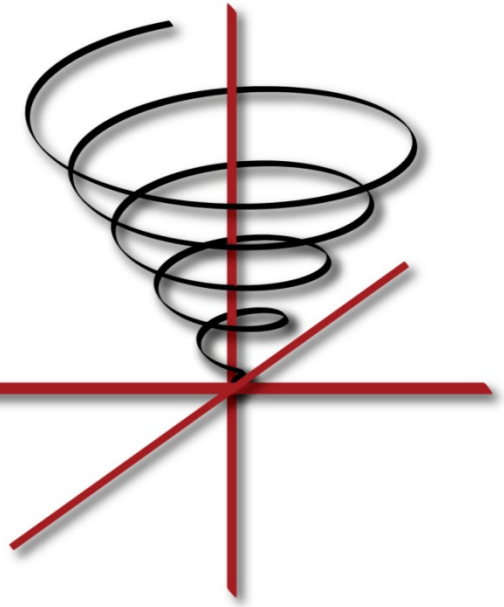
Updates on FFTX and NTTX



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ECP EXASCALE COMPUTING PROJECT

Have You Ever Wondered About This?

Numerical Linear Algebra

LAPACK
ScaLAPACK
LU factorization
Eigensolves
SVD

BLAS, BLACS
BLAS-1
BLAS-2
BLAS-3

Spectral Algorithms

Convolution
Correlation
Upsampling
Poisson solver
…

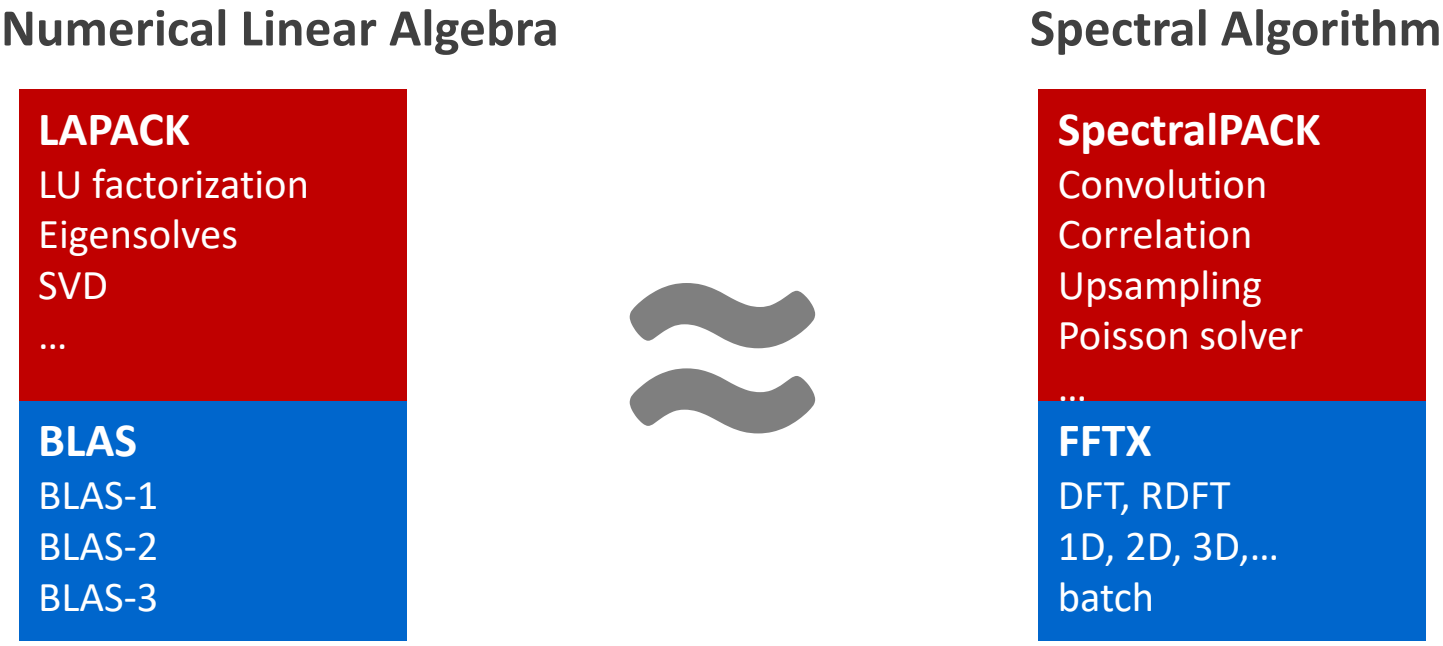
?

FFTW
DFT, RDFT
1D, 2D, 3D,…
batch

No LAPACK equivalent for spectral methods

- **Medium size 1D FFT (1k—10k data points) is most common library call**
  applications break down 3D problems themselves and then call the 1D FFT library
- **Higher level FFT calls rarely used**
  FFTW *guru* interface is powerful but hard to used, leading to performance loss
- **Low arithmetic intensity and variation of FFT use make library approach hard**
  Algorithm specific decompositions and FFT calls intertwined with non-FFT code

FFTX and SpectralPACK



Define the LAPACK equivalent for spectral algorithms

- **Define FFTX as the BLAS equivalent**
  provide user FFT functionality as well as algorithm building blocks
- **Define class of numerical algorithms to be supported by SpectralPACK**
  PDE solver classes (Green's function, sparse in normal/k space,…), signal processing,…
- **Library front-end, code generation and vendor library back-end**
  mirror concepts from FFTX layer

