Adaptive Transpose Algorithms for Distributed Multicore Processors

John C. Bowman and Malcolm Roberts

University of Alberta and Université de Strasbourg

April 15, 2016

www.math.ualberta.ca/∼bowman/talks

Acknowledgement: Wendell Horton, Institute for Fusion Studies

Matrix Transposes

- The matrix transpose is an essential primitive of high-performance parallel computing.

Matrix Transposes

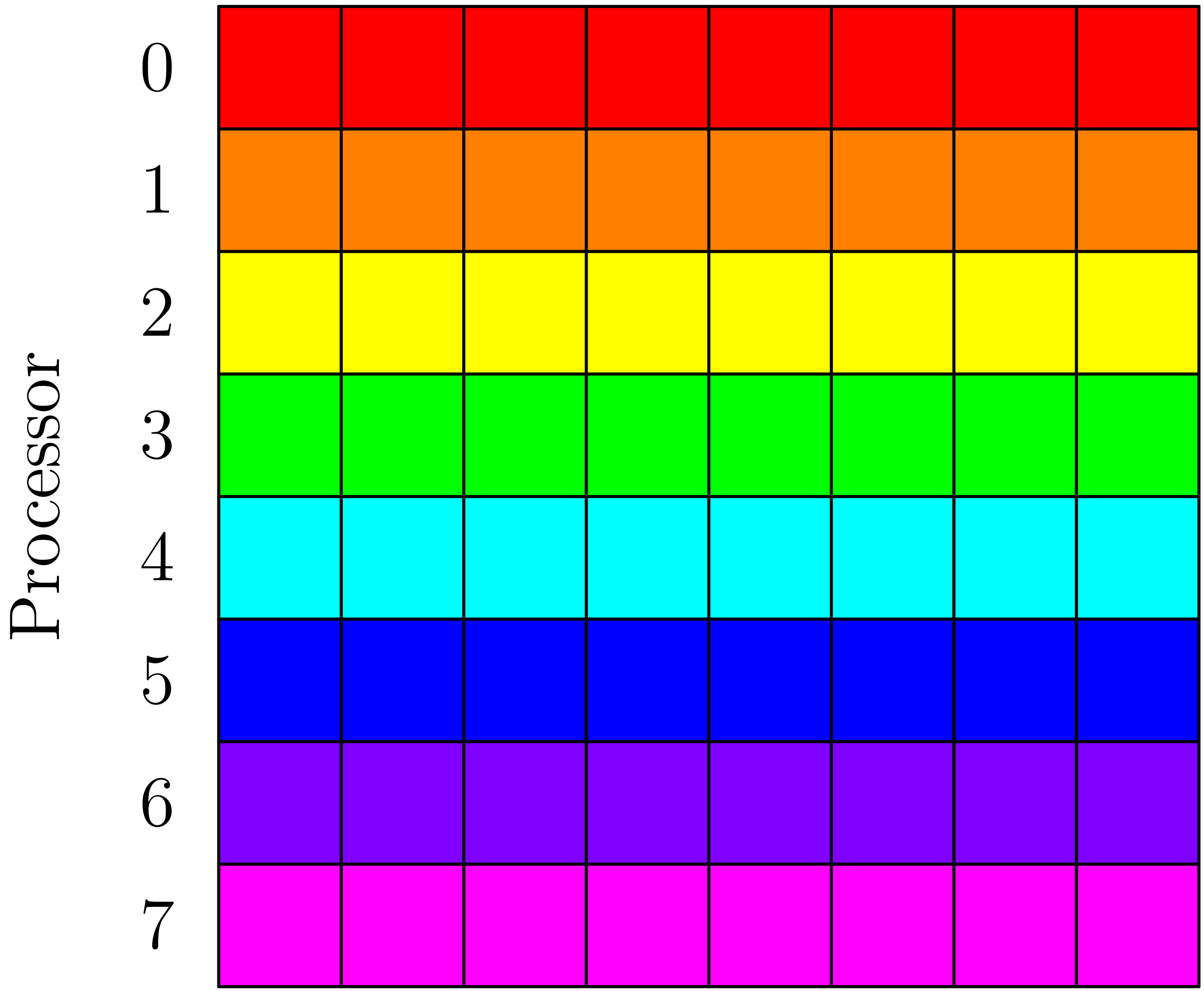
- The matrix transpose is an essential primitive of high-performance parallel computing.
- Transposes are used to localize the computation of multi-dimensional fast Fourier transforms onto individual processors.

- The performance of various transpose algorithms depends on:
  - communication bandwidth
  - communication latency
  - network congestion
  - communication packet size
  - local cache size
  - network topology

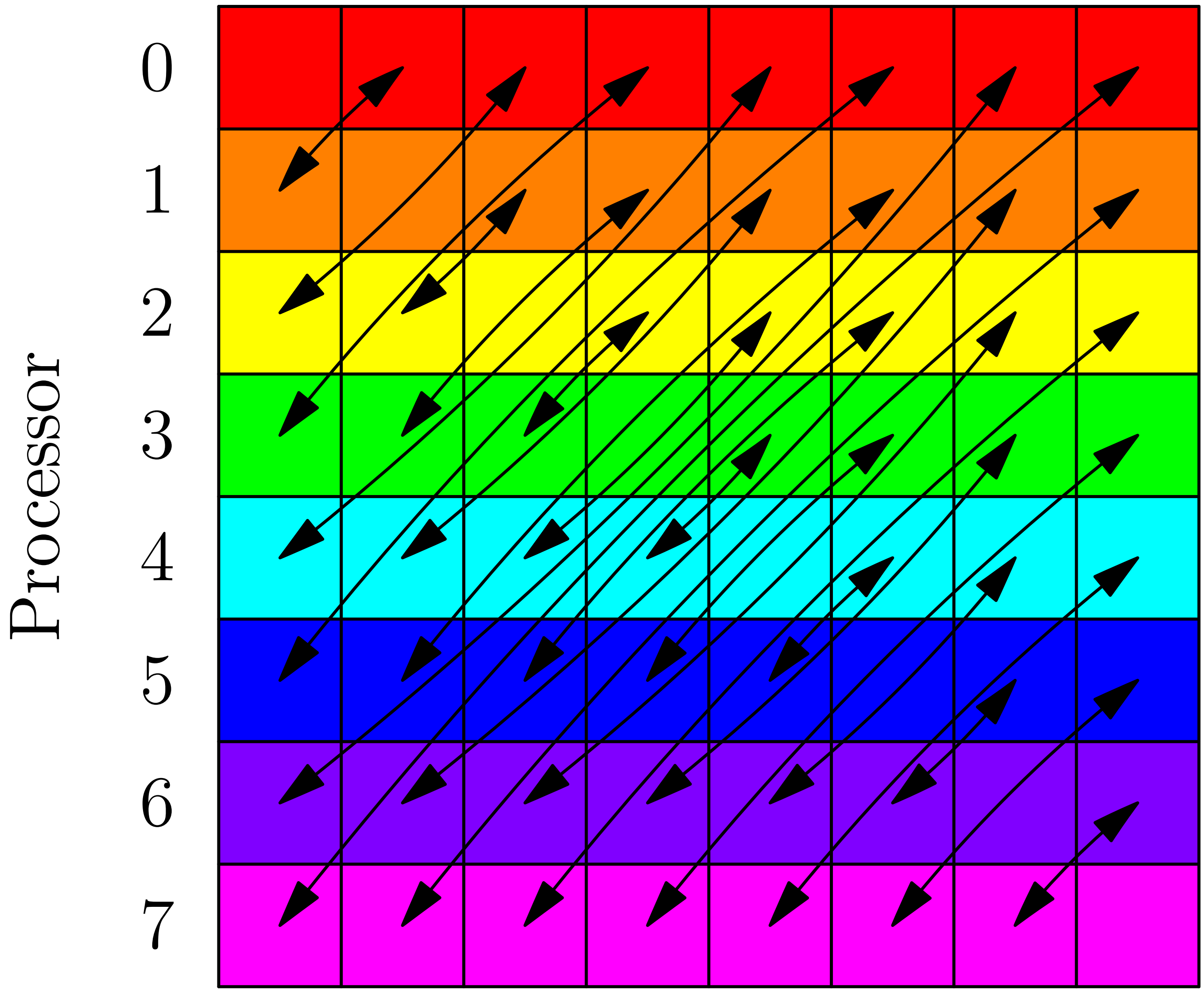
- The performance of various transpose algorithms depends on:
  - communication bandwidth
  - communication latency
  - network congestion
  - communication packet size
  - local cache size
  - network topology
- It is hard to estimate the relative importance of these factors at compilation time.

