

# The Design of FFTX

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#### in collaboration with

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## Have You Ever Wondered About This?



#### **Spectral Algorithms**



### 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**

**Numerical Linear Algebra** 

LAPACK LU factorization Eigensolves SVD 	
BLAS	
BLAS-1	
BLAS-2	
BLAS-3	

**Spectral Algorithms** 

SpectralPACK Convolution Correlation Upsampling Poisson solver ... FFTX DFT, RDFT 1D, 2D, 3D,... batch

#### 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)

Solution characterization

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

 $Q = \int_{D} \rho d\vec{x}$ 

$$\Delta(\Phi) = \rho$$
$$\rho : \mathbb{R}^3 \to \mathbb{R}$$

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

Poisson's equation.  $\boldsymbol{\Delta}$  is the Laplace operator

#### **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:  $\phi(.) = \text{convolution of RHS } \rho(.)$  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

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

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**



*Hockney: Convolution + problem specific zero padding and output subset* 

## FFTX C++ Code: Hockney Free Space Convolution

box\_t<3> inputBox(point\_t<3>({{0,0,0}}),point\_t<3>({32,32,32}));
array\_t<3, double> rho(inputBox);
// ... set input values.

```
box_t<3> transformBox(point_t<3>({{0,0,0}}),point_t<3>({{129,129,129}));
box_t<3> outputBox(point_t<3>({33,33,33}),point_t<3>({129,129,129}));
```





```
std::ofstream splFile("hockney.spl");
export_spl(context, solver, splFile, "hockney33_97_130");
splFile.close();
// Offline codegen.
auto fptr = import_spl<3, double, double>("hockney33_97_130");
array_t<3, double> Phi(inputBox);
fptr(&rho, &Phi, 1);
```



## **FFTX C Code: Hockney Free Space Convolution**



Looks like FFTW calls, but is a specification for SPIRAL



65

### **FFTX C Code: Describing The Hockney Symmetry**

Gk

65

65

```
// Access is to four octants of a symmetric cube.
// Cube size is N^3 and M = N/2.
fftx iodimx oct00[] = {
  \{ M+1, 0, 0, 0, 1, 1, 1 \},\
  \{ M+1, 0, 0, 0, M+1, 2*M, 1 \},\
                                                       oct10
                                                                 oct11
  \{ M+1, 0, 0, 0, (M+1)*(M+1), 4*M*M, 1 \} \},
  oct01[] = {
  \{ M-1, M-1, M+1, 0, -1, 1, 1 \},\
  \{ M+1, 0, 0, 0, M+1, 2*M, 1 \},\
  \{ M+1, 0, 0, 0, (M+1) * (M+1), 4 * M * M, 1 \} \},
  oct10[] = {
  \{ M+1, 0, 0, 0, 1, 1, 1 \},\
                                                       oct00 oct01
  \{ M-1, M-1, M+1, 0, -(M+1), 2*M, 1 \},
  \{ M+1, 0, 0, 0, (M+1) * (M+1), 4 * M * M, 1 \} \},
                                                      \tilde{G}_k = \frac{1}{4\pi ||k - N\vec{u}||_2^2} \quad \text{if } k \neq N\vec{u}
 oct11[] = {
  \{ M-1, M-1, M+1, 0, -1, 1, 1 \},\
  \{ M-1, M-1, M+1, 0, -(M+1), 2*M, 1 \},
  { M+1, 0, 0, 0, (M+1)*(M+1), 4*M*M, 1} };
fftx temp complex half G k = fftx create zero temp complex (rk, f d);
plans[2] = fftx plan guru copy complex(rk, oct00, G k, half G k, FFTX MODE SUB);
plans[3] = fftx plan guru copy complex(rk, oct01, G k, half G k, MY FFTX MODE SUB);
plans[4] = fftx plan quru copy complex(rk, oct10, G k, half G k, MY FFTX MODE SUB);
```

// FFTX data access descriptors.

plans[5] = fftx plan guru copy complex(rk, oct11, G k, half G k, MY FFTX MODE SUB);

#### We are a developing higher-level more natural geometric API



## **FFTX Backend: SPIRAL**



## C/C++ FFTX Program Trace





## **SPIRAL Script Captures Performance Engineering**

# Pruned 3D Real Convolution Pattern
Import(realdft);
Import(filtering);

# set up algorithms needed for multi-dimensional pruned real convolution opts opts PR **Recognizes pattern and applies code generation** opts IP **Developed by** opts opts 1; performance engineer + application specialist opts # sp Casts FFTX call sequence as SPIRAL non-terminal [N, # de Does code generation and autotuning n\_fr # pr Clear separation of concerns frontend/backend sym t := # generate code and autotune rt := DP(t, opts)[1].ruletree; c := CodeRuleTree(rt, opts);

```
# create files
PrintTo(name::".c", PrintCode(name, c, opts));
```



