heFFTe Tutorial

Stan Tomov, Miroslav Stoyanov (ORNL),
Alan Ayala (AMD), Azzam Haidar (NVIDIA), and Jack Dongarra

students and outside collaborators

Innovative Computing Laboratory
University of Tennessee, Knoxville

Exascale Computing Project
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The Fast Fourier Transform (FFT)

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- Considered one of the top 10 algorithms of the 20th century

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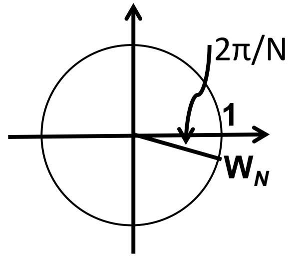
  - **FFT computes the Discrete Fourier Transform (DFT) of a series:**
    Let $x = x_0, \ldots, x_{N-1}$ are complex numbers. The DFT of x is the sequence $\mathbf{X} = \mathbf{X}_0, \ldots, \mathbf{X}_{N-1}$

$$X_k = \sum_{n=0}^{N-1} x_n e^{-i2\pi kn/N} \qquad k = 0, \ldots, N-1.$$



, i.e., $\mathbf{X} = F_N\, x$, where

$$F_N = \begin{bmatrix} 1 & 1 & \cdots & 1 \\ w_N^{1.1} & w_N^{1.2} & \cdots & w_N^{1.(N-1)} \\ \vdots & & & \\ w_N^{(N-1).1} & w_N^{(N-1).2} & \cdots & w_N^{(N-1).(N-1)} \end{bmatrix}, \quad w_N = e^{-(2\pi i/N)}$$

$= \cos(2\pi/N) - i \sin(2\pi/N)$

is a primitive N^{th} root of unity

*** DFT can be computed as GEMV in $2N^2$ flops but FFT can do it in $5\,N \log_2 N$ flops!**

  - The Inverse Discrete Fourier Transform (IDFT) is similarly defined except that the **e** exponents are taken as $i\, 2\pi\, k\, n / N$, and elements divided by N

The Fast Fourier Transform (FFT)

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Discrete Fourier Transform (DFT)

Let x be an m-dimensional array of size $N := N_1 \times N_2 \times \cdots \times N_m$. Its DFT is defined by $y := DFT(x)$, obtained as:

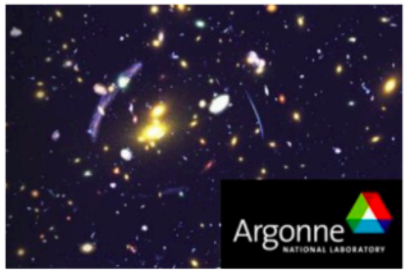
$$y(k_1, k_2, \ldots, k_m) := \sum_{n_1=0}^{N_1-1} \sum_{n_2=0}^{N_2-1} \cdots \sum_{n_m=0}^{N_m-1} \tilde{x} \cdot e^{-2\pi i \left(\frac{k_1 n_1}{N_1} + \frac{k_2 n_2}{N_2} \cdots + \frac{k_m n_m}{N_m} \right)},$$

where $\tilde{x} := x(n_1, n_2, \ldots, n_m)$.

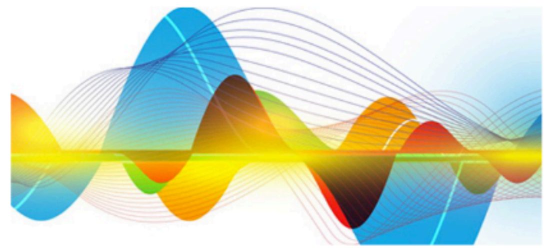
- A naive DFT costs $\mathcal{O}(N^2)$
- Using the FFT, the cost can be reduced to $\mathcal{O}(N \log_2 N)$.

Applications Relying on Parallel FFTs

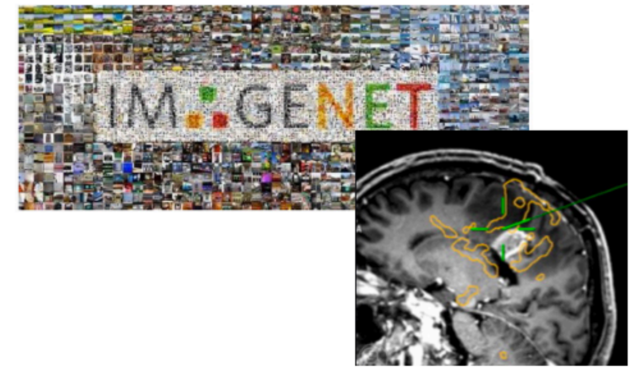
Cosmology
ECP **ExaSky - HACC**

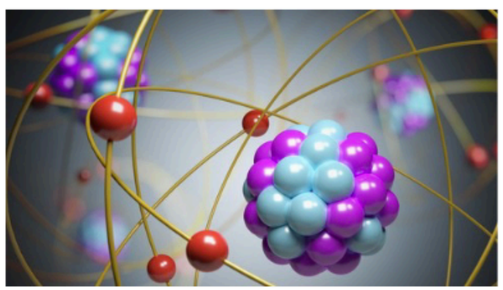


Signal processing,
***ECP* WARPX**

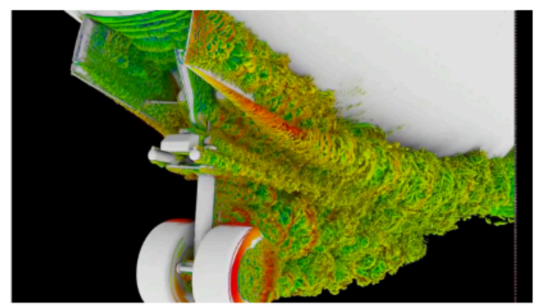


Deep Learning

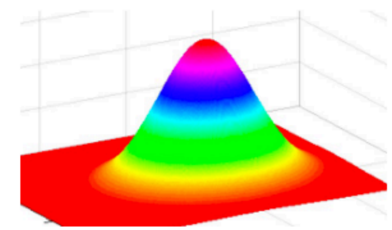




Molecular Dynamics
***ECP* EXAALT**



Particle Simulations
***ECP* CoPa / Cabana**



PDE solutions, **MASSIF**

Figure: Several applications from the U.S. ECP project heavily rely on FFTs.

Examples of FFT use

- **Spectral methods to solve PDEs**

Δ u(x, y) = f(x, y),
where f is periodic in x and y, i.e., f(x + 2π, y) = f(x, y + 2π)

Take Fourier transform **F** on both sides, so

F Δ u(x, y) = F f(x, y)

=> $-(j^2+k^2)\,(F\,u)_{j,k} = (F\,f)_{j,k}$

=> $(F\,u)_{j,k} = -1/(j^2+k^2)\ \ (F\,f)_{j,k}$

=> $u = F^{-1}\,(-\,1/(j^2+k^2)$.* F f)

Examples of FFT use

- Compression

```
>> A = imread( 'Fourier' , 'jpeg' );
>> imshow(A);
>> [nx,ny,nz] = size(A)
   512    417    3

>> FA = fft( A );
>> thresh=0.01*max(abs(FA(:))); ind=abs(FA)>thresh; cFA=FA.*ind;
>> count=nx*ny*nz-sum(ind(:)); percent = 100-count/(nx*ny*nz)*100
   percent = 8.59

>> Afilt = ifft( cFA );
>> imshow(uint8(Afilt));
```

Examples of FFT use

- Convolution

Convolutions f * g of images f and filers g can be accelerated through FFT, as shown by the following equality, consequence of the convolution theorem:

$$f * g = FFT^{-1} \left[FFT(f) .* FFT(g) \right],$$

where .* is the Hadamard (component-wise) product, following the '.*' Matlab notation

