BLUE WATERS

SUSTAINED PETASCALE COMPUTING

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Toward petaflop 3D FFT on clusters of SMPs

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GREAT LAKES CONSORTIUM FOR PETASCALE COMPUTATION

Petaflop parallel 3D FFT, why?

NSF petascale turbulence benchmark required petaflop performance of 3D FFT of 12288^3 on BW

- Demands 10% of BW's peak including communication

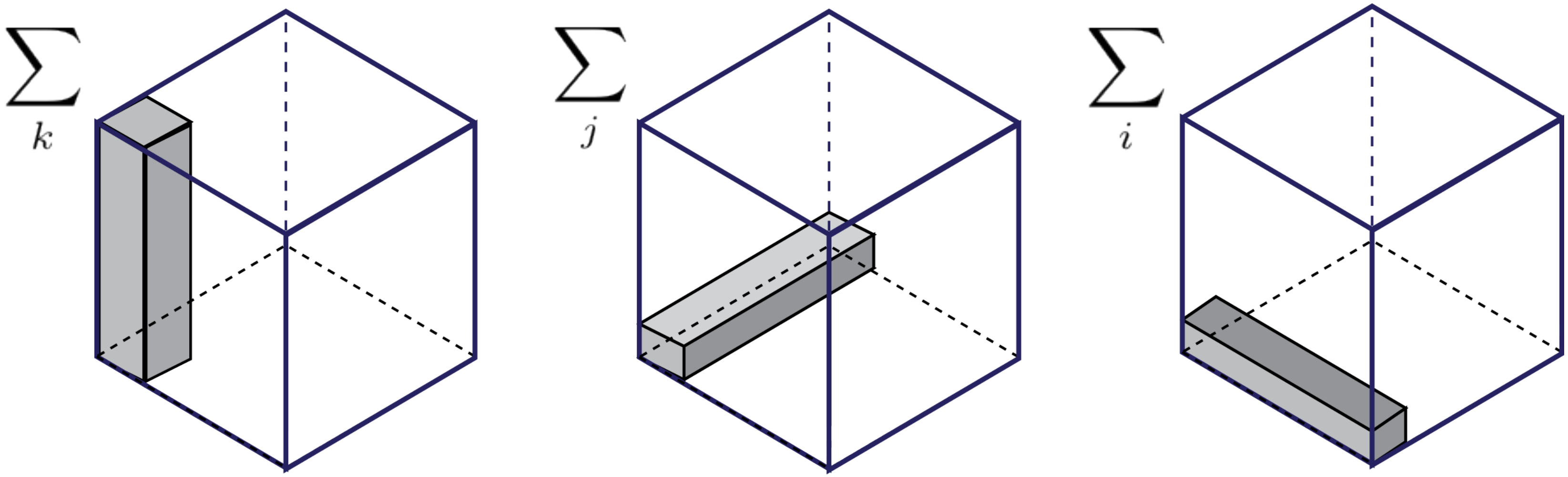
Disclaimers

- The results on P7 were obtained on early hardware and software and do not represent the true performance of BW; the conclusions are subject to change.
- All the test codes are available upon request and distributed under UIUC/NCSA open-source (a BSD) license.
- Opinions are solely mine and not NCSA's.

Outline

- 3D FFT, basic algorithm and use cases
- Slab distribution on clusters of SMPs
- Performance Analysis of 2D FFT on P7
  - PDCFT2 in PESSL, MPI
  - DCFT2 in ESSLSMP using OpenMP
  - OpenMP/TLS: transpose with get operation (TLS=thread-local storage)
  - OpenMP/Mix: no transpose
- Further improvements
- Requirements of 3D FFT library

3D FFT $u^x_{\mathbf{k}} \leftarrow \sum_i \sum_j \sum_k \exp^{i\mathbf{k}\cdot\mathbf{r}_{i,j,k}} u^x(\mathbf{r}_{i,j,k})$