Electrical & Computer

## **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





## **Inspiration: Symbolic Integration**

- Rule based AI system basic functions, substitution
- May not succeed not all expressions can be symbolically integrated
- Arbitrarily extensible

define new functions as integrals Γ(.), distributions, Lebesgue integral

- Semantics preserving rule chain = formal proof
- Automation

Mathematica, Maple

#### **Table of Integrals**

#### BASIC FORMS

- $(1) \qquad \int x^n dx = \frac{1}{n+1} x^{n+1}$
- (2)  $\int \frac{1}{x} dx = \ln x$
- (3)  $\int u dv = uv \int v du$
- $(4) \qquad \int u(x)v'(x)dx = u(x)v(x) \int v(x)u'(x)dx$

#### RATIONAL FUNCTIONS

- (5)  $\int \frac{1}{ax+b} dx = \frac{1}{a} \ln(ax+b)$
- (6)  $\int \frac{1}{(x+a)^2} dx = \frac{-1}{x+a}$
- (7)  $\int (x+a)^n dx = (x+a)^n \left(\frac{a}{1+n} + \frac{x}{1+n}\right), \ n \neq -1$
- (8)  $\int x(x+a)^n dx = \frac{(x+a)^{1+n}(nx+x-a)}{(n+2)(n+1)}$



TABLE OF INTEGRALS, SERIES, AND PRODUCTS SEVENTH EDITION

I. M. RYZHIK







## **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**

 $\underline{n-1}^{\mathsf{ir}}$ 

#### Linear Transforms

#### $\mathbf{DFT}_n \rightarrow (\mathbf{DFT}_k \otimes \mathbf{I}_m) \mathsf{T}_m^n(\mathbf{I}_k \otimes \mathbf{DFT}_m) \mathsf{L}_k^n, \quad n = km$ $\mathbf{DFT}_n \rightarrow P_n(\mathbf{DFT}_k \otimes \mathbf{DFT}_m)Q_n, \quad n = km, \ \mathsf{qcd}(k,m) = 1$ $\mathbf{DFT}_p \rightarrow R_p^T(\mathbf{I}_1 \oplus \mathbf{DFT}_{p-1})D_p(\mathbf{I}_1 \oplus \mathbf{DFT}_{p-1})R_p, p \text{ prime}$ $\mathbf{DCT}$ - $\mathbf{3}_n \rightarrow (\mathbf{I}_m \oplus \mathbf{J}_m) \, \mathbf{L}_m^n(\mathbf{DCT}$ - $\mathbf{3}_m(1/4) \oplus \mathbf{DCT}$ - $\mathbf{3}_m(3/4))$ $\cdot (\mathsf{F}_2 \otimes \mathrm{I}_m) \begin{bmatrix} \mathrm{I}_m & 0 \oplus -\mathsf{J}_{m-1} \\ \frac{1}{\sqrt{2}} (\mathrm{I}_1 \oplus 2 \, \mathrm{I}_m) \end{bmatrix}, \quad n = 2m$ DCT-4<sub>n</sub> $\rightarrow$ S<sub>n</sub>DCT-2<sub>n</sub> diag<sub>0 < k < n</sub>(1/(2 cos((2k + 1)\pi/4n))) $\mathbf{IMDCT}_{2m} \rightarrow (\mathsf{J}_m \oplus \mathrm{I}_m \oplus \mathrm{I}_m \oplus \mathsf{J}_m) \left( \left( \begin{bmatrix} 1\\-1 \end{bmatrix} \otimes \mathrm{I}_m \right) \oplus \left( \begin{bmatrix} -1\\-1 \end{bmatrix} \otimes \mathrm{I}_m \right) \right) \mathsf{J}_{2m} \mathbf{DCT} \mathsf{-4}_{2m}$ $\mathbf{WHT}_{2^k} \rightarrow \prod_{i=1}^{\circ} (\mathbf{I}_{2^{k_1+\cdots+k_{i-1}}} \otimes \mathbf{WHT}_{2^{k_i}} \otimes \mathbf{I}_{2^{k_{i+1}+\cdots+k_t}}), \quad k = k_1 + \cdots + k_t$ $DFT_2 \rightarrow F_2$ DCT-2<sub>2</sub> $\rightarrow$ diag $(1, 1/\sqrt{2})$ F<sub>2</sub> DCT-4<sub>2</sub> $\rightarrow$ J<sub>2</sub>R<sub>13 $\pi$ /8</sub>

### **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)

### **Program Transformations**



## Autotuning in Constraint Solution Space



## Translating an OL Expression Into Code





## Get Going Quickly: Hockney with OpenACC

```
void ioprunedconv 130 0 62 72 130(double *Y, double *X, double * S) {
    static double D84[260] = \{65.5, 0.0, (-0.500000000001132), (-20.686114762237267), \}
      (-0.500000000000000000), (-10.337014680426078), (-0.50000000000000455),
for(int i18899 = 0; i18899 <= 1; i18899++) {</pre>
    for(int i18912 = 0; i18912 <= 4; i18912++) {
        a9807 = ((2*i18899) + (4*i18912));
                                             FFTX/SPIRAL with OpenACC backend
        a9808 = (a9807 + 1);
                                             Compared to cuFFT expert interface
        a9809 = (a9807 + 52);
        a9810 = (a9807 + 53);
        a9811 = (a9807 + 104);
        a9812 = (a9807 + 105);
        s3295 = (*((X + a9807)) + *((X + a9809)))
                                                                            15% faster
            + *((X + a9811)));
        s3296 = (*((X + a9808)) + *((X + a9810)))
                                                                            on TITAN V
            + *((X + a9812)));
```

```
s3297 = (((0.3090169943749474**((X + a9809)))
- (0.80901699437494745**((X + a9811))))
```

```
+ *((X + a9807)));
```

