OpenFFT: An Open-Source Package for 3-D FFTs with Minimal Volume of Communication

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1. Adaptive decomposition
- Translate the multi-dimensional data into one-dimensional data, and divide the resultant one-dimensional data equally to the processes using a block distribution.
- Treat the dimensions in a specific order: abc, cba, bca, etc.
- Decompose in the lowest possible dimensions depending on the number of processes.

2. Transpose-order awareness
- The adaptive decomposition provides plenty of transpose orders.
- Different order results in different volumes of communication.
- Choosing a proper order reduces the volume of communication.

3. Transpose order and volume of communication
- $(M!-1)! M$ transpose orders for $M$-dimensional FFTs.
- 8, 1296, and 7962624 transpose orders for 3-D, 4-D, and 5-D FFTs, respectively.
- Analyses of the volume are computationally performed.

Summary
Our OpenFFT package
- Adaptive decomposition + Transpose-order awareness.
- Decompose in the lowest dimensions, and follow the most communication-efficient transpose orders.
- Numerical results show good performance and scaling property.
- Freely available at http://www.openmx-square.org/openfft

Future work
- Extend our implementation to M-D FFTs.

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References