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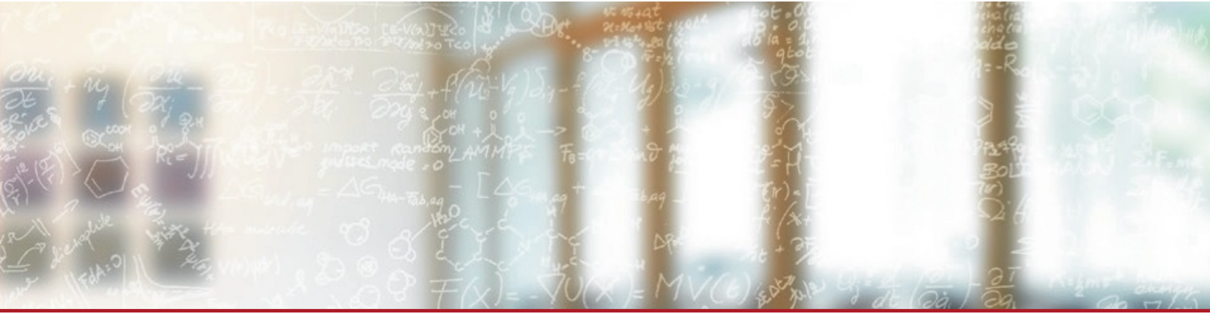

Improved scaling of massively parallel FFTs on modern supercomputers

Cray User Group Meeting (CUG) 2021

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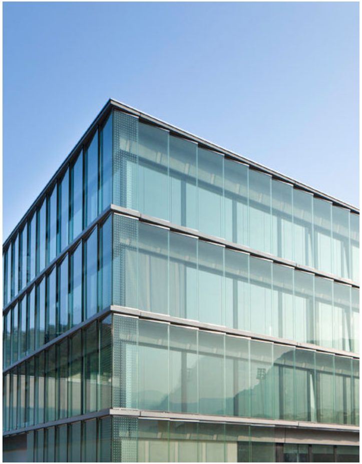
Improved scaling of massively parallel FFTs on modern supercomputers



- Motivation
- Parallelisation approaches
- Implementation of the parallelisation
- Alternative decompositions
- More flexibility, resolution
- Distributed 1D FFT
- Benchmarks
- Conclusions and outlook

Motivation

- Fast Fourier Transform (FFT) algorithm part of many HPC applications
  - Plasma physics
  - Chemistry and material science
- Mostly 2D or 3D Fourier transforms
- Distributed computation is communication intensive, scaling is a challenge
- Optimised MPI collective routines are available – applied to FFTs

Parallelisation approaches

- Example of 3D FFT, applies also to 2D and 1D FFTs
- Slab decomposition (preferred decomposition)
- Pencil decomposition (more tasks than number of grid points in one direction)
- Higher order decompositions (rarely used)
- Binary exchange

Parallelisation approaches contd.

- Slab and pencil decomposition require all-to-all communication
- Binary exchange requires point-to-point communication
- Large message sizes: communication and computation overlap
- We focus on strong scaling – small message sizes

Implementation of the parallelisation

- Multiple processing units with shared memory on the node, data transfer within the node assumed to have zero cost
- High speed network between nodes assumed to be fully connected (good approximation for current Cray machines with Aries or Slingshot network), bandwidth-latency cost model
- Computer networks might support more than one port per node, message size dependent, on Aries network short messages many ports and long messages one port
- For pure MPI solutions latency is reduced by collecting all messages on the nodes before sending them and distributing them after receiving (presented at CUG 2018) $\longrightarrow$ reduction of number of messages
- Efficient `MPI_Alltoall` or `MPI_Alltoallv` required, persistent MPI well suited (initialisation phase for setup of the communication algorithms), no performance difference between these two collectives

FFTs with pencil decomposition

- Comparison between our `all-to-all` routine from “ext_mpi”
  https://github.com/eth-cscs/ext_mpi_collectives
  and standard MPI `all-to-all` as reference
- Strong scaling for pencil decomposed 3D FFT (FFTW) 600^3, 768^3 and 1200^3 grid-points double precision real numbers, 12 (3×4) tasks per node
- Benefits for small message sizes (large number of nodes) visible in the strong scaling experiments

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- A totally revised version of the library will be published soon

FFTs with pencil decomposition contd.

