Parallel Optimization Methods for Direct Numerical Simulation of High Reynolds Number Wall Turbulence with a Grid Size of 100 Billion

Jiabin Xie, Guangnan Feng, Han Huang, Junxuan Feng, Yutong Lu*

中山大學 SUN YAT-SEN UNIVERSITY

国家超级计算广州中心 NATIONAL SUPERCOMPUTER CENTER IN GUANGZHOU

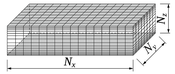
Abstract

Direct numerical simulation (DNS) is a technique that directly solves the fluid Navier-Stokes equations with high spatial and temporal resolutions. However, its utility in studying high Reynolds number (*Re*) wall turbulence of particular interest is limited by the rapidly growing grid size (i.e., the memory and computation requirement) with Re^3.

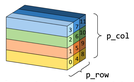
We present PowerLLEL, a high-performance finite difference solver tailored for the challenging DNS of incompressible wall turbulence at extreme scales. An adaptive multi-level parallelization strategy is proposed to fully exploit the multi-level parallelism of various architectures and enhance computational performance. The communication performance of global transpose and halo exchange is significantly improved by a tridiagonal solver based on the parallel diagonal dominant (PDD) algorithm and three RDMA-implemented communication optimizations.

Strong scaling tests on the Tianhe-2A supercomputer show that PowerLLEL achieves nearly 92% parallel efficiency with up to 31,104 cores on a grid size of 143.3 billion.

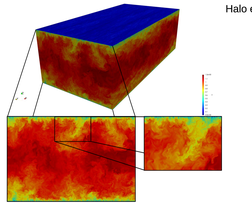
Background



Computational domain and grid



2D domain decomposition (p_row×p_col MPI ranks)

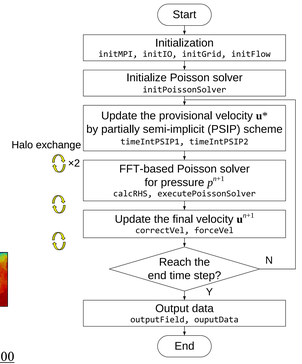


Turbulent channel flow at $Re_\tau \approx 5200$ (25.8 B grid size)

$$\nabla \cdot \mathbf{u} = 0$$

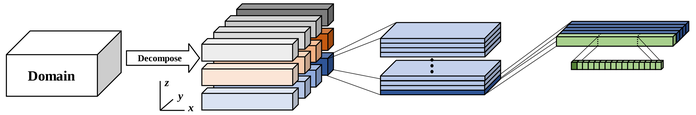
$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} = -\nabla p + \frac{1}{\mathrm{Re}} \nabla^2 \mathbf{u}$$

Navier-Stokes equation



Algorithm flowchart

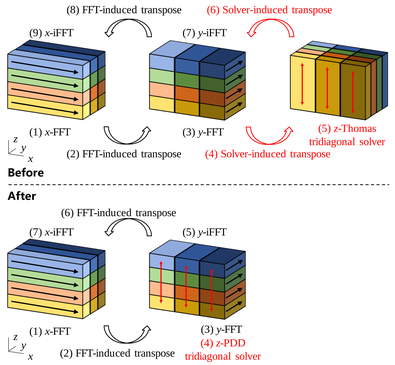
Optimization 1: Multi-level Parallelization Strategy



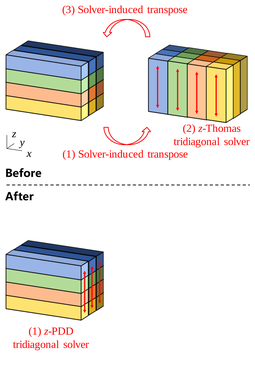
Decomposed domain:	**Pencil**	**Slab/Sub-pencil**	**X-segment**
	⇕	⇕	⇕
Programming model:	**Process**	**Thread**	**SIMD**
	⇕	⇕	⇕
Architecture:	**Device**	**Processor**	**Compute Unit**

