Leveraging Optimized FFT on Intel Platforms

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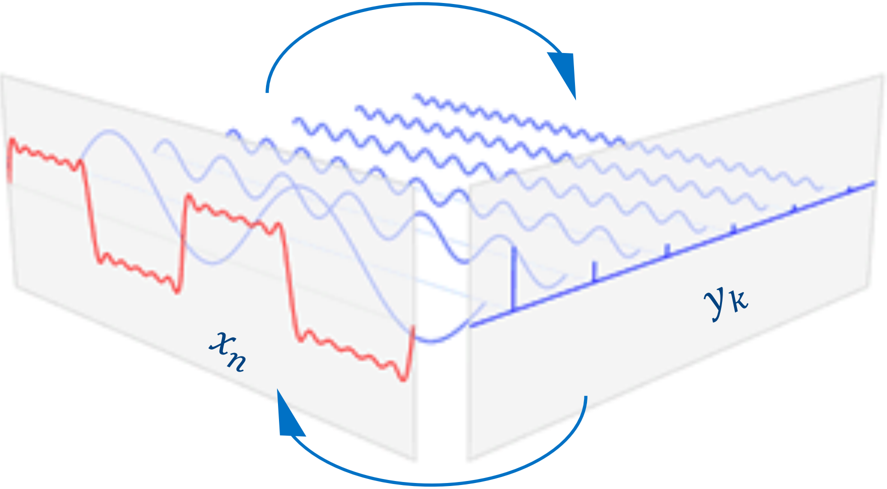
Rev. 7/17/13

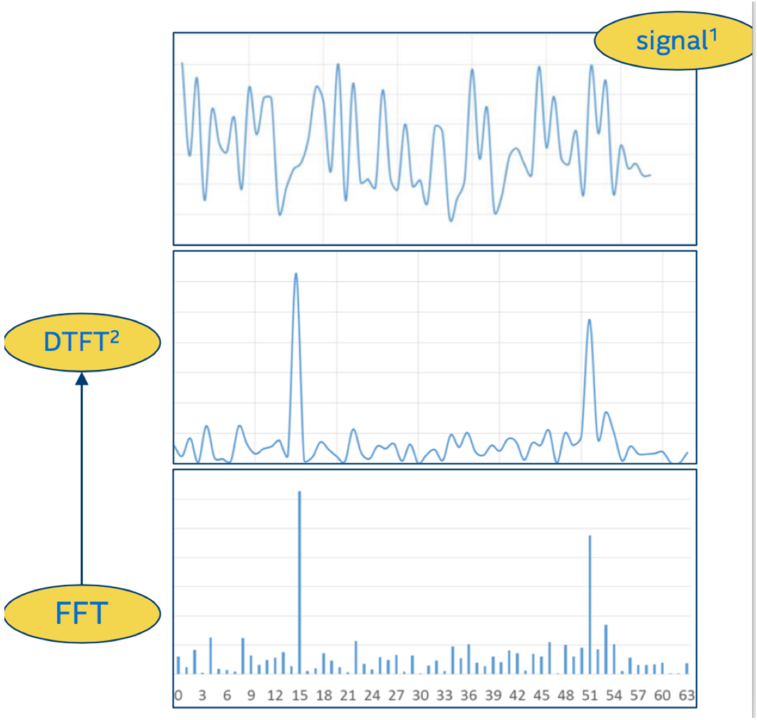
Agenda

- Discrete Fourier Transform in applications
- Fast Fourier Transform (FFT) in a nutshell
- FFTW & MKL DFT
- 3D FFT in applications
- Summary

Discrete Fourier transforms (DFT)