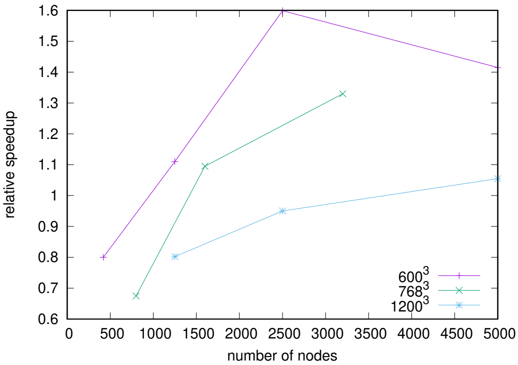
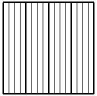
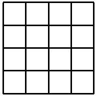


Figure: Relative speedup of our pencil decomposed 3D FFTs ("ext_mpi" `all-to-all` plus FFTW) with respect to standard MPI (FFTW), 12 (3×4) tasks per node, 600^3, 768^3 and 1200^3 grid-points, Cray XC50, presented at CUG 2018

Alternative decompositions

- In many cases decompositions enforced by constraints of the solver
- For particle in cell (PIC) method minimum communication volume for particles is obtained by division of domain (cube) in three directions

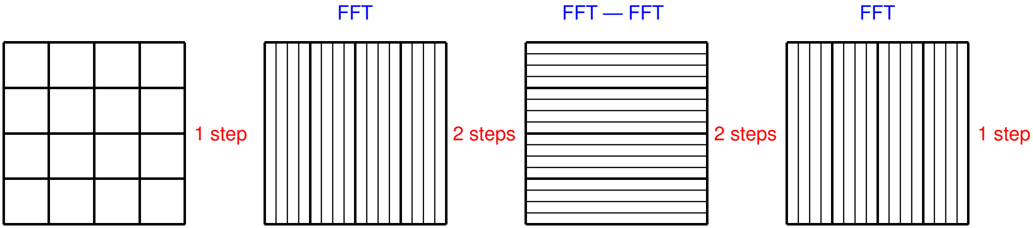
in 2D:  versus 

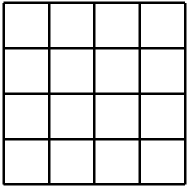
- Either additional communication steps are required for rearrangement of data or FFTs are applied directly to the decomposition $\longrightarrow$ parallelisation of the FFT algorithm in higher dimension than necessary for resolution and number of nodes given

More flexibility, resolution

- FFT kernels for large prime numbers solved in parallel (parallel discrete Fourier transform DFT)
- Parallel DFT solve with `MPI_Allgather` or `MPI_Reduce_scatter_block`
- Optimised routines exploiting multiple communication ports per node
- `allgather` might also be applied to non-prime numbers, if no proper decomposition can be made, or the prime factors are small and many ports are available
- Example: 4×4 distributed 2D mesh and 3 ports per node; Poisson equation

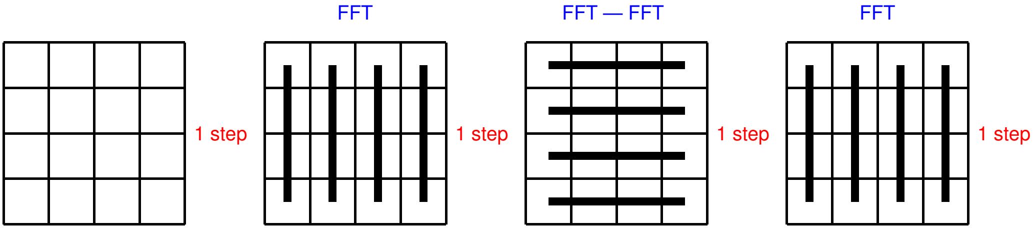
More flexibility, resolution contd.