FFTX and SpectralPACK solve the "spectral motif" long term

Example: Poisson's Equation in Free Space

Partial differential equation (PDE)

$$\Delta(\Phi) = \rho$$

$$\rho : \mathbb{R}^3 \to \mathbb{R}$$

$$D = \text{supp}(\rho) \subset \mathbb{R}^3$$

Poisson's equation. Δ is the Laplace operator

Solution characterization

$$\Phi : \mathbb{R}^3 \to \mathbb{R}$$

$$\Phi(\vec{x}) = \frac{Q}{4\pi||\vec{x}||} + o\left(\frac{1}{||\vec{x}||}\right) \text{ as } ||\vec{x}|| \to \infty$$

$$Q = \int_D \rho d\vec{x}$$

Approach: Green's function

$$\Phi(\vec{x}) = \int_D G(\vec{x} - \vec{y})\rho(\vec{y})d\vec{y} \equiv (G * \rho)(\vec{x}), \quad G(\vec{x}) = \frac{1}{4\pi||\vec{x}||_2}$$

Solution: ϕ(.) = convolution of RHS *ρ*(.) with Green's function *G*(.). Efficient through FFTs (frequency domain)

Method of Local Corrections (MLC)

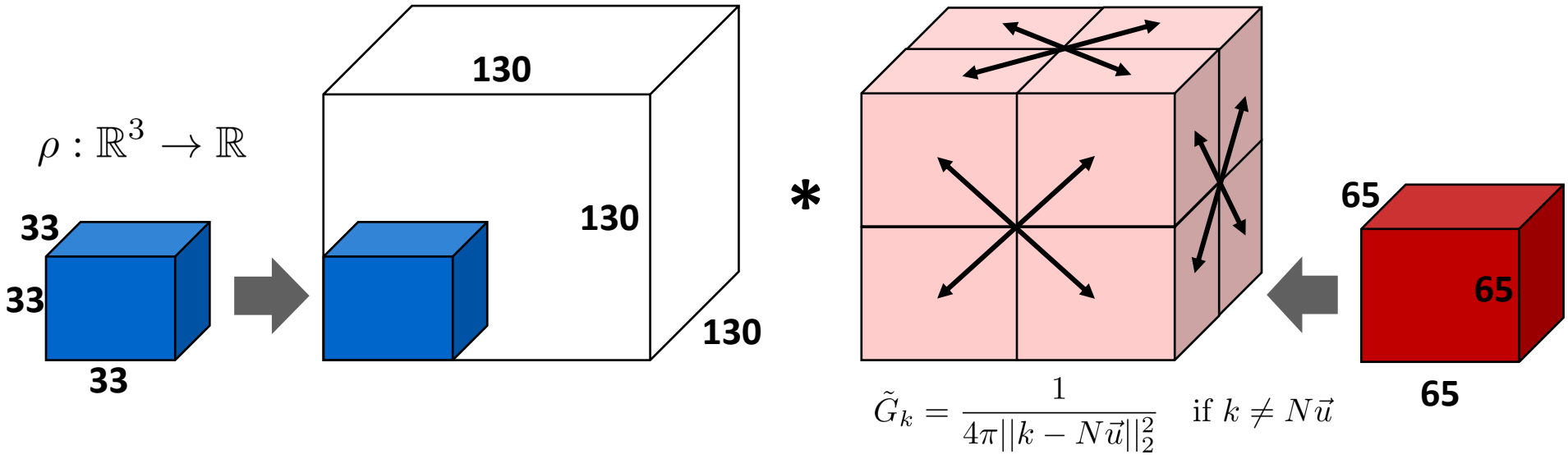
$$\tilde{G}_k = \frac{1}{4\pi||k - N\vec{u}||_2^2} \quad \text{if } k \neq N\vec{u}$$

Green's function kernel in frequency domain

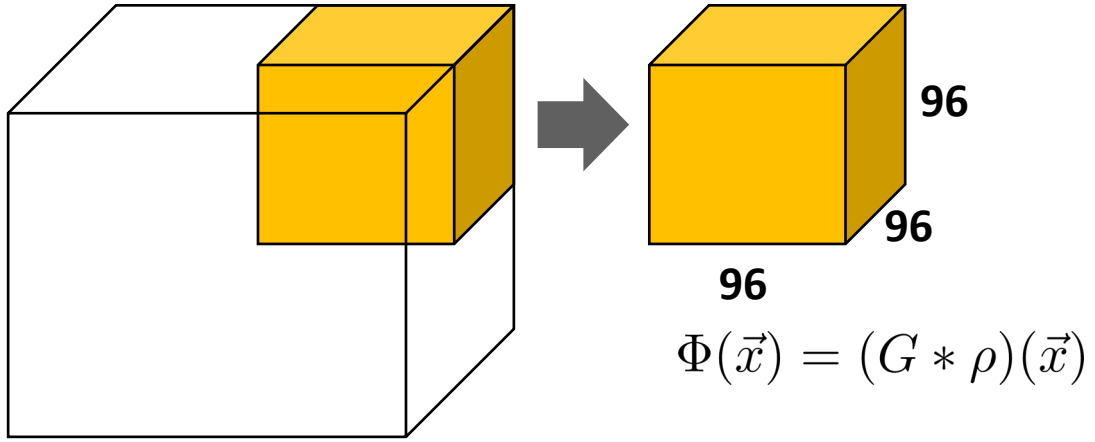
P. McCorquodale, P. Colella, G. T. Balls, and S. B. Baden: **A Local Corrections Algorithm for Solving Poisson's Equation in Three Dimensions.** Communications in Applied Mathematics and Computational Science Vol. 2, No. 1 (2007), pp. 57-81., 2007.

C. R. Anderson: **A method of local corrections for computing the velocity field due to a distribution of vortex blobs.** Journal of Computational Physics, vol. 62, no. 1, pp. 111–123, 1986.