- The performance of various transpose algorithms depends on:
  - communication bandwidth
  - communication latency
  - network congestion
  - communication packet size
  - local cache size
  - network topology
- It is hard to estimate the relative importance of these factors at compilation time.
- An adaptive algorithm, dynamically tuned to take advantage of these specific architectural details, is desirable.

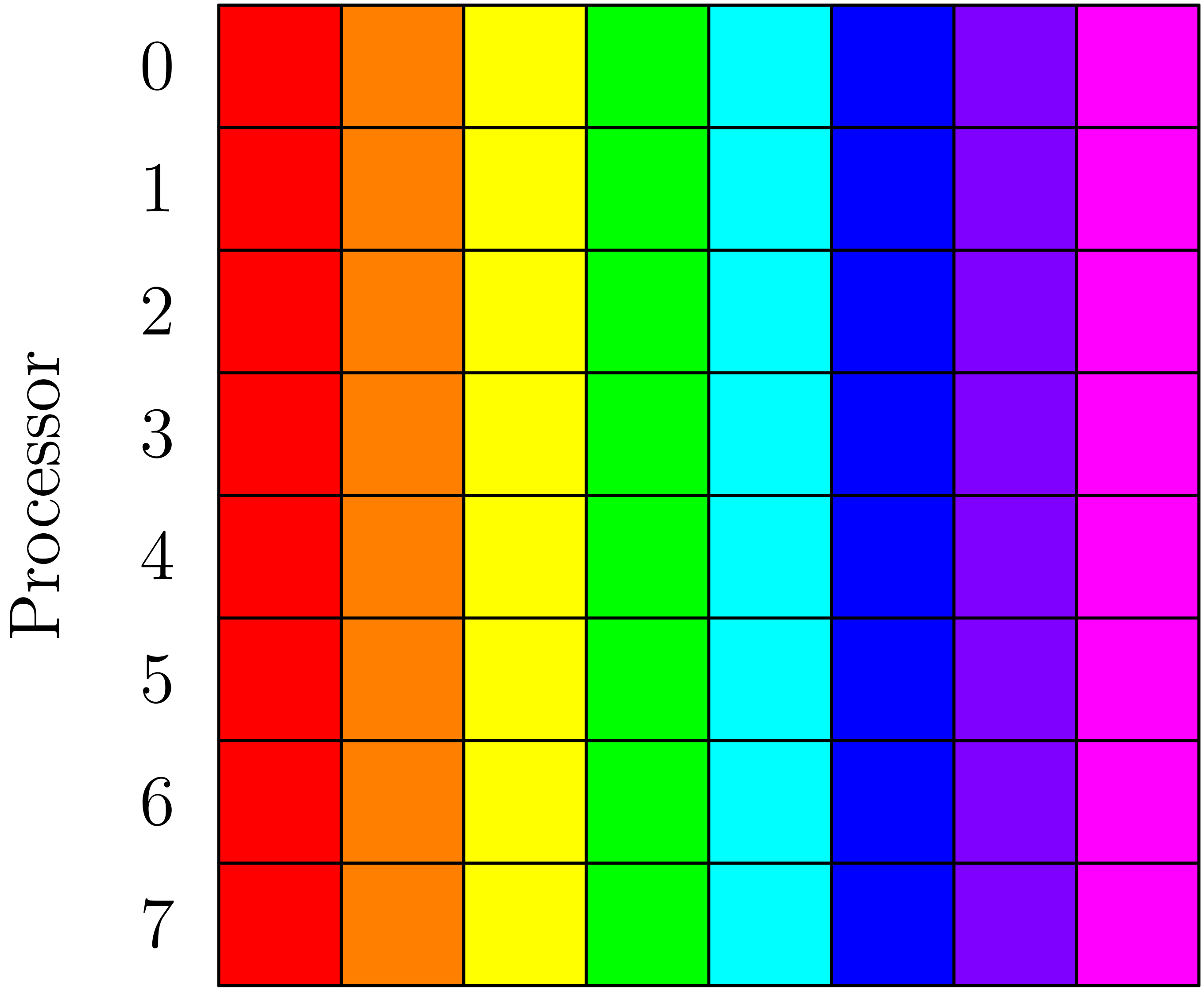
8×8 Matrix Transpose over 8 Processors



8×8 Matrix Transpose over 8 Processors



8×8 Matrix Transpose over 8 Processors



Direct (All-to-All)

- Advantages:
  - efficient for $N \gg P$ (large messages);
  - most direct.

Direct (All-to-All)

- Advantages:
  - efficient for $N \gg P$ (large messages);
  - most direct.
- Disadvantages:
  - many small message sizes when $P \geq N$.

Direct (All-to-All)

- Advantages:
  - efficient for $N \gg P$ (large messages);
  - most direct.
- Disadvantages:
  - many small message sizes when $P \geq N$.
- Implementation:
  - `MPI_ALLTOALL`, `MPI_SEND`/`MPI_RECV`.

Recursive (Butterfly)

- Advantages:
  - efficient for $N \ll P$ (small messages);
  - recursively subdivides transpose into smaller block transposes;
  - $\log N$ phases;
  - groups messages together to reduce communication latency.