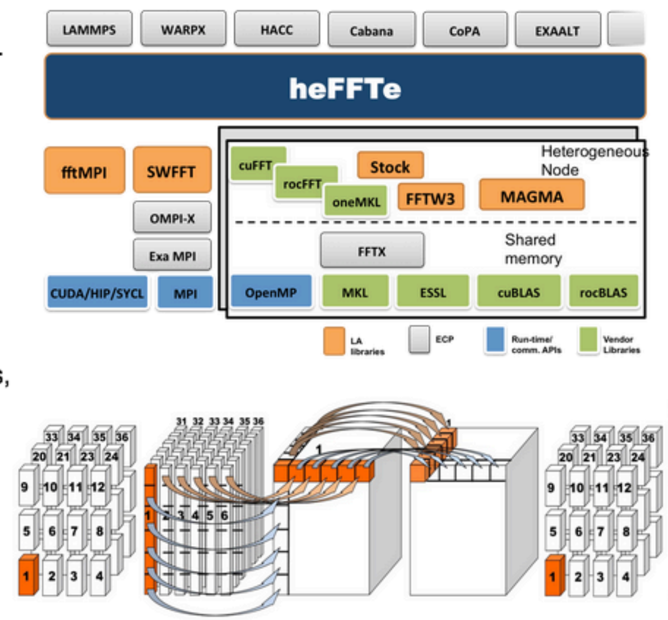
```
>> m = 100;            n = 50;
>> f = rand(m, 1);     g = rand(n, 1);

>> F = fft(f, m+n-1); G = fft(g, m+n-1);
>> norm( conv(f, g)  -  ifft( F .* G))
    ans =
    5.769457742102946e-14
```

heFFTe
Highly Efficient FFTs for Exascale

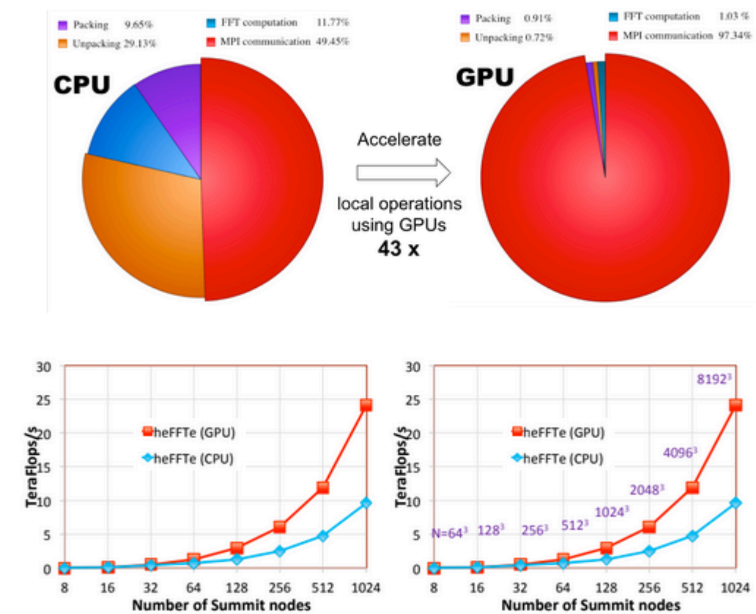
THEN

- The fast Fourier transform (FFT) is used in many domain applications - more than a dozen ECP applications use FFTs in their codes;
- State-of-the-art libraries like FFTW were no longer actively developed for emerging platforms;
- No GPU support for distributed multi-dimensional FFTs at the time;
- Some ECP application constructed their own FFTs directly in applications, e.g., fftMPI for LAMMPS and SWFFT for HACC;
- Features and application-specific needs were not supported uniformly;
- The goal was to leverage the existing FFT capabilities and build a sustainable FFT library for Exascale.



NOW

- GPUs (e.g., V100 on Summit) accelerate local FFT computations more than 40 x
- heFFTe supports multiple backends for Nvidia GPUs, AMD GPUs, Intel GPUs and multicore CPUs;
- Novel features such as Batched 2-D and 3-D FFTs
- Support FFT convolution, sine, and cosine transforms;
- Support for real and complex FFTs, multiple precisions and approximate FFT;
- Very good strong and weak scalability (Figure on right);
- FFT benchmark for MPI collectives and other FFT libraries.



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heFFTe
Highly Efficient FFTs for Exascale

THEN

- There were many FFT libraries but no GPU support for large-scale distributed systems
- HeFFTe did not exist and goal was to add GPU support while leveraging and extending existing capabilities
  - Added quickly support for NVIDIA GPUs to cover fftMPI and SWFFT functionalities
  - Still explored design choices on language, precisions, versions, how to add other architectures, how to leverage other FFTs, etc.
  - Decided to move from LAPACK/MAGMA software engineering and develop in C++ to easily handle data types, parameterizations, architectures, and configurable use of multiple FFT libraries

NOW

- C++ library with backends for Nvidia GPUs, AMD GPUs, Intel GPUs, and multicore CPUs (with framework to easily add others, if needed)
- Backends are used not just for architectures but also for leveraging 3rd party FFT libraries (e.g., Stock, FFTW3, MKL, oneMKL, cuFFT, rocFFT)
- Support for multiple precisions, real and complex
- Support for many FFT-based functionalities

heFFTe

CURRENT DEVELOPMENTS

- Amongst the very few parallel FFT libraries that support GPUs, heFFTe provides unique functionalities that cover a large number of features from the state-of-the-art, making it ubiquitous for a wide range of applications

	Library	Pencil Decomp	Brick Decomp	Slab Decomp	Transpose Reshape	Stride Reshape	R2C Transform	Single precision	Mixed precision	Multiple backends	Nonblocking All-to-All
CPU	FFTW3	✓				✓	✓	✓			
CPU	FFTMPI	✓	✓		✓			✓		✓	
CPU	2DECOMP	✓				✓	✓				
CPU	SWFFT		✓		✓						
CPU	PFFT	✓			✓		✓				
CPU	P3DFFT	✓		✓	✓		✓	✓			✓
GPU	AccFFT	✓			✓	✓	✓	✓		✓	
GPU	FFTE	✓		✓	✓		✓	✓			
GPU	heFFTe	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓

heFFTe

Highly Efficient FFT for Exascale (heFFTe). Scalable, high-performance multidimensional FFTs; Flexible; User-friendly interfaces (C++/C/Fortran/python); Examples & benchmarks; Testing; Modified BSD license.

Capabilities:

- Multidimensional FFTs
- C2C, R2C, C2R
- DCS, DST, and convolution
- Batched FFTs
- Support flexible user data layouts
- Leverage and build on existing **FFT capabilities** through multiple backends

Pre-exascale environment:

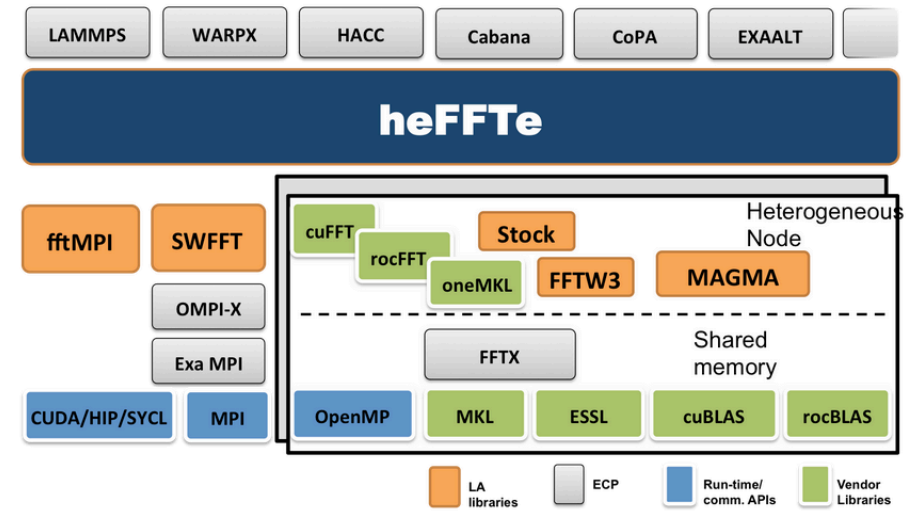
- **Summit @ OLCF (Nvidia GPUs)**
- **Crusher / Frontier (AMD GPUs), and others**
- **Florentia / Aurora (Intel GPU)**

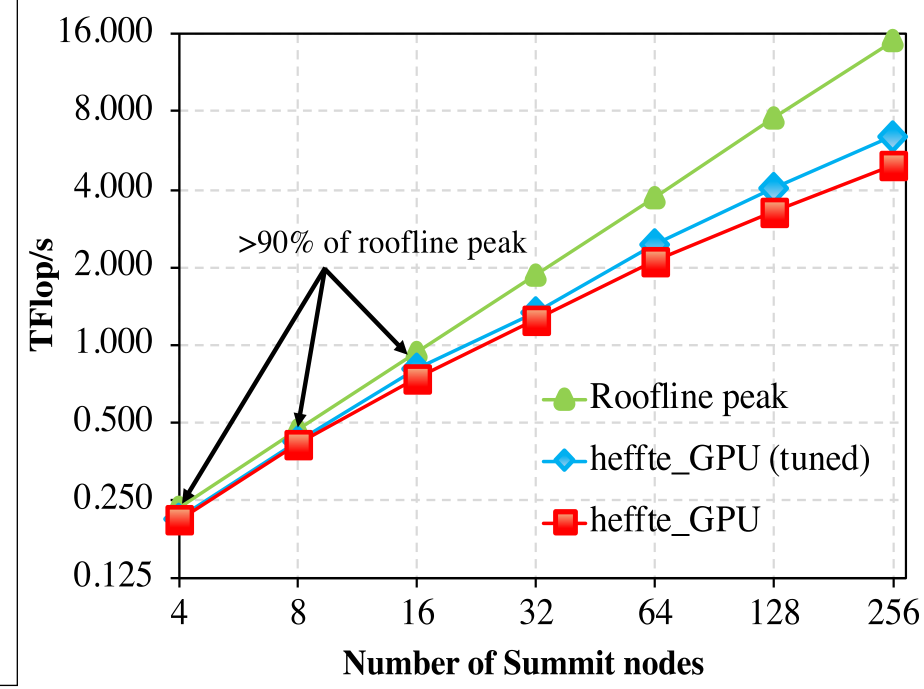
Current status:

- **heFFTe 2.3** with support for CPUs, Nvidia GPUs, AMD GPUs, and Intel GPUs
- Very good strong and weak scaling, reaching up to 90% of roofline peak

Open Source Software

- **spack** installation and integration in xSDK
- Homepage: http://icl.utk.edu/fft/
  Repository: https://bitbucket.org/icl/heffte/





heFFTe Availability

Availability

- http://icl.utk.edu/fft/ download, documentation
- https://bitbucket.org/icl/heffte Git repo
- Latest release is heFFTe 2.3

Support

- Linux
- CPU, Nvidia GPUs, AMD GPUs, Intel GPUs
- CUDA >= 7.0; recommend latest CUDA
- CUDA architecture >= 2.0 (Fermi, Kepler, Maxwell, Pascal, Volta, Ampere, Hopper)
- 1D FFTs: Stock, cuFFT, FFTW, oneMKL, IBM ESSL, rocFFT, ...

Installation options

1. Cmake
   - `heffte> mkdir build && cd build`

   To install GPU-enabled heFFTe, e.g., for NVIDIA GPUs:
   - `heffte/build> cmake –DHeffte_ENABLE_CUDA=ON ..`
   - `heffte/build> make –j && make install`
2. Spack
   - `Part of xSDK and E4S`
   - `spack install heffte`
3. Dependencies are 1D FFTs (open source or vendor) libraries

   `Stock, CUFFT (NVIDIA), oneMKL (Intel), FFTW3, ROCFFT (AMD)`

For further detail see: https://bitbucket.org/icl/heffte/src/master/doxygen/

Installation options ...

Typical CMake build command:

```
cmake \
    -D CMAKE_BUILD_TYPE=Release \
    -D BUILD_SHARED_LIBS=ON      \
    -D CMAKE_INSTALL_PREFIX=<path-for-installation> \
    -D Heffte_ENABLE_AVX=ON \
    -D Heffte_ENABLE_FFTW=ON \
    -D FFTW_ROOT=<path-to-fftw3-installation> \
    -D Heffte_ENABLE_CUDA=ON \
    -D CUDA_TOOLKIT_ROOT_DIR=<path-to-cuda-installation> \
    <path-to-heffte-source-code>
```

Additional heFFTe options:

```
Heffte_ENABLE_ROCM=<ON/OFF>       (enable the rocFFT backend)
Heffte_ENABLE_ONEAPI=<ON/OFF>     (enable the oneMKL backend)
Heffte_ENABLE_MKL=<ON/OFF>        (enable the MKL backend)
Heffte_ENABLE_AVX512=<ON/OFF>     (enable AVX512 instructions in the stock backend)
MKL_ROOT=<path>                   (path to the MKL folder)
Heffte_ENABLE_DOXYGEN=<ON/OFF>    (build the documentation)
Heffte_ENABLE_TRACING=<ON/OFF>    (enable the even logging engine)
```

Additional language interfaces and helper methods:

```
-D Heffte_ENABLE_PYTHON=<ON/OFF>   (configure the Python module)
-D Heffte_ENABLE_FORTRAN=<ON/OFF>  (build the Fortran modules)
-D Heffte_ENABLE_SWIG=<ON/OFF>     (generate new Fortrans source files)
-D Heffte_ENABLE_MAGMA=<ON/OFF>    (link to MAGMA for helper methods)
```

GPU-Aware MPI

Different implementations of MPI can provide GPU-Aware capabilities, where data can be send/received directly in GPU memory. OpenMPI provided CUDA aware capabilities if compiled with the corresponding options, e.g., see CUDA-Aware OpenMPI. Both CUDA and ROCm support such API; however, the specific implementation available to the user may not be available for various reasons, e.g., insufficient hardware support. HeFFTe can be compiled without GPU-Aware capabilities with the CMake option:

```
-D Heffte_DISABLE_GPU_AWARE_MPI=ON
```

Note: Only one of the GPU backends can be enabled (CUDA, ROCM, or ONEAPI) since the three backends operate with arrays allocated in GPU device memory (or alternatively shared/managed memory). By default when using either GPU backend, heFFTe assumes that the MPI implementation is GPU-Aware, see the next section.

```
-D Heffte_ENABLE_CUDA=ON
-D CUDA_TOOLKIT_ROOT_DIR=<path-to-cuda-installation>
```

```
-D CMAKE_CXX_COMPILER=hipcc
-D Heffte_ENABLE_ROCM=ON
```

```
-D CMAKE_CXX_COMPILER=dpcpp
-D Heffte_ENABLE_ONEAPI=ON
-D Heffte_ONEMKL_ROOT=<path-to-onemkl-installation>
```

For further detail see: https://bitbucket.org/icl/heffte/src/master/doxygen/

heFFTe backends

Single-Device FFT Libraries

Library	Language	Developer	GPU support	Open Source	2D & 3D support	Stride data support
CUFFT	C	NVIDIA	✓		✓	✓
ESSL	C++	IBM			✓	✓
FFTE	Fortran	Riken		✓	✓	✓
FFTPACK	Fortran	NCAR		✓		
FFTS	C	U. Waikato		✓		
FFTW3	C	MIT		✓	✓	✓
FFTX	C	LBNL	✓	✓	✓	✓
KFR	C++	KFR		✓		✓
KISS	C++	Sandia		✓	✓	✓
OneMKL	C	Intel	✓		✓	✓
ROCM	C++	AMD	✓	✓	✓	✓
VkFFT	C++	D. Tolmachev	✓	✓	✓	✓

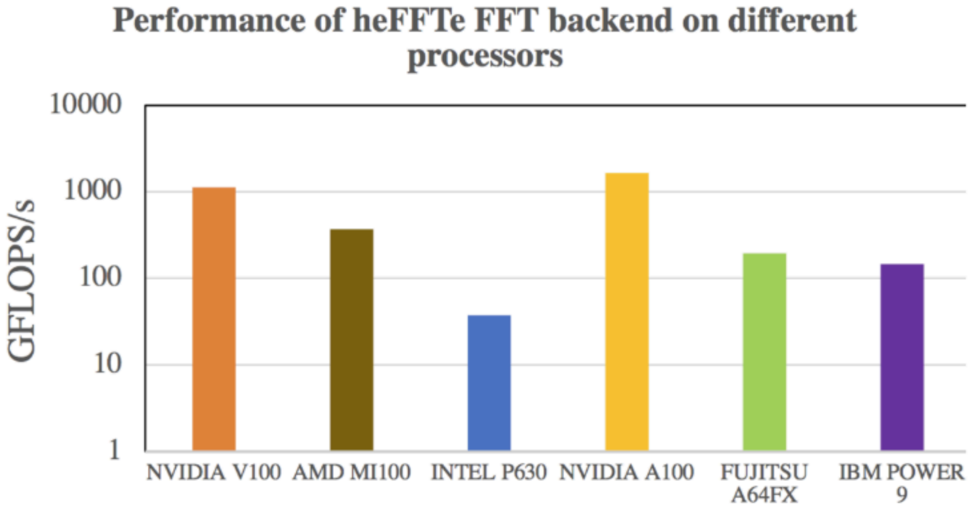
Figure: State-of-the-art of FFT libraries targeting a single-device unit.

Ref.: Interim Report on Benchmarking FFT Libraries on High Performance Systems
Ayala et al., ICL Tech Report 2021.

heFFTe backends

Single-Device FFT Comparison

- Useful when input data is small or can be batched.
- heFFTe provides portability to run FFT experiment on different devices.



