

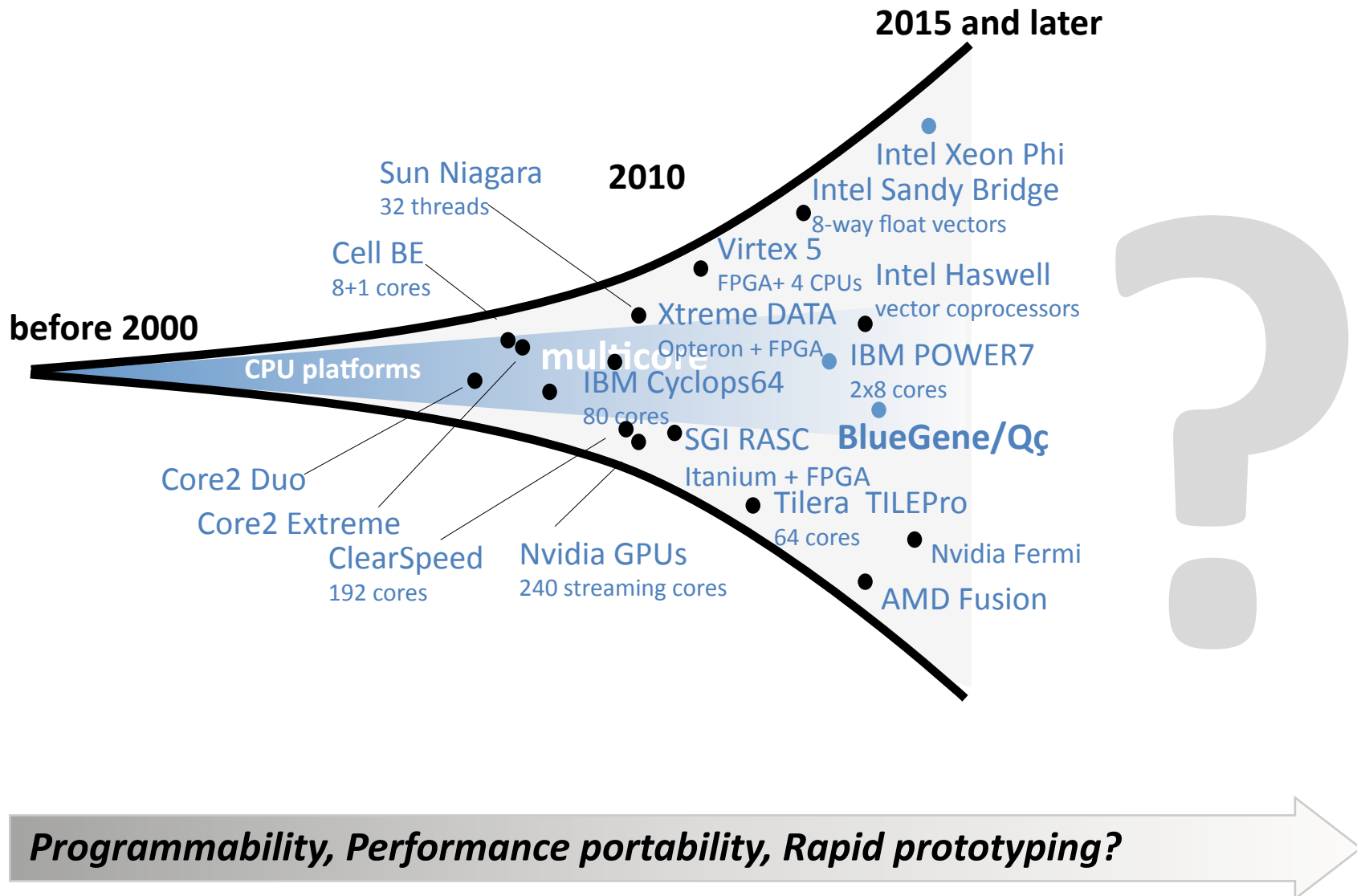


Presented by
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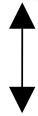
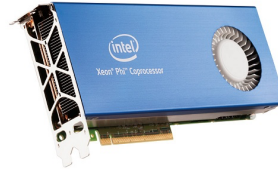
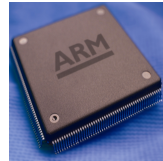


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The (Future) Present is Parallel and Heterogeneous