$$y_k = \sum_{n=0}^{N-1} e^{-2\pi i k n/N}\, x_n$$

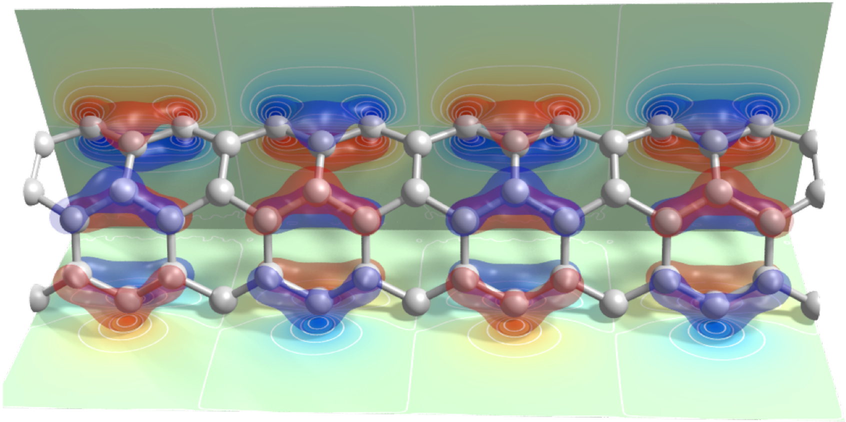


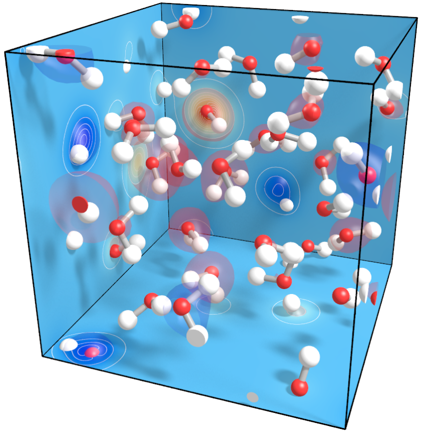


$$x_k = (1/N) \sum_{n=0}^{N-1} e^{+2\pi i k n/N}\, y_n$$

DFT in Applications

- Signal processing, spectroscopy, magnetic resonance imaging, ….
- Speech and image recognition
- Simulations of periodic systems
- Quantum computing





"It's hard to explain what sort of impact Fourier's had," because the Fourier transform is such a fundamental concept that by now, "it's part of the language," Demanet, http://news.mit.edu/2009/explained-fourier

Fourier transform as matrix-vector product: $O(N^2)$

$$x_k = (1/N)\sum_{n=0}^{N-1} e^{+2\pi ikn/N}\, y_n$$

$$\omega = e^{-2\pi i/N} = \cos\frac{2\pi}{N} - i\sin\frac{2\pi}{N}$$

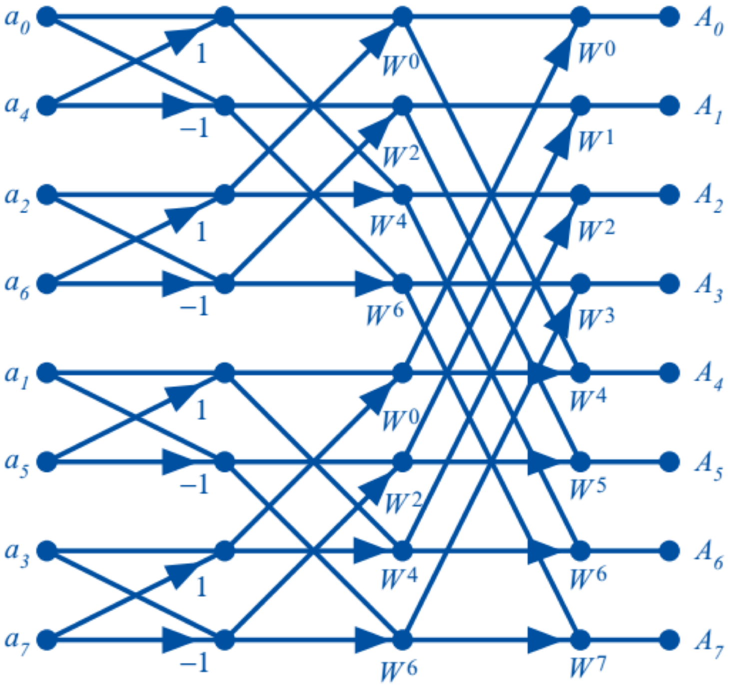
$$y = \left(\quad \omega^{jk} \quad\right) x \quad \Longleftrightarrow \quad y_k = \sum_{n=0}^{N-1} e^{-2\pi ikn/N}\, x_n$$

Fast Fourier Transform (FFT): a fast way to compute DFT

Fast Fourier Transformation (FFT), *O(N log(N))*
The Cooley-Tukey algorithm

8-point FFT

$$FFT8 = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & \omega & -i & -i\omega & -1 & -\omega & i & i\omega \\ 1 & -i & -1 & i & 1 & -i & -1 & i \\ 1 & -i\omega & i & \omega & -1 & i\omega & -i & -\omega \\ 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 \\ 1 & -\omega & -i & i\omega & -1 & \omega & i & -i\omega \\ 1 & i & -1 & -i & 1 & i & -1 & -i \\ 1 & i\omega & i & -\omega & -1 & -i\omega & -i & \omega \end{bmatrix}$$



$$W = \omega = e^{-2\pi i/8} = (1-i)/\sqrt{2}$$

Twiddle factors: $W^0, W^1, \ldots, W^7$

Typical Ways to Compute FFT

Cooley-Tukey

- Recursively split the FFT into smaller equal sizes

Split-Radix

- Radix 4:2:2

Stockham

- Eliminates the need for rearranging the inputs/outputs that is specific to Cooley-Tukey

