heFFTe: Highly Efficient Exascale FFTs Library for Heterogeneous Architectures

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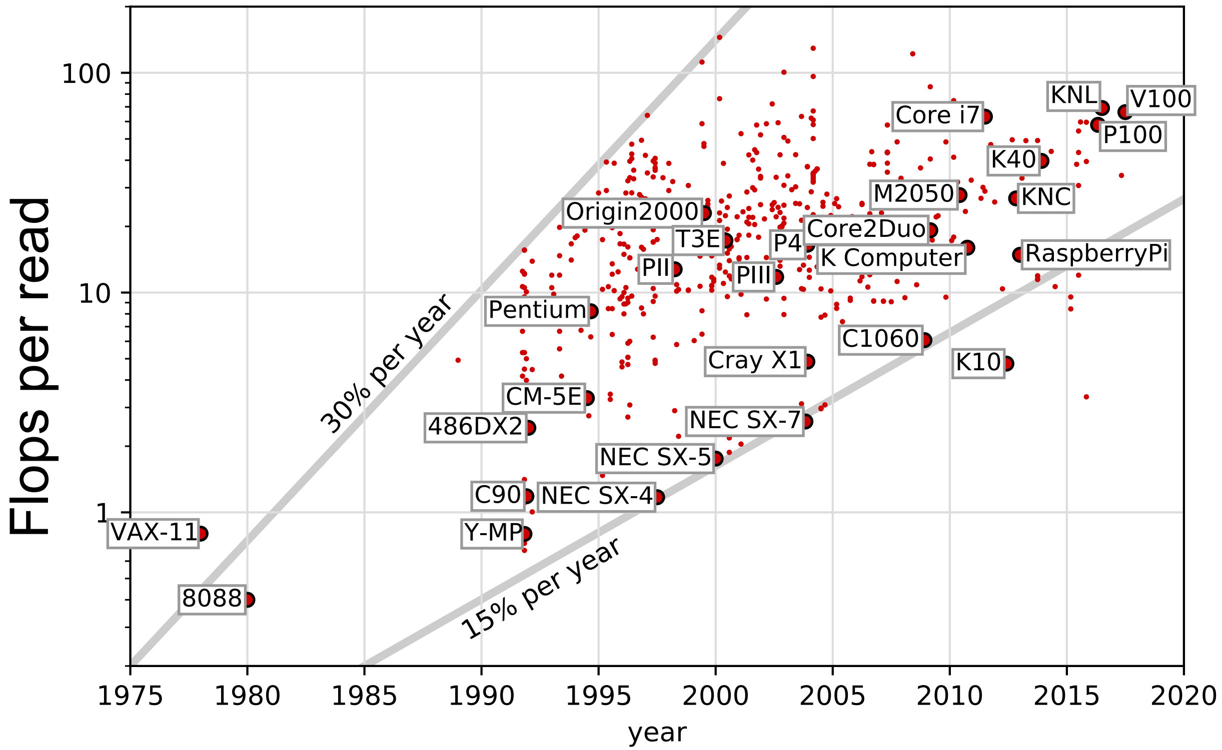
Hardware evolution motivates software redesigns

Hardware trends
compute vs. bandwidth peak



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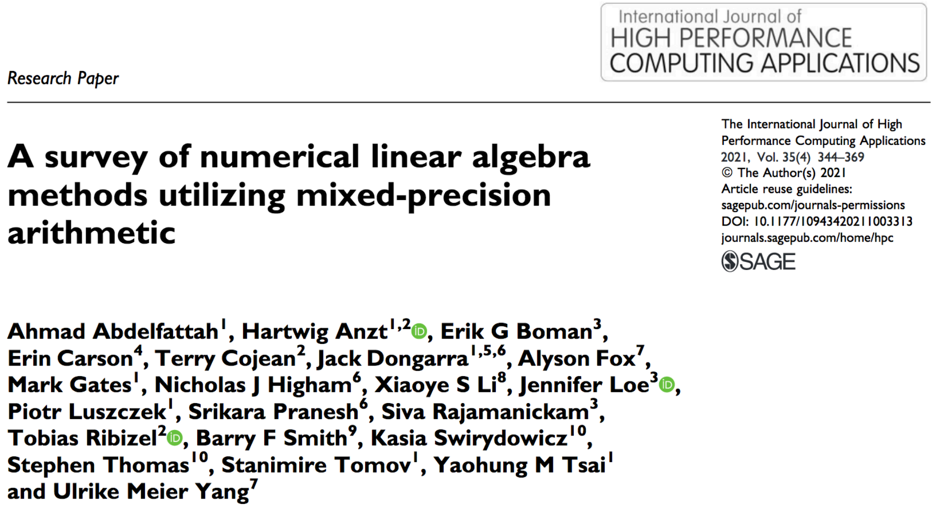
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A survey of numerical linear algebra methods utilizing mixed-precision arithmetic

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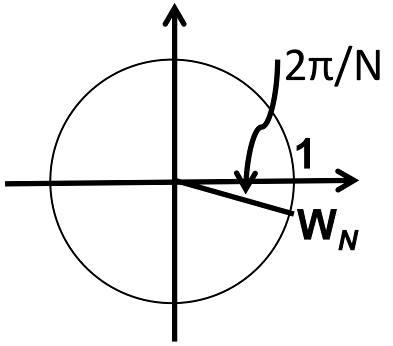
- **Need highly parallel algorithms**
- **Need algorithms with increased data reuse**
  (or reduced communication)
  - Currently, need more than 100x reuse for algorithm to remain compute bound

Fast Fourier Transform (FFT)

- **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

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

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

is a primitive N^{th} root of unity

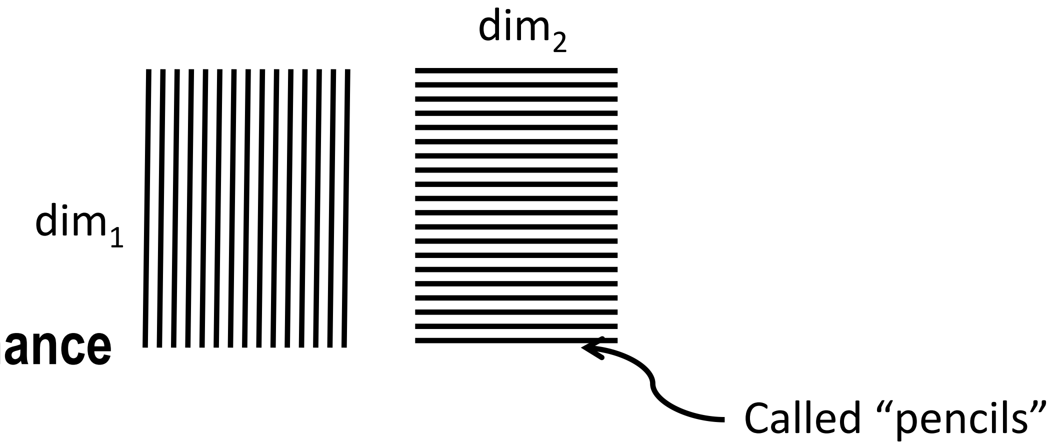
* **DFT can be computed as GEMV in $2N^2$ flops but FFT can do it in $5\, N \log_2 N$ flops!**

- 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

Computing multidimensional FFTs with heFFTe

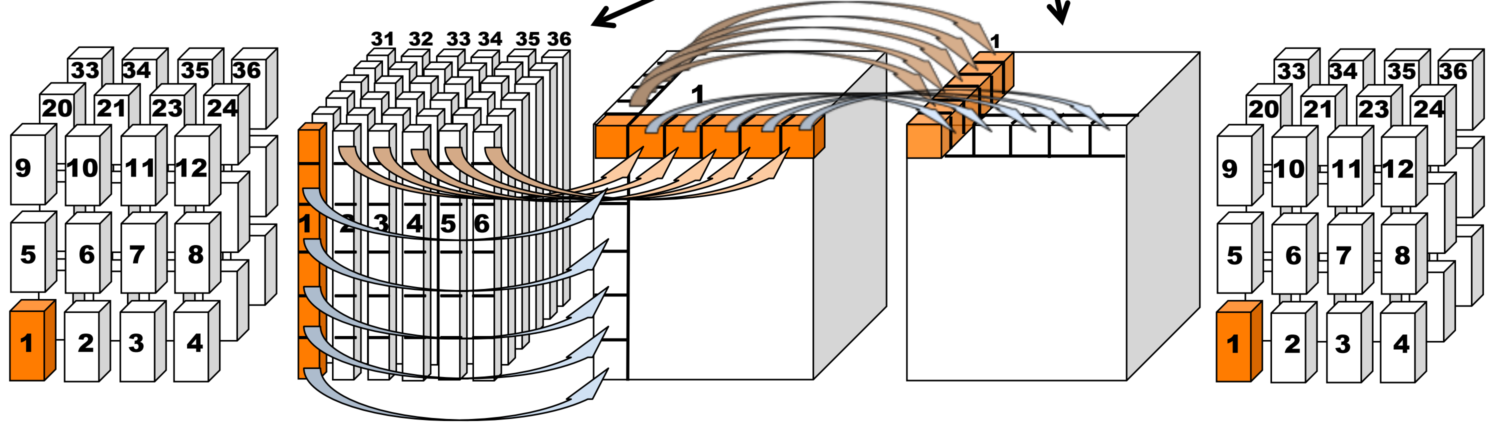
- **D-dimensional FFT algorithm**

```
for i in {dim_j , j = 1 .. D }
        Compute batch of ∏(dim != i) 1D FFTs of size dim_i
```