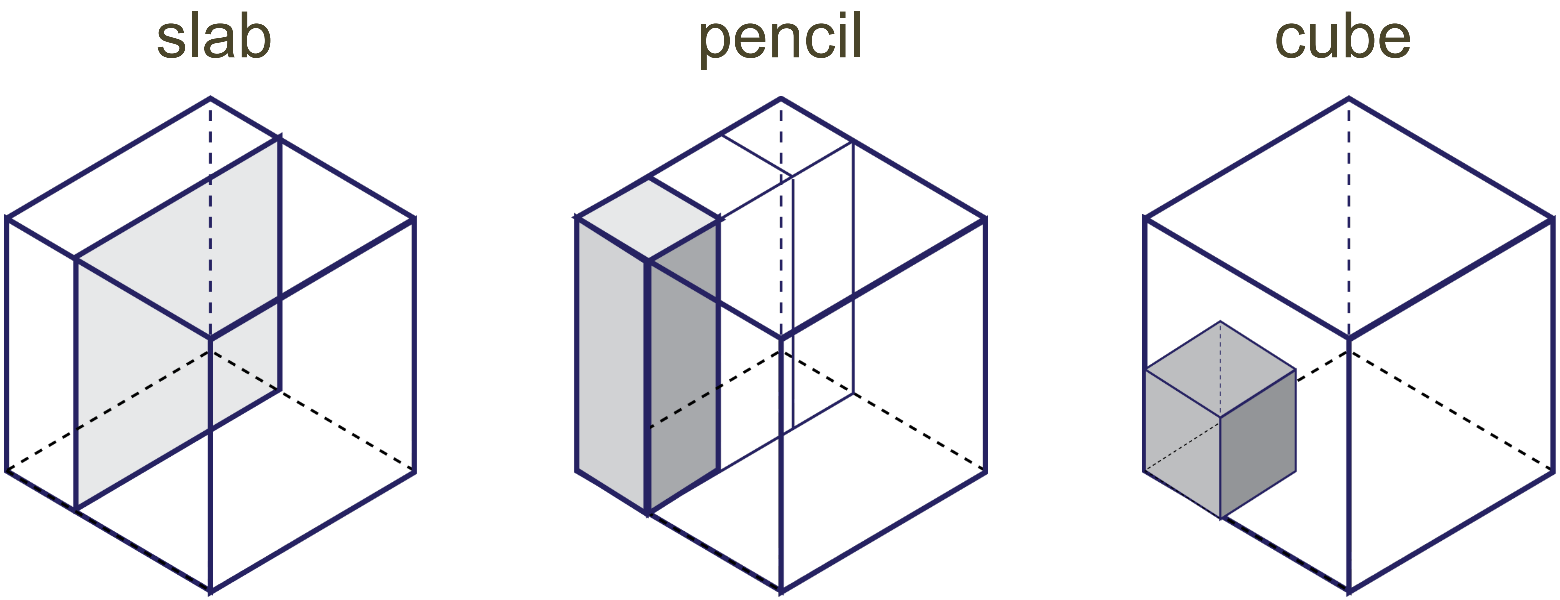
- Commonly using 1D FFT, variants of Cooley–Tukey algorithm
- Applications using 3D FFT
  - Coulomb potential for MD, e.g., NAMD, LAMMPS …
  - CFD: Turbulence with direct numerical solver (DNS)
  - Electronic structure methods, e.g.,Qbox, OpenAtom …

Status of parallel 3D FFT

Parallel 3D FFT libraries including P3DFFT use 1D FFTs and perform transposes. Why?