Prime-factor

- Decompose into **relatively** prime numbers

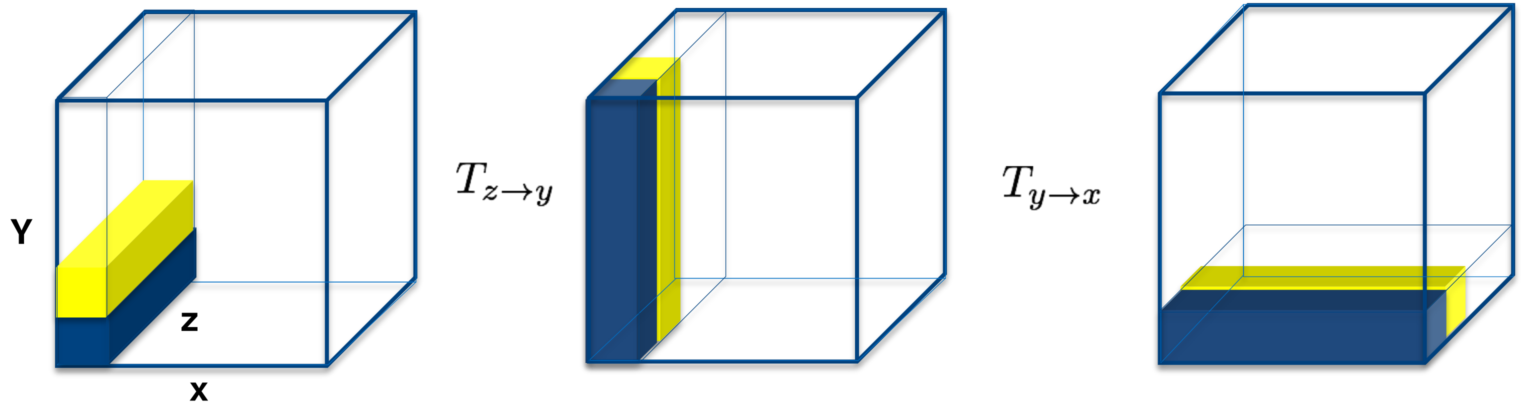
Bluestein (Chirp-Z)

- For arbitrary sizes, uses Cooley-Tukey and convolution theorem

many others…

Basic 3D FFT using stride-1 1D FFT

$$\hat{f}(k_x, k_y, k_z) = \sum_x \sum_y \sum_z e^{i2\pi(k_x x + k_y y + k_z z)} f(x, y, z) = \sum_x e^{i2\pi k_x x} \left[\sum_y e^{i2\pi k_y y} \left[\sum_z e^{i2\pi k_z z} f(x, y, z) \right] \right]$$



- Optimized 1D FFT on stride-1 for each direction
- Transpose to transform the data for 1D FFT

We have libraries for FFT

- MKL-FFT, FFTW …
- Highly optimized 1D FFT $2^p 3^q 5^r \cdots P^z$
- Optimized N-dim FFT and transposes
- Building blocks for DIY FFT

How to use FFT libraries to maximize the productivity!

FFTW and MKL DFT

- Both implement 1 to multi-dimensional FFT
  - Complex-to-Complex
  - Complex-to-Real and Real-to-Complex
  - Double & single precision
  - Threaded on SMP nodes and distributed FFT on multi SMP nodes
- FFTW www.fftw.org
  - Introduced FFT plan concepts
  - Novel code-generation and runtime self-optimization techniques
- Intel® MKL Fast Fourier Transforms (next)
  - Highly optimized on Intel platforms
  - Provide FFTW Wrapper

Intel® MKL Fast Fourier Transforms (FFTs)

FFTW Interfaces support	C, C++ and FORTRAN source code wrappers provided for FFTW2 and FFTW3. FFTW3 wrappers are already built into the library
Cluster FFT	Perform Fast Fourier Transforms on a cluster Interface similar to DFTI Multiple MPIs supported
Parallelization	Thread safe with automatic thread selection
Storage Formats	Multiple storage formats such as CCS, PACK and Perm supported
Batch support	Perform multiple transforms in a single call
Additional Features	Perform FFTs on partial images Padding added for better performance Transform combined with transposition mixed-language usage supported

Intel® MKL 2018 New FFT Features & Optimizations

- MKL_VERBOSE support for FFT starting from MKL 2018 Update 1

  set MKL_VERBOSE=1. The verbose information in the program will be shown up:

  MKL_VERBOSE Intel(R) MKL 2018.0 Update 1 Product build 20170712 for Intel(R) 64 architecture Intel(R) Advanced Vector Extensions 2 (Intel(R) AVX2) enabled processors, Lnx 2.30GHz gnu_thread NMICDev:0
  MKL_VERBOSE FFT: MAIN_DESC | sro4:5:3x5:1:1 | THR_LIMIT = 1 | 0.00s CNR:OFF Dyn:1 FastMM:1 TID:0 NThr:36 WDiv:HOST:+0.000

- Significantly improved 1D and 3D FFT performance for Intel® Xeon® Processor supporting Intel® Advanced Vector Extensions 512 (Intel® AVX-512)

  https://software.intel.com/en-us/mkl/features/benchmarks

Typical FFT use in applications

FFTW APIs

```
void do_fftw(){

  const int N=3;
  int ngrid[]={64,64,64};
  const int howmany=4;
  const size_t distance=64*64*64;
  fftw_complex in[howmany*distance];
  fftw_complex out[howmany*distance];

  fftw_plan for_plan=fftw_plan_many_dft(N,ngrid,howmany,
      in,ngrid,1,distance,out,ngrid,1,distance,
      FFTW_FORWARD, FFTW_MEASURE);

  fftw_plan back_plan=fftw_plan_many_dft(N,ngrid,howmany,
      out,ngrid,1,distance,in,ngrid,1,distance,
      FFTW_BACKWARD, FFTW_MEASURE);

  //FFT
  fftw_execute_dft(for_plan,in,out);

  //inverse FFT
  fftw_execute_dft(back_plan,out,in);

  fftw_destroy_plan(back_plan);
  fftw_destroy_plan(for_plan);
}
```

1. Create plans for forward FFT and inverse FFT
   - Require addresses of In/Out
   - Select (FFTW_ESTIMATE, FFTW_MEASURE, FFTW_ PATIENT,…)
   - Alternative APIs
2. Execute Forward FFT
3. Execute backward (Inverse) FFT
4. Cleanup

Using MKL DFT APIs

```
void do_mkl_dfti(){

  const int N=3;
  int ngrid[]={64,64,64};
  const int howmany=4;
  const size_t distance=64*64*64;
  _MKL_Complex16 in[howmany*distance];
  _MKL_Complex16 out[howmany*distance];

  DFTI_DESCRIPTOR_HANDLE mkl_plan;

  MKL_LONG status = DftiCreateDescriptor(&mkl_plan,
      DFTI_DOUBLE,DFTI_COMPLEX,N,ngrid);
  status=DftiSetValue(mkl_plan,DFTI_NUMBER_OF_TRANSFORMS,howmany);
  status=DftiSetValue(mkl_plan,DFTI_INPUT_DISTANCE,distance);
  DftiCommitDescriptor(mkl_plan);

  //FFT
  DftiComputeForward(mkl_plan,in,out);

  //inverse FFT
  DftiComputeBackward(mkl_plan,out,in);

  DftiFreeDescriptor(&mkl_plan);

}
```

1. Create a descriptor
2. Set configuration parameters (optional)
3. Commit a descriptor
4. Execute Forward FFT
5. Execute backward (Inverse) FFT
6. Cleanup

FFTW Wrapper in MKL

- No code modification necessary.
- Include the header file: `-I${MKLROOT}/include/fftw`
- Link MKL as usual, e.g., -mkl

Mapping between FFTW and Intel MKL Interfaces

- https://software.intel.com/en-us/articles/the-intel-math-kernel-library-and-its-fast-fourier-transform-routines

3D FFT in electronic structure codes

PW DFT on Parallel Computers

Clarke, Stich & Payne, CPC, 72, 14 (1992)

Computer Physics Communications 72 (1992) 14–28
North-Holland

Computer Physics Communications

Large-scale ab initio total energy calculations on parallel computers

L.J. Clarke
Edinburgh Parallel Computer Centre, University of Edinburgh, Mayfield Road, Edinburgh, EH9 3JZ, UK

I. Štich [1] and M.C. Payne
Cavendish Laboratory (TCM), University of Cambridge, Madingley Road, Cambridge, CB3 0HE, UK

Received 30 March 1992

An implementation of a set of total energy plane-wave pseudopotential codes on a parallel computer is described which allows calculations to be performed for systems containing many hundreds of atoms in the unit cell. Possible parallelisation strategies are discussed and it is shown that assigning parts of real and Fourier space across the processors is the least restricted approach. The performance of our parallel codes is demonstrated by timing tests carried out on several i860-based parallel machines and these are compared with tests performed on conventional sequential supercomputers. Ab initio computations on systems which are beyond the power of conventional supercomputers as well as new perspectives for first-principles molecular dynamics are discussed.

