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INCREASING ARITHMETIC INTENSITY IN ALGEBRA-BASED CFD

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Abstract. Algebra-based CFD provides a natural route towards portable DNS and LES solvers on modern heterogeneous supercomputers by expressing the numerical method in terms of sparse operators and a reduced set of algebraic kernels. This separation between discretization and hardware-dependent implementation improves maintainability and portability, but it also exposes a central bottleneck: the dominant sparse matrix-vector products have low arithmetic intensity and are often limited by memory bandwidth. In this work, we revisit the minimal-kernel strategy for algebra-based CFD from the point-of-view of arithmetic intensity. We discuss how repeated applications of the same sparse operators to multiple fields, vector components or time blocks arising in parallel-in-time formulations can be reorganized to increase data reuse without changing the underlying numerical formulation. Within this framework, we also address key algorithmic ingredients required by practical DNS and LES solvers, including boundary conditions, CFL-based time-step estimation, Poisson solvers exploiting spatial symmetries, and repeated block structures. The resulting approach links symmetry-preserving discretizations with portable and efficient implementations for scale-resolving CFD on contemporary HPC architectures.

1 INTRODUCTION AND ANTECEDENTS

Modern heterogeneous supercomputers are enabling increasingly large and detailed DNS and LES of turbulent flows. However, exploiting these machines efficiently remains challenging for CFD solvers, whose performance is often limited by data movement, memory bandwidth and the ability to expose sufficient parallelism across different hardware architectures.