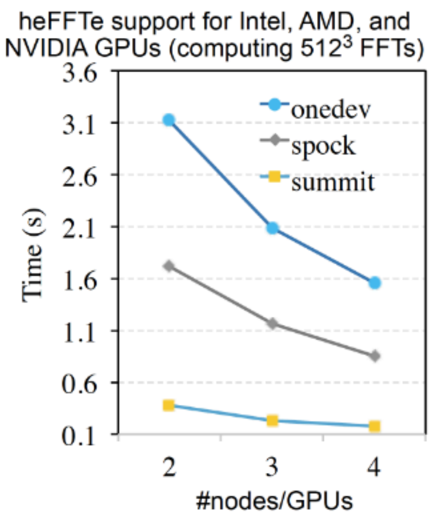


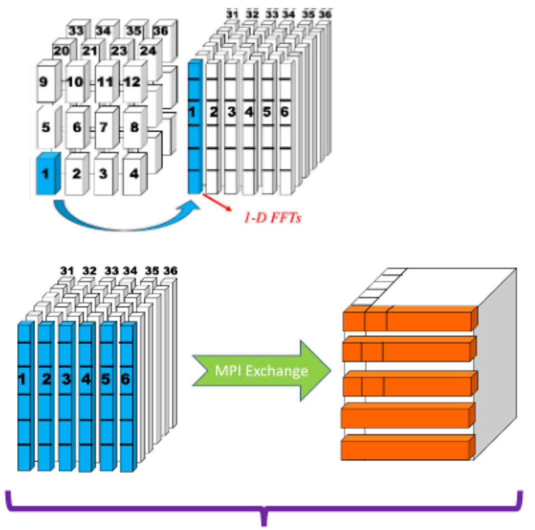
Figure: Comparison of single-device performance for a 512^3 FFT.

heFFTe implementation

Parallel FFT implementation

Algorithm 1 Parallel 3-D FFT computation on GPUs

Input: 3-D array, processor grids: P_{in}, P_{out}
Transfer data from P_{in} to a pencil or slab grid
Define processor grids (MPI groups) for each direction
for $r \leftarrow 1, \cdots, n_{\text{exchanges}}$ **do**
    Compute local 1-D or 2-D FFTs on the GPUs
    Pack data in contiguous memory
    for P on my MPI group **do**
        Transfer computed data to neighbor processes
    end for
    Unpack data in contiguous memory
end for
Transfer data from the pencil or slab grid to P_{out}

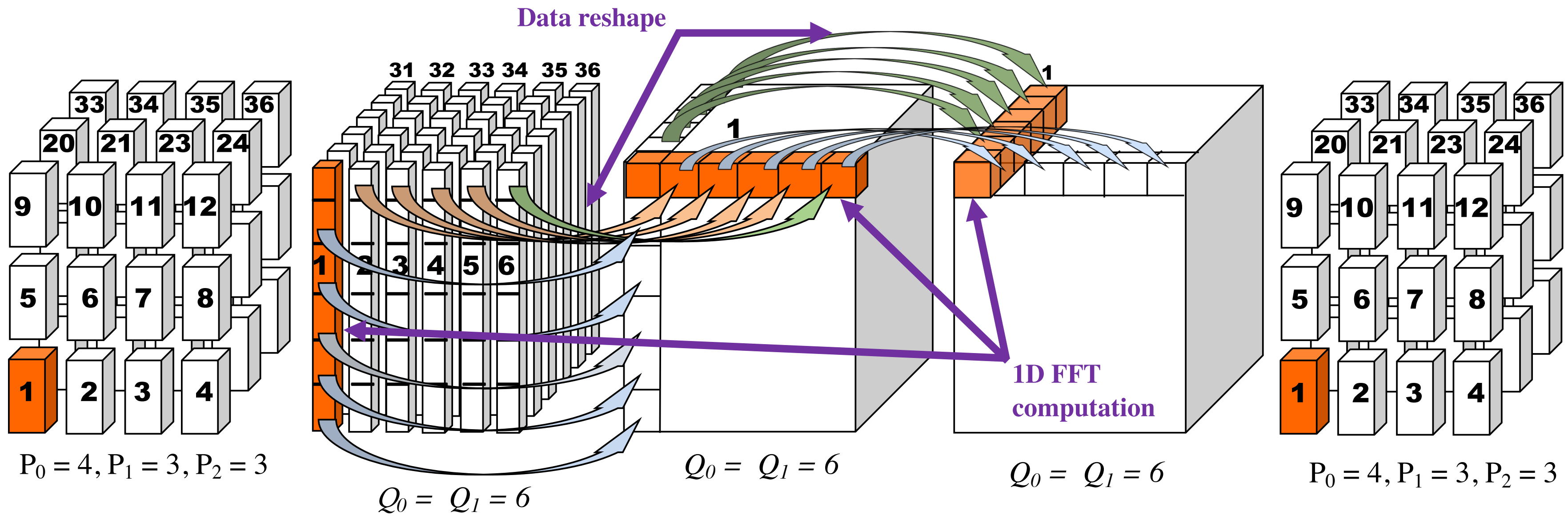


These 3 tasks can be replaced by 1 via MPI_Alltoallw

Communication can be accelerated by enabling Mixed-Precision, c.f., Advances in Mixed Precision Algorithms: 2021 Edition. *Abdelfattah et al., LLNL-TR-825909*

heFFTe Overview

Support flexible user data layout input/output (pencils/cubes/slabs)



2-D and 3-D FFTs
C2C, R2C, and C2R transformations
DCS, DST, and convolution
Batched FFTs
CPU and GPUs (Nvidia, AMD, and Intel)
Multi-precision FFTs

