Design and Specification of Large-scale Simulations for GPUs using FFTX

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Porting Scientific codes to GPUs

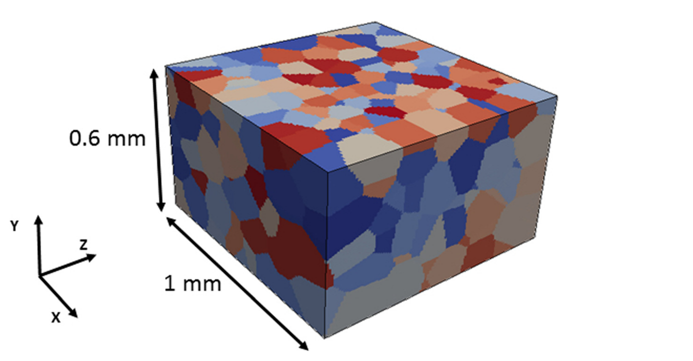
Common characteristics of scientific codes:
- Usually in Fortran
- FFT-based simulations involve all-to-all communication
- High memory requirement

Incompatibility with GPUs:
- GPUs haves small on-chip memory (~16GB max)
- Various communication latencies

Solutions for porting code:
- Domain decomposition (regular or irregular)
- Exploit properties of data and convolution kernel
- Sampling/ pruning used so that domain results fit on GPU memory

Case study: MASSIF
- Hooke's law simulation
- Partial Differential Equation solved by Green's function method
- FFT-based convolution and tensor contraction between rank-2 tensors and rank-4 Green's function

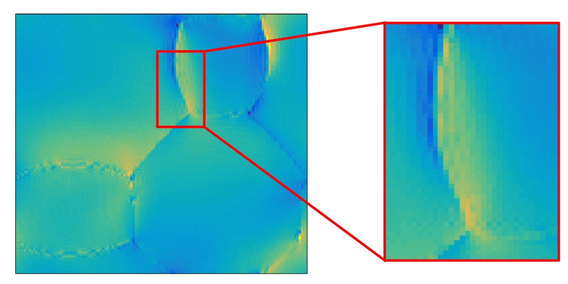
MASSIF simulates Composite microstructure made up of grains



Algorithm 1 MASSIF Inner loop

Initialize: $\epsilon^0 \leftarrow E$, $\sigma^0_{mn}(\mathbf{x}) \leftarrow C_{mnk\ell}(\mathbf{x}) : \epsilon^0_{k\ell}(\mathbf{x})$
while $e_s > e_{tol}$ **do**
$\hat{\sigma}^{(i)}_{mn}(\xi) \leftarrow \text{FFT}(\sigma^{(i)}_{mn}(\mathbf{x}))$
Check convergence
$\Delta\hat{\epsilon}^{(i+1)}_{k\ell}(\xi) \leftarrow \hat{\Gamma}_{k\ell mn}(\xi) : \hat{\sigma}^{(i)}_{mn}(\xi)$
Update strain: $\hat{\epsilon}^{(i+1)}_{k\ell}(\xi) \leftarrow \hat{\epsilon}^{(i)}_{k\ell}(\xi) - \Delta\hat{\epsilon}^{(i+1)}_{k\ell}(\xi)$
$\epsilon^{(i+1)}_{k\ell}(\mathbf{x}) \leftarrow \text{iFFT}(\hat{\epsilon}^{(i+1)}_{k\ell}(\xi))$
Update stress: $\sigma^{(i+1)}_{mn}(\mathbf{x}) \leftarrow C_{mnk\ell}(\mathbf{x}) : \epsilon^{(i+1)}_{k\ell}(\mathbf{x})$

Stress field at grain boundary



Proposed solution:
- Domain decomposition with grains are domains
- Domain-local FFT followed by convolution and tensor contraction
- Green's function computed on-the-fly to avoid storage
- Adaptive sampling of dense convolution result to fit problem on GPU memory

Complex data mappings! How to get maximum performance on various platforms?