Abinit
BigDFT
CASTEP
CPMD
GPAW
NWChem-PW
Qbox
Quantum Espresso
VASP
……

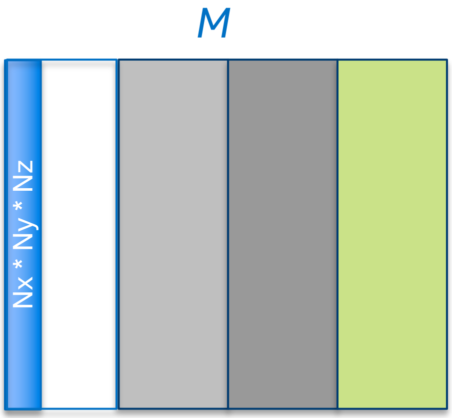
Algorithm 8: A pseudo PW KS-DFT code

```
C(:,:) = random
Orthonormalize all the columns:  C^H C=I  // Gram-Scmidth

for step=1,...,Nstep
{
  //compute density
  rhoR=0                              //memet
  for n=1,..,N
    Cr(:,n)=iFFT(C(:,n))              //iFFT
    rhoR(:) += f*conj(Cr(:,n))*Cr(:,n) //DOT
  endfor
  rhoG=FFT(rhoR)                      //FFT

  rhoG_old=rhoG

  do {

    B=0                          //memset
    for n=1,...,M
      B(:,n) += Gsq(:) C(:n)     //DOT
      B(:,n) += Vh(:) C(:,n)     //DOT

      Vtmp(:)=Vxc(rhoR(:))*Cr(:,n) //interpolation,DOT
      B(:,n) += FFT(Vtmp)(:)     //FFT

      B(:,n) += Vloc+Vnl         //small GEMM
    endfor

    E=C^H B                      //zgemm
    Diagonalize(E)               //zheev family
    Update C <- EC               //zgemm

    Compute rhoR and rhoG        //DOT,FFT

  } while(||rhoG - rhoG_old||>eps)

  Compute forces on ions: C^H F C
  Move ions
}
```

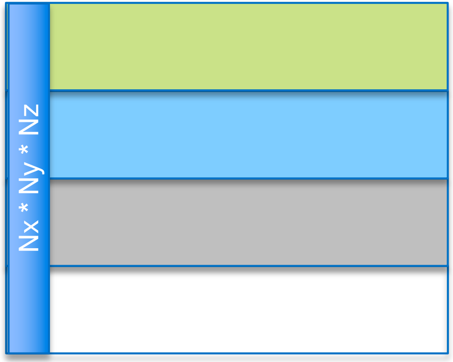
C(Ng, N), the solution
Ng=Nx * Ny * Nz, FFT grid
N= number of KS orbials

Data parallelization (FORTRAN convention)

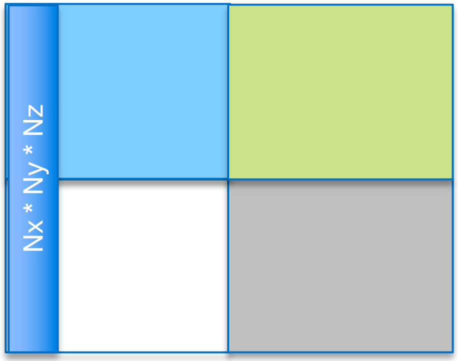
Band distribution
- Distribute M
- FFT within a task; exploit optimized FFT library
- Choice for HF, GW & RPA



FFT distribution
- Distribute Ng
- Cluster FFT
- Choice for DFT in many codes

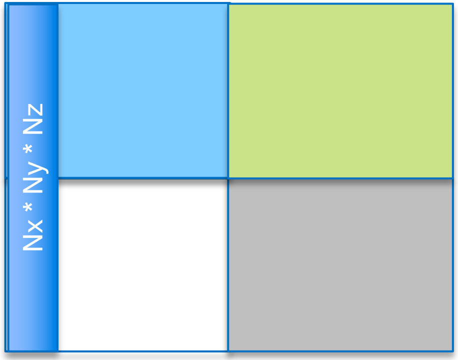


Mixed
- FFT groups
- Band groups



Colors=MPI tasks

Band & FFT distribution



Distribute M and Ng
Distribute FFT
Parallel GEMM (aka Scalapack)