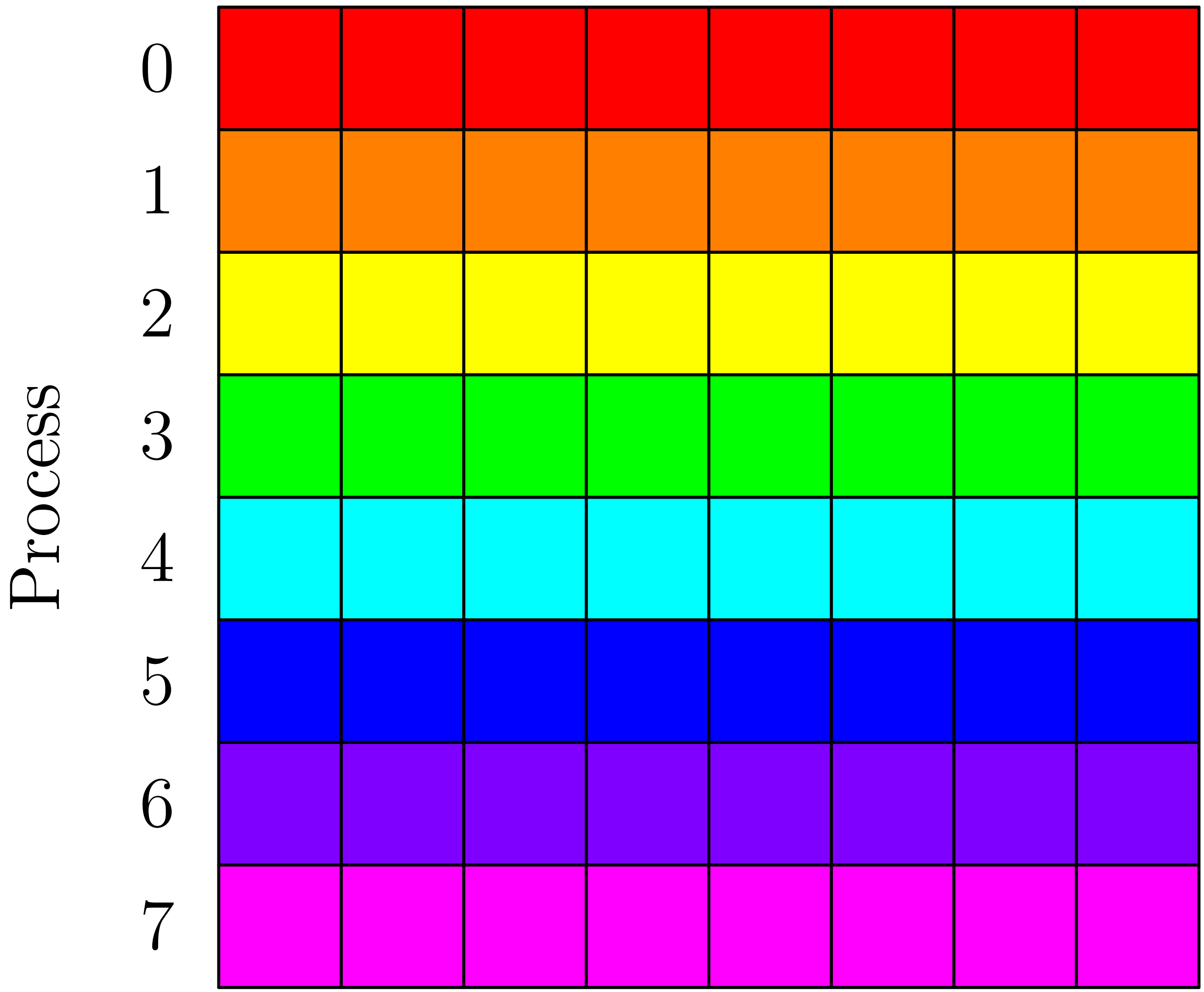
Recursive (Butterfly)

- Advantages:
  - efficient for $N \ll P$ (small messages);
  - recursively subdivides transpose into smaller block transposes;
  - $\log N$ phases;
  - groups messages together to reduce communication latency.
- Disadvantages:
  - requires intermediate communications.

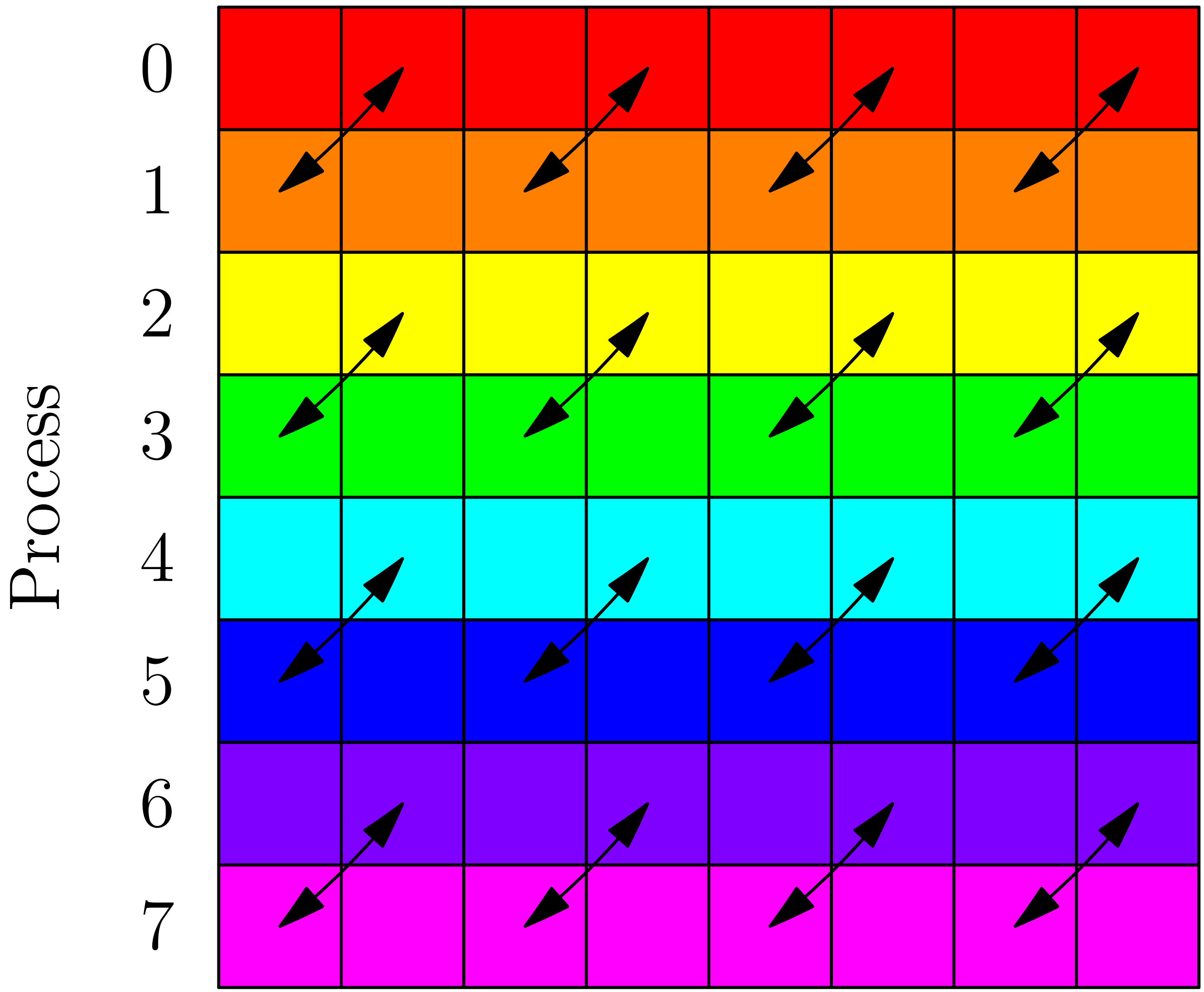
Recursive (Butterfly)

- Advantages:
  - efficient for $N \ll P$ (small messages);
  - recursively subdivides transpose into smaller block transposes;
  - $\log N$ phases;
  - groups messages together to reduce communication latency.
- Disadvantages:
  - requires intermediate communications.
- Implementation:
  - FFTW