Spiral FFT: One Frontend, Many Backends



K Computer



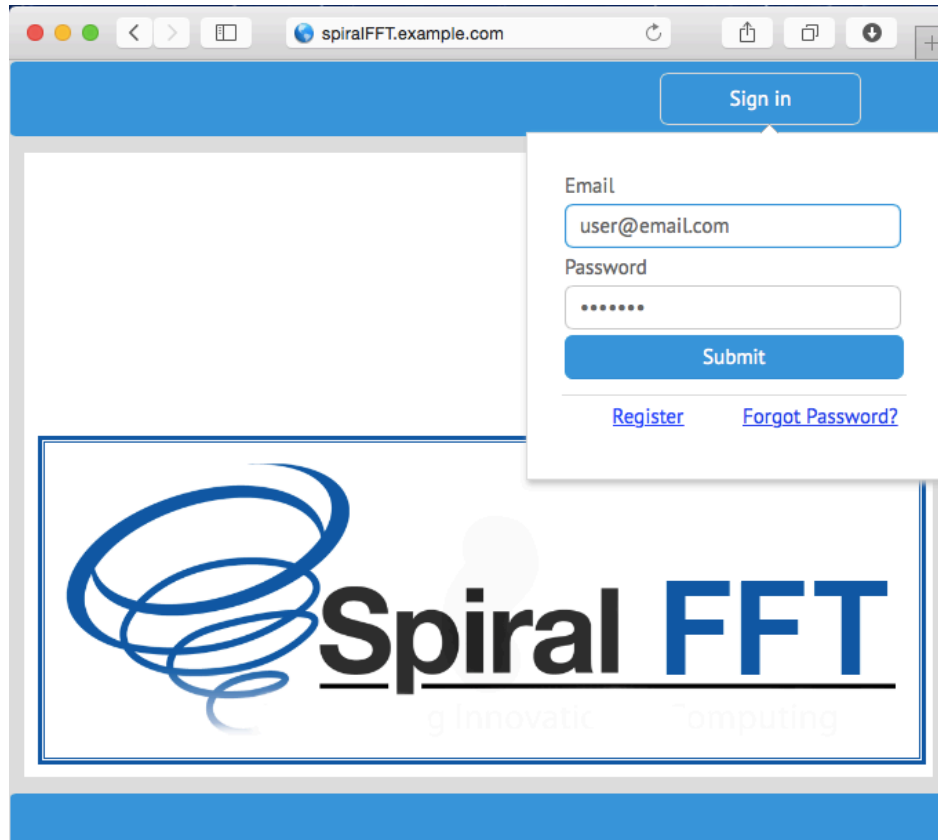
BlueGene/P



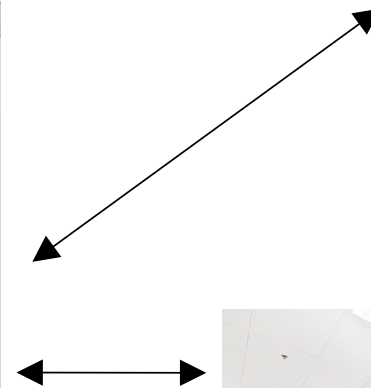
BlueGene/Qc



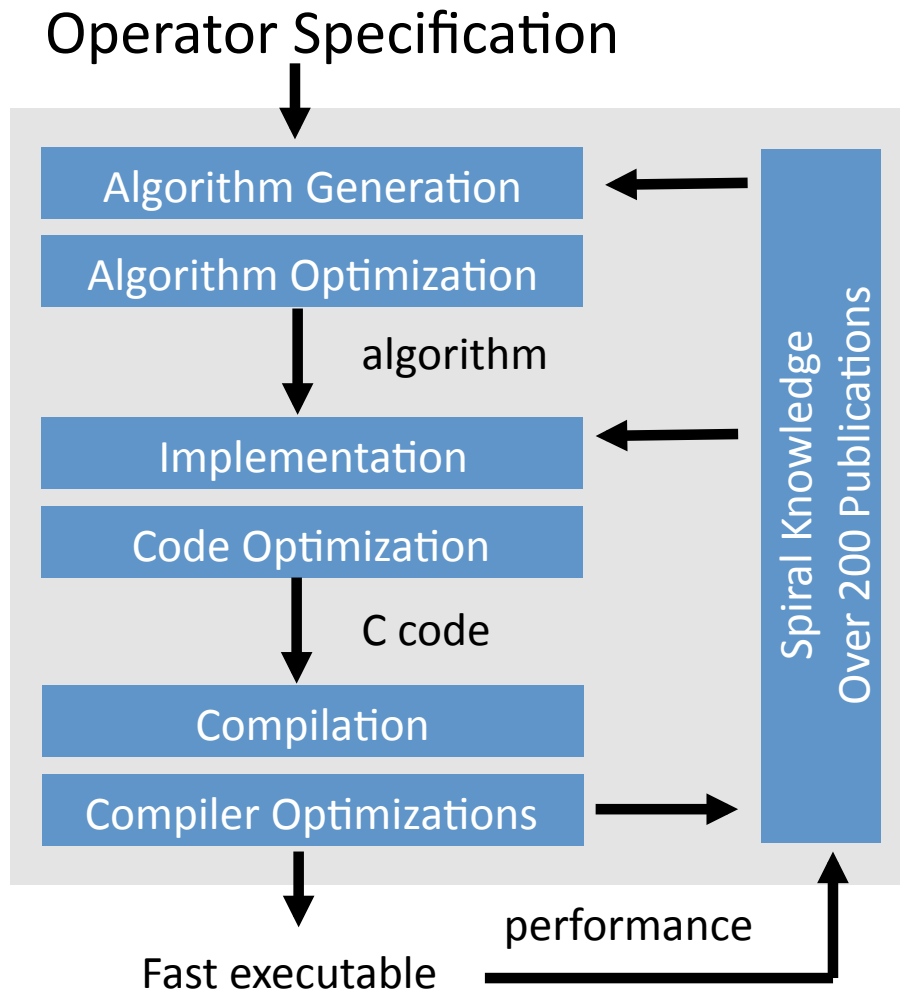
Blue Waters



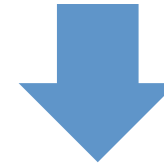
The screenshot shows a web browser window with the URL `spiralFFT.example.com`. The page features a blue header with a "Sign in" button. Below the header is a sign-in form with fields for "Email" (containing `user@email.com`) and "Password" (masked with dots). A blue "Submit" button is positioned below the password field. At the bottom of the form are links for "Register" and "Forgot Password?". The main content area displays the "Spiral FFT" logo, which consists of a blue spiral graphic and the text "Spiral FFT" in a bold, blue font. Below the logo, the tagline "g Innovatic omputing" is visible in a smaller, lighter blue font.



Spiral FFT: Automated Optimization/Implementation



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