heFFTe Strong Scalability – Summit

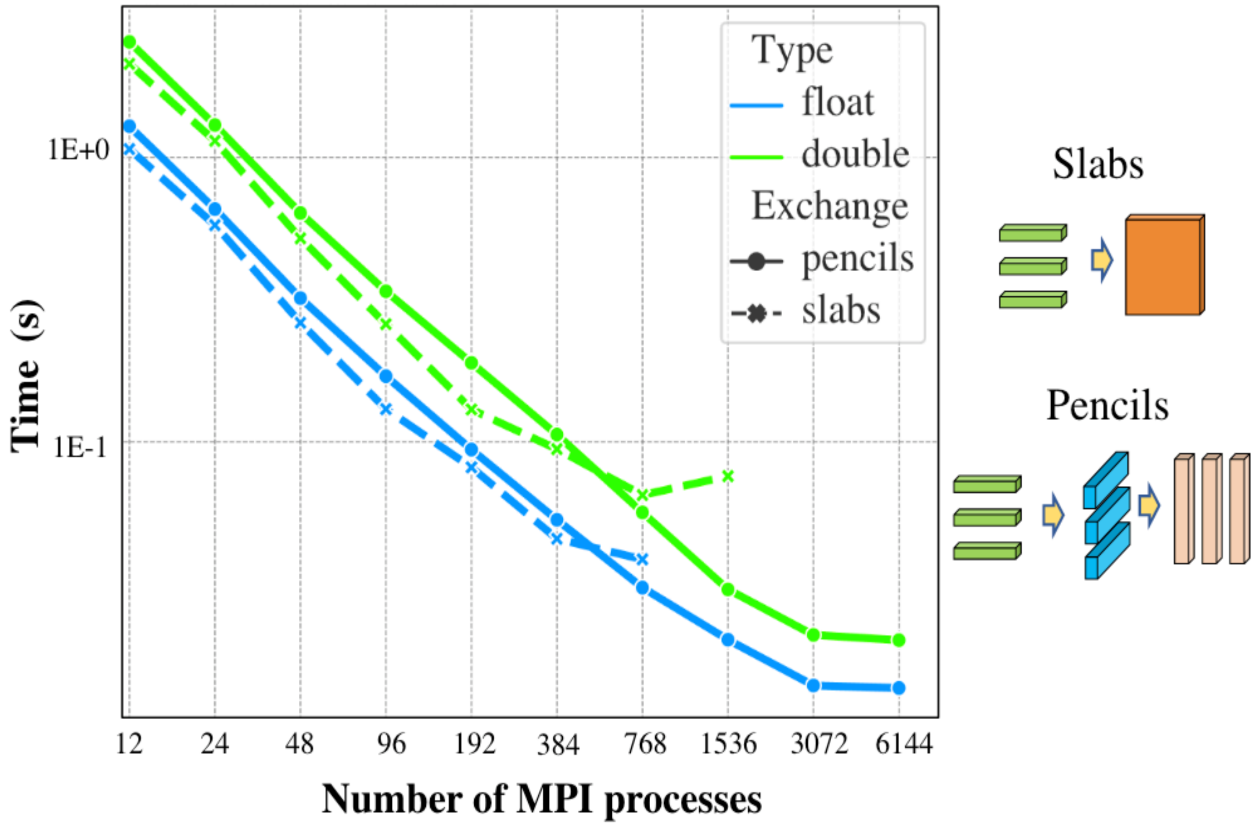
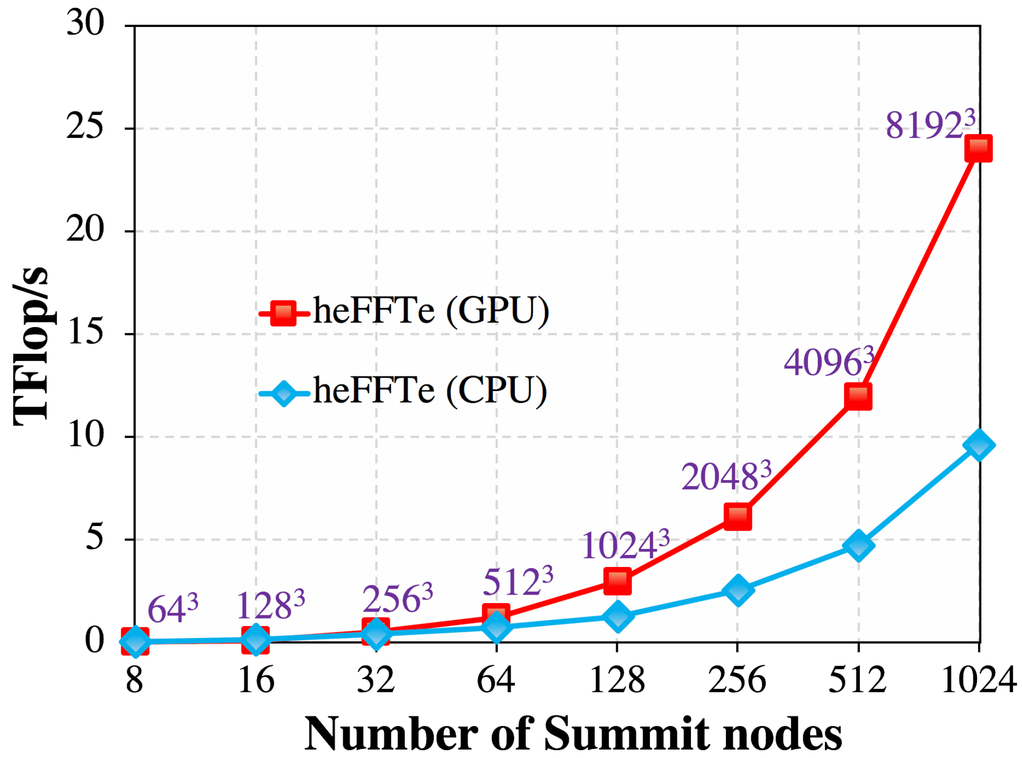
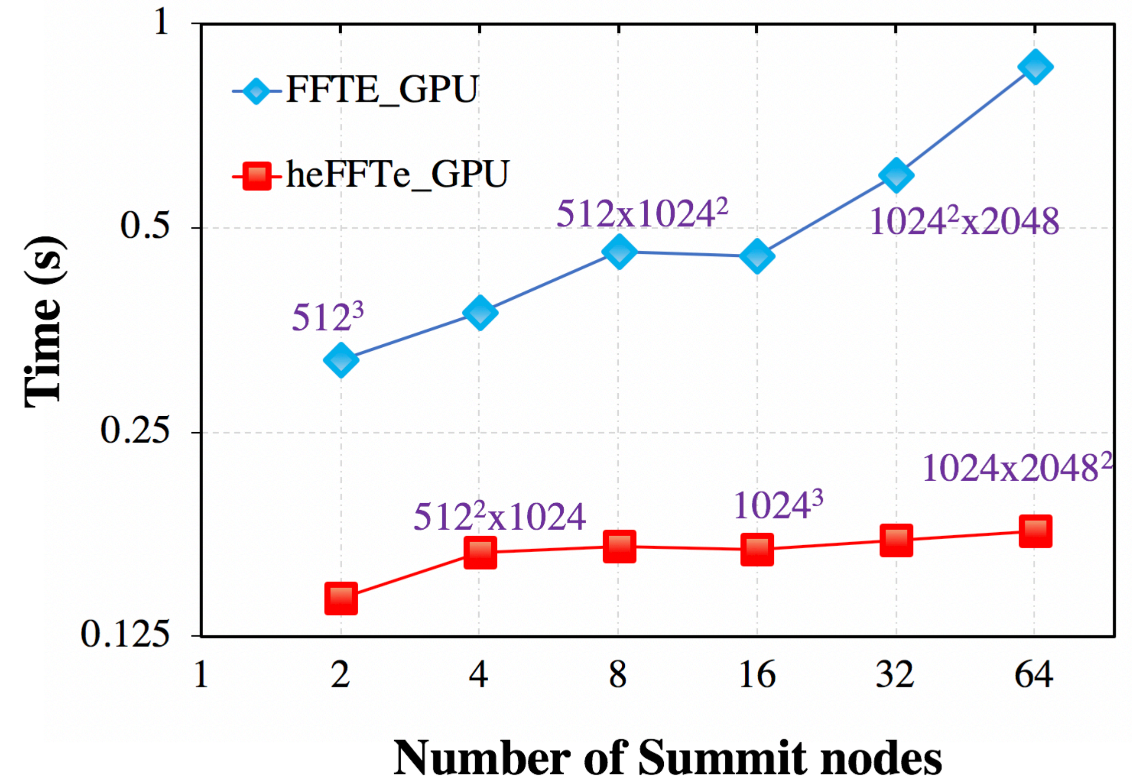


Fig. 6. Comparison of pencil and slab decompositions for strong scaling of a 3-D FFT of size 1024^3. Using *heFFTe* with cuFFT backend, 6 MPI processes (1 MPI processes per GPU-V100) per node, and single-precision complex data.

heFFTe Weak Scalability

- 2x speedup over state-of-the-art CPU libraries, FFTMPI, SWFFT
- 2x speedup over GPU library FFTE.