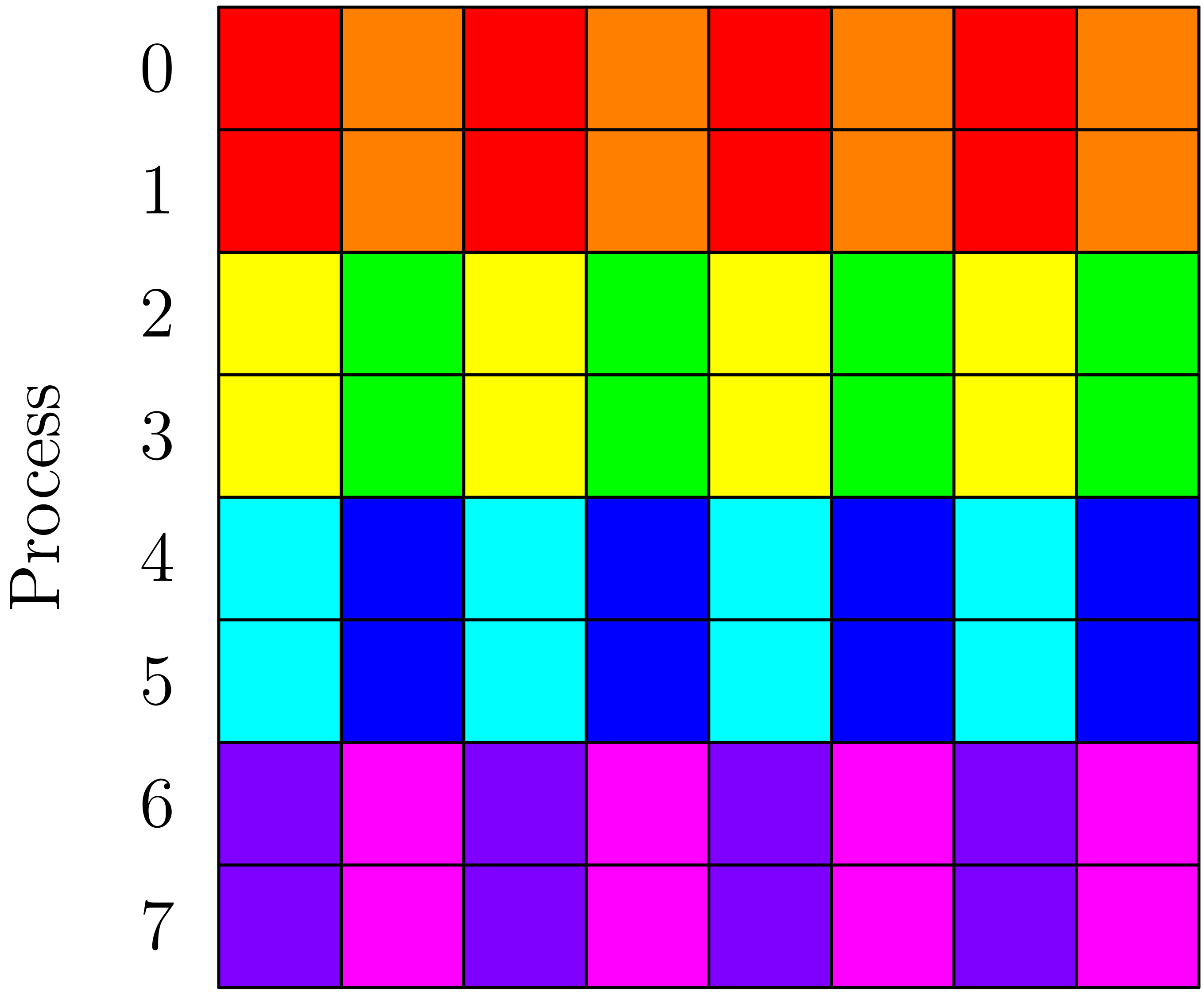
8×8 Block Transpose over 8 processors



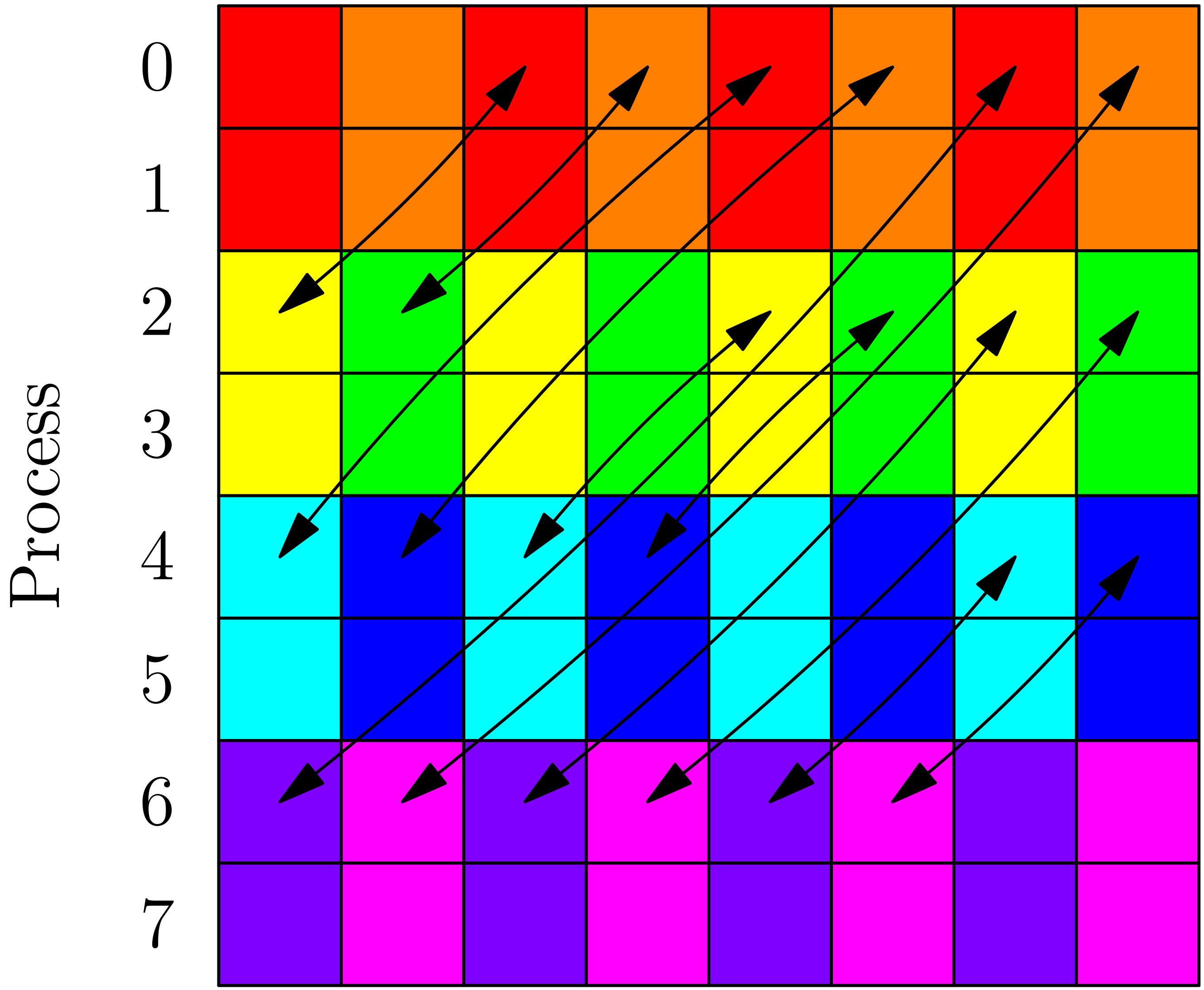
8×8 Block Transpose over 8 processors



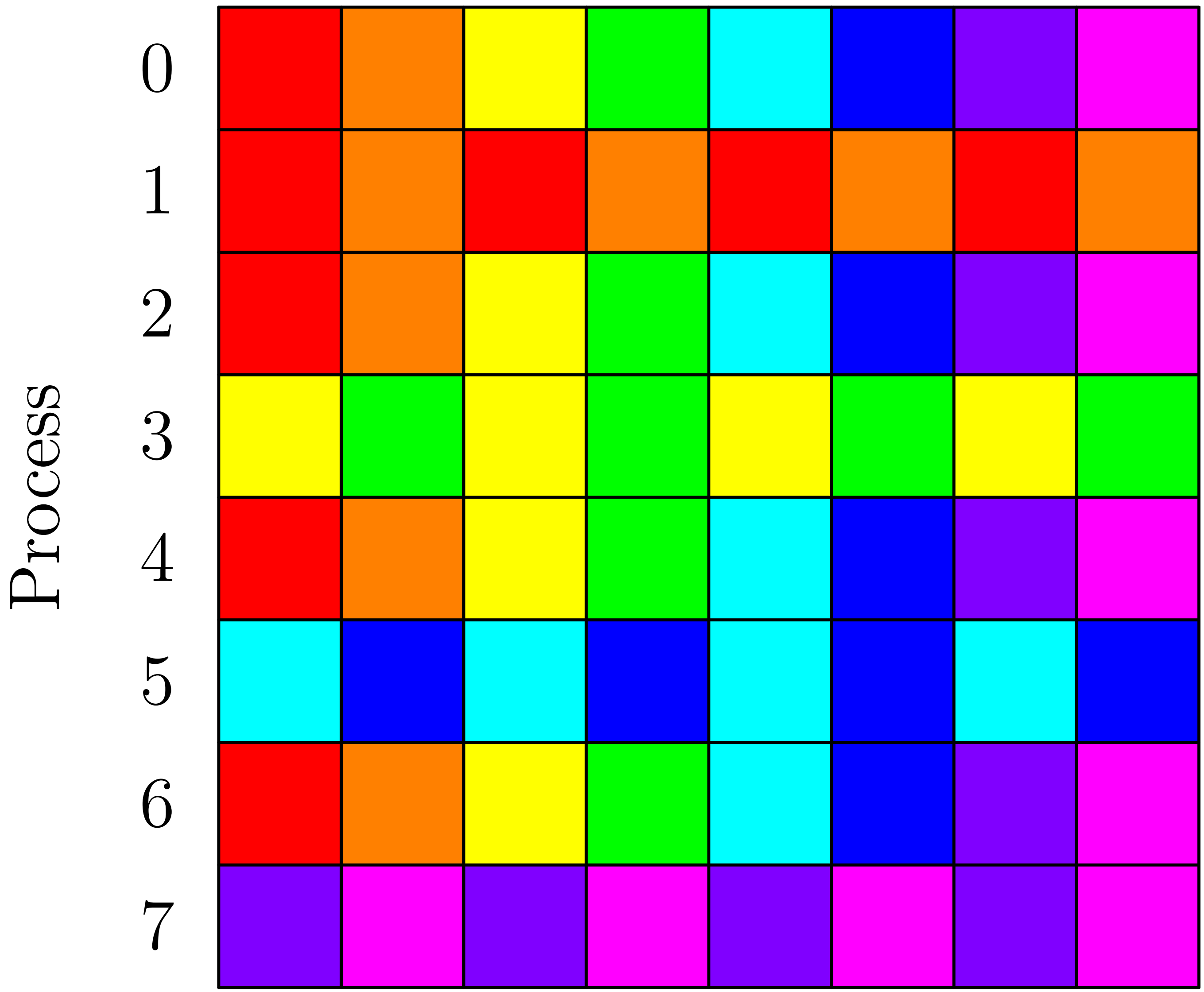
8×8 Block Transpose over 8 processors



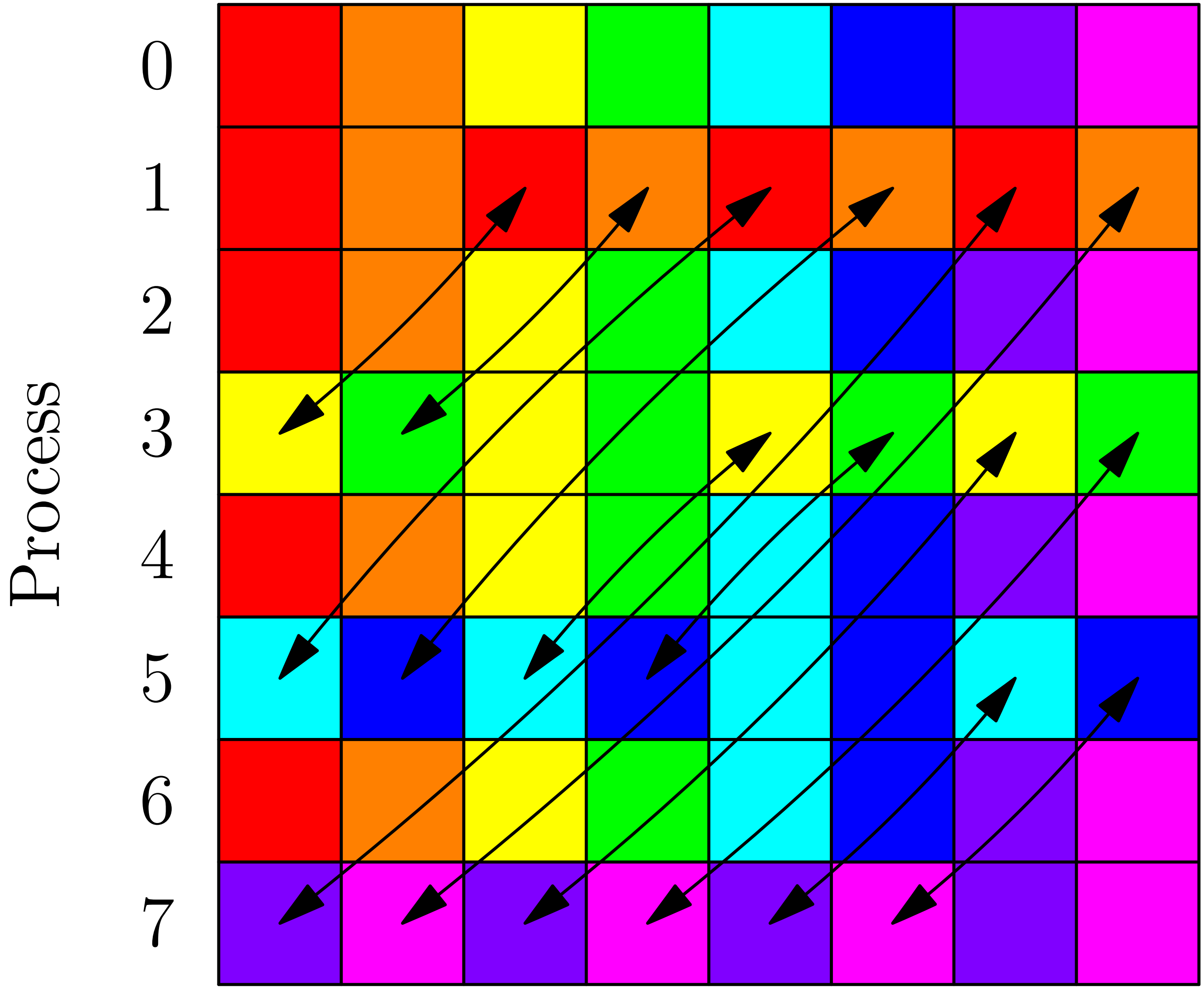
8×8 Block Transpose over 8 processors



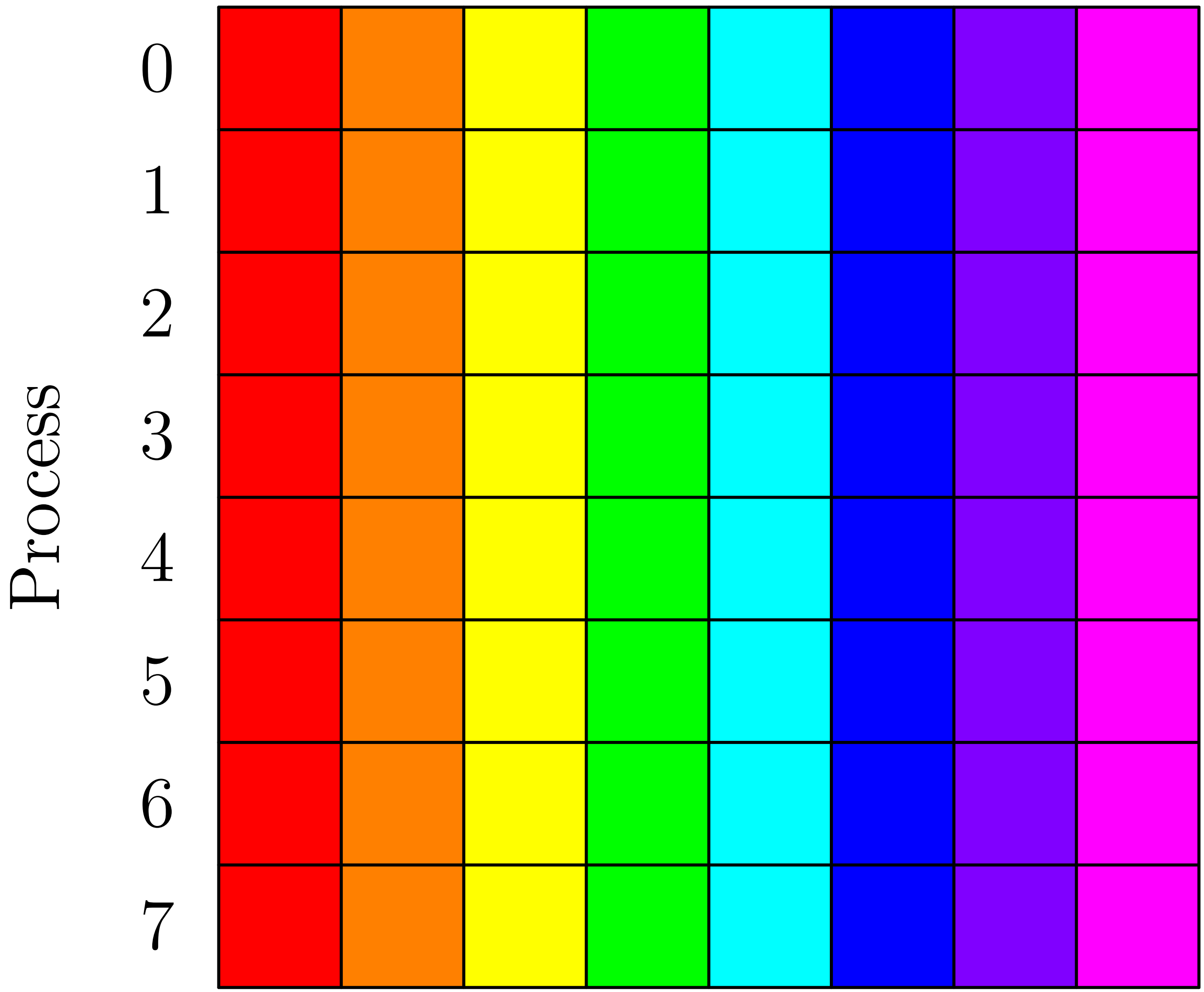
8×8 Block Transpose over 8 processors



8×8 Block Transpose over 8 processors



8×8 Block Transpose over 8 processors



Adaptive

- Advantages:

  – best of both worlds

  – uses subdivision at highest level to increase communication block size;

  – *optimally* groups messages together to reduce communication latency.

  – directly communicates several sub-blocks at a time.

Adaptive

- Advantages:
  - best of both worlds
  - uses subdivision at highest level to increase communication block size;
  - *optimally* groups messages together to reduce communication latency.
  - directly communicates several sub-blocks at a time.
- Implementation:
  - FFTW (sub-optimal), FFTW++ (quasi-optimal).

Hybrid Parallel Architectures (nodes $\times$ threads)

- Advantages:
  - MPI between nodes / OpenMP within node;
  - exploits modern multicore architectures;
  - many algorithms can use memory striding to avoid local transposition within a node;
  - compatible with modern trend of less memory/core;

Hybrid Parallel Architectures (nodes $\times$ threads)

- Advantages:
  - MPI between nodes / OpenMP within node;
  - exploits modern multicore architectures;
  - many algorithms can use memory striding to avoid local transposition within a node;
  - compatible with modern trend of less memory/core;
- Disadvantages:
  - requires both OpenMP and MPI support.

Communication Costs: Direct Transpose

- Suppose an $N \times N$ matrix is distributed over P processes with $P \mid N$.

Communication Costs: Direct Transpose