- **Order could be any, but particular order may impact performance**
- **Main building blocks**
  - **1D FFTs**
  - **Data reshuffles/transpositions**
  - **MPI communications**

Steps in preparing "pencils" in the different dimensions and computing batches of 1D FFTs locally on each node/GPU



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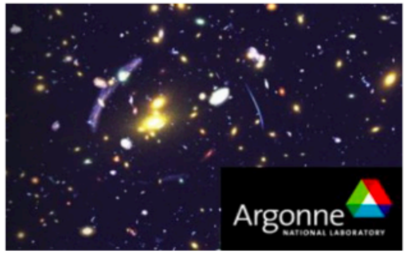
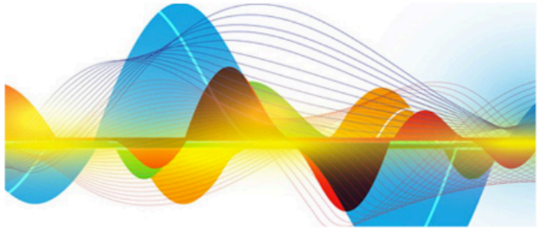
Applications Relying on Parallel FFTs

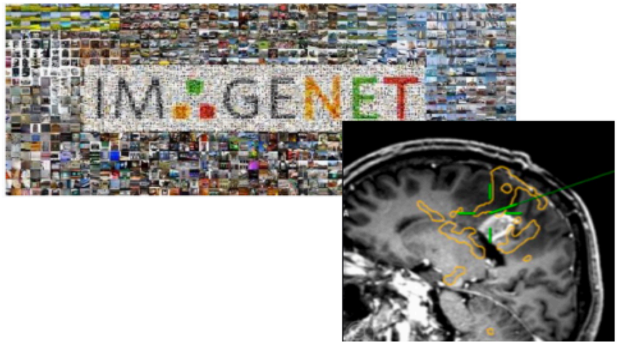
Cosmology
***ECP* ExaSky - HACC**

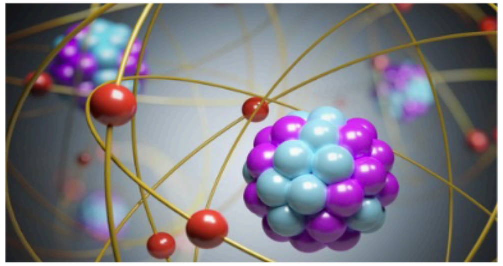


Signal processing,
***ECP* WARPX**

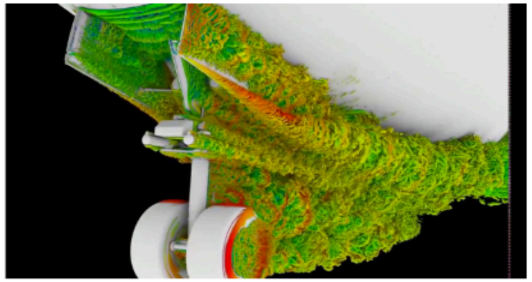


Deep Learning

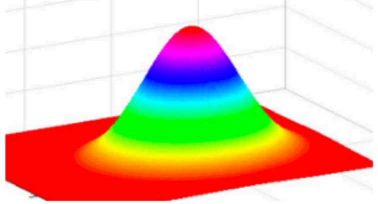




Molecular Dynamics
***ECP* EXAALT**



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



PDE solutions, **MASSIF**

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

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Examples of FFT use

- **Spectral methods to solve PDEs**

$$\Delta u(x, y) = f(x, y),$$

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

$$F \;\Delta u(x, y) = F\, f(x, y)$$

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

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

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

Algorithm 2 Solve $-\nabla u + u = f$ in $\Omega = [0..2\pi]$ using FFTs.

Input : function f, smooth and periodic on the boundary
Output: solution u
1. Sample $f[i] = f(x_i)$ at N grid points $x_i = i * h$, $h = 2\pi/N$ and error tolerance e_{tol}
2. Compute g = FFT (f, e_{tol})
3. Scale g point-wise, $g[i] = g(i)/(1+(ih)^2)$
4. Compute u = IFFT(g, e_{tol})

Particle Simulations
CoPa – Cabana - Cajita

Cosmology
HACC

Molecular Dynamics **Exaalt**

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 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:

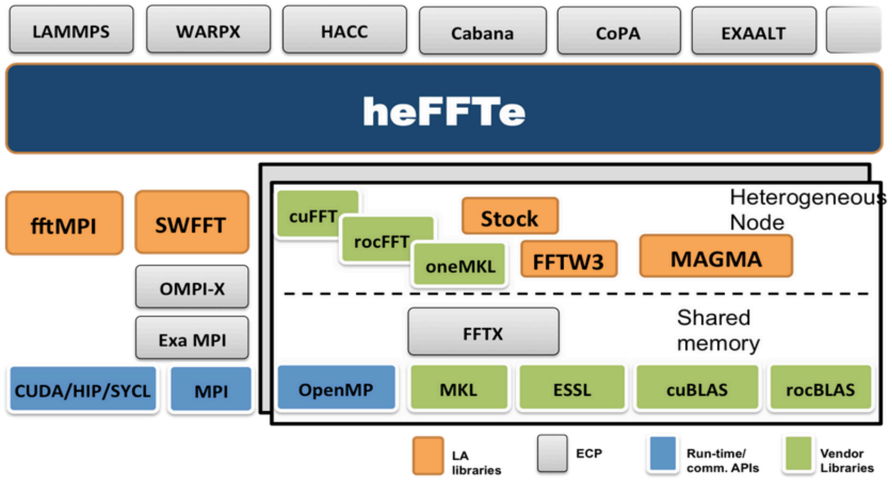
- **Summit @ OLCF (Nvidia GPUs)**
- **Crusher / Frontier (AMD GPUs), and others**
- **Florentia / Aurora (Intel GPU)**

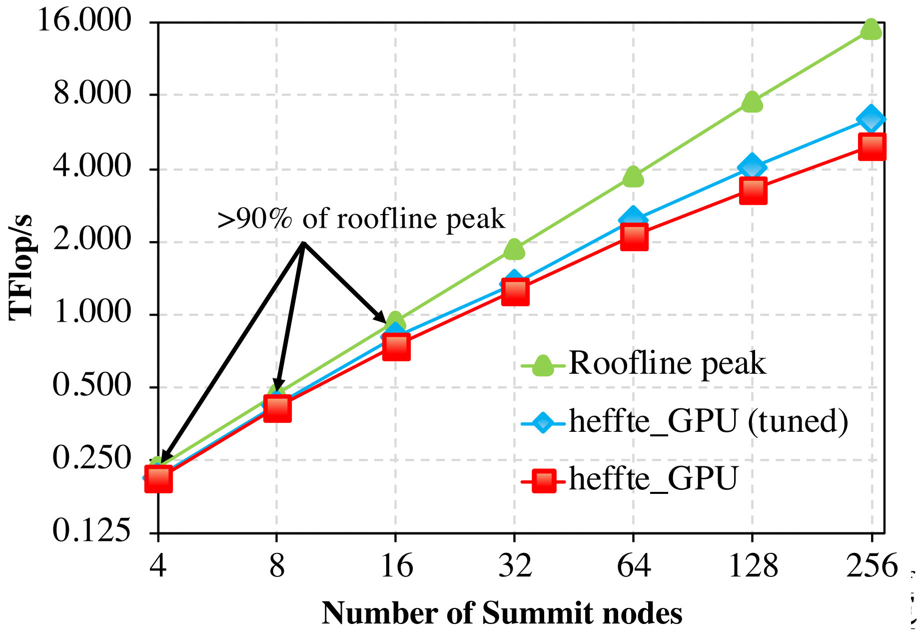
Current status:

- **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://github.com/icl-utk-edu/heffte**





heFFTe

Highly Efficient FFT for Exascale

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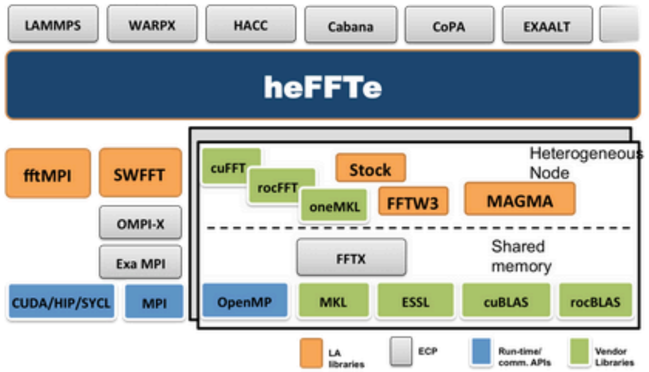
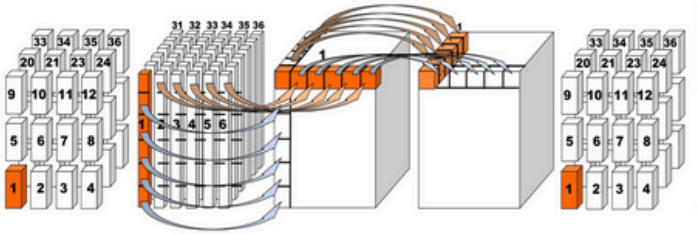
Azzam Haidar (NVIDIA)
Jack Dongarra (UTK)

THEN

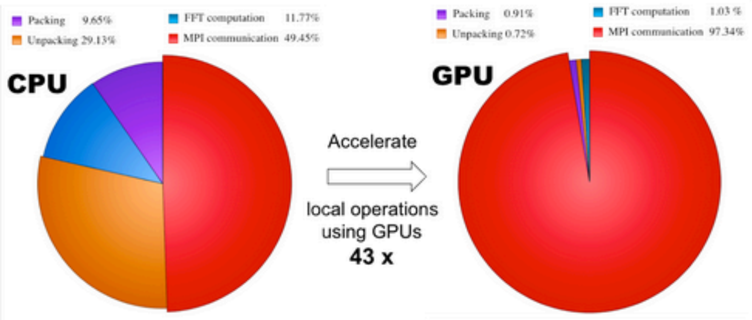
- The fast Fourier transform (FFT) is used in many domain applications - more than a dozen ECP applications use FFTs in their codes;
- State-of-the-art libraries like FFTW were no longer actively developed for emerging platforms;
- No GPU support for distributed multi-dimensional FFTs at the time;
- 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.

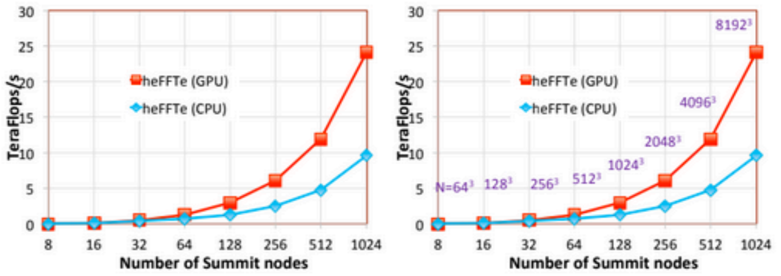




NOW

- 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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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

Experiences preparing for Aurora and Frontier

- Use of abstractions &standards (FFTs) helped with both functional & performance portability
- GPU kernel functional portability was helped by auto-generation tools
- xSDK policies helped the software engineering – heFFTe is xSDK compatible (regarding configuring, installing, testing, MPI usage, portability, contact and version information, open source licensing, namespacing, and repository access)
- Interactions and collaborations with diverse ST developers through xSDK and specialized xSDK PCRs were extremely helpful (xSDK mixed-precision techniques, batched sparse solvers, etc.)
- Interactions with vendors and early access to new and pre-released hardware helped
- To add efficient and sustainable support for many architectures, a large numerical library will inevitably need some auto-tuning capabilities; Libraries are parameterized but more may be needed

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 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.

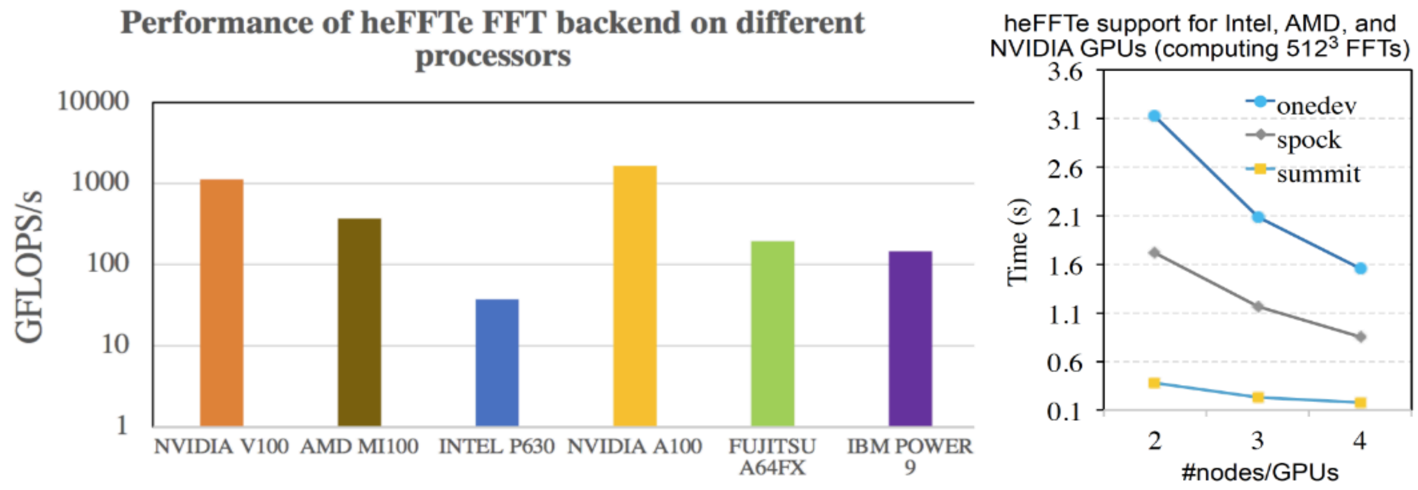


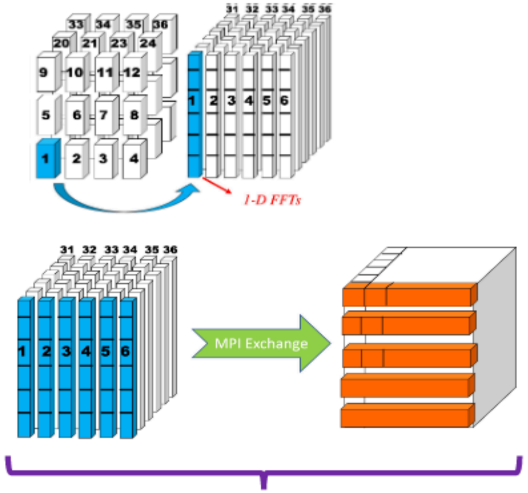
Figure: Comparison of single-device performance for a 512^3 FFT.