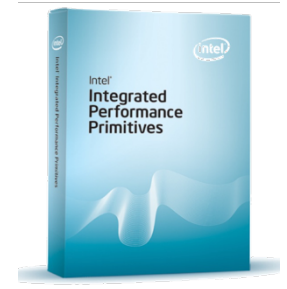


```

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



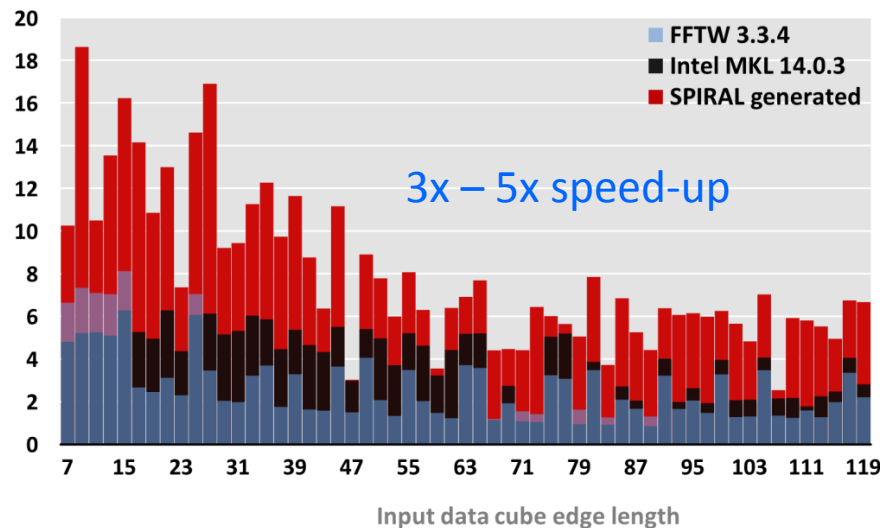
Spiral FFT: Performance, Driven by Machine/Project

- 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

Spiral

Fast executable

- Multithreading (Multicore)
- Vector SIMD (SSE, VMX/Altivec,...)
- Message Passing (Clusters, MPP)
- Streaming/multibuffering (Cell)
- Graphics Processors (GPUs)

$$I_p \otimes_{\parallel} A_{\mu n}, \quad L_m^{mn} \bar{\otimes} I_{\mu}$$

$$A \hat{\otimes} I_{\nu} \quad \underbrace{L_2^{2\nu}}_{isa}, \quad \underbrace{L_{\nu}^{2\nu}}_{isa}, \quad \underbrace{L_{\nu}^{\nu^2}}_{isa}$$

$$I_p \otimes_{\parallel} A_n, \quad \underbrace{L_p^{p^2} \bar{\otimes} I_{n/p^2}}_{\text{all-to-all}}$$

$$I_n \otimes_2 A_{\mu n}, \quad L_m^{mn} \bar{\otimes} I_{\mu}$$

$$\prod_{i=0}^{n-1} A_i, \quad A_n \hat{\otimes} I_w, \quad P_n \otimes Q_w$$

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

Questions?



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