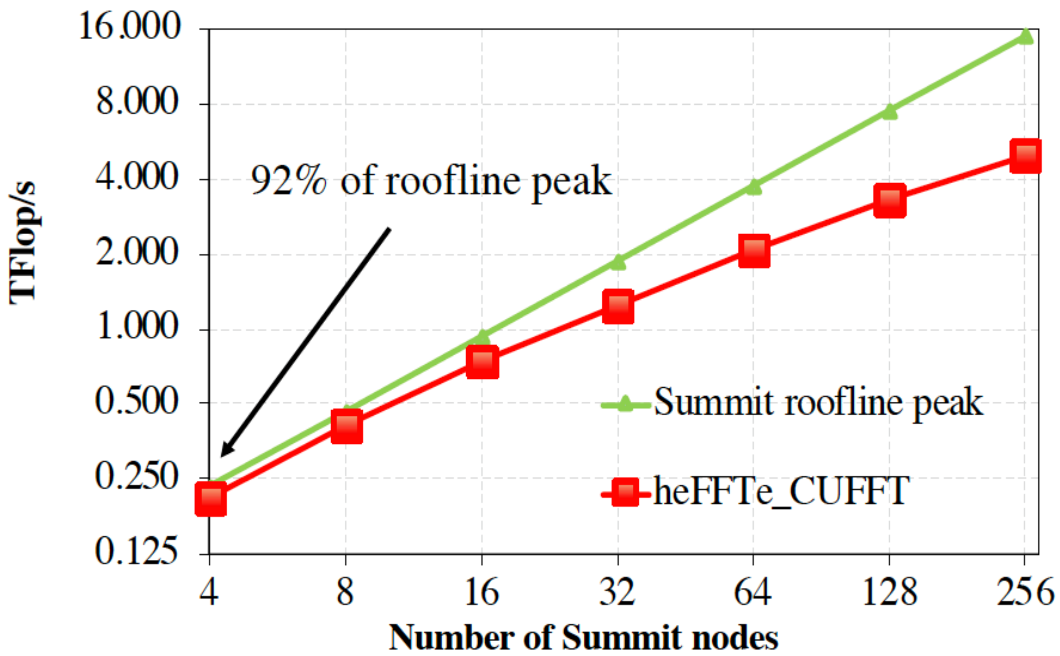


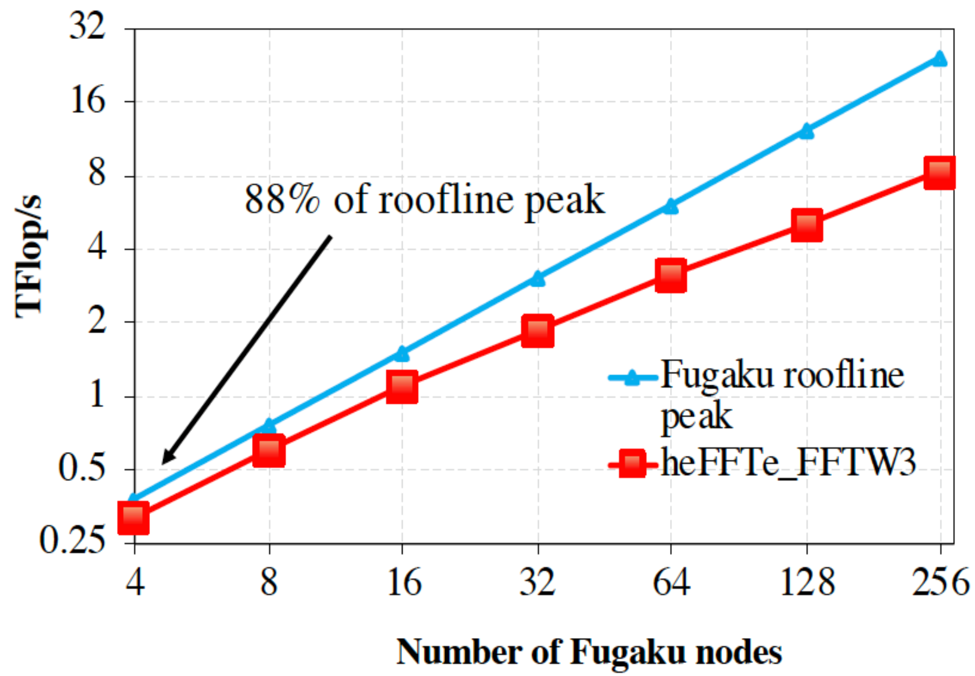


Forward and backward FFT on a Complex 3D array in double precision.

Using 6,144 NVIDA V100 GPUs (6/node) and 40,960 IBM Power 9 cores (40/node).

heFFTe Roofline analysis





Roof-line performance model – heFFTe performance on a 3-D FFT of size 1024^3 using 6 MPI/node, 1 GPU-Volta100 per MPI for Summit, and 48 A64FX per node on Fugaku.

FIBER FFT benchmark (https://github.com/icl-utk-edu/fiber)

Parallel FFT Libraries

Library	Developer	Language	CPU Backend	GPU Backend	Real-to-Complex	Slab Decomp.	Brick Decomp.
2DECOMP&FFT	NAG	Fortran	FFTW3, ESSL	-	✓	✓	
AccFFT	Georgia Tech	C++	FFTW3	CUFFT	✓		
Cluster FFT	Intel	Fortran	MKL	-			
CRAFFT	Cray	Fortran	FFTW3	-	✓		
cuFFTMp	NVIDIA	C	-	CUFFT	✓		
FFTE	U. Tsukuba / Riken	Fortran	FFTE	CUFFT	✓	✓	
fftMPI	Sandia	C++	FFTW3, MKL, KISS	-			✓
FFTW3	MIT	C	FFTW3	-	✓	✓	
heFFTe	ICL - UTK	C++	FFTW3, MKL, Stock	CUFFT, ROCM, OneMKL	✓	✓	✓
nb3DFFT	RWTH Aachen	Fortran	ESSL	-	✓		
P3DFFT	UC San Diego	C++	FFTW3	-	✓	✓	
spFFT	ETH	C++	FFTW3	CUFFT, ROCM	✓	✓	
SWFFT	Argonne	C++	FFTW3	-			✓

Figure: State-of-the-art of FFT libraries targeting parallel systems.

Ref.: Interim Report on Benchmarking FFT Libraries on High Performance Systems
Ayala et al., ICL Tech Report 2021.

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FIBER FFT benchmark (https://github.com/icl-utk-edu/fiber)

Scaling FFT on top Supercomputers

- Similar behavior is observed for state-of-the-art FFT libraries.

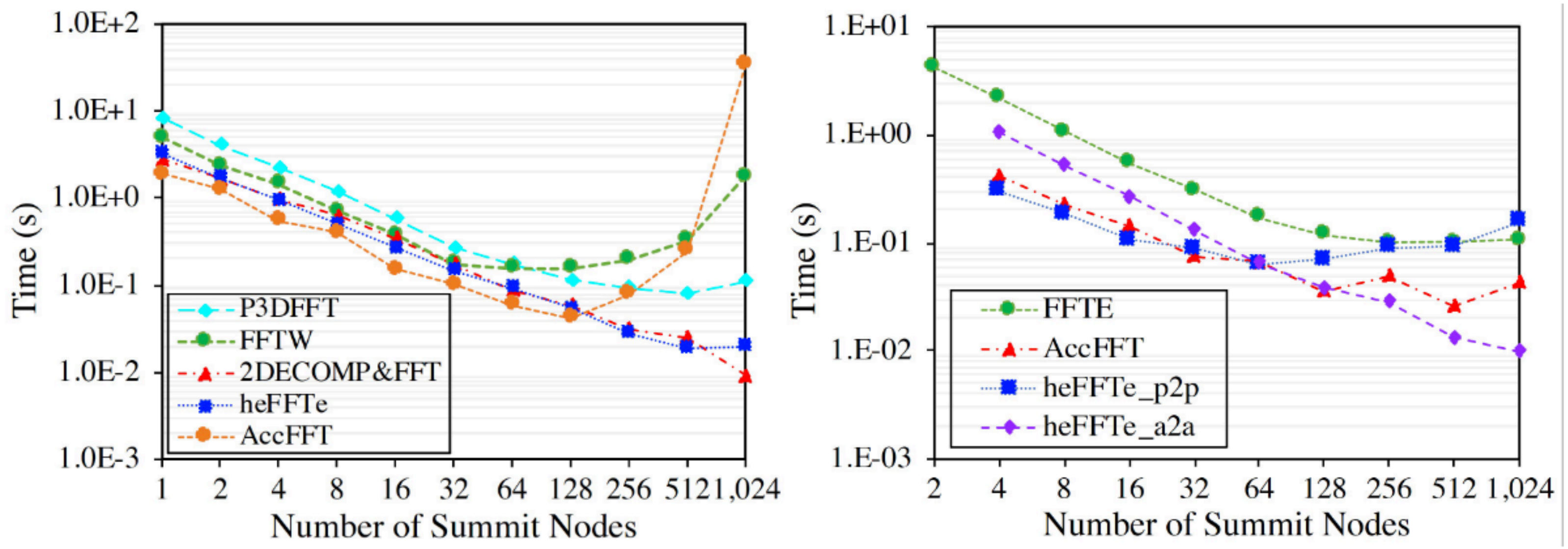
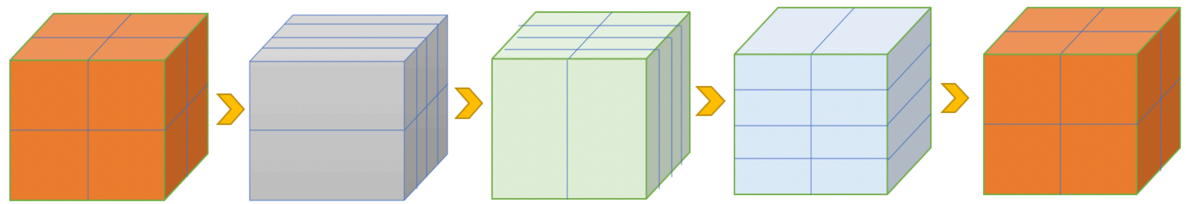


Figure: Strong Scalability on 32K Power9 cores for CPU-based libraries (left), and 4096 V-100 for GPU-based libraries (right).

Ref.: FFT Benchmark Performance Experiments on Systems Targeting Exascale. *Ayala et al., ICL Tech Report 2022.*

heFFTe API

1. Definition of input/output processors grids (normally provided by users):



Input processor grid

```
std::array<int,3>  proc_i
```

Output processor grid

```
std::array<int,3>  proc_o
```

If user only has their MPI communicator and number of processors, we provide a routine to generate above grid of processors:

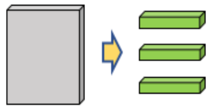
```
heffte ::proc_setup_min_surface(my_mpi_comm, nprocs);
```

2. Distribute data among processors using ***box3D*** *objects at input and output :*

```
std::vector<box3d<index>> inboxes   = heffte::split_world(world, proc_i);
std::vector<box3d<index>> outboxes = heffte::split_world(world, proc_o);
```

3. Select type of FFT intermediate reshape, via one of the following flags:

--slabs



--pencils

heFFTe API

4. Create FFT plan:

```
auto fft = heffte :: make_fft3d<backend_tag>(inboxes[me], outboxes[me], my_mpi_comm, options);
```

backend_tag: Corresponds to the FFT library for local computations (e.g., FFTW3, CUFFT, MKL)
options: Contains information from flags set by users

5. Compute an in-place parallel 3D FFT:

```
std::complex<my_precision_type> *output_array;

fft.forward(output_array, output_array, workspace.data(), scale::full);
fft.backward(output_array, output_array, workspace.data() );
```

workspace.data(): Can be given by the user or calculated by heFFTe for stablishing a computation workspace
scale::… : The scaling options are *full*, *none* and *symmetric*

