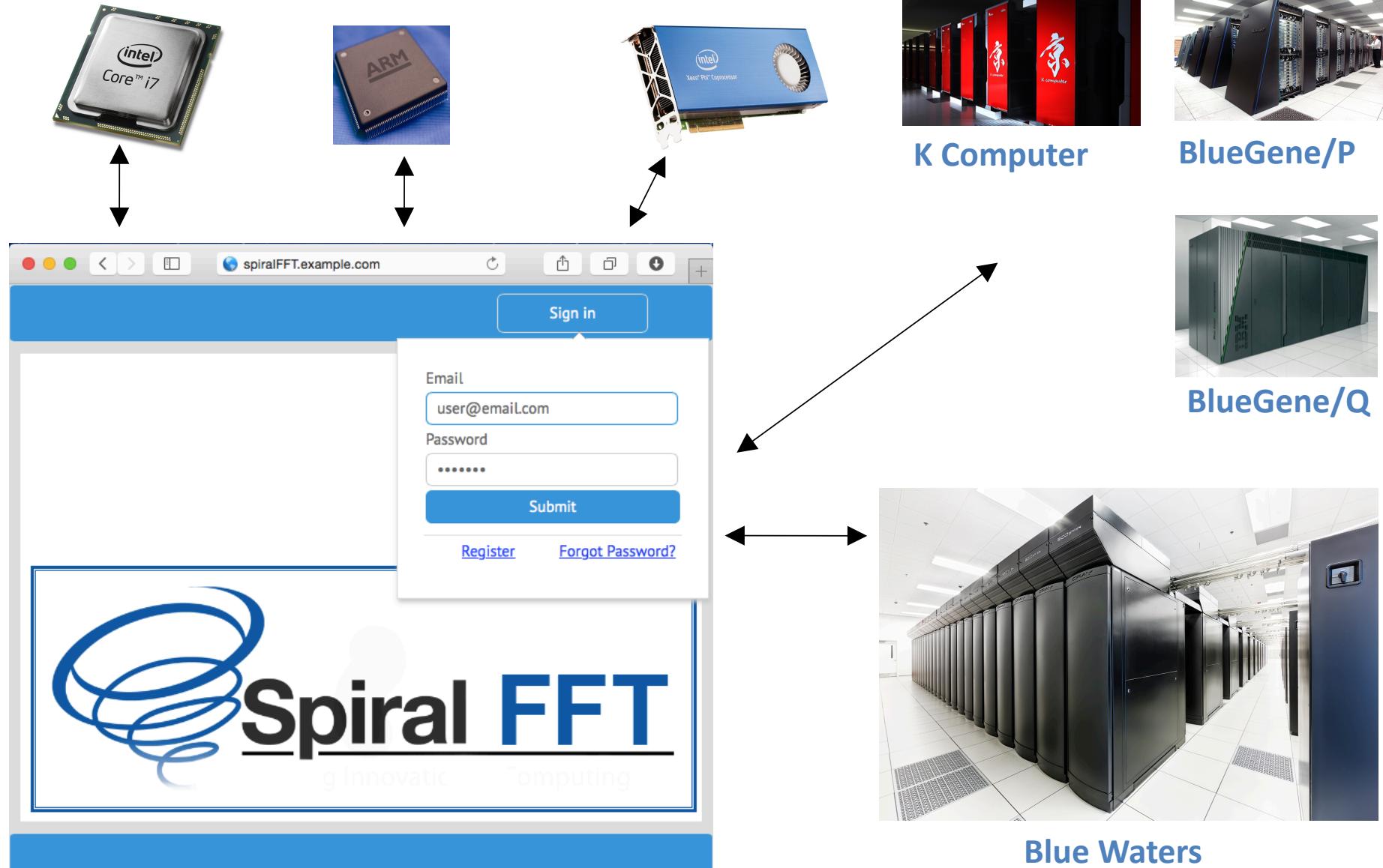
This research is part of the Blue Waters sustained-petascale computing project, which is supported by the National Science Foundation (awards OCI-0725070 and ACI-1238993) and the state of Illinois. Blue Waters is a joint effort of the University of Illinois at Urbana-Champaign and its National Center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