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}

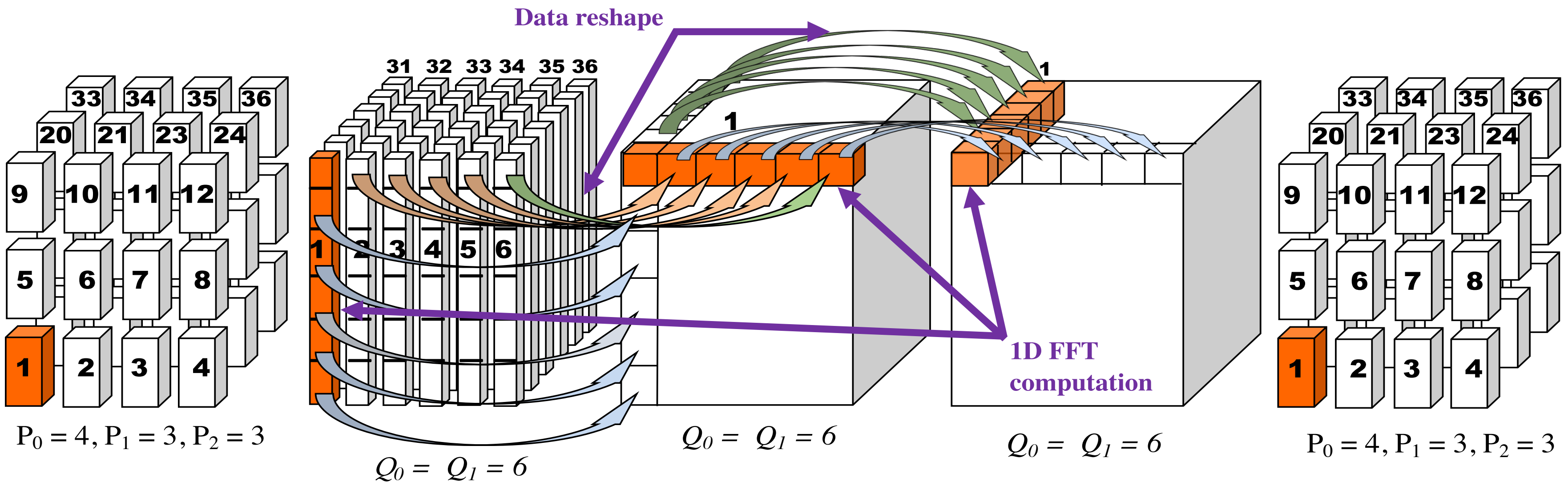


These 3 tasks can be replaced by 1 via MPI_Alltoallw

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

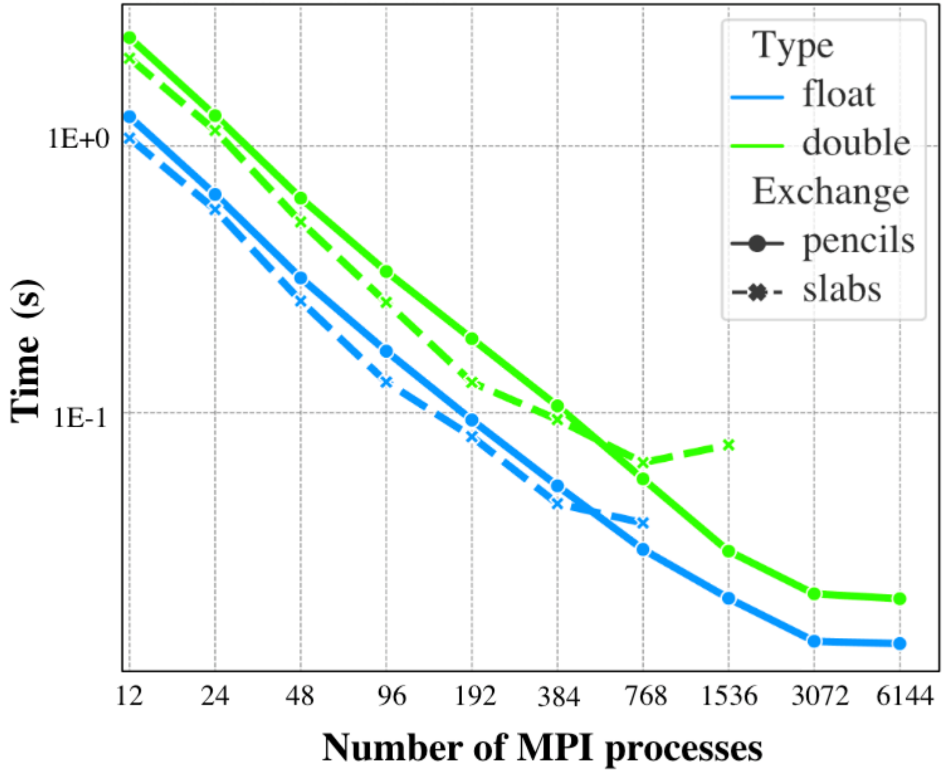
heFFTe Overview

- 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



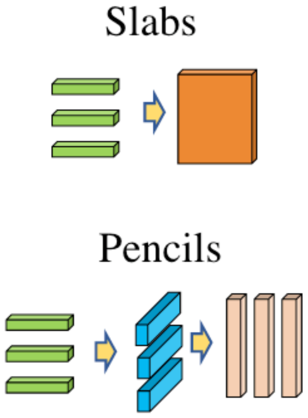
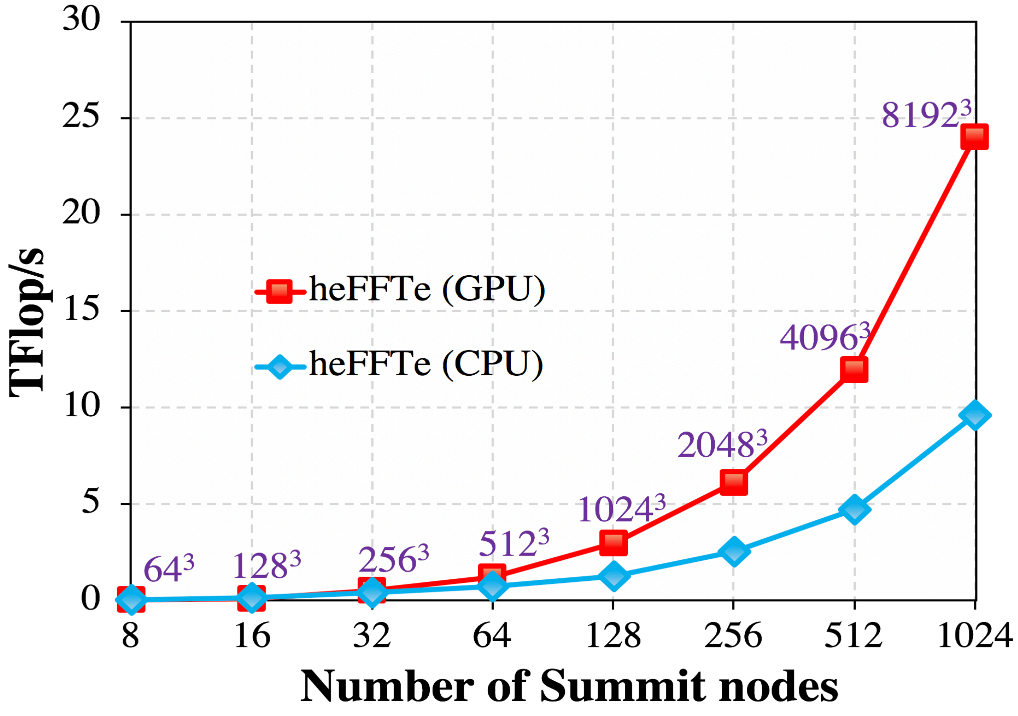
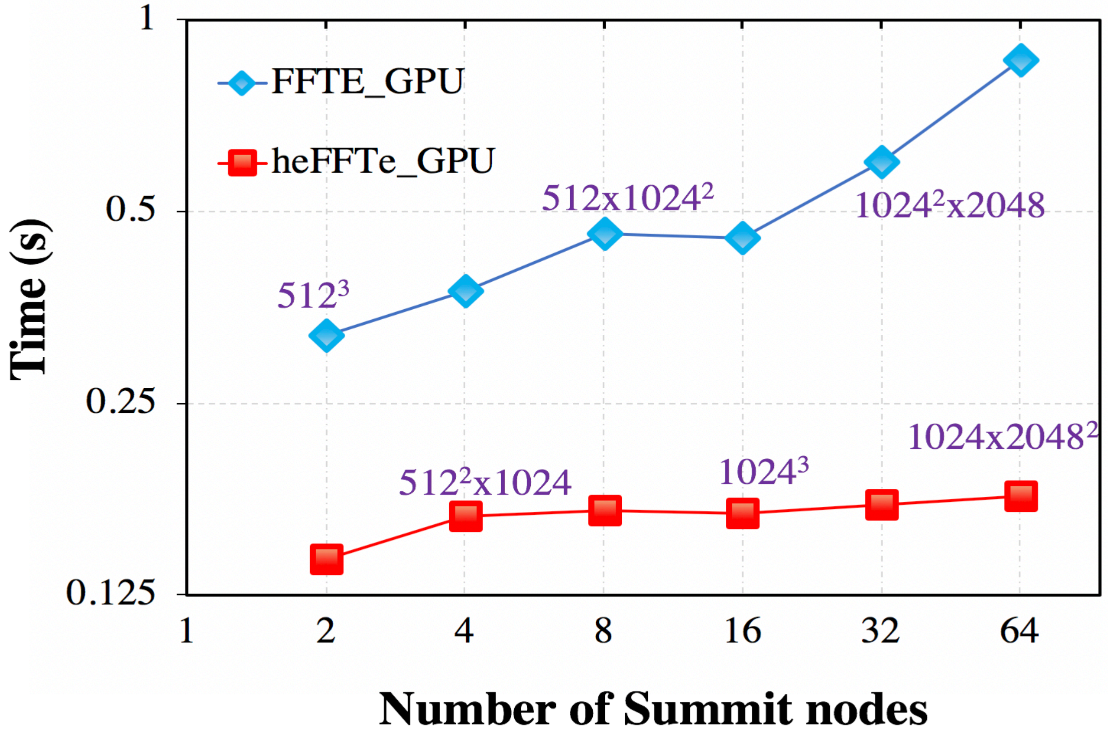