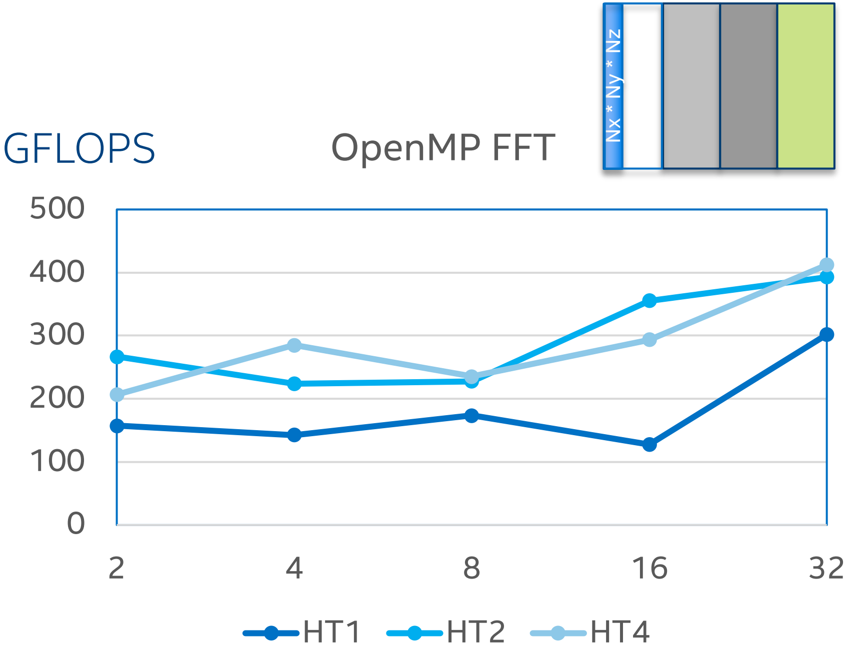
- Implemented in VASP, Qbox, NWCHEM-PW
- Necessary for small-memory systems (e.g., Blue Gene L/P/Q): Qbox 2006 Gordon Bell
- Maybe needed for big problems
- May provide the best compromise between FFT and GEMM efficiency
- Can leverage **TSGEMM** and **TSQR**

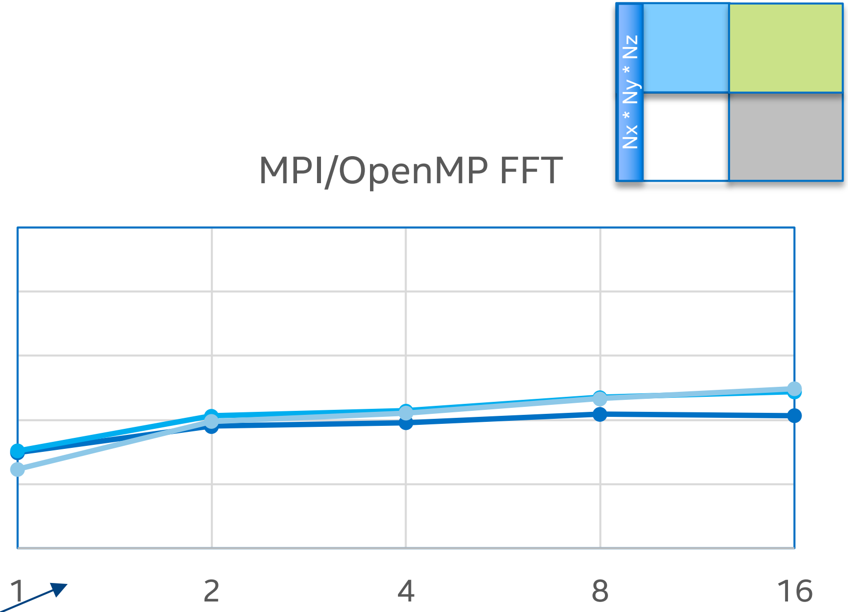
Optimizing 3D FFT use

- Many concurrent FFTs of *Nx*Ny*Nz*
  - M=10-1000
  - FFT grid Nx=10-200 for typical problems of today
- Memory bandwidth or network bandwidth limited
- Cache blocking, SIMD and overlap of the data movement and computation: critical for high performance
- Leverage “many (batched)” FFT
- Moving data efficiently via optimized transpose
- Overlap with other computations