6. Tracing functionality can be added within your code to generate a runtime trace for performance analysis.

```
heffte::add_trace(“Initiating tracing”);

    ---Code to be traced ---

heffte::add_trace(“Ending tracing”);
```

heFFTe API

Test drivers / examples / benchmarks

Directory benchmarks provides speed3d_c2c, speed3d_r2c, speed3d_r2r, and convolution benchmarks

```
Usage:
mpirun -np x <bench_executable> <backend> <precision> <size-x> <size-y> <size-z> <args>

       backend is the 1-D FFT library
       precision is either float or double
         use float-long or double-long to enable 64-bit indexing
       size-x/y/z are the 3D array dimensions
       args is a set of optional arguments that define algorithmic tweaks and variations
        -reorder: reorder the elements of the arrays so that each 1-D FFT will use contiguous data
        -no-reorder: some of the 1-D will be strided (non contiguous)
        -a2a: use MPI_Alltoall() communication method
        -a2av: use MPI_Alltoallv() communication method (default)
        -p2p: use MPI_Send() and MPI_Irecv() communication methods
        -p2p_pl: use MPI_Isend() and MPI_Irecv() communication methods
        -no-gpu-aware: move the data to the cpu before doing gpu operations (gpu backends only)
        -pencils: use pencil reshape logic
        -slabs: use slab reshape logic
        -io_pencils: if input and output proc grids are pencils, useful for comparison with other libraries
        -ingrid x y z: specifies the processor grid to use in the input, x y z must be integers
        -outgrid x y z: specifies the processor grid to use in the output, x y z must be integers
        -subcomm num_ranks: specifies the number of ranks to use in intermediate reshapes
        -batch batch_size: specifies the size of the batch to use in the benchmark
        -r2c_dir dir: specifies the r2c direction for the r2c tests, dir must be 0 1 or 2
        -mps: for the cufft backend and multiple gpus, associate the mpi ranks with different cuda devices
        -nX: number of times to repeat the run, accepted variants are -n5 (default), -n10, -n50

Examples:
   mpirun -np  4  speed3d_r2r  fftw-cos  double 128 128 128 -p2p
   mpirun -np  8  speed3d_r2r  cufft-cos float  256 256 256
   mpirun -np 12  speed3d_r2r  fftw-sin  double 512 512 512 -slabs

   mpirun -np  4  speed3d_c2c  fftw  double 128 128 128 -no-reorder
   mpirun -np  8  speed3d_c2c  cufft float  256 256 256
   mpirun -np 12  speed3d_r2c  fftw  double 512 512 512 -p2p -slabs
```

heFFTe API

Test drivers / examples / benchmarks

/* mpirun */
mpirun -np 2 speed3d_c2c fftw float 4 2 2 –a2a

```
-----------------------------------------------------------------------------------------------------------------
                                              Testing HEFFTE library
-----------------------------------------------------------------------------------------------------------------
Test summary:
-------------
        Computation of 3D FFT
        1 forward and 1 backward 3D-FFTs on 2 procs on a 4x2x2 grid
        1D FFT library       : FFTW3
        Precision            : SINGLE
        Comunication type    : ALL2ALL
        Scaling after forward: YES
Memory comsuption:
------------------
        Memory usage (per-proc) for FFT grid   = 6.1e-05 MB
        Memory usage (per-proc) by FFT library = 0.00076 MB
        Total memory comsuption                = 0.0015 MB
Processor grids for FFT stages:
-------------------------------
        Initial grid    1st-direction   2nd-direction   3rd-direction
            2 1 1           1 1 2          2 1 1           2 1 1
                                                        (Final grid)

-----------------------------------------------------------------------------------------------------------------
 ID      np        nx       ny       nz        Gflops/s       One FFT (s)    Initialisation (s)       Max Error
_3D_      2         4        2        2        0.06804         3.26e-06          0.001659          6.917283e-08
-----------------------------------------------------------------------------------------------------------------
```

heFFTe API

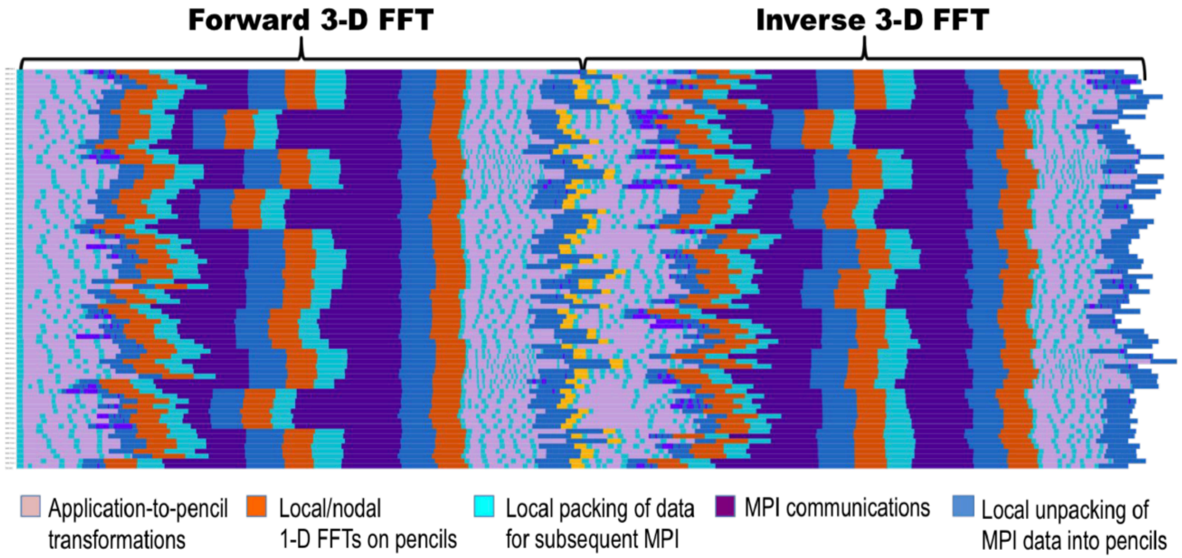
Test drivers / examples / benchmarks

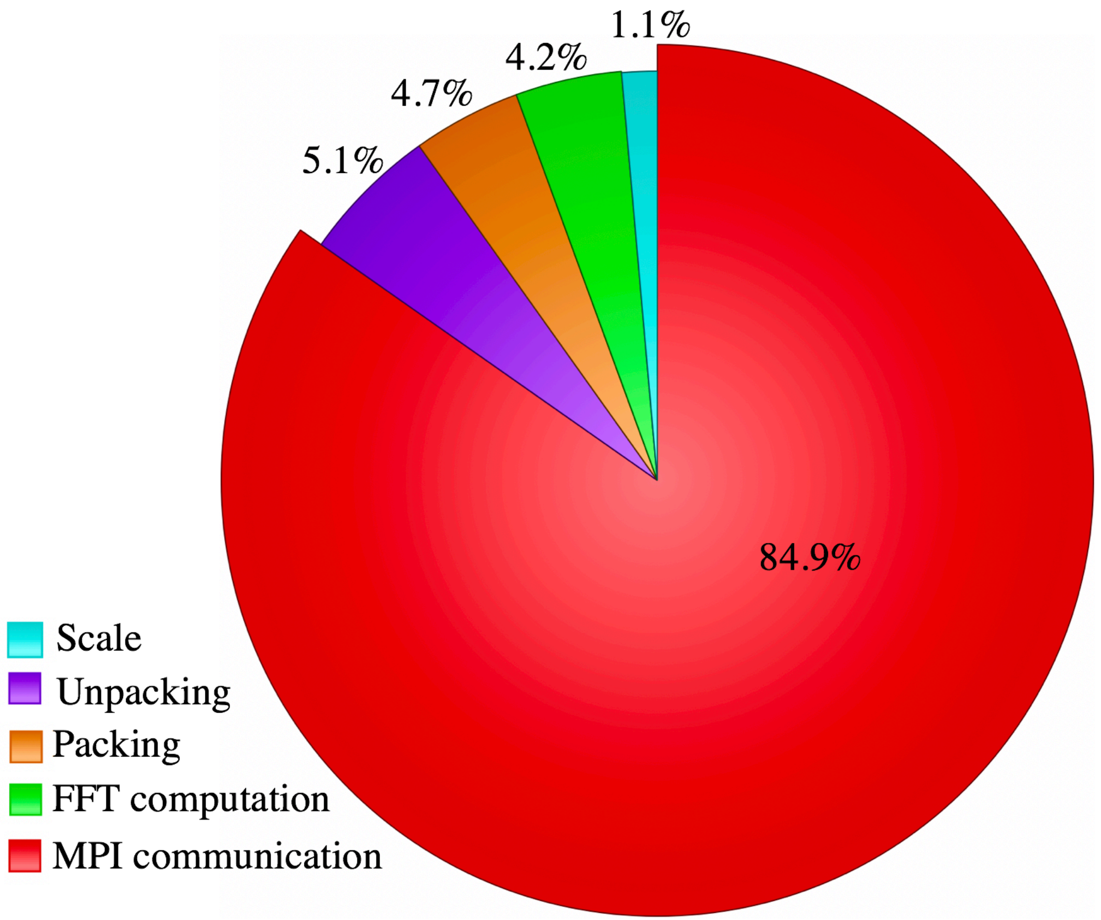
Should you have questions about the use of flags, please refer to `flags.md` for detailed information. For systems, such as Summit supercomputer, which support execution with `jsrun` by default, follow the examples:

```
jsrun  -n1280 -a1 -c1 -r40 ./speed3d_r2c fftw double 1024 256 512 -pencils
jsrun --smpiargs="-gpu" -n192 -a1 -c1 -g1 -r6 ./speed3d_c2c cufft double 1024 1024 1024 -p2p -reorder
```