Fig. 6. Comparison of pencil and slab decompositions for strong scaling of a 3-D FFT of size 1024^3. Using *heFFTe* with cuFFT backend, 6 MPI processes (1 MPI processes per GPU-V100) per node, and single-precision complex data.

heFFTe Weak Scalability

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

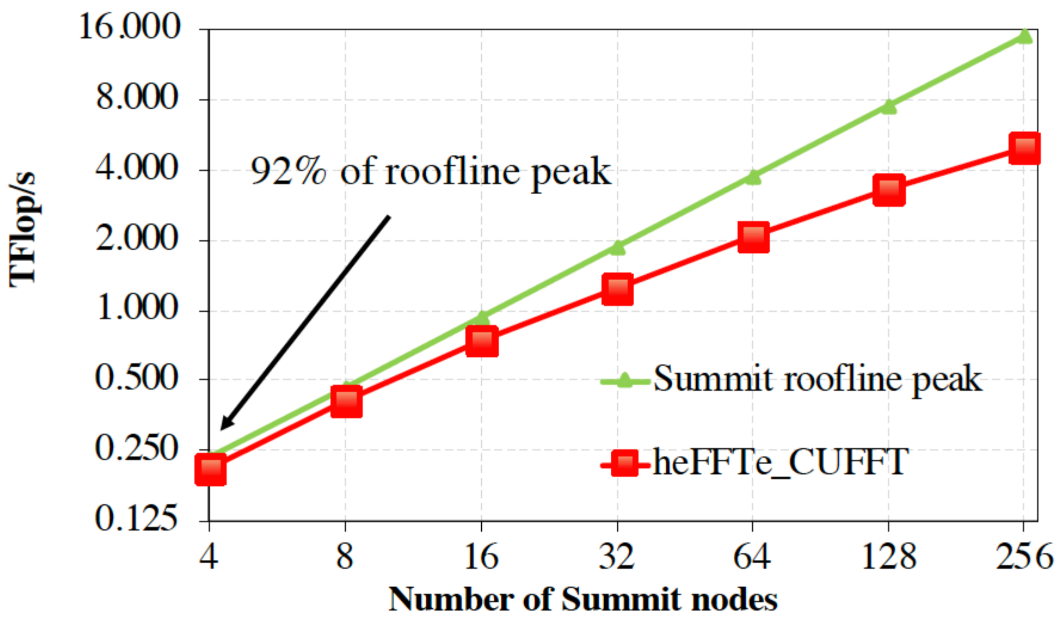


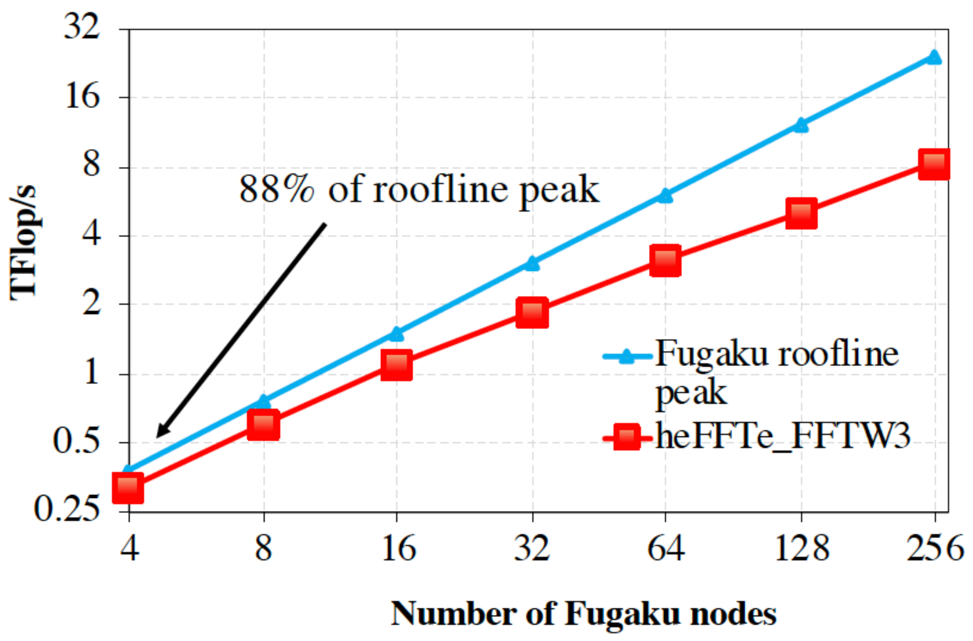


Forward and backward FFT on a Complex 3D array in double precision.

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.

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HPFFT benchmark (https://github.com/icl-utk-edu/hpfft)

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	-			✓

HPFFT benchmark (https://github.com/icl-utk-edu/hpfft)

Scaling FFT on top Supercomputers

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

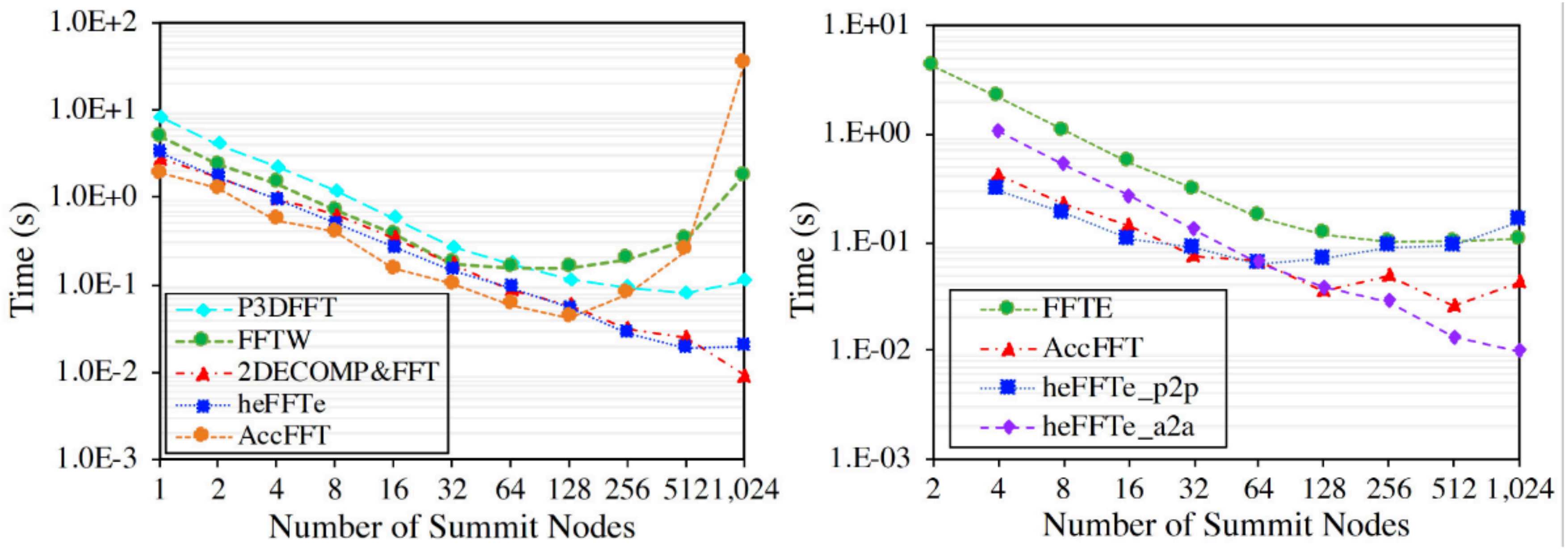
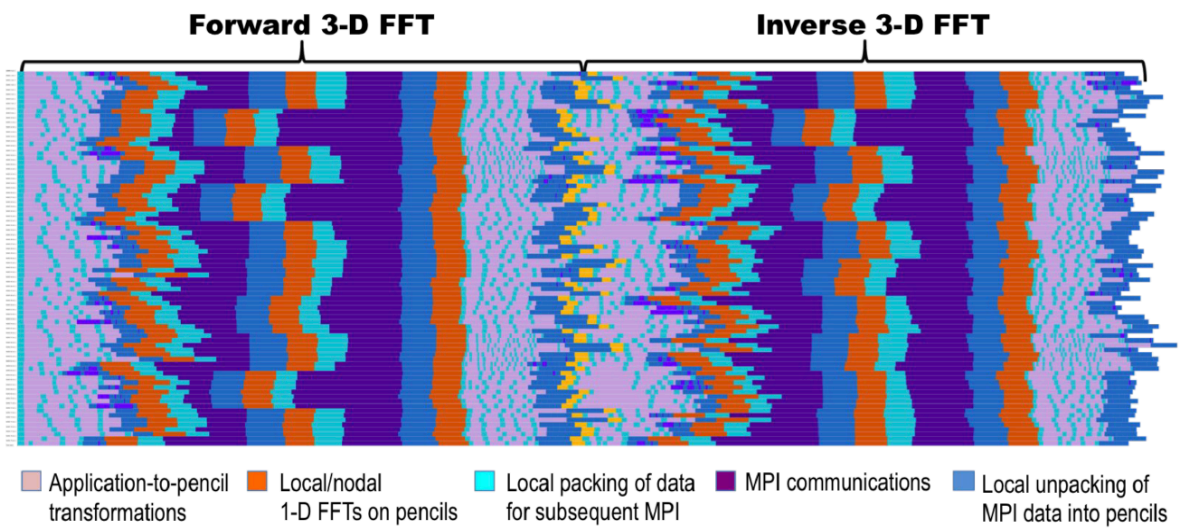