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

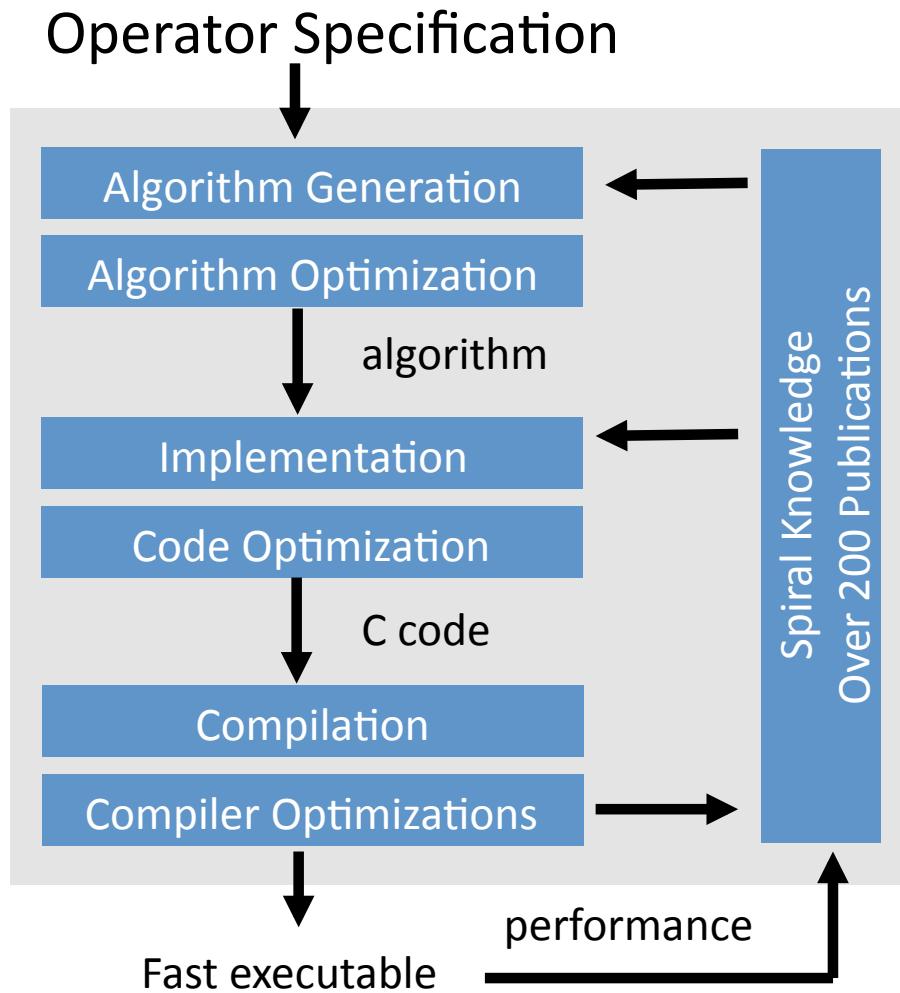


Programmability, Performance portability, Rapid prototyping?

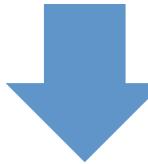
Spiral FFT: One Frontend, Many Backends



Spiral FFT: Automated Optimization/Implementation



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

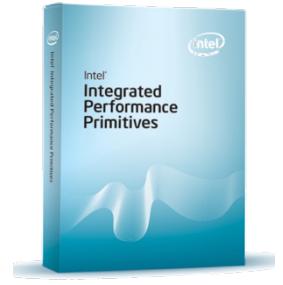


```

void sub(double *y, double *x) {
    double f0, f1, f2, f3, f4, f7, f8, f10, f11;
    f0 = x[0] - x[3];
    f1 = x[0] + x[3];
    f2 = x[1] - x[2];
    f3 = x[1] + x[2];
    f4 = f1 - f3;
    y[0] = f1 + f3;
    y[2] = 0.7071067811865476 * f4;
    f7 = 0.9238795325112867 * f0;
    f8 = 0.3826834323650898 * f2;
    y[1] = f7 + f8;
    f10 = 0.3826834323650898 * f0;
    f11 = (-0.9238795325112867) * f2;
    y[3] = f10 + f11;
}
    
```

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: 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].