- 1D FFTs can be and are highly tuned on a target architecture.
  - No special data structure: regular 1D arrays.
- Requirements of applications widely vary and supporting many special cases at **high** efficiency is hard.
  - How many variables to be transformed: 1, few and many?
  - Computations on each domain and their relative operations counts dictate how to distribute the data.
    - E.g., real-space computations are much less critical than the rest for turbulence or DFT and are ignored.
- HPC architectures are evolving and so are the optimal data distribution for a target problem: BG, XT, and PERCS

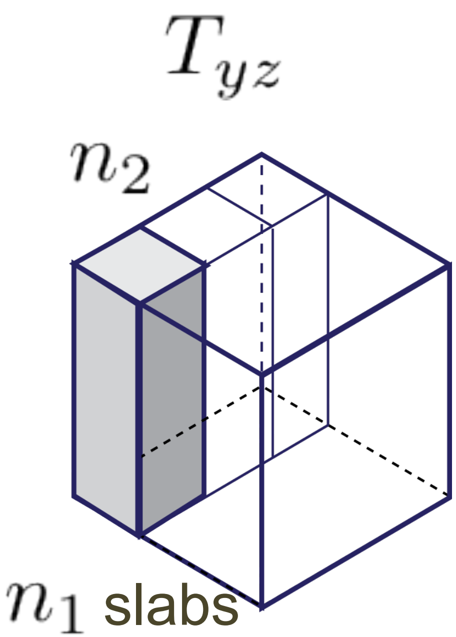
Parallel 3D FFT: data distribution over n_p PE



$n_p < N$ | $N < n_p < N^2$ | $N^2 < n_p$

What is n_p on BW? → more than 300 K cores; → about 10K SMP nodes

Pencil distribution using MPI: P3DFFT*



n_p MPI tasks with $n_p = n_1 n_2$

- Can exploit efficient 1D FFT on *N* elements of stride 1 by FFT libraries, e.g., ESSL, FFTW
- But, need to transpose the pencils twice

$$u(i,j,\underline{k}) \xrightarrow[T_{yz}]{} u(i,k,\underline{j}) \xrightarrow[T_{xy}]{} u(j,k,\underline{i})$$

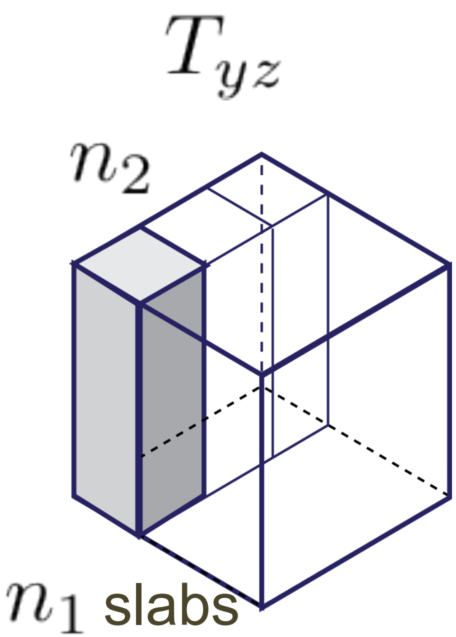
n_1 communicator groups (YZ slabs) of n_2 tasks

n_2 communicator groups (XY slabs) of n_1 tasks

Array syntax in C convention.

* P3DFFT library, http://code.google.com/p/p3dfft/, D. Pekurovsky, SDSC

Optimal distribution for clusters of SMPs: back to slabs



2D FFT on a SMP

$$u(i,j,\underline{k}) \underset{T_{yz}}{\longrightarrow} u(i,k,\underline{j}) \underset{T_{xy}}{\longrightarrow} u(j,k,\underline{i})$$

- BW's SMP node is powerful
  - 32 cores, > 64 GB memory
  - High memory bandwidth
  - A lot of threads : 128=4x32 threads
- 2D FFT on a SMP
  - MPI can be optimized to exploit SMPs
  - OpenMP (any threading) will work