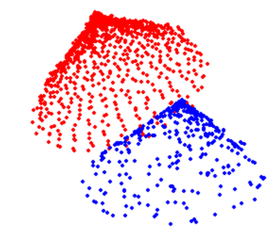
DGX-2 Source: NVIDIA

Summit Source: ORNL

Challenges FFTW

FFTW is de-facto standard interface for FFT
- **Vendor libraries support the FFTW 3.X interface:** Intel MKL, IBM ESSL, AMD ACML (end-of-life), Nvidia cuFFT, Cray LibSci/CRAFFT

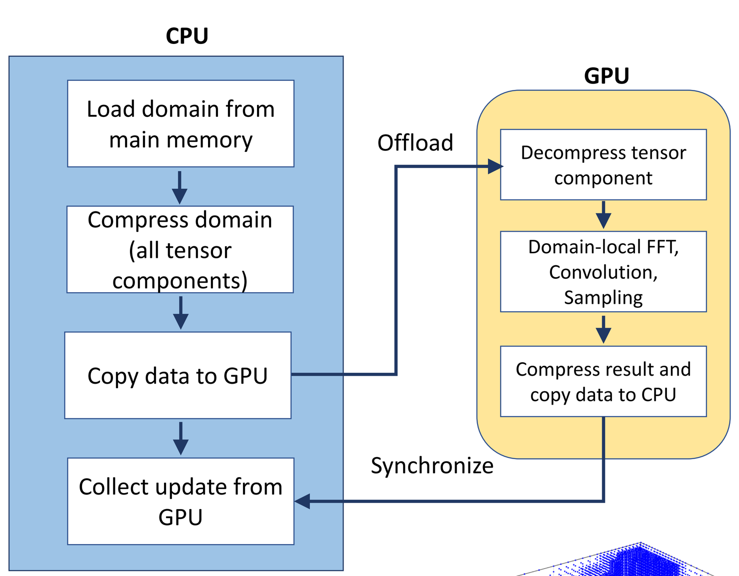
Some Issues:
- No native support for accelerators (GPUs, Xeon PHI, FPGAs) and SIMT
- Parallel/MPI version does not scale beyond 32 nodes
- No analogue to LAPACK for spectral method

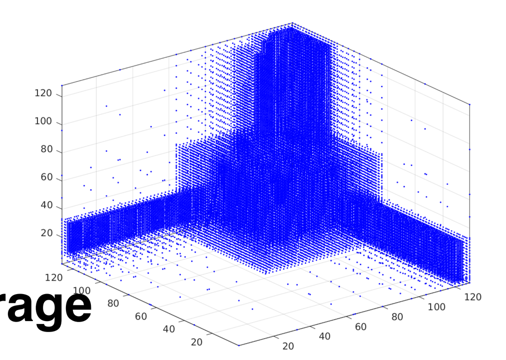


Complex data patterns may need to be expressed, FFTW currently falls short. But, extensions like FFTX could add new descriptors.