Algorithm: Hockney Free Space Convolution



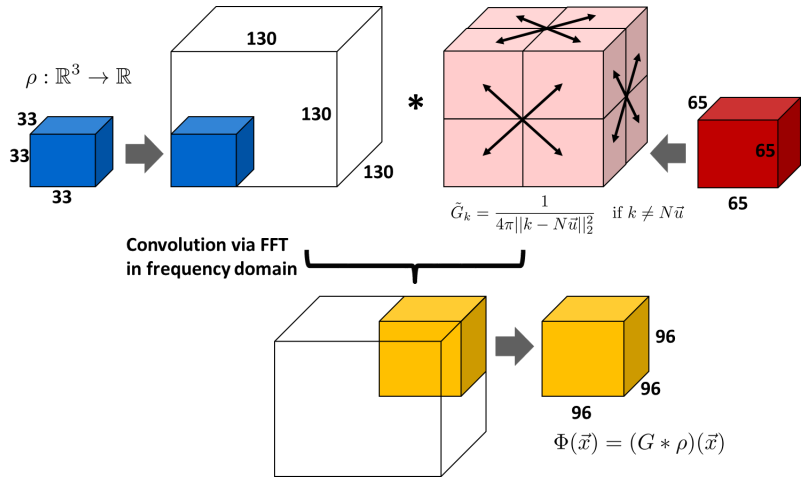
Convolution via FFT in frequency domain



Hockney: Convolution + problem specific zero padding and output subset

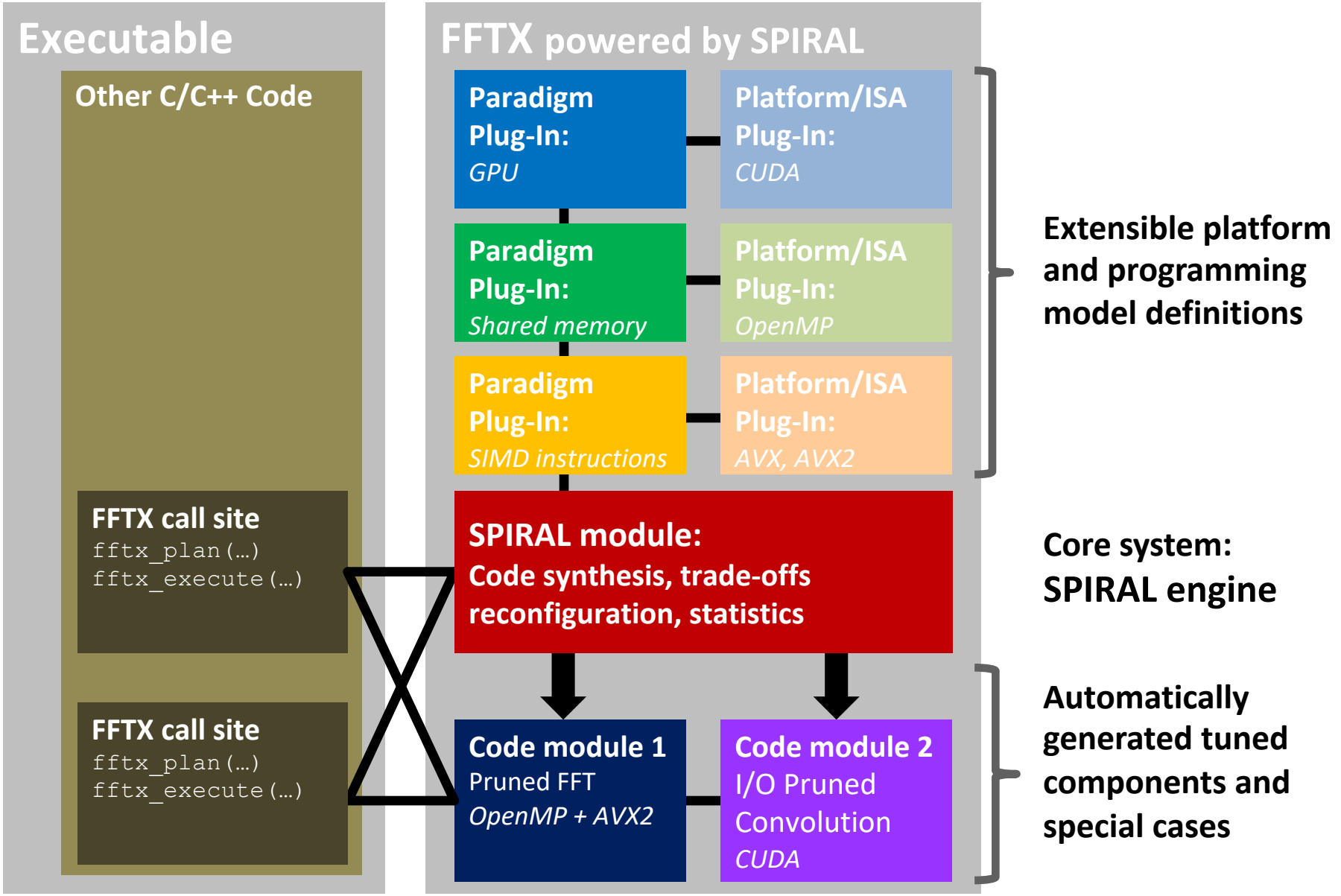
3D Convolution in FFTX/C++

```
#include "fftx3.hpp"
...
int main(int argc, char* argv[])
{
  int nx, ny, nz;
  box_t<3> domain(point_t<3>({{1,1,1}}), point_t<3>({{nx,ny,nz}}));

  array_t<3,std::complex<double>> input(domain);
  array_t<3,std::complex<double>> symbol(domain);
  array_t<3,std::complex<double>> output(domain);
  std::array<array_t<3,std::complex<double>>,2> temp {domain};

  MDDFT(domain.extents(), temp[0], input);
  RCDiag(domain.extents(), temp[1], temp[0], symbol);
  IMDDFT(domain.extents(), output, temp[1]);
}
```