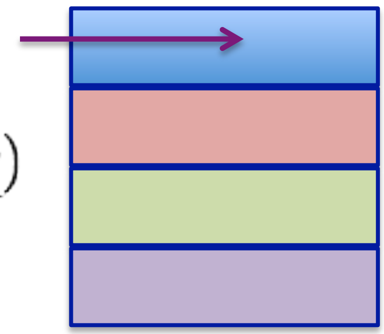
2DFFT on a SMP

- Use optimized 1DFFT: ESSL, FFTW, MKL
  - Multiple 1DFFTs: e.g., guru interface of FFTW
  - 20-50% of peak for N>1000
- On P7, analyze the performance of
  - PESSL: MPI reference implementation
  - ESSLSMP
  - MPI: alltoall implementation
  - OpenMP/TLS
  - OpenMP/Mix

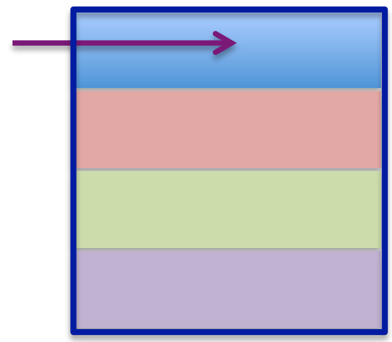
Memory access pattern of 2D FFT: no reordering