FFT 3D on SMP: OpenMP vs MPI

GLOPS=Theoretical Cooley-Tukey



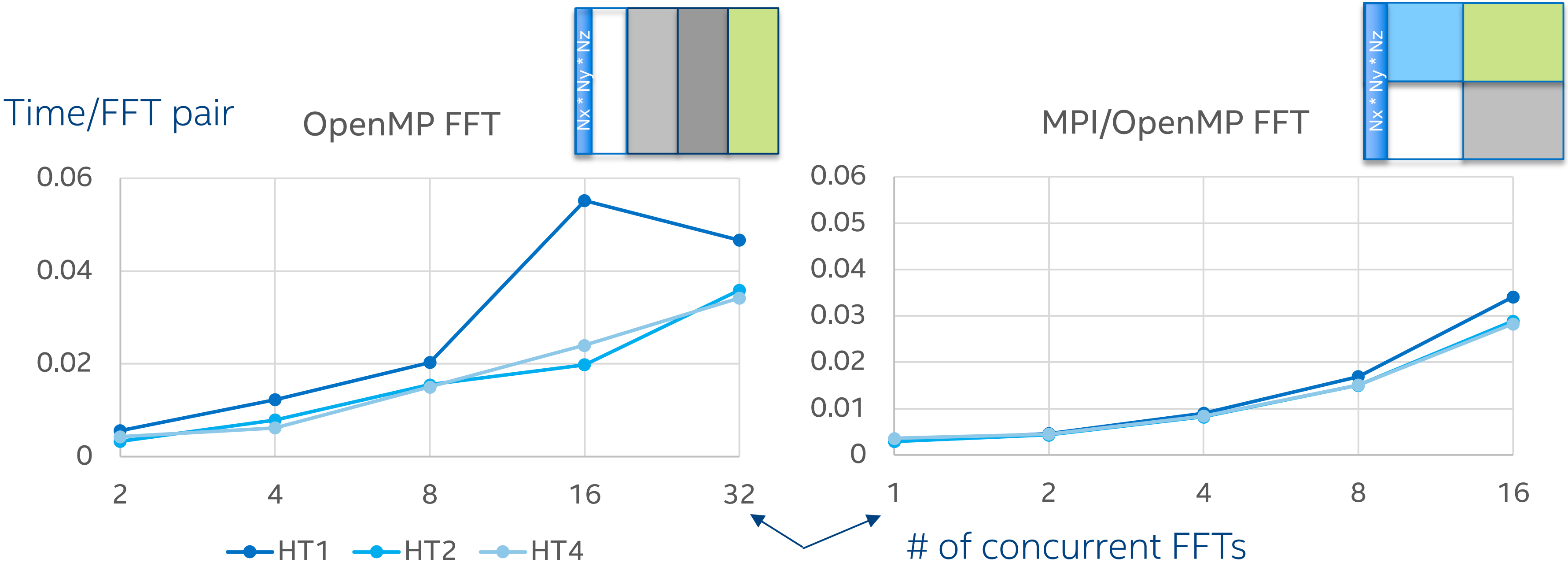


# of concurrent FFTs

- Using 64 cores of 72-core Intel(R) Xeon Phi(TM) CPU 7250 @ 1.40GHz
- I_MPI_PIN_DOMAIN= 64*4/MPI
- KMP_AFFINITY=(scatter,balanced,compact), granularity=fine

FFT 3D on SMP: OpenMP vs MPI

$128 \times 128 \times 128$

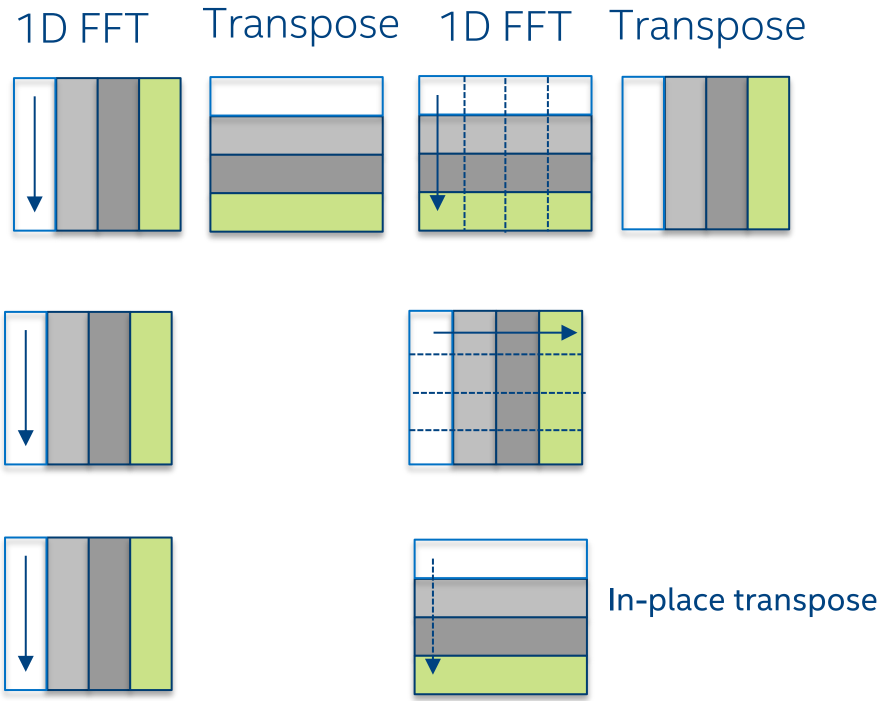


- Optimize either throughputs (how many FFT/s) or time (strong scaling)
- Using 64 cores of 72-core Intel(R) Xeon Phi(TM) CPU 7250 @ 1.40GHz
- I_MPI_PIN_DOMAIN= 64*4/MPI; KMP_AFFINITY=(scatter,balanced,compact), granularity=fine