Decomposed domain	Programming model - Architecture	CPU	MT-3000	Sunway 26010Pro
Pencil	Process - Device	MPI - Processor	MPI - Acc Zone	MPI - Core-group
Slab/Sub-pencil	Thread - Processor	OpenMP/pthread - Core	hthreads - Acc Array	Athread - CPE
X-segment	SIMD - Compute Unit	SIMD - SIMD Unit	SIMD - Acc Cores	SIMD - SIMD Unit

Optimization 2: PDD-based Tridiagonal Solver

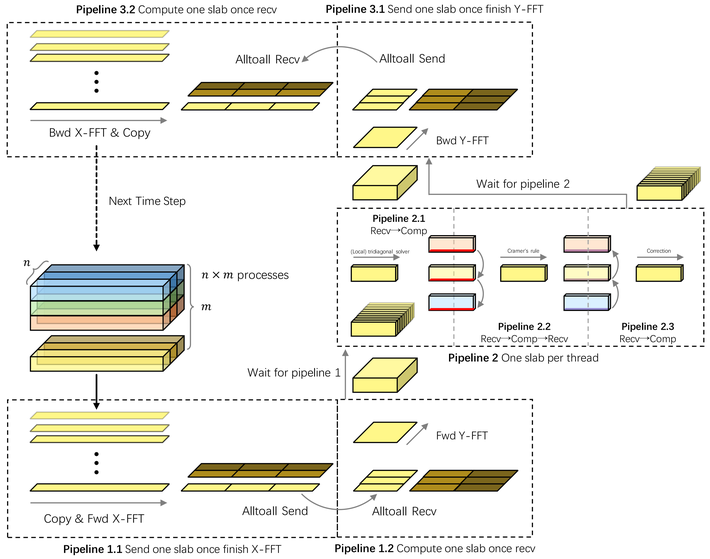


Optimization 3.1: Application of the PDD-based tridiagonal solver to the pressure Poisson solver

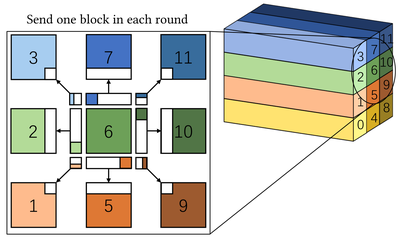


Optimization3.2: Application of the PDD-based tridiagonal solver to the PSIP step

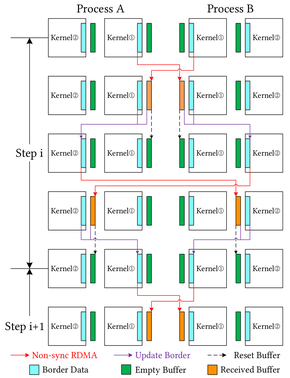
Optimization 3: RDMA-based Communication



Optimization 4.1: Pipeline Overlap

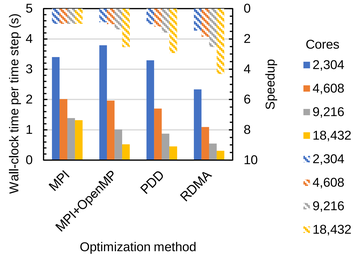


Optimization 4.2: Round-robin Halo Exchange

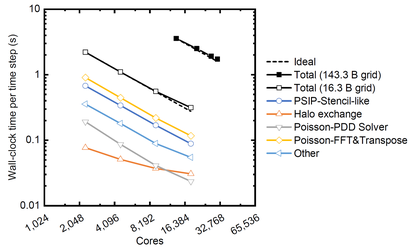


Optimization 4.3: Non-sync RDMA

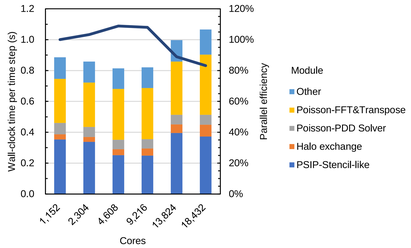
Evaluation



Speedup of proposed optimization methods



Strong scaling test results



Weak scaling test results (2.66 M grid points/core)