Distributed memory, OpenMP/TLS

$FFT(x,\underline{y})$



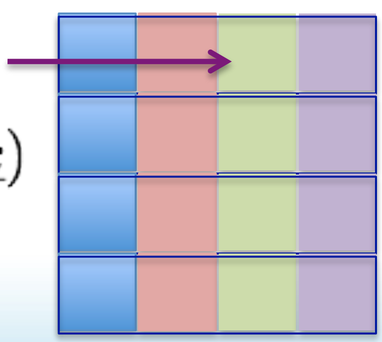
OpenMP/Mix

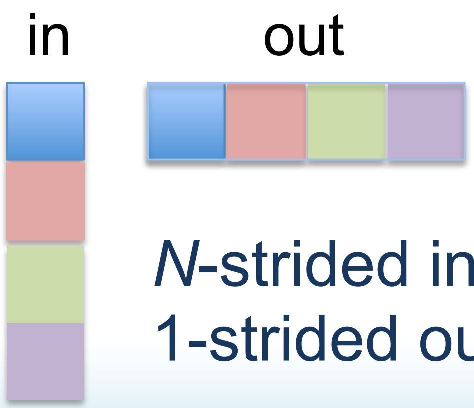


ESSPSMP

Transpose

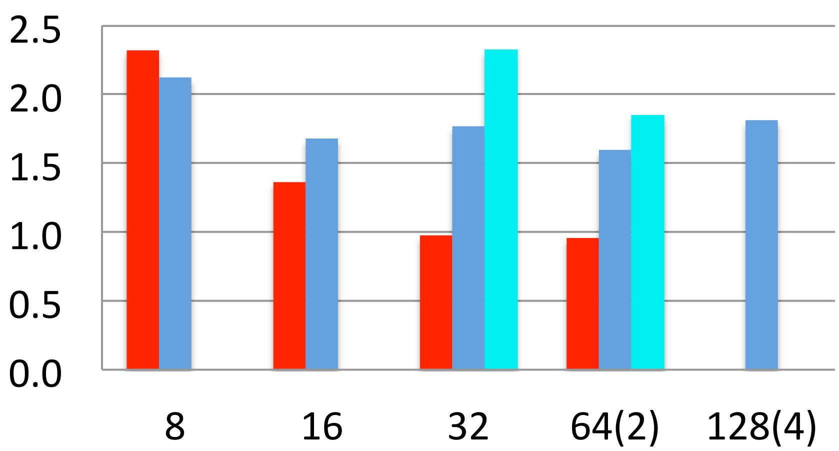
$FFT(y,\underline{x})$



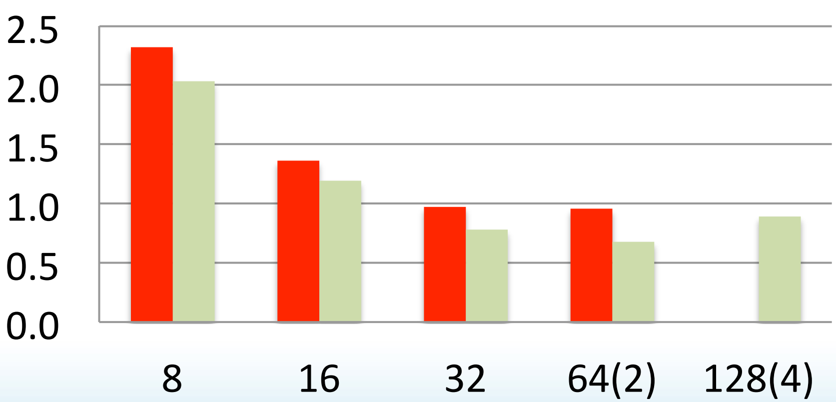


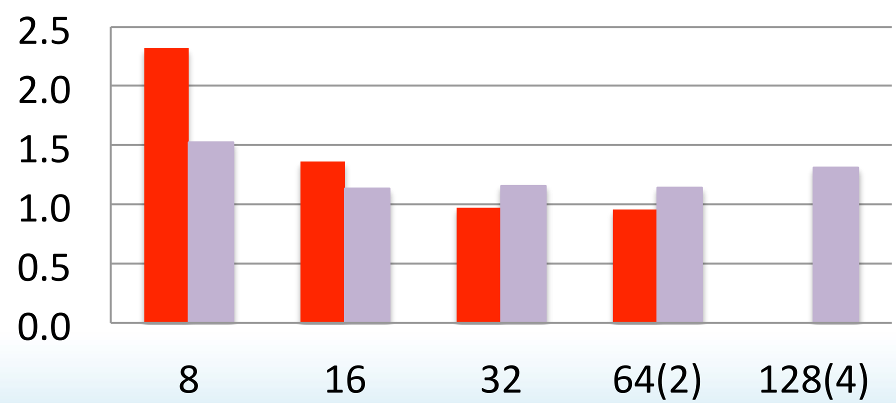
N-strided in,
1-strided out

Timing on BlueDrop: *N*=12288

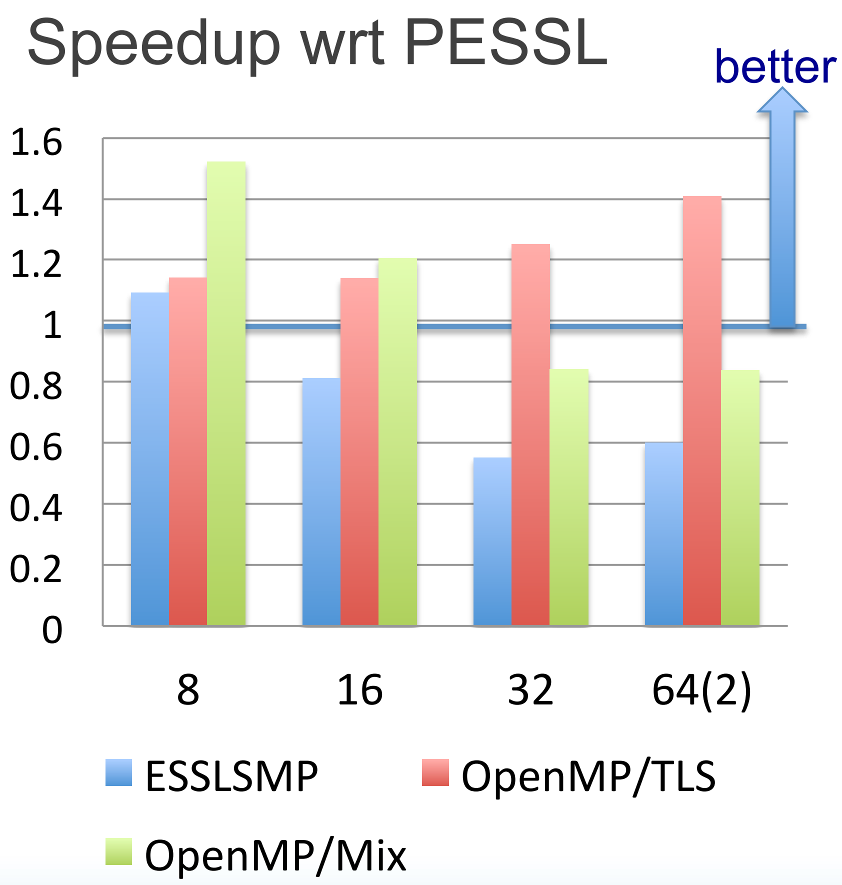


PESSL
ESSLSMP
MPI (not showing 8 and 16)
OpenMP/TLS Best
OpenMP/Mix





Effects of memory hierarchy of BlueDrop



- BD node: not a pure SMP but NUMA with two-level memory hierarchy