- Suppose an $N \times N$ matrix is distributed over P processes with $P \mid N$.
- Direct transposition involves $P - 1$ communications per process, each of size N^2/P^2, for a total per-process data transfer of

$$\frac{P-1}{P^2}N^2.$$

Block Transpose

- Let $P = ab$. Subdivide $N \times M$ matrix into $a \times a$ blocks each of size $N/a \times M/a$.

Block Transpose

- Let $P = ab$. Subdivide $N \times M$ matrix into $a \times a$ blocks each of size $N/a \times M/a$.

- Inner: Over each team of b processes, transpose the a individual $N/a \times M/a$ matrices, grouping all a communications with the same source and destination together.

  – Requires b communications per process, each of size $(NM/a)/b^2 = aNM/P^2$, for a total per-process data transfer of $(b-1)aNM/P^2$.

Block Transpose

- Let $P = ab$. Subdivide $N \times M$ matrix into $a \times a$ blocks each of size $N/a \times M/a$.

- Inner: Over each team of b processes, transpose the a individual $N/a \times M/a$ matrices, grouping all a communications with the same source and destination together.

  – Requires b communications per process, each of size $(NM/a)/b^2 = aNM/P^2$, for a total per-process data transfer of $(b-1)aNM/P^2$.

- Outer: Over each team of a processes, transpose the $a \times a$ matrix of $N/a \times M/a$ blocks.

  – Requires a communications per process, each of size $(NM/b)/a^2 = bNM/P^2$, for a total per-process data transfer of $(a-1)bNM/P^2$.

Communication Costs

- Let τ_ℓ be the typical latency of a message and τ_d be the time required to send each matrix element, so that the time to send a message consisting of n matrix elements is

$$\tau_\ell + n\tau_d$$

.

Communication Costs

- Let τ_ℓ be the typical latency of a message and τ_d be the time required to send each matrix element, so that the time to send a message consisting of n matrix elements is