Shown as source code, implemented as delayed execution in via run time compilation

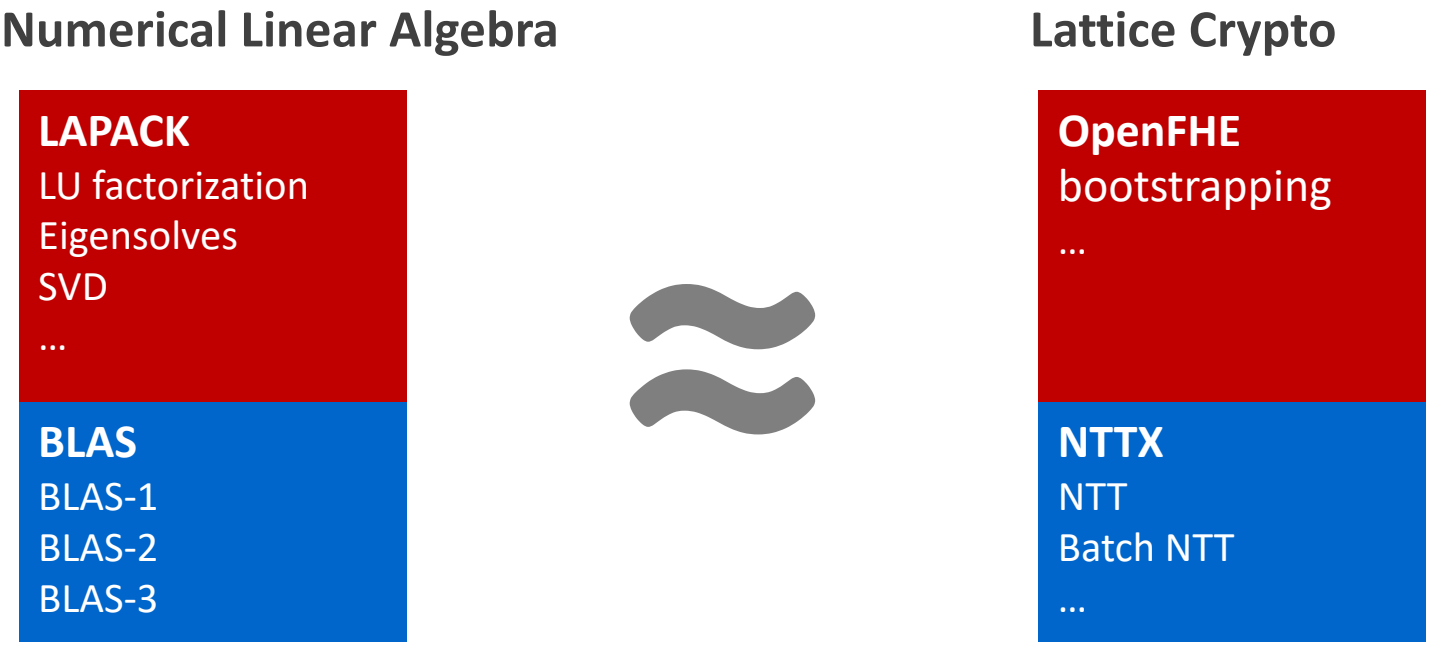
FFTX Backend: SPIRAL



In Development: Delayed Execution in FFTX C++ Code

```
#include "fftx3.hpp"
...
int main(int argc, char* argv[])
{
  int nx, ny, nz;
  box_t<3> domain(point_t<3>({{1,1,1}}), point_t<3>({{nx,ny,nz}}));

  array_t<3,std::complex<double>> input(domain);
  array_t<3,std::complex<double>> symbol(domain);
  array_t<3,std::complex<double>> output(domain);

  // will not be materialized
  fftx::tmp_array<array_t<3,std::complex<double>>,2> temp {domain};
  // no-op, just collect calling parameters, delayed execution
  MDDFT(domain.extents(), temp[0], input);
  // no-op, just collect calling parameters, delayed execution
  RCDiag(domain.extents(), temp[1], temp[0], symbol);
  // passing in the output triggers RTC and execution of the entire delayed sequence
  IMDDFT(domain.extents(), output, temp[1]);
  // output now contains the correct result, but temp[] was never materialized
}
```