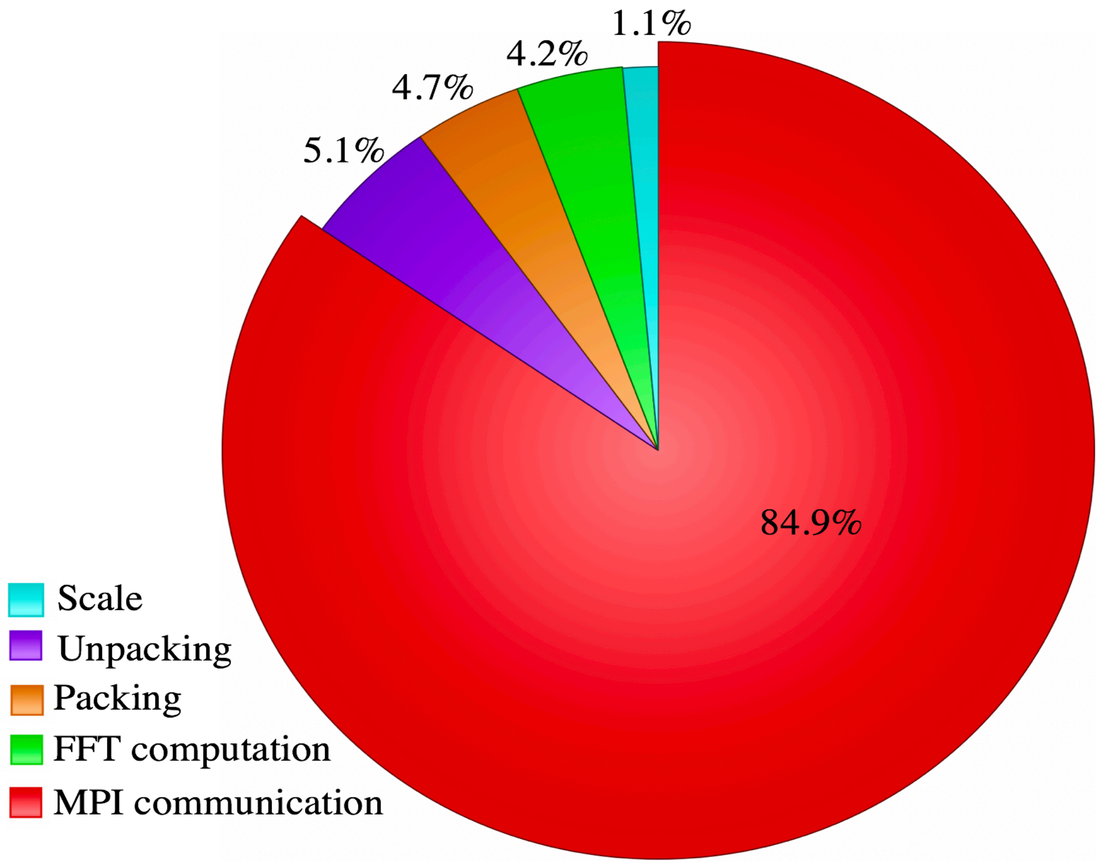
Figure: Strong Scalability on 32K Power9 cores for CPU-based libraries (left), and 4096 V-100 for GPU-based libraries (right).

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

heFFTe 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×.

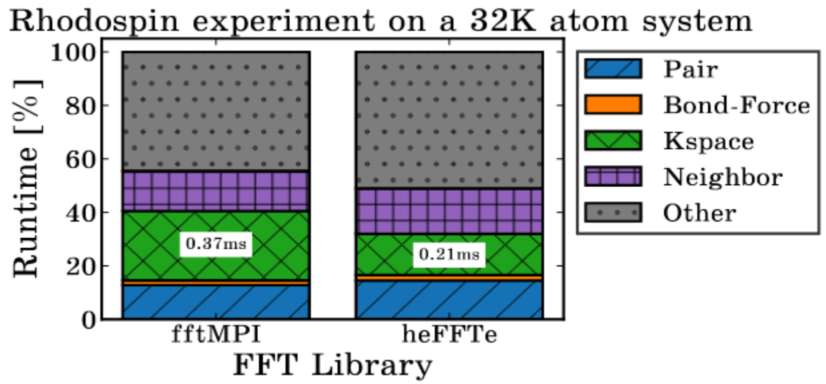


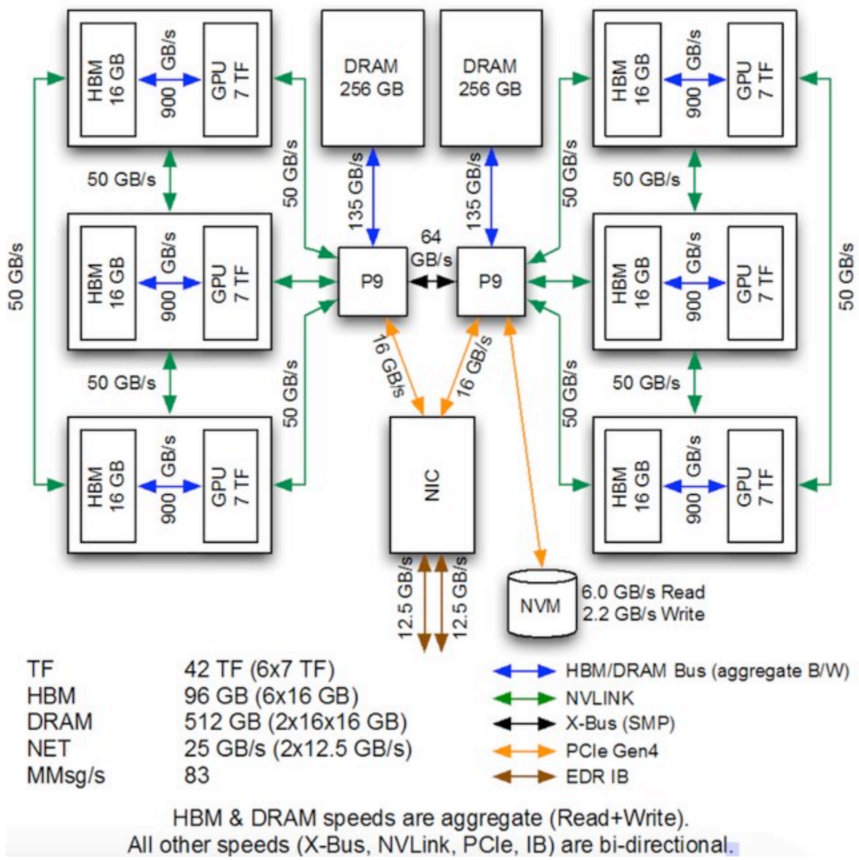
Figure: Breakdown for the LAMMPS Rhodopsin experiment. Using 32 Summit nodes, 6 V-100 GPUs per node, and 1 MPI per GPU.

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

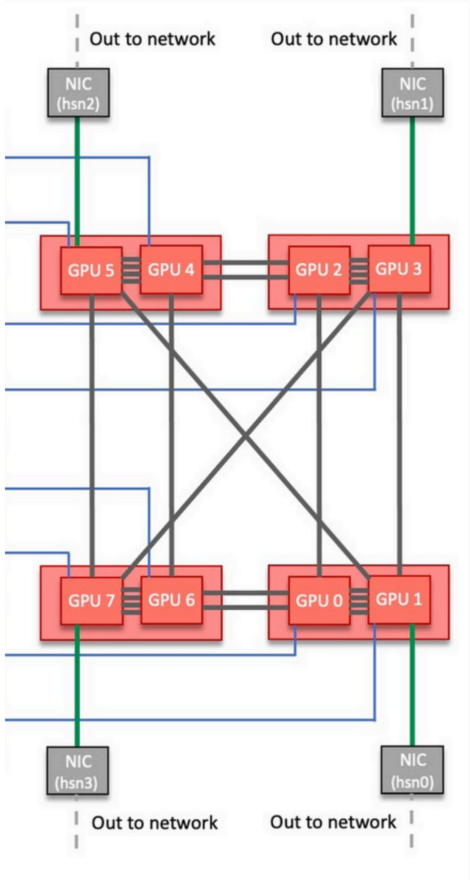
heFFTe on Frontier

- How should performance compare to Summit ?