$$\tau_\ell + n\tau_d$$

.

- The time required to perform a direct transpose is

$$T_D = \tau_\ell(P-1) + \tau_d \frac{P-1}{P^2} NM = (P-1)\left(\tau_\ell + \tau_d \frac{NM}{P^2}\right),$$

whereas a block transpose requires

$$T_B(a) = \tau_\ell\left(a + \frac{P}{a} - 2\right) + \tau_d\left(2P - a - \frac{P}{a}\right)\frac{NM}{P^2}.$$

Communication Costs

- Let τ_ℓ be the typical latency of a message and τ_d be the time required to send each matrix element, so that the time to send a message consisting of n matrix elements is

$$\tau_\ell + n\tau_d$$

.

- The time required to perform a direct transpose is

$$T_D = \tau_\ell(P-1) + \tau_d \frac{P-1}{P^2} NM = (P-1)\left(\tau_\ell + \tau_d \frac{NM}{P^2}\right),$$

whereas a block transpose requires

$$T_B(a) = \tau_\ell\left(a + \frac{P}{a} - 2\right) + \tau_d\left(2P - a - \frac{P}{a}\right)\frac{NM}{P^2}.$$

- Let $L = \tau_\ell/\tau_d$ be the effective communication block length.

Direct vs. Block Transposes

- Since

$$T_D - T_B = \tau_d \left(P + 1 - a - \frac{P}{a} \right) \left(L - \frac{NM}{P^2} \right),$$

we see that a direct transpose is preferred when $NM \geq P^2 L$, whereas a block transpose should be used when $NM < P^2 L$.

Direct vs. Block Transposes

- Since

$$T_D - T_B = \tau_d \left(P + 1 - a - \frac{P}{a} \right) \left(L - \frac{NM}{P^2} \right),$$

  we see that a direct transpose is preferred when $NM \geq P^2 L$, whereas a block transpose should be used when $NM < P^2 L$.

- To find the optimal value of a for a block transpose consider

$$T_B'(a) = \tau_d \left(1 - \frac{P}{a^2} \right) \left(L - \frac{NM}{P^2} \right).$$

Direct vs. Block Transposes

- Since

$$T_D - T_B = \tau_d \left(P + 1 - a - \frac{P}{a} \right) \left(L - \frac{NM}{P^2} \right),$$

  we see that a direct transpose is preferred when $NM \geq P^2 L$, whereas a block transpose should be used when $NM < P^2 L$.