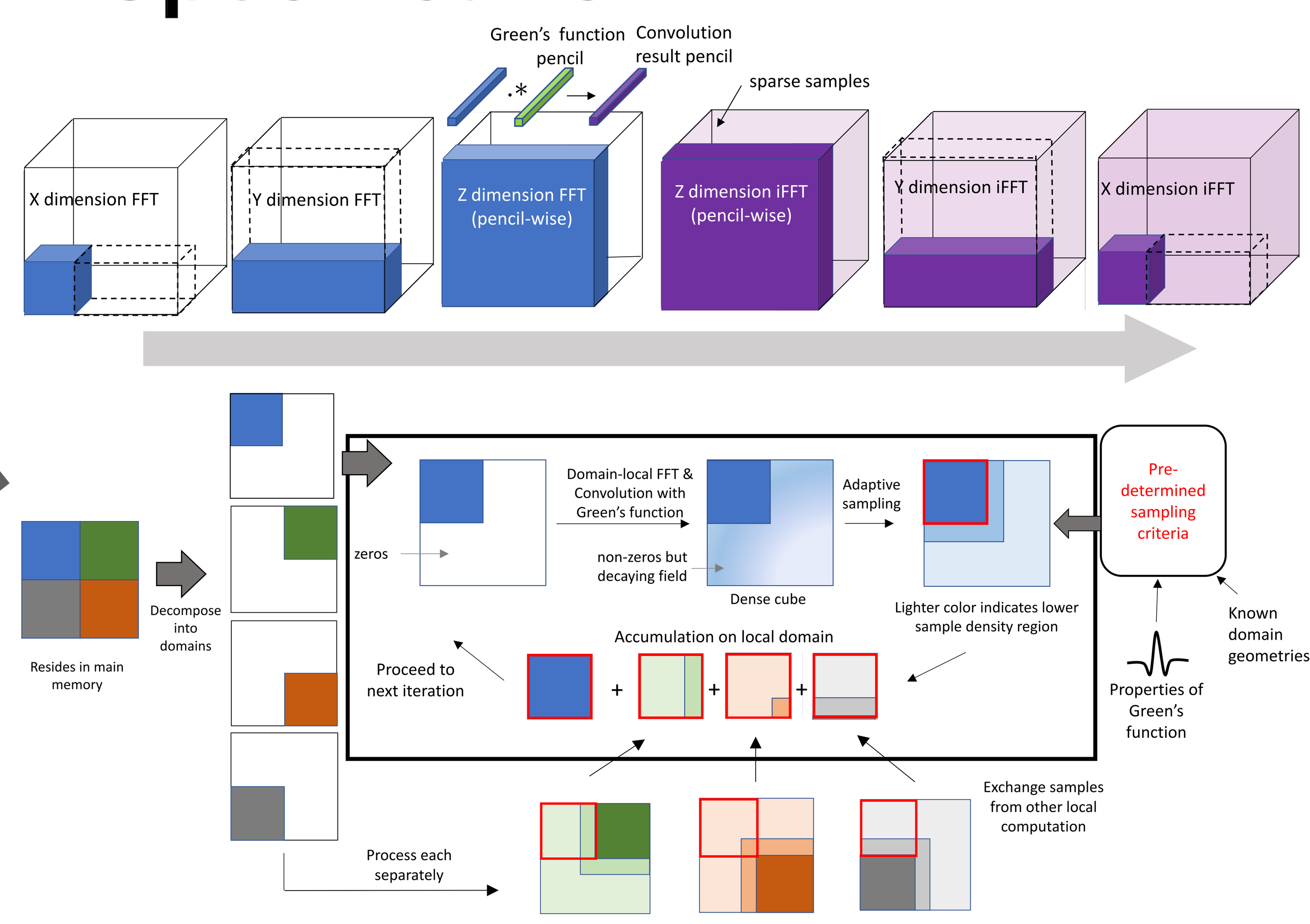
Solution: Emerging interfaces like FFTX, extension of FFTW, enables algorithm specification as composition of sub-plans

Front end: Algorithm Specification





Octree Sampling reduces storage on GPU



FFT, tensor contraction and sampling

```
//GPU side, compute on individual domain
#define NUMSUBPLANS 5
plan subplans[NUMSUBPLANS];
plan p; // top-level plan
//... Initialize ....

// create zero-initialized temporary
// n x n x n array with 3 x 3 tensor at each point
tmp1 = create_zero_temp(cube_size, tensor_size);

// copy k x k x k input domain into n x n x n tmp1
subplans[0] = copy_plan(domain, tmp1);// (from, to)

// DFT on the input
tmp2 = create_complex_temp(size_tmp1);
subplans[1] = dft_plan(tmp1);

//Tensor contraction
//In this case we know that output size is the same as tmp2
tmp3 = create_zero_temp(size_tmp2);
subplans[2] = tensor_contraction_plan(tmp2, data, tmp3,
      dimensions_to_contract);//(in,data,out,info)

// iDFT on the contracted output
tmp4 = create_complex_temp(size_tmp3);
subplans[3] = inverse_dft_plan(tmp3, tmp4);

//The next plans apply adaptive sampling
subplans[4] = plan_sample(tmp4, final_output, Octree_S); // (from, to ,
      Octree_descriptor)

// create the top level plan. this copies the sub-plan pointers
p = plan_compose(NUMSUBPLANS, subplans);

// plan to be used with execute()
return p;
```