Application-tailored FFT

- Data structure and distribution set by the entire application
- Can interleave FFT and other computations
- **Can reduce data movement**
- Can overlap communications/computations

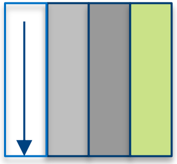
2D FFT example



Using MKL FFT configuration parameters for customized FFT: composed 3D FFT=2D + 1D

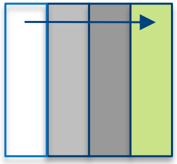
Create 2D FFT plan

```
MKL_LONG ngrid_2d[]={ngrid[1],ngrid[2]};

DFTI_DESCRIPTOR_HANDLE plan_yz, plan_x;
MKL_LONG status = DftiCreateDescriptor(&plan_yz,dfti_get_precision(real_type()),DFTI_COMPLEX,2,ngrid_2d);
status=DftiSetValue(plan_yz,DFTI_NUMBER_OF_TRANSFORMS,ngrid[0]);
status=DftiSetValue(plan_yz,DFTI_INPUT_DISTANCE,ngrid[1]*ngrid[2]);
DftiCommitDescriptor(plan_yz);
```



Create 1D FFT plan

```
MKL_LONG strides[2]={0,ngrid[1]*ngrid[2]};
status=DftiCreateDescriptor(&plan_x,dfti_get_precision(real_type()),DFTI_COMPLEX,1,ngrid[0]);
status=DftiSetValue(plan_x,DFTI_NUMBER_OF_TRANSFORMS,ngrid[1]*ngrid[2]);
status=DftiSetValue(plan_x,DFTI_INPUT_DISTANCE,1);
status=DftiSetValue(plan_x,DFTI_OUTPUT_DISTANCE,1);
status=DftiSetValue(plan_x,DFTI_INPUT_STRIDES,strides);
status=DftiSetValue(plan_x,DFTI_OUTPUT_STRIDES,strides);
DftiCommitDescriptor(plan_x);
```



Forward 3D FFT

```
DftiComputeForward(plan_yz,g[0]);
DftiComputeForward(plan_x,g[0]);
```

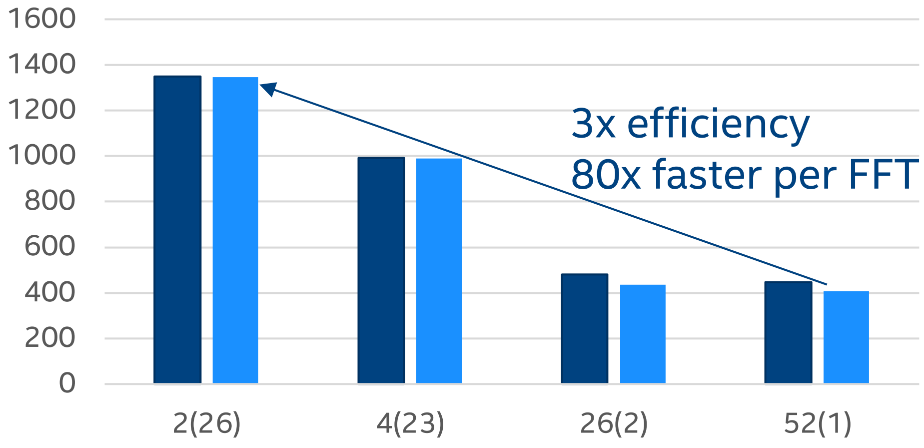
Backward 3D FFT

```
DftiComputeBackward(plan_x,g[0]);
DftiComputeBackward(plan_yz,g[0]);
```

https://software.intel.com/en-us/mkl-developer-reference-c-configuration-settings

Performance of “many” 3D FFT of 128^3

GFLOPS, higher the better



# of FFT (threads)

# of FFT = # of MPI ranks
Theoretical Cooley-Tukey GFLOPS

Intel® Xeon® Platinum 8170 CPU, 2S, 26C/S

Reducing BW needs

- Multiple threads for each FFT : SMP optimization and no MPI communications
- Cache/register optimization via in-place, on-the-fly transpose and SIMD optimization in MKL
- A FFT is 80 times faster using Composed methods using 26 threads than the baseline using 1 thread.

Summary

- Overview of FFT capabilities in MKL
- Considerations to maximize FFT performance in applications
  - Allocation
  - Computation
  - Data movement
- Adapt FFT use for application-specific data structures and algorithms based on FFT primitives

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