- To find the optimal value of a for a block transpose consider

$$T_B'(a) = \tau_d \left(1 - \frac{P}{a^2} \right) \left(L - \frac{NM}{P^2} \right).$$

- For $NM < P^2 L$, we see that T_B is convex, with a minimum at $a = \sqrt{P}$.

Optimal Number of Threads

- The minimum value of T_B is

$$\begin{aligned} T_B(\sqrt{P}) &= 2\tau_d\left(\sqrt{P}-1\right)\left(L+\frac{NM}{P^{3/2}}\right) \\ &\sim 2\,\tau_d\sqrt{P}\left(L+\frac{NM}{P^{3/2}}\right), \qquad P \gg 1. \end{aligned}$$

Optimal Number of Threads

- The minimum value of T_B is

$$T_B(\sqrt{P}) \;=\; 2\tau_d\left(\sqrt{P}-1\right)\left(L+\frac{NM}{P^{3/2}}\right)$$
$$\sim 2\,\tau_d\sqrt{P}\left(L+\frac{NM}{P^{3/2}}\right), \qquad P \gg 1.$$

- The global minimum of T_B over both a and P occurs at

$$P \approx (2NM/L)^{2/3}.$$

Optimal Number of Threads

- The minimum value of T_B is

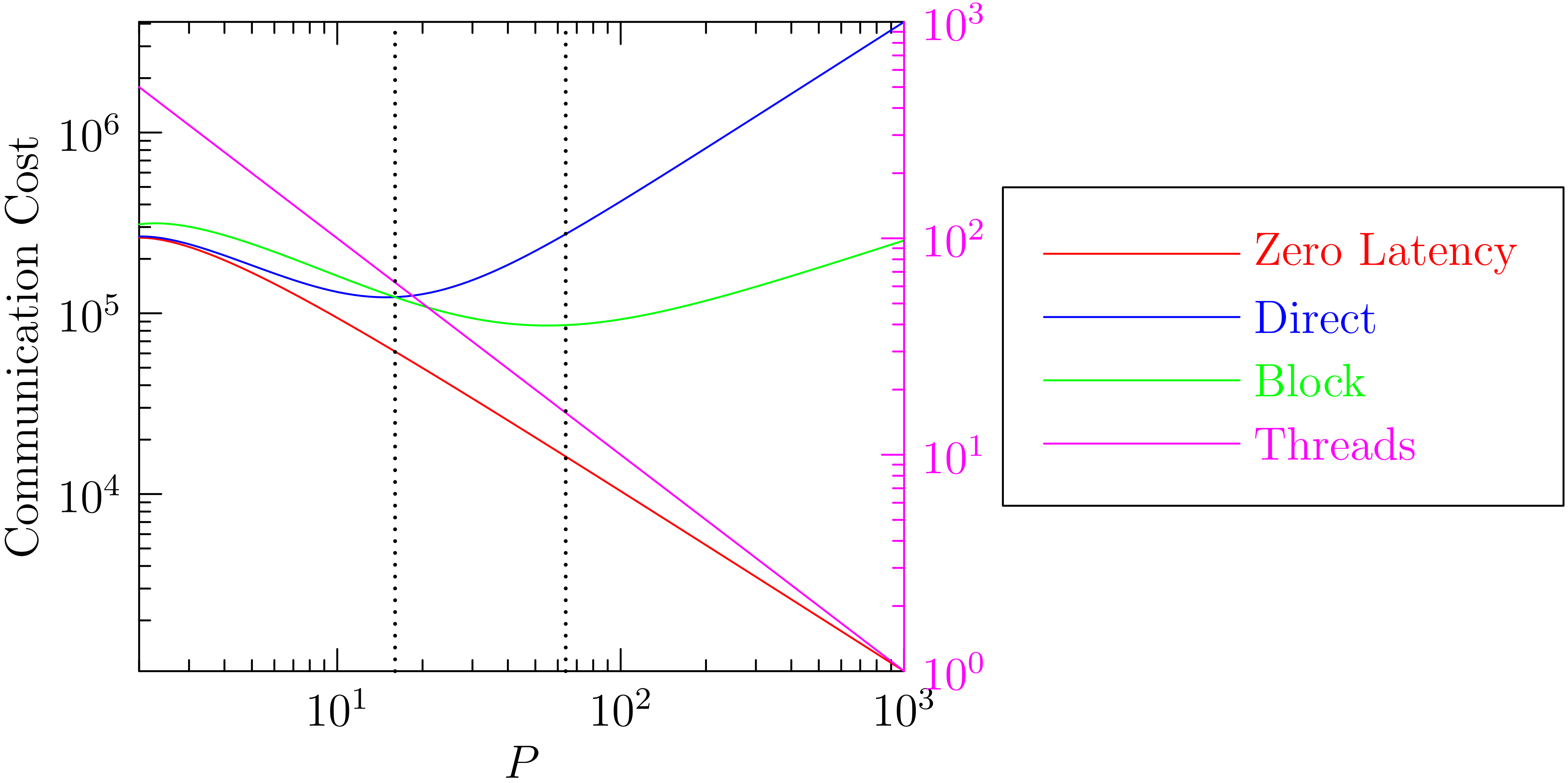
$$\begin{aligned} T_B(\sqrt{P}) &= 2\tau_d\left(\sqrt{P}-1\right)\left(L+\frac{NM}{P^{3/2}}\right) \\ &\sim 2\,\tau_d\sqrt{P}\left(L+\frac{NM}{P^{3/2}}\right), \qquad P \gg 1. \end{aligned}$$

- The global minimum of T_B over both a and P occurs at

$$P \approx (2NM/L)^{2/3}.$$

- If the matrix dimensions satisfy $NM > L$, as is typically the case, this minimum occurs above the transition value $(NM/L)^{1/2}$.

Transpose Communication Costs



Implementation

- Choose optimal block size b that minimizes effects of communication latency.

Implementation

- Choose optimal block size b that minimizes effects of communication latency.

- Use hybrid OpenMPI/MPI with the optimal number of threads:

  – yields larger communication block size;

  – local transposition is not required within a single MPI node;

  – allows smaller problems to be distributed over a large number of processors;

  – for 3D FFTs, allows for more slab-like than pencil-like models, reducing the size of or even eliminating the need for a second transpose.

Implementation

- Choose optimal block size b that minimizes effects of communication latency.
- Use hybrid OpenMPI/MPI with the optimal number of threads:

  – yields larger communication block size;