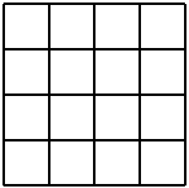




- 2 additional steps for data rearrangement (3 ports per node)
- Minimum computational cost

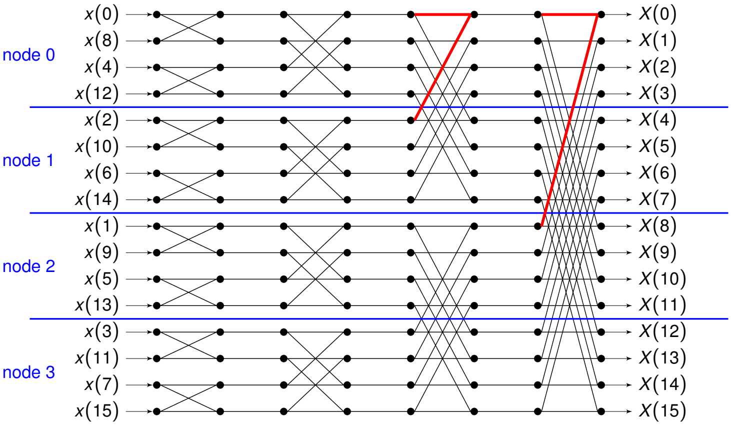
More flexibility, resolution contd.





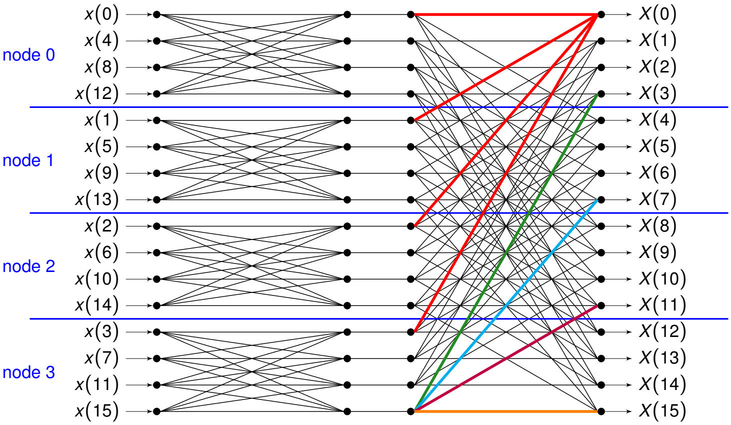
- 1 communication step per FFT (3 ports per node)
- Minimum computational cost for `alltoall` solution
- More restrictive with respect to resolutions
- `allgather` solution also with 1 communication step per FFT/DFT

Distributed 1D FFT



Radix 2, decimation in time

Distributed 1D FFT contd.

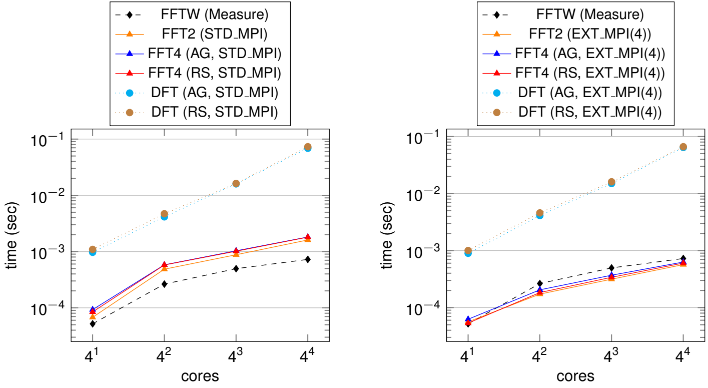


Radix 4, decimation in time

Benchmarks

- Distributed 1D FFT radix 2 and 4 and comparison with FFTW
- Reordering of the data before execution included in the benchmark
- 4 MPI tasks per node communicating with each other using shared memory ("ext_mpi" library)
- Both, `allgather` and `reduce_scatter_block` approach for small DFTs (FFT kernels)
- Local FFTs within the node computed with FFTW

Benchmarks contd.