Accumulation

```
//CPU side, accumulate over all domains

#define NUMSUBPLANS 3
plan subplans[NUMSUBPLANS];
plan accum; // top-level accumulate plan

// n x n x n array with 3 x 3 tensor at each point
temp = create_zero_temp(cube_size, tensor_size);

//smaller temp arrays
output_cube = create_zero_temp( domain_d_size, tensor_size);
net_output_cube = create_zero_temp( domain_d_size, tensor_size);

for j in [1,...,D] except d:

 subplans[0] = plan_decode_octree(S[j], data_array, temp); //decode octree.
       copy into temp

 subplans[1]= plan_multires_interpolate( S[j], temp, domain_d, output_cube
       ,output_size);
 //descriptor, input cube (samples missing), filter (only interpolate that
       region), outputcube, outputsize

 subplan[2] = plan_sum(output_cube, net_output_cube);

 // create the top level plan
 accum = plan_compose(NUMSUBPLANS, subplans);

 // plan to be used with execute()
 return accum;
```

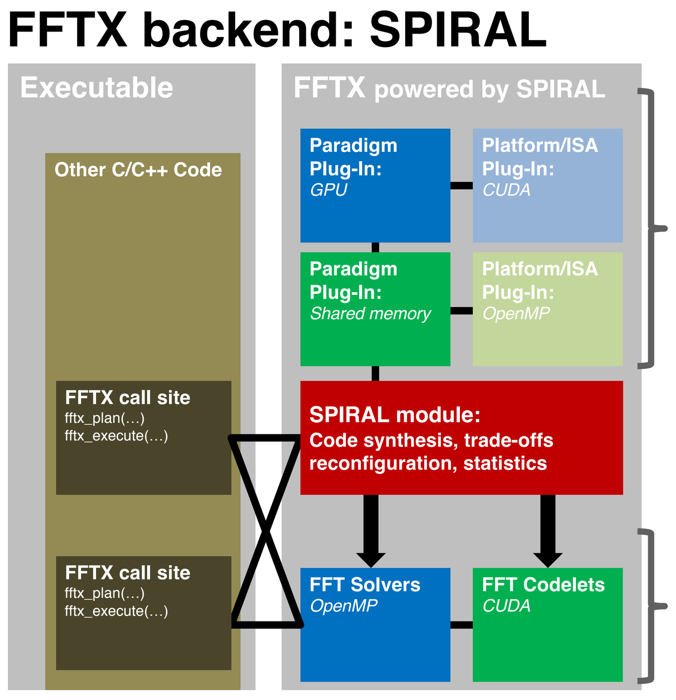
Back end: Code Optimization

FFTX is..

Modernized FFTW-style interface
- **Backwards compatible to FFTW 2.X and 3.X**
- **Small number of new features, familiar interface**

Code generation backend using SPIRAL
- **Library/application kernels are interpreted as specifications in DSL** extract semantics from source code and known library semantics
- **Compilation and advanced performance optimization** cross-call and cross library optimization, accelerator off-loading,…
- **Reference library implementation and bindings to vendor libraries**