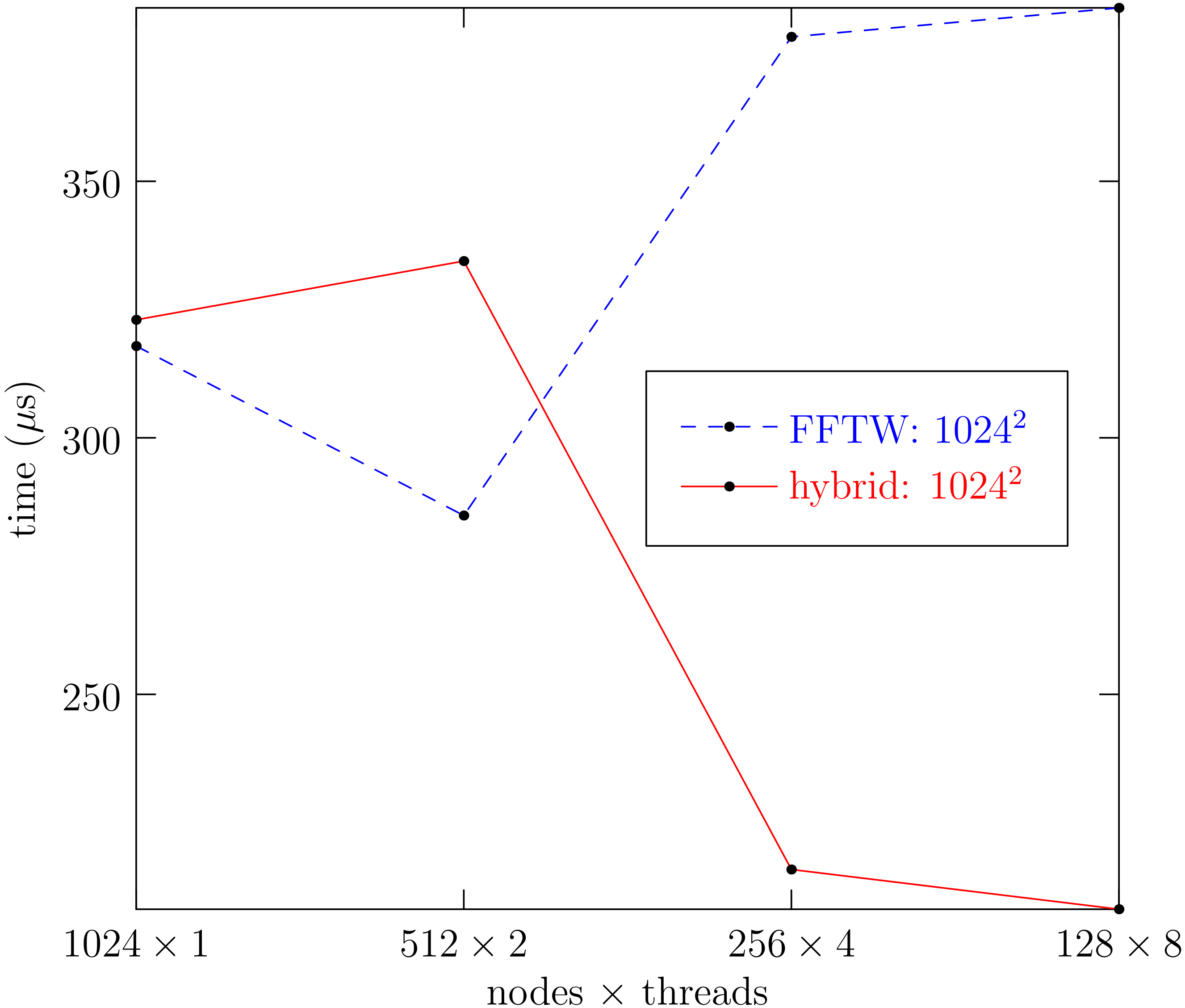
  – local transposition is not required within a single MPI node;

  – allows smaller problems to be distributed over a large number of processors;

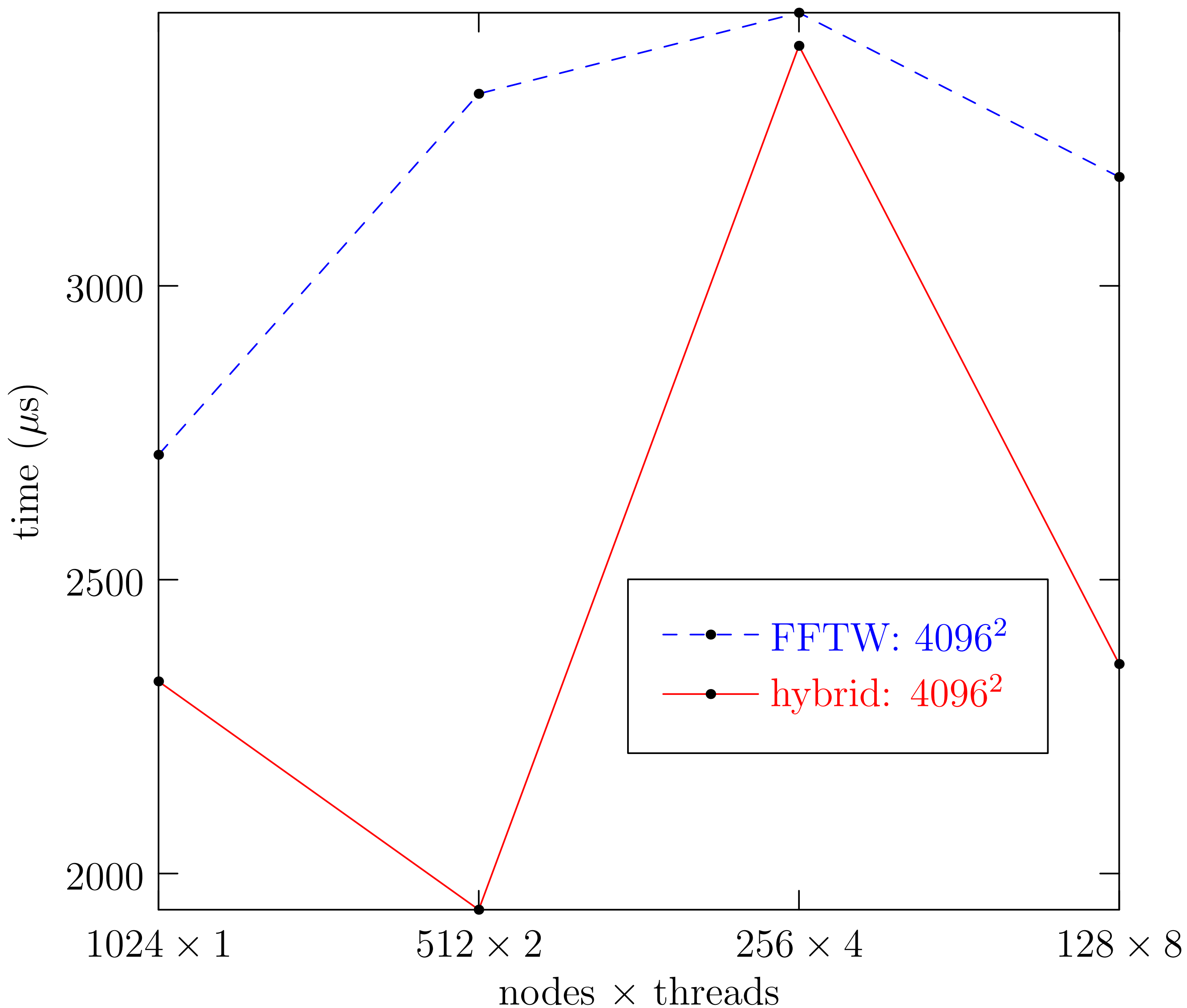
  – for 3D FFTs, allows for more slab-like than pencil-like models, reducing the size of or even eliminating the need for a second transpose.

- The use of nonblocking MPI communications allows us to overlap computation with communication: this can yield an additional 10–30% performance gain for 3D convolutions.

1024×1024 Transpose over 1024 Processors



4096×4096 Transpose over 4096 Processors



Applications

- FFT in 2 & higher dimensions

Applications

- FFT in 2 & higher dimensions
- Pseudospectral Collocation
  - Explicit Dealiasing via Zero Padding
  - Implicit Dealiasing

Conclusions

- Hybrid MPI/OpenMP is often more efficient than pure MPI for distributed matrix transposes.

Conclusions

- Hybrid MPI/OpenMP is often more efficient than pure MPI for distributed matrix transposes.

- The hybrid paradigm provides an optimal setting for nonlocal computationally intensive operations found in applications like the fast Fourier transform.

Conclusions

- Hybrid MPI/OpenMP is often more efficient than pure MPI for distributed matrix transposes.
- The hybrid paradigm provides an optimal setting for nonlocal computationally intensive operations found in applications like the fast Fourier transform.
- The advent of implicit dealiasing of convolutions makes overlapping transposition with FFT computation feasible.

References

[Bowman & Roberts 2011] J. C. Bowman & M. Roberts, SIAM J. Sci. Comput., **33**:386, 2011.