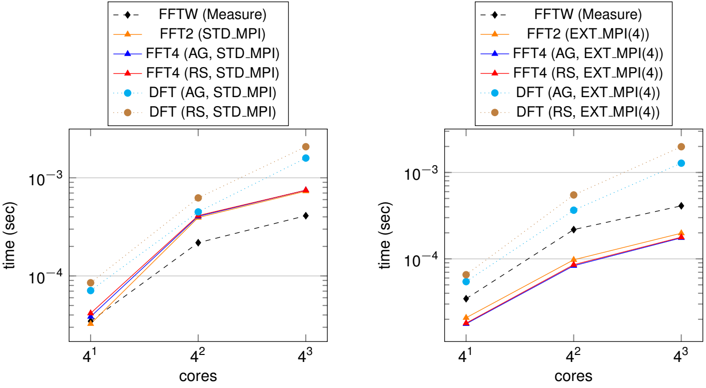


(a) 256 points per core (STD_MPI)

(b) 256 points per core (EXT_MPI(4))

Figure: Weak scalability of various FFT and DFT implementations on Cray XC40 KNL, using standard MPI (left), and ext_mpi with shared memory between every 4 cores (right) in the custom implementations.

Benchmarks contd.



(a) 64 points per core (STD_MPI)

(b) 64 points per core (EXT_MPI(4))

Figure: Weak scalability of various FFT and DFT implementations on Cray XC40 KNL, using standard MPI (left), and ext_mpi with shared memory between every 4 cores (right) in the custom implementations.

Benchmarks contd.

- 256 grid points per task (core) is the break even for the `allgather` / `reduce_scatter_block` (ext_mpi) approach versus the `alltoall` (standard MPI) method
- Large part of the speedup of “ext_mpi” compared to “standard MPI” comes form the data reordering before the execution of the FFTs, done with `all-to-all` (ext_mpi), not necessary for solution of the Poisson equation

Literature

- Andreas Jocksch, Matthias Kraushaar and David Daverio: Optimised all-to-all communication on multicore architectures applied to FFTs with pencil decomposition, Concurrency Computat Pract Exper., 2018
- Andreas Jocksch, Noe Ohana and Emmanuel Lanti and Vasileios Karakasis and Laurent Villard: Optimised allgatherv, reduce_scatter and allreduce communication in message-passing systems, arXiv, 2020

Conclusions and outlook

- For pure MPI solutions short messages all-to-all communication can be accelerated by using shared memory on the node
- Optimised `Allgather` and `Reduce_scatter_block` provide more degrees of freedom to parallelise FFTs (DFTs)
- Improved strong scaling properties of parallel FFTs
- Work in progress, library will be further developed

Acknowledgements

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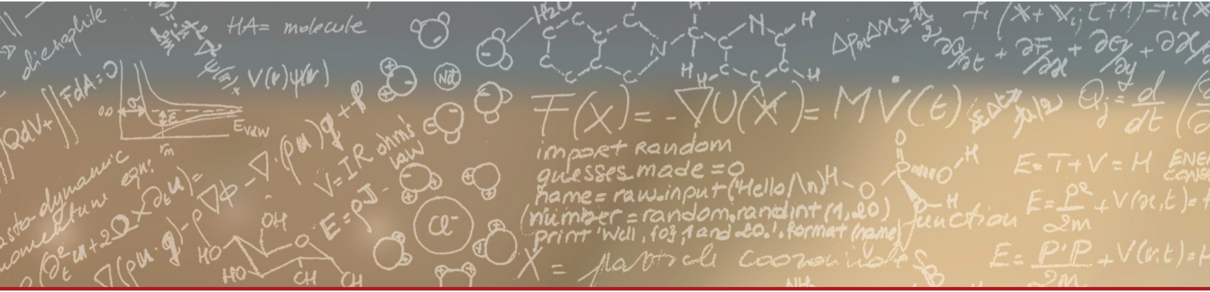

Thank you for your attention.

https://github.com/eth-cscs/ext_mpi_collectives