FFTX backend: SPIRAL



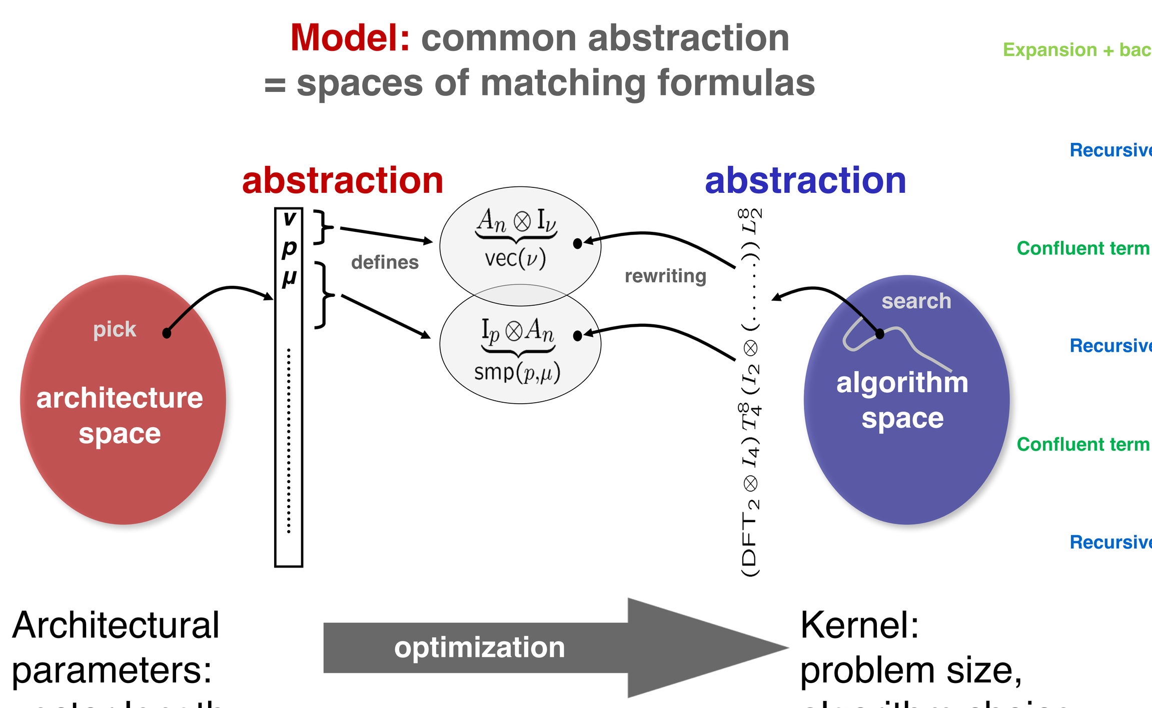
Extensible platform and programming model definitions

Core system: SPIRAL engine

Automatically generated FFTW-like library components

DARPA BRASS

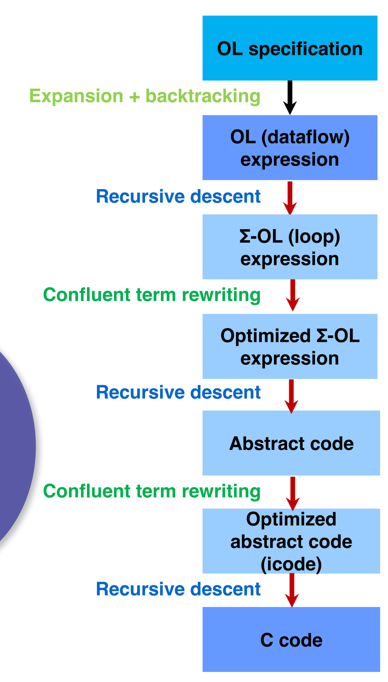
Platform-aware formal program synthesis



Architectural parameters: vector length, #processors, …

Kernel: problem size, algorithm choice

Translating an OL expression into code



Constraint Solver Input: DFT_8 AVX(2-way ℂ)

Output = Ruletree, expanded into

OL expression:

$$\left((F_2 \bar{\otimes} I_2) T_2^4 (I_2 \otimes F_2) L_2^4 \bar{\otimes} I_2\right) \; T_2^8 \; \left(I_2 \otimes \; L_2^4 \; (F_2 \bar{\otimes} I_2)\right)\left(L_2^4 \bar{\otimes} I_2\right)$$

Σ-OL:

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

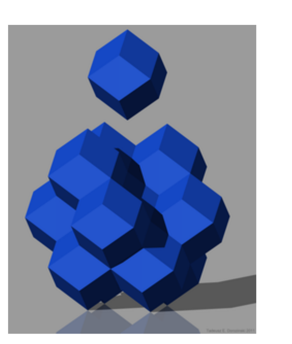
C code:

```
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;
}
```

Future Plans + Other Applications

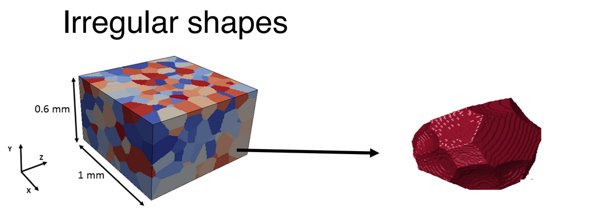
Future work: MASSIF

- Irregular domain decomposition
- Extension of adaptive sampling for irregular domains