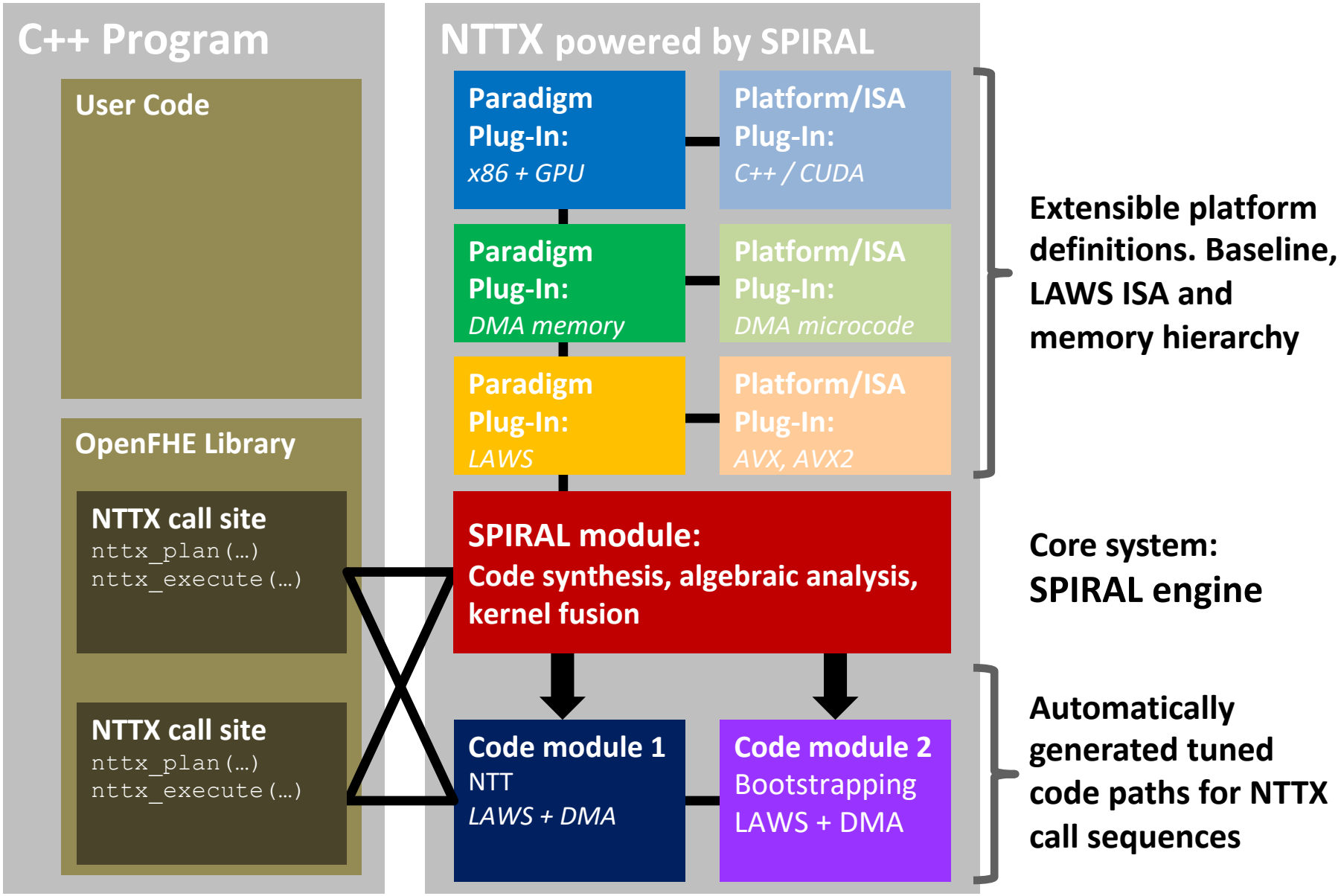
NTTX and OpenFHE



NTTX as lower layer for OpenFHE

- **Define NTTX as the BLAS/FFTW equivalent**
  platform independent high performance NTTs
- **Define higher level cross kernel operations**
  imul/imod, bootstrapping etc. expressed as composable NTTX calling sequence
- **Library front-end, SPIRAL code generation backend**
  mirror concepts from FFTX and GBTLX:
  library API + code gen = performance portability

NTTX and SPIRAL



NTT in NTTX/C++

```
// C/C++ NTTX API example: compute a singel NTT
#include "nttx.h"
nttx_plan *p;
p = nttx_plan_ntt(in, out, n, modulus, NTTX_FORWARD);
nttx_execute(p);
nttx_free(p);
```

```
#include <rpu.h>
void _ntt1024x512_b1() {
    enter(OP_DEFAULT);
    _vload_512x128i(REG_V60, REG_A1, 0);
    _vload_512x128i(REG_V20, REG_A1, 8192);
    _vbroadcast_512x128i(REG_V19, REG_A3, 1, 1);
    _vimulmod_512x128i(REG_V59, REG_V20, REG_V19, REG_M1);
    _vaddmod_512x128i(REG_V58, REG_V60, REG_V59, REG_M1);
    _vsubmod_512x128i(REG_V57, REG_V60, REG_V59, REG_M1);
    _vunpacklo_512x128i(REG_V56, REG_V58, REG_V57);
    _vunpackhi_512x128i(REG_V18, REG_V58, REG_V57);
    _vbroadcast_512x128i(REG_V17, REG_A3, 2, 2);
    _vimulmod_512x128i(REG_V55, REG_V18, REG_V17, REG_M1);
    ...
    _vstores_512x128i(REG_A2, 16, REG_V21, 2);
    leave(OP_DEFAULT);
}
```

Radix-2 1,024-point NTT code using shuffle instructions for ASIC

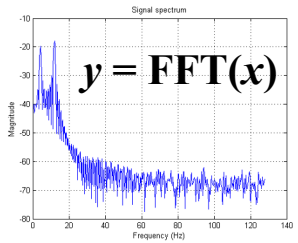
SPIRAL: Go from Mathematics to Software

Given:

- **Mathematical problem specification**
  core mathematics does not change
- **Target computer platform**
  varies greatly, new platforms introduced often

Wanted:

- **Very good implementation of specification on platform**
- **Proof of correctness**



on

automatic

```
void fft64(double  *Y, double  *X) {
    ...
    s5674 = _mm256_permute2f128_pd(s5672, s5673, (0) | ((2) << 4));
    s5675 = _mm256_permute2f128_pd(s5672, s5673, (1) | ((3) << 4));
    s5676 = _mm256_unpacklo_pd(s5674, s5675);
    s5677 = _mm256_unpackhi_pd(s5674, s5675);
    s5678 = *((a3738 + 16));
    s5679 = *((a3738 + 17));
    s5680 = _mm256_permute2f128_pd(s5678, s5679, (0) | ((2) << 4));
    s5681 = _mm256_permute2f128_pd(s5678, s5679, (1) | ((3) << 4));
    s5682 = _mm256_unpacklo_pd(s5680, s5681);
    s5683 = _mm256_unpackhi_pd(s5680, s5681);
    t5735 = _mm256_add_pd(s5676, s5682);
    t5736 = _mm256_add_pd(s5677, s5683);
    t5737 = _mm256_add_pd(s5670, t5735);
    t5738 = _mm256_add_pd(s5671, t5736);
    t5739 = _mm256_sub_pd(s5670, _mm256_mul_pd(_mm_vbroadcast_sd(&(C22)), t5735));
    t5740 = _mm256_sub_pd(s5671, _mm256_mul_pd(_mm_vbroadcast_sd(&(C22)), t5736));
    t5741 = _mm256_mul_pd(_mm_vbroadcast_sd(&(C23)), _mm256_sub_pd(s5677, s5683));
    t5742 = _mm256_mul_pd(_mm_vbroadcast_sd(&(C23)), _mm256_sub_pd(s5676, s5682));
    ...
}
```

performance

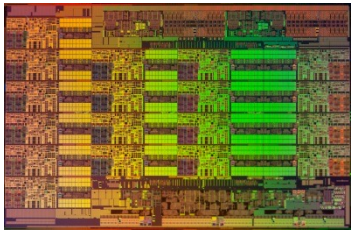
+

PROOF

QED.

SPIRAL's Target Computing Landscape

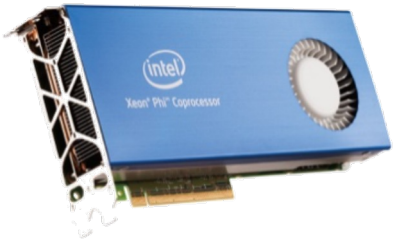
1 Gflop/s = one billion floating-point operations (additions or multiplications) per second



Intel Xeon 8180M
2.25 Tflop/s, 205 W
28 cores, 2.5—3.8 GHz
2-way—16-way AVX-512

IBM POWER9
768 Gflop/s, 300 W
24 cores, 4 GHz
4-way VSX-3

Nvidia Tesla V100
7.8 Tflop/s, 300 W
5120 cores, 1.2 GHz
32-way SIMT



Intel Xeon Phi 7290F
1.7 Tflop/s, 260 W
72 cores, 1.5 GHz
8-way/16-way LRBni

Snapdragon 835
15 Gflop/s, 2 W
8 cores, 2.3 GHz
A540 GPU, 682 DSP, NEON

Intel Atom C3858
32 Gflop/s, 25 W
16 cores, 2.0 GHz
2-way/4-way SSSE3

Dell PowerEdge R940
3.2 Tflop/s, 6 TB, 850 W
4x 24 cores, 2.1 GHz
4-way/8-way AVX

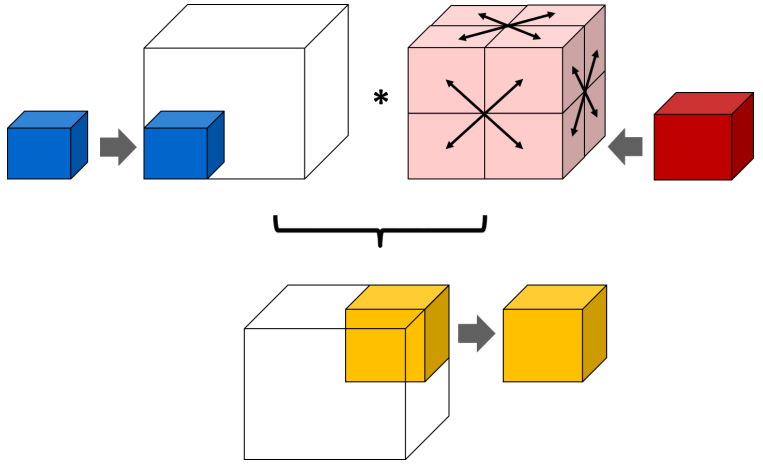
Summit
187.7 Pflop/s, 13 MW
9,216 x 22 cores POWER9
+ 27,648 V100 GPUs