}

```
...
*((104 + Y + a12569)) = ((s3983 - s3987)
        + (0.80901699437494745*t6537)
        + (0.58778525229247314*t6538));
*((105 + Y + a12569)) = (((s3984 - s3988)));
```

```
+ (0.80901699437494745*t6538))
```

```
- (0.58778525229247314*t6537));
```



### 1,000s of lines of special GPU code, transparently used

## **Backend: SPIRAL Code Generation**

```
global void ker code0(int *D48, double *D49, double *D50, double *D51, int *D52, double *X) {
   shared double T235[260];
                                           FFTX/SPIRAL with
  . . .
  if (((threadIdx.x < 13))) {
      for(int i96 = 0; i96 <= 4; i96++) { CUDA backend</pre>
          int a31, a32, a33, a34;
                                                                           Early result:
          a31 = (2*i96);
          a32 = (threadIdx.x + (13*a31));
                                                                          220 Gflop/s
          a33 = (threadIdx.x + (13*((a31 + 5) % 10)));
                                                                          70% faster than cuFFT
          a34 = (4 \times i96);
          *((((T_{235} + 0) + a_{34}) + (20*threadIdx.x))) = (*((T_{6} + a_{32})) + *((T_{6} + a_{33})));
          *(((1 + (T235 + 0) + a34) + (20*threadIdx.x))) = 0.0;
          *(((2 + (T235 + 0) + a34) + (20*threadIdx.x))) = (*((T6 + a32)) - *((T6 + a33)));
          *(((3 + (T235 + 0) + a34) + (20*threadIdx.x))) = 0.0;
      double t261, t262, t263, t264, t265, t266, t267, t268;
      int a129;
      t_{263} = (*(((T_{235+0})+12)+(20*threadIdx.x)))+*((((T_{235+0})+8)+(20*threadIdx.x))));
      t_{264} = (*(((T_{235+0})+12)+(20*threadIdx.x))) - *((((T_{235+0})+8)+(20*threadIdx.x))));
      . . .
      *((3 + T5 + a129)) = ((0.58778525229247314*t268) - (0.95105651629515353*t266));
  }
    syncwarp();
  if (((threadIdx.x < 1))) {
      double t305, t306, t307, t308, t309, t310, t311, t312, t313, t314, t315, t316;
      int a387;
      t305 = (*((T5 + 12)) + *((T5 + 144)));
       . . .
```

### *3,000 lines of code, kernel fusion, cross call data layout transforms*

## **Selected Results: FFTs and Spectral Algorithms**



#### Performance of 2x2x2 Upsampling on Haswell

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

Performance [Pseudo Gflop/s]





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

#### **PFA SAR Image Formation on Intel platforms**

performance [Gflop/s]



## **SPIRAL: Success in HPC/Supercomputing**

- NCSA Blue Waters
   PAID Program, FFTs for Blue Waters
- RIKEN K computer
   FFTs for the HPC-ACE ISA
- LANL RoadRunner
   FFTs for the Cell processor
- PSC/XSEDE Bridges
   Large size FFTs
- LLNL BlueGene/L and P FFTW for BlueGene/L's Double FPU

## ANL BlueGene/Q Mira Early Science Program, FFTW for BGQ QPX











Carnegie Mellon

2006 Gordon Bell Prize (Peak Performance Award) with LLNL and IBM 2010 HPC Challenge Class II Award (Most Productive System) with ANL and IBM

#### Global FFT (1D FFT, HPC Challenge)

performance [Gflop/s]



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

## SPIRAL 8.1.0: Available Under Open Source

#### Open Source SPIRAL available

- non-viral license (BSD)
- Initial version, effort ongoing to open source whole system
- Commercial support via SpiralGen, Inc.
- Developed over 20 years
  - Funding: DARPA (OPAL, DESA, HACMS, PERFECT, BRASS), NSF, ONR, DoD HPC, JPL, DOE, CMU SEI, Intel, Nvidia, Mercury
- Open sourced under DARPA PERFECT, continuing under DOE ECP
- Tutorial material available online
   www.spiral.net



F. Franchetti, T. M. Low, D. T. Popovici, R. M. Veras, D. G. Spampinato, J. R. Johnson, M. Püschel, J. C. Hoe, J. M. F. Moura: <u>SPIRAL: Extreme Performance Portability</u>, Proceedings of the IEEE, Vol. 106, No. 11, 2018.

Special Issue on From High Level Specification to High Performance Code