8 core – 16 core – 32 core
chip enclosure

- OpenMP/TLS & OpenMP/Mix outperform PESSL on a16-core enclosure
- OpenMP/TLS wins as the threads increase
- Similar trends with N=4096,6144,and 8192

Will OpenMP 2D FFT work on BW?

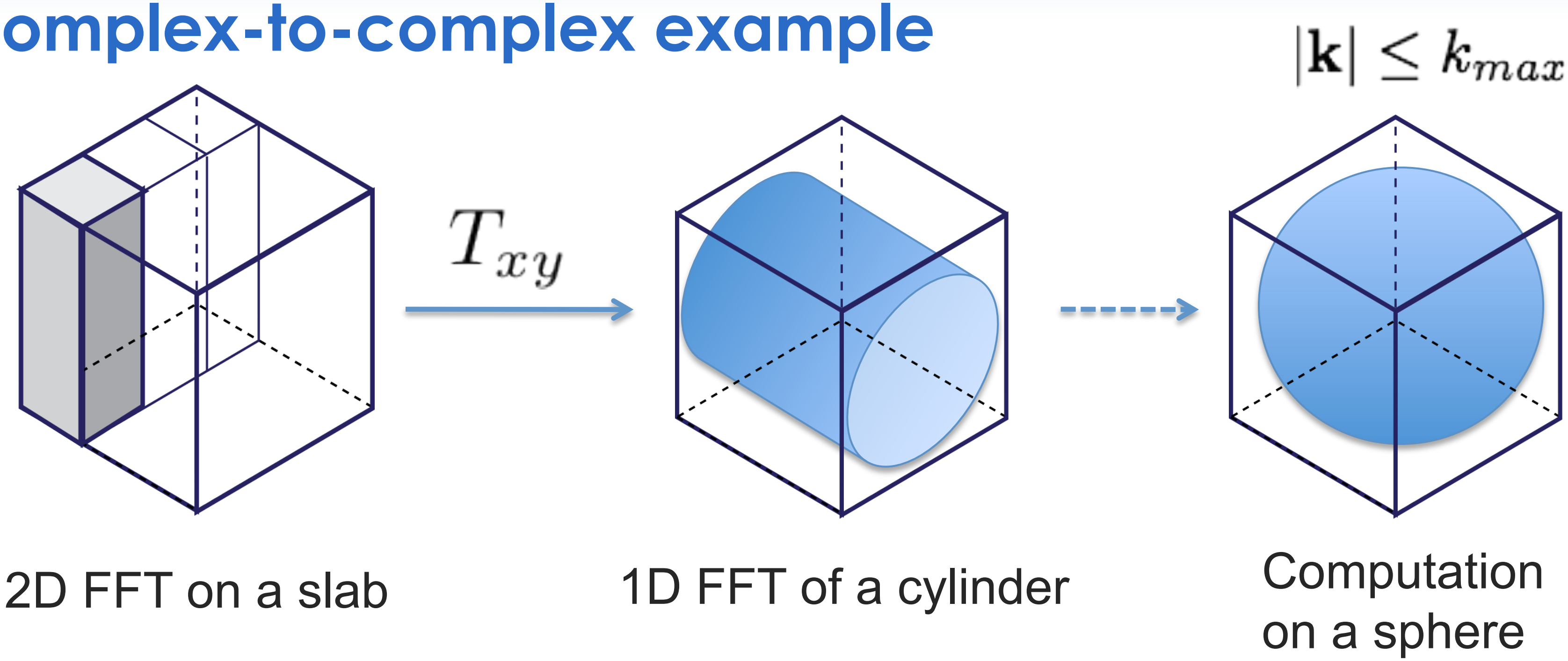
- Parallel execution of *N* 1DFFTs on *N* elements for *N* >> 1
- Some or all explicit memory copies can be eliminated.
  - 4 copies of naïve MPI : one or no copy with OpenMP
  - Possible to eliminate 2 copies with MPI with MPI_Datatype
- Memory and thread locality can be managed: OpenMP/TLS
- SMT 2/4 may further hide memory latency
- Synchronization not necessary