Rules in Internal Domain Specific Language

Linear Transforms

$$\begin{aligned}
\mathbf{DFT}_n &\rightarrow (\mathbf{DFT}_k \otimes \mathrm{I}_m)\, \mathrm{T}^n_m (\mathrm{I}_k \otimes \mathbf{DFT}_m)\, \mathrm{L}^n_k, \quad n = km \\
\mathbf{DFT}_n &\rightarrow P_n(\mathbf{DFT}_k \otimes \mathbf{DFT}_m)Q_n, \quad n = km,\ \gcd(k,m) = 1 \\
\mathbf{DFT}_p &\rightarrow R_p^T(\mathrm{I}_1 \oplus \mathbf{DFT}_{p-1})D_p(\mathrm{I}_1 \oplus \mathbf{DFT}_{p-1})R_p, \quad p \text{ prime} \\
\mathbf{DCT\text{-}3}_n &\rightarrow (\mathrm{I}_m \oplus \mathrm{J}_m)\, \mathrm{L}^n_m (\mathbf{DCT\text{-}3}_m(1/4) \oplus \mathbf{DCT\text{-}3}_m(3/4)) \\
&\quad \cdot (\mathrm{F}_2 \otimes \mathrm{I}_m) \begin{bmatrix} \mathrm{I}_m & 0 \oplus -\mathrm{J}_{m-1} \\ \frac{1}{\sqrt{2}}(\mathrm{I}_1 \oplus 2\,\mathrm{I}_m) & \end{bmatrix}, \quad n = 2m \\
\mathbf{DCT\text{-}4}_n &\rightarrow S_n \mathbf{DCT\text{-}2}_n\, \mathrm{diag}_{0 \le k < n}(1/(2\cos((2k+1)\pi/4n))) \\
\mathbf{IMDCT}_{2m} &\rightarrow (\mathrm{J}_m \oplus \mathrm{I}_m \oplus \mathrm{I}_m \oplus \mathrm{J}_m)\left(\left(\begin{bmatrix} 1 \\ -1 \end{bmatrix} \otimes \mathrm{I}_m\right) \oplus \left(\begin{bmatrix} -1 \\ -1 \end{bmatrix} \otimes \mathrm{I}_m\right)\right) \mathrm{J}_{2m}\, \mathbf{DCT\text{-}4}_{2m} \\
\mathbf{WHT}_{2^k} &\rightarrow \prod_{i=1}^{t} (\mathrm{I}_{2^{k_1+\cdots+k_{i-1}}} \otimes \mathbf{WHT}_{2^{k_i}} \otimes \mathrm{I}_{2^{k_{i+1}+\cdots+k_t}}), \quad k = k_1 + \cdots + k_t \\
\mathbf{DFT}_2 &\rightarrow \mathrm{F}_2 \\
\mathbf{DCT\text{-}2}_2 &\rightarrow \mathrm{diag}(1, 1/\sqrt{2})\, \mathrm{F}_2 \\
\mathbf{DCT\text{-}4}_2 &\rightarrow \mathrm{J}_2\, \mathrm{R}_{13\pi/8}
\end{aligned}$$

Spectral Domain Algorithms



Hardware

- Multithreading (Multicore)
- Vector SIMD (SSE, VMX/Altivec,…)
- Message Passing (Clusters, MPP)
- Streaming/multibuffering (Cell)
- Graphics Processors (GPUs)
- Gate-level parallelism (FPGA)
- HW/SW partitioning (CPU + FPGA)

$$\mathrm{I}_p \otimes_{\parallel} A_{\mu n}, \quad \mathbf{L}^{mn}_m \bar{\otimes} \mathrm{I}_\mu$$

$$A \bar{\otimes} \mathrm{I}_\nu \quad \underbrace{\mathbf{L}^{2\nu}_2}_{\text{isa}}, \quad \underbrace{\mathbf{L}^{2\nu}_\nu}_{\text{isa}}, \quad \underbrace{\mathbf{L}^{\nu^2}_\nu}_{\text{isa}}$$

$$\mathrm{I}_p \otimes_{\parallel} A_n, \quad \underbrace{\mathbf{L}^{p^2}_p \bar{\otimes} \mathrm{I}_{n/p^2}}_{\text{all-to-all}}$$

$$\mathrm{I}_n \otimes_2 A_{\mu n}, \quad \mathbf{L}^{mn}_m \bar{\otimes} \mathrm{I}_\mu$$

$$\prod_{i=0}^{n-1} A_i, \quad A_n \bar{\otimes} \mathrm{I}_w, \quad P_n \otimes Q_w$$

$$\prod_{i=0}^{n-1^{\text{ir}}} A, \quad \mathrm{I}_s \bar{\otimes} A, \quad \underbrace{\mathbf{L}^m_n}_{\text{bram}}$$

$$\underbrace{A_1}_{\text{fpga}}, \quad \underbrace{A_2}_{\text{fpga}}, \quad \underbrace{A_3}_{\text{fpga}}, \quad \underbrace{A_4}_{\text{fpga}}$$

Program Transformations

$$\begin{aligned}
\underbrace{AB}_{\text{smp}(p,\mu)} &\rightarrow \underbrace{A}_{\text{smp}(p,\mu)}\ \underbrace{B}_{\text{smp}(p,\mu)} \\
\underbrace{A_m \otimes \mathrm{I}_n}_{\text{smp}(p,\mu)} &\rightarrow \underbrace{\left(\mathrm{L}^{mp}_m \otimes \mathrm{I}_{n/p}\right)\left(\mathrm{I}_p \otimes (A_m \otimes \mathrm{I}_{n/p})\right)\left(\mathrm{L}^{mp}_p \otimes \mathrm{I}_{n/p}\right)}_{\text{smp}(p,\mu)} \\
\underbrace{\mathrm{L}^{mn}_m}_{\text{smp}(p,\mu)} &\rightarrow \begin{cases} \underbrace{\left(\mathrm{I}_p \otimes \mathrm{L}^{mn/p}_{m/p}\right)}_{\text{smp}(p,\mu)} \underbrace{\left(\mathrm{L}^{pn}_p \otimes \mathrm{I}_{m/p}\right)}_{\text{smp}(p,\mu)} \\ \underbrace{\left(\mathrm{L}^{pm}_m \otimes \mathrm{I}_{n/p}\right)}_{\text{smp}(p,\mu)} \underbrace{\left(\mathrm{I}_p \otimes \mathrm{L}^{mn/p}_m\right)}_{\text{smp}(p,\mu)} \end{cases}
\end{aligned}$$

Recursive rules

$$\begin{aligned}
\underbrace{\mathrm{I}_m \otimes A_n}_{\text{smp}(p,\mu)} &\rightarrow \mathrm{I}_p \otimes_{\parallel} \left(\mathrm{I}_{m/p} \otimes A_n\right) \\
\underbrace{(P \otimes \mathrm{I}_n)}_{\text{smp}(p,\mu)} &\rightarrow \left(P \otimes \mathrm{I}_{n/\mu}\right) \overline{\otimes}\, \mathrm{I}_\mu
\end{aligned}$$