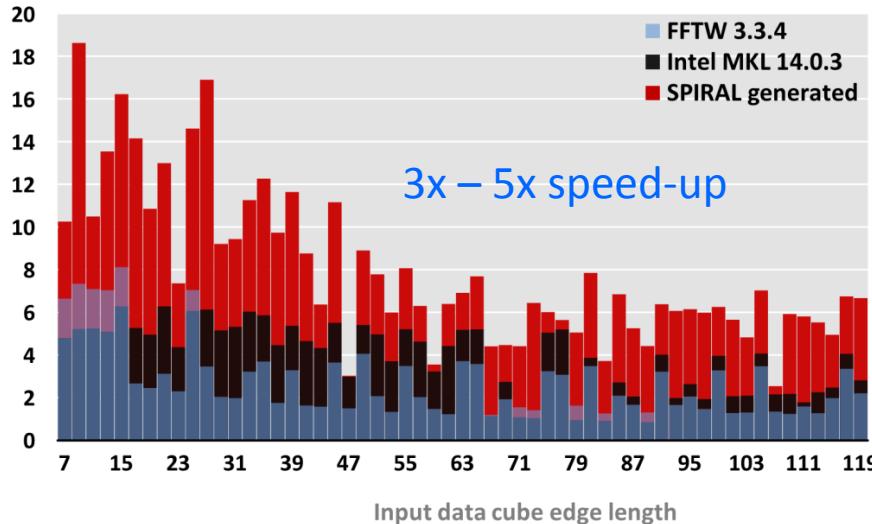
- **2010 HPC Challenge Class II Award (Most Productive System):**

“Automatic Generation of the HPC Challenge’s Global FFT Benchmark for BlueGene/P” [2].

Performance of 2x2x2 Upsampling on Haswell

3.5 GHz, AVX, double precision, interleaved input, single core

Performance [Pseudo Gflop/s]



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.*

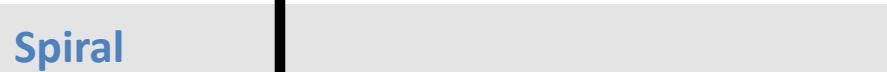
[1] F. Gygi, F. Franchetti, et. al., In Proceedings of Supercomputing, 2006.

[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)

Spiral FFT: Capabilities and Blue Waters

Operator Specification



Fast executable

- Multithreading (**Multicore**) $I_p \otimes_{\parallel} A_{\mu n}, \quad L_m^{mn} \bar{\otimes} I_{\mu}$
- Vector SIMD (**SSE, VMX/Altivec,...**) $A \bar{\otimes} I_{\nu}, \quad \underbrace{L_2^{2\nu}}_{\text{isa}}, \quad \underbrace{L_{\nu}^{2\nu}}_{\text{isa}}, \quad \underbrace{L_{\nu}^{\nu^2}}_{\text{isa}}$
- Message Passing (**Clusters, MPP**) $I_p \otimes_{\parallel} A_n, \quad \underbrace{L_p^{p^2} \bar{\otimes} I_{n/p^2}}_{\text{all-to-all}}$
- Streaming/multibuffering (**Cell**) $I_n \otimes_2 A_{\mu n}, \quad L_m^{mn} \bar{\otimes} I_{\mu}$
- Graphics Processors (**GPUs**) $\prod_{i=0}^{n-1} A_i, \quad A_n \bar{\otimes} I_w, \quad P_n \otimes Q_w$

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

Questions?



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