Summit node



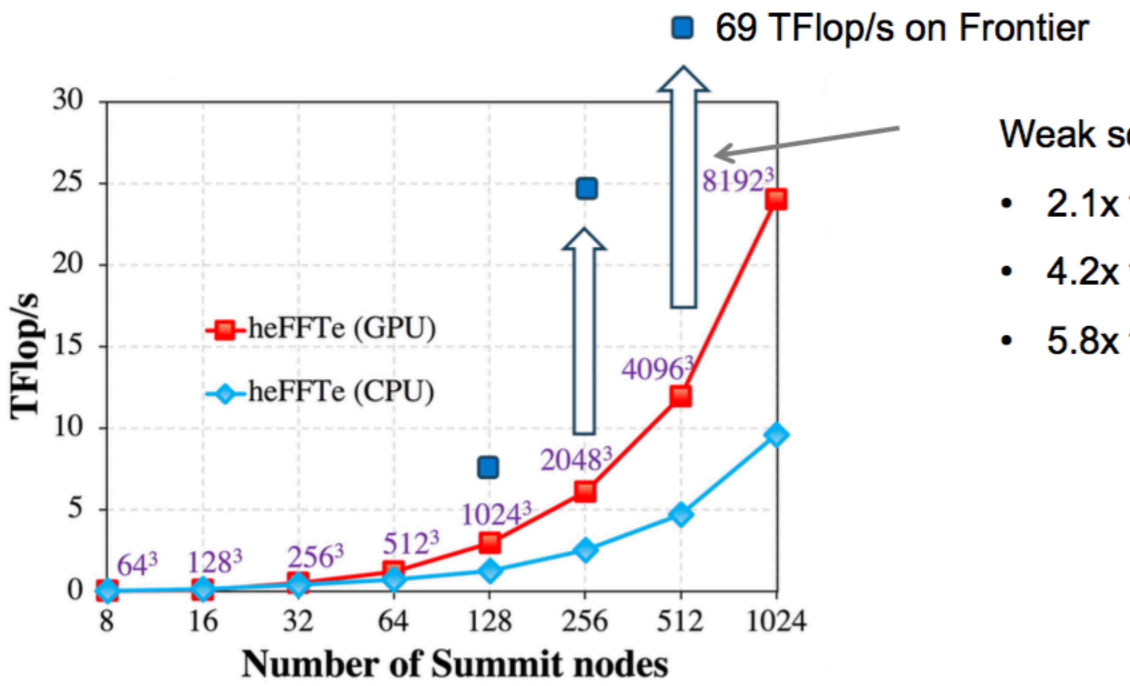
Frontier node



- 4 NICs (25 GBs + 25 GBs) in Frontier vs.
  1 NIC (25 GBs + 25 GBs) in Summit
- Expect to see 4 x speedup on Frontier vs. Summit on communication-bound codes like FFT (asymptotically for the same number of nodes)

heFFTe on Frontier

- **How do we compare to Summit?**

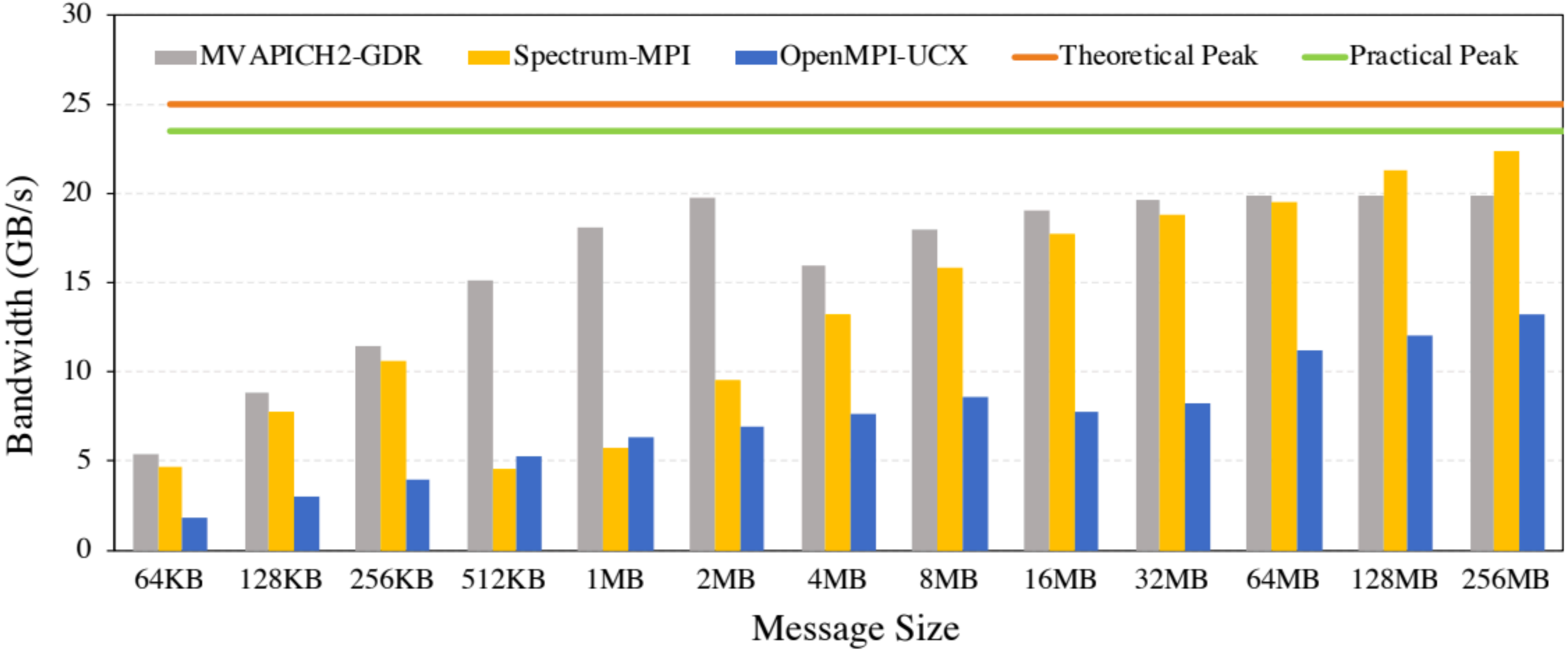


Weak scaling comparison

- 2.1x faster than on summit for 128 nodes
- 4.2x faster than on summit for 256 nodes
- 5.8x faster than on summit for 512 nodes

heFFTe using MVAPICH

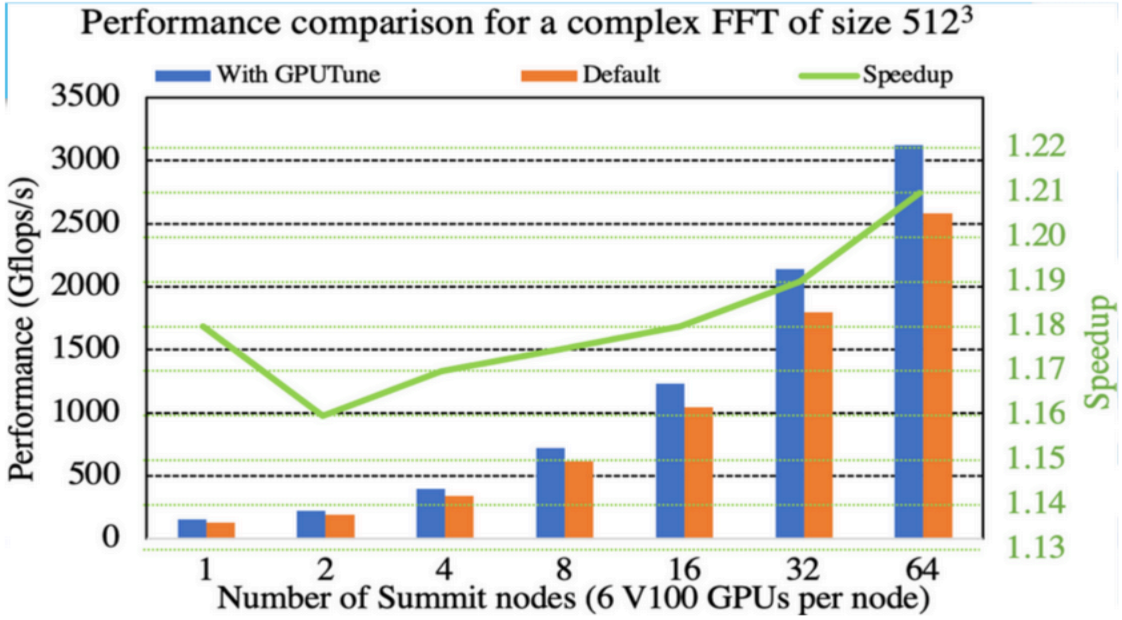
Strong scalability on 3D FFTs of size 1024^3, using 24 MPI processes (1 MPI per Power9 core) per node (blue), and 24 MPI processes (4 MPI per GPU-V100) per node (red)



Tuning heFFTe

Parameterize FFT implementation and expose parameters for tuning (a2a, a2av, a2aw, p2p, blocking/non-blocking, grid sizes, layouts, etc.)