heFFTe tracing tools

- We provide our own tracing function and scripts for direct link with vendor profilers.






```
heffte_tracing("start");
  heffte_execute(fft, work, work, FORWARD);
  heffte_execute(fft, work, work, BACKWARD);
heffte_tracing("stop"));
```

```
mpirun -np 2 ./vampir_trace.sh ./heffte_exec -my_options ...
```

Integration to ECP EXAALT

LAMMPS Rhodopsin Benchmark using heFFTe

- Molecular dynamics apps heavily rely on FFTs, and often have their own parallel FFT implementation (e.g., fftMPI, SWFFT).
- Using heFFTe real-to-complex accelerates LAMMPS Kspace kernel around 1.76×.

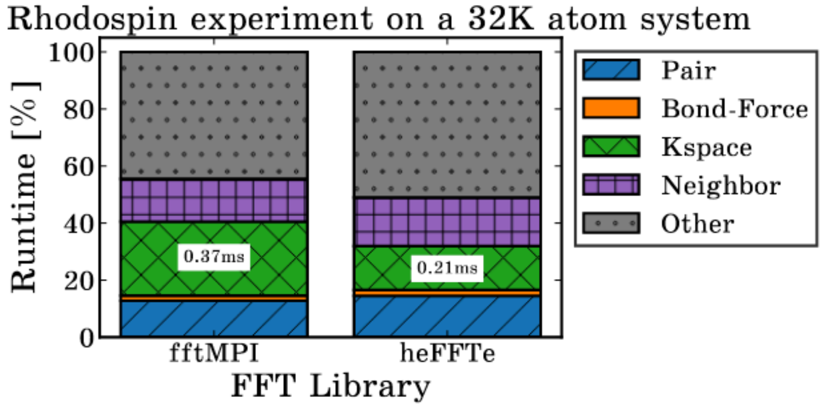


Figure: Breakdown for the LAMMPS Rhodopsin experiment. Using 32 Summit nodes, 6 V-100 GPUs per node, and 1 MPI per GPU.

Ref.: Performance Analysis of Parallel FFT on Large Multi-GPU Systems. *Ayala et al., IEEE IPDPS 2022.*

Integration to ECP EXAALT

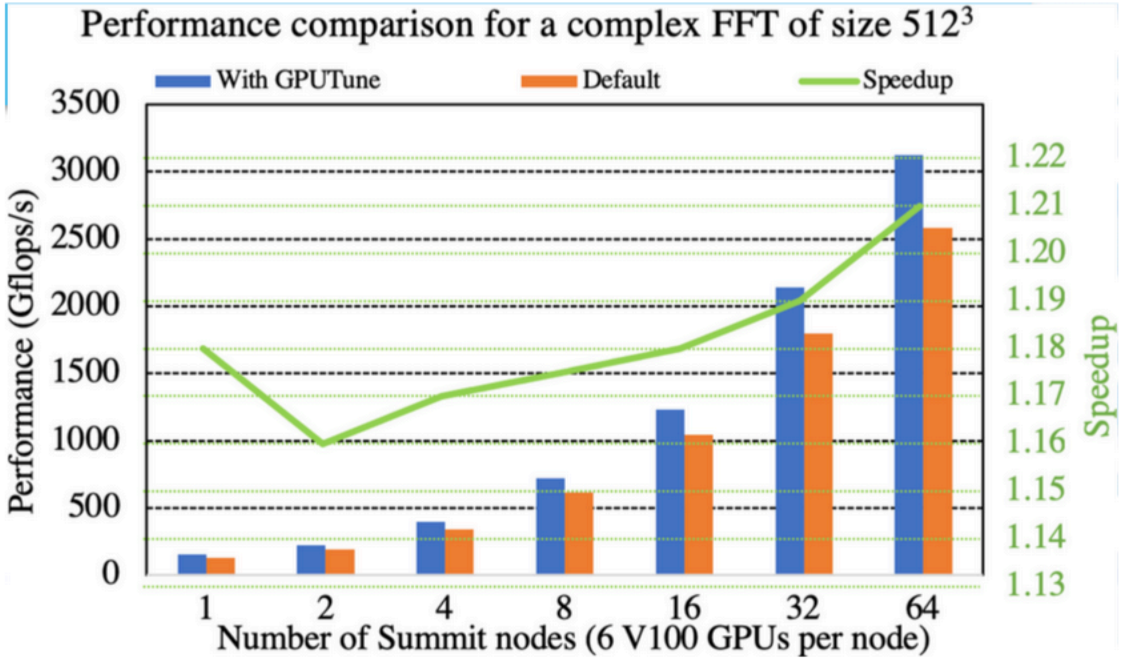
```
FFT3d::FFT3d(LAMMPS *lmp, MPI_Comm comm, int nfast, int nmid, int nslow,
             int in_ilo, int in_ihi, int in_jlo, int in_jhi,
             int in_klo, int in_khi,
             int out_ilo, int out_ihi, int out_jlo, int out_jhi,
             int out_klo, int out_khi,
             int scaled, int permute, int *nbuf, int usecollective) : Pointers(lmp)
{
  #ifndef HEFFTE
  plan = fft_3d_create_plan(comm,nfast,nmid,nslow,
                            in_ilo,in_ihi,in_jlo,in_jhi,in_klo,in_khi,
                            out_ilo,out_ihi,out_jlo,out_jhi,out_klo,out_khi,
                            scaled,permute,nbuf,usecollective);
  if (plan == nullptr) error->one(FLERR,"Could not create 3d FFT plan");
  #else
  heffte::plan_options options = heffte::default_options<heffte_backend>();
  options.algorithm = (usecollective == 0) ?
                        heffte::reshape_algorithm::p2p_plined
                      : heffte::reshape_algorithm::alltoallv;
  options.use_reorder = (permute != 0);
  hscale = (scaled == 0) ? heffte::scale::none : heffte::scale::full;

  heffte_plan = std::unique_ptr<heffte::fft3d<heffte_backend>>(
        new heffte::fft3d<heffte_backend>(
                heffte::box3d<>({in_ilo,in_jlo,in_klo}, {in_ihi, in_jhi, in_khi}),
                heffte::box3d<>({out_ilo,out_jlo,out_klo}, {out_ihi, out_jhi, out_khi}),
                comm, options)
    );
  *nbuf = heffte_plan->size_workspace();
  heffte_workspace.resize(heffte_plan->size_workspace());
  #endif
```

```
void FFT3d::compute(FFT_SCALAR *in, FFT_SCALAR *out, int flag)
{
  #ifndef HEFFTE
  fft_3d((FFT_DATA *) in,(FFT_DATA *) out,flag,plan);
  #else
  if (flag == 1)
      heffte_plan->forward(reinterpret_cast<std::complex<FFT_SCALAR>*>(in),
                           reinterpret_cast<std::complex<FFT_SCALAR>*>(out),
                           reinterpret_cast<std::complex<FFT_SCALAR>*>(heffte_workspace.data())
                          );
  else
      heffte_plan->backward(reinterpret_cast<std::complex<FFT_SCALAR>*>(in),
                            reinterpret_cast<std::complex<FFT_SCALAR>*>(out),
                            reinterpret_cast<std::complex<FFT_SCALAR>*>(heffte_workspace.data()),
                            hscale
                           );
  #endif
}
```

Tuning heFFTe

- Auto-tuning heFFTe using GPTune (https://gptune.lbl.gov/), we were able to increase performance by tuning FFT input parameters and communication settings
- Shown is performance improvements and speedup on Summit (~15 - 20%)



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- Collaborators:
    - A. Haidar (NVIDIA)
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