Yes, any threading model that exploits shared memory would work well on BW or clusters of SMPs.

2D FFT on IH-Drawer:
really early results and need NDA

- Nearly flat memory on a P7 node (*almost* perfect SMP)
  - OpenMP methods all outperform PESSL
  - OpenMP/Mix works best *so far*
  - ESSLSMP and OpenMP/TLS similar
  - PESSL scales beyond a node but 64-task on 64 cores is not better than OpenMP implementations on 32 cores
- OpenMP/TLS, most likely the method of choice
  - Can improve transpose using VSX/SSE and thread scheduling
  - Can hide NUMAness
  - Can perform multiple 2D FFTs simultaneously
  - Especially useful as a component of 3DFFT

Improvement of 3D FFT algorithm:
complex-to-complex example



Physics dictates and always de-aliasing imposed in applications

- Depending upon k_{max} , optimal data in the spectral space varies
- Often, real-to-complex and only half of a sphere needed

Common usecases of 3D FFT

Apps	N_v	N	Datatype	Spectral data
NAMD, LAMMPS	1	10^2-10^3	real	Cubic
DNS	~3	> 10^3	real	Cylinder
Qbox, OpenAtom	>> 1	> 10^2	real/complex	Sphere

for i $= 1 \cdots N_v$ **do**
    1D FFT $\mathbf{v}_i$ on z
    transpose on yz slab
    1D FFT $\mathbf{v}_i$ on y
    transpose on xy slab
    1D FFT $\mathbf{v}_i$ on x
end for

for i $= 1 \cdots N_v$ **do**
    2D FFT $\mathbf{v}_i$ on yz
    transpose on xy slab
    1D FFT $\mathbf{v}_i$ on x
end for

Blocking

2D FFT $\mathbf{V}$ on yz
transpose on xy slab
1D FFT $\mathbf{V}$ on x

???

My wish list for a parallel 3D FFT library

- Hybrid: threads on SMP and MPI-like over SMPs
- Allow maximum overlap
  - Non-blocking alltoall(v) on a team of SMPs
  - One-sided get from *M*-strided to *1*-strided data
- Portable: use optimized 1D FFT and maybe 2D FFT
- Allocators!!!
- Efficient APIs to access the data and memory layout
- Learn from FFTW and MKL and provide
  - Basic and “guru” APIs
  - APIs to tune the run-time variables, BUT auto-tuning and compile-time optimization much preferred

Conclusions

- 3D FFT in the era of clusters of SMPs
  - Back to slabs
  - Exploit shared memory and threads
- But, global communication (a.k.a. alltoall) ultimately limits the performance.
- Other related works
  - Takahashi (previous talk)
  - Chen *et al* (PKUFFT, 3D FFT on clusters of GPUs)
  - …