- 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%)



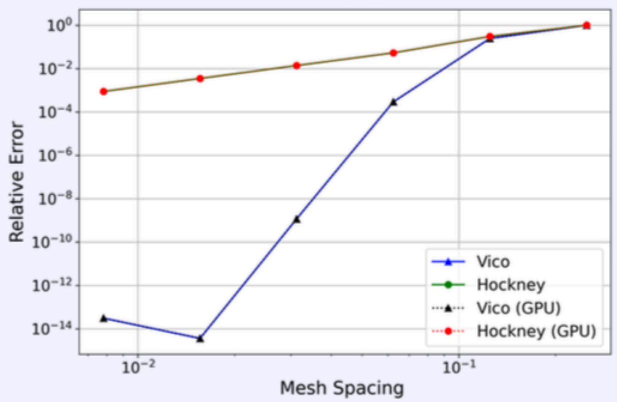
Approximate FFT with run-time lossy data compression

- Some solvers do not require full FP64 accuracy FFTs

Novel Poisson solver: Problem

What do we gain?

Convergence for smooth Gaussian source:



- These solvers are in IPPL and require Discrete Cosine Transform of type 1 Montanaro et al. (ETH)

FFT API for approximate FFTs

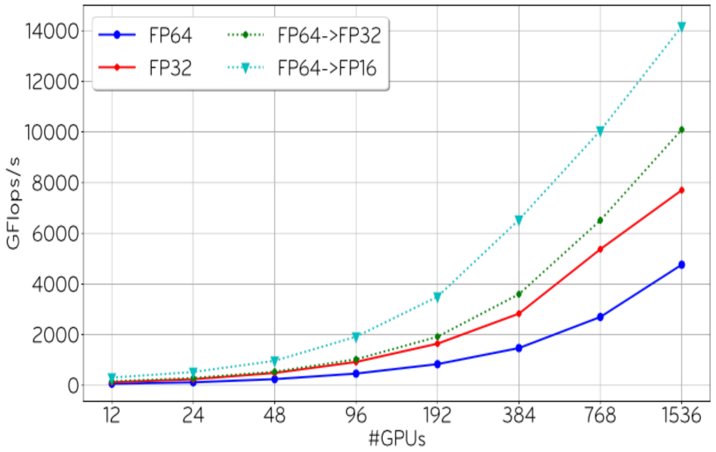
Algorithm 1 Approximate 3D FFT with lossy compression.

Input : 3D data $D_{x,y,z}$ in FP64 precision and error tolerance e_{tol}

Output: Approximate 3D FFT of $D_{x,y,z}$ stored in FP64 within error tolerance e_{tol}

1: **for** $i := x, y, z$ **do**
2: Custom Alltoall (Algorithm 3) combined with data $D_{x,y,z}$ compression/decompression within an error tolerance of e_{tol} in direction i
3: Batched 1D FFTs for direction i in FP64
4: **end for**

Speedup and accuracy of FFT using casting



Accuracy of approximate FFTs in heFFTe for 1024^3 FFTs

#GPU	FP64	FP32	FP64 → FP32
12	6.00e-15	4.96e-06	1.94e-07
24	6.17e-15	4.91e-06	2.20e-07
48	5.92e-15	4.49e-06	3.01e-07
96	6.00e-15	3.47e-06	3.90e-07
192	5.11e-15	3.54e-06	3.99e-07
384	5.25e-15	4.44e-06	5.09e-07
768	5.29e-15	3.13e-06	5.44e-07
1536	5.38e-15	3.06e-06	5.57e-07

TABLE II

COMPARISON OF THE FFT ACCURACY WHEN USING CASTING OPERATION FROM FP64 TO FP32 IN THE COMMUNICATION WITH THE TWO REFERENCES. EACH REFERENCE CORRESPONDS TO AN EXECUTION USING A UNIQUE PRECISION WHICH IS EITHER FP64 OR FP32.

PROJECT OVERVIEW

TITLE
Collaborative Research: Frameworks: Performance Engineering Scientific Applications with MVAPICH and TAU using Emerging Communication Primitives

SPONSOR
NSF CSSI

TEAM MEMBERS
PI: Dhabaleswar K. (DK) Panda,
Lead Institution: The Ohio State University
Aamir Shafi, Hari Subramoni, Mustafa Abduljabbar (**OSU**)
Sameer Shende (**UO**)
Yifeng Cui, Daniel Roten (**SDSC**)
Stan Tomov (**UTK**)

GRAPHICAL REPRESENTATION

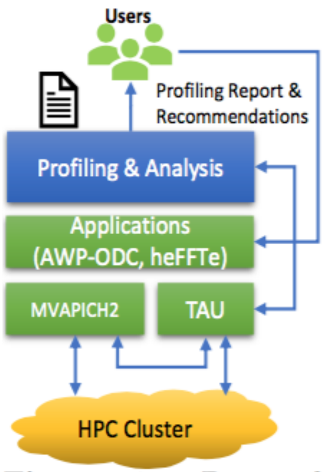
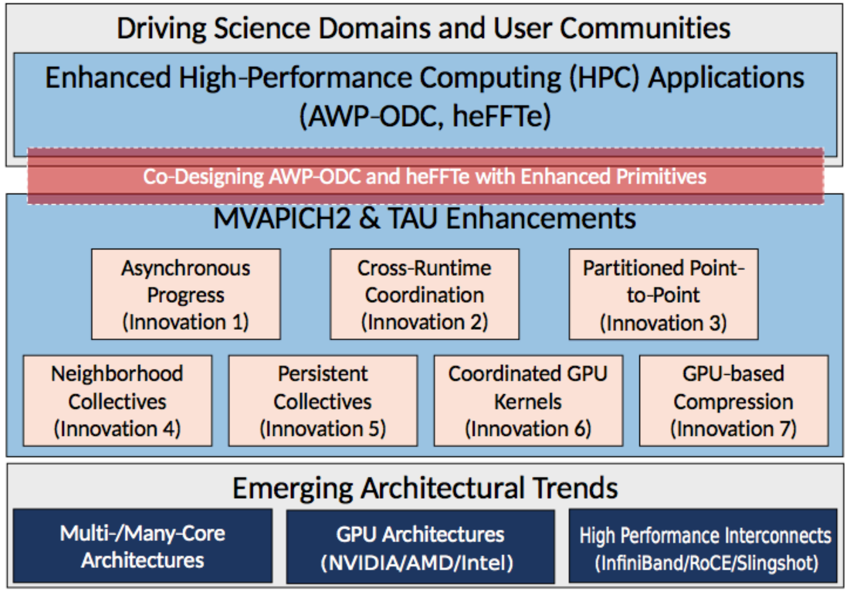


Figure 1: Proposed Profiling Framework



TECHNICAL DETAILS

OVERALL PROJECT OBJECTIVE
Co-design using the MPI_T API—in the MVAPICH2 and TAU libraries with scientific applications. Focus is on two popular HPC applications spanning multiple domains and representing various communication patterns - Anelastic Wave Propagation (AWP-ODC) and heFFTe. AWP-ODC is a highly scalable parallel finite-difference application with point-to-point operations that enables 3D earthquake calculations.

UTK CONTRIBUTION
HeFFTe, dominated by collective operations, is a massively parallel application that provides a scalable and efficient implementation of the widely used Fast Fourier Transform (FFT) operations.

IMPACT AND IMPLEMENTATION

BROADER IMPACT
Impact on driving guidelines for designing, deploying, and utilizing next-generation HPC systems for various application domains.

SCIENTIFIC IMPACT
Develop the next generation innovations by co-designing MVAPICH2 and TAU libraries to scale driving science domains—including AWP-ODC and heFFTe

NEXT STEPS & TIMELINE
3 years project, integrating heFFTe with innovations in MPI and TAU

Collaborators and Support

- heFFTe is funded by the Department of Energy (DoE) Exascale Project WBS 2.3.3.13.
- Collaborators:
  - A. Haidar (NVIDIA)
  - ICL OpenMPI Team (UTK)
  - ICL FIBER Team (UTK)
  - Network-Based Computing Research (DK. Panda's group, OSU)
  - ECP X-Tune (Sherry Li's group, LBNL)
  - D. Takahashi (U. Tsukuba)
  - D. Pekurovsky (SDSC)