Tesselated polytopes

Irregular shapes



Future work: FFTX and SpectralPACK

Numerical Linear Algebra	Spectral Algorithms
LAPACK LU factorization Eigensolves SVD …	**SpectralPACK** Convolution Correlation Upsampling Poisson solver …
BLAS BLAS-1 BLAS-2 BLAS-3	**FFTX** DFT, RDFT 1D, 2D, 3D,… batch

LAPACK for spectral algorithms
- **Define FFTX as the analogue to BLAS**
- **Define class of numerical algorithms to be supported by SpectralPACK** PDE solver classes (Green's function, sparse in normal/k space,…), signal processing
- **Define SpectralPACK functions** circular convolutions, NUFFT, Poisson solvers, free space convolution

Other FFT-based simulations

Poisson's equation in free space

Partial differential equation (PDE) Solution

$\Delta(\Phi) = \rho \qquad \Phi : \mathbb{R}^3 \rightarrow \mathbb{R}$
$\rho : \mathbb{R}^3 \rightarrow \mathbb{R}$
$D = \text{supp}(\rho) \subset \mathbb{R}^3$

Poisson's equation. Δ is the Laplace operator

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

Approach: Green's function

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

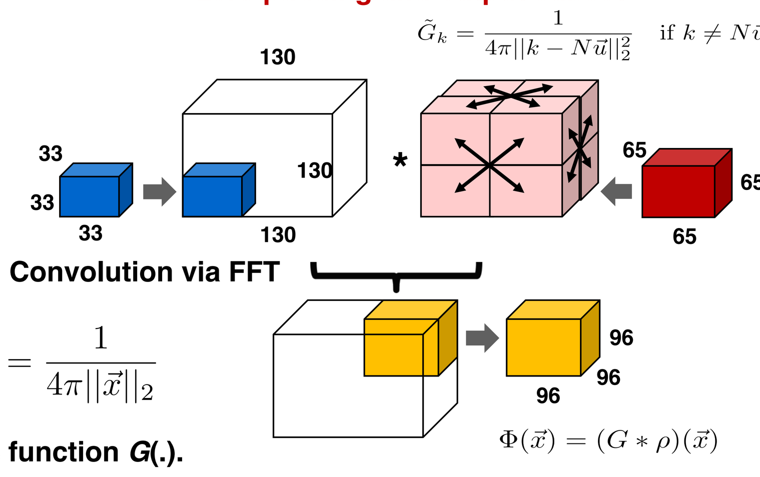
Solution: φ(.) = convolution of RHS ρ(.) with Green's function G(.). Efficient through FFTs (frequency domain)

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

Green's function kernel in frequency domain

Hockney free-space convolution

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

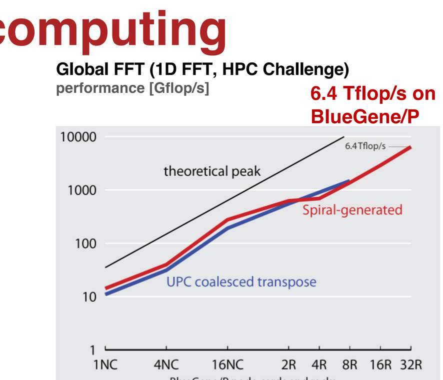


$\tilde{G}_k = \frac{1}{4\pi||k - N\vec{u}||_2^2}$ if $k \neq N\vec{u}$

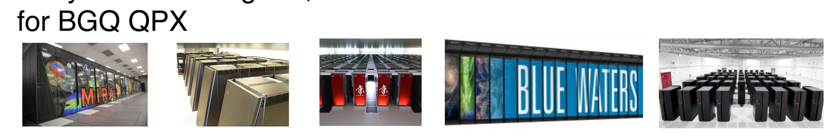
$\Phi(\vec{x}) = (G * \rho)(\vec{x})$

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



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



2006 Gordon Bell Prize (Peak Performance Award) with LLNL and IBM

2010 HPC Challenge Class II Award (Most Productive System) with ANL and IBM

Carnegie Mellon | SpiralGen Accelerating Innovation in Computing | ECP EXASCALE COMPUTING PROJECT

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