Base case rules

Translating an OL Expression Into Code

Constraint Solver Input: $\underbrace{DFT_8}_{AVX(2\text{-way } \mathbb{C})}$

Output =

Ruletree, expanded into

OL Expression:

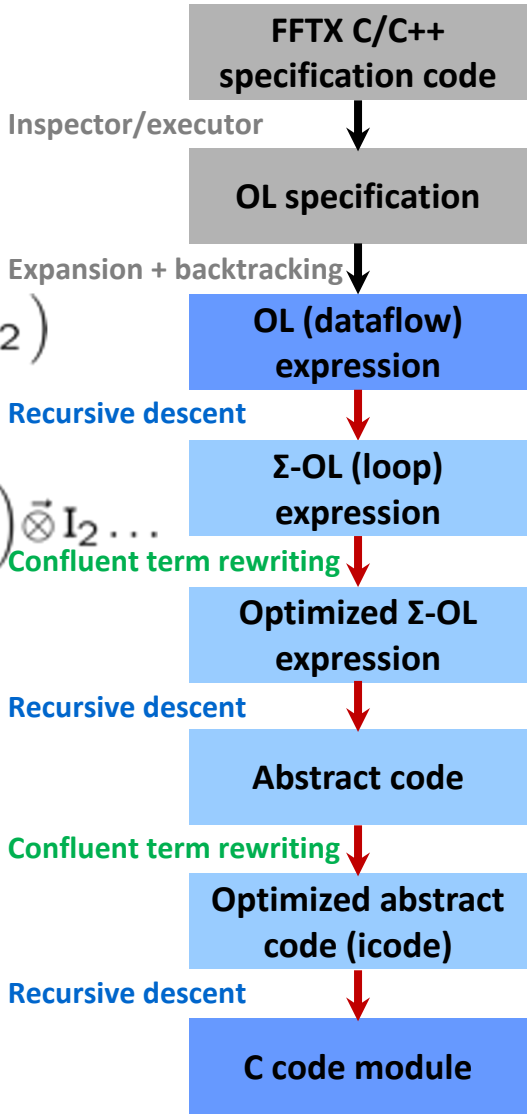
$$\left((F_2 \otimes I_2) T_2^4 (I_2 \otimes F_2) L_2^4 \vec{\otimes} I_2\right) \underbrace{T_2^8}_{vec(2)} \left(I_2 \otimes \underbrace{L_2^4}_{vec(2)} (F_2 \vec{\otimes} I_2)\right)\left(L_2^4 \vec{\otimes} I_2\right)$$

∑-OL:

$$\left(\sum_{j=0}^{1} \left(S_{\imath_2 \otimes (j)_2} F_2 \mathrm{Map}^2_{x \mapsto \omega_4^{2i+j_x}} G_{\imath_2 \otimes (j)_2}\right) \sum_{j=0}^{1} \left(S_{(j)_2 \otimes \imath_2} F_2 G_{\imath_2 \otimes (j)_2}\right)\right) \vec{\otimes} I_2 \ldots$$

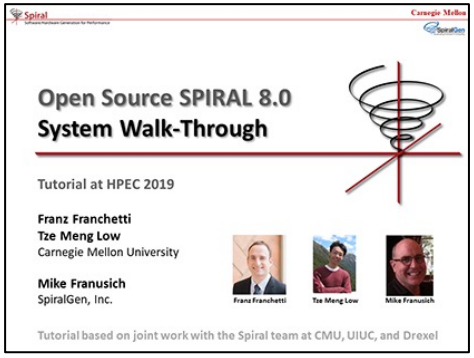
C Code:

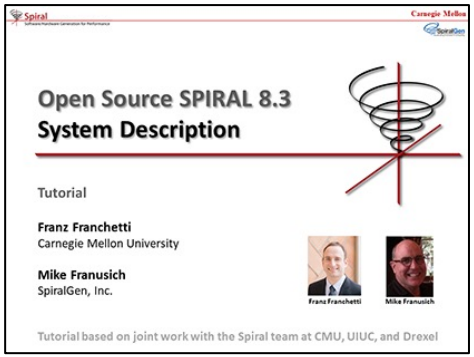
```
void dft8(_Complex double *Y, _Complex double *X) {
    __m256d s38, s39, s40, s41,...
    __m256d  *a17, *a18;
    a17 = ((__m256d  *) X);
    s38 = *(a17);
    s39 = *((a17 + 2));
    t38 = _mm256_add_pd(s38, s39);
    t39 = _mm256_sub_pd(s38, s39);
    ...
    s52 = _mm256_sub_pd(s45, s50);
    *((a18 + 3)) = s52;
}
```



SPIRAL 8.4.0: Available Under Open Source

- **Release of FFTX 1.0.0**
- **Open Source SPIRAL available**
  - non-viral license (BSD)
  - Initial version, effort ongoing to open source whole system
  - Commercial support via SpiralGen, Inc.
- **Tutorial material available online**





- **FFTX and SPIRAL available via GitHub**

spiral-software	8.4.0-release	https://github.com/spiral-software/spiral-software
spiral-package-fftx	1.1.0-release	https://github.com/spiral-software/spiral-package-fftx
spiral-package-simt	1.1.0-release	https://github.com/spiral-software/spiral-package-simt
spiral-package-mpi	1.0.0-release	https://github.com/spiral-software/spiral-package-mpi
FFTX	1.0.0-release	https://github.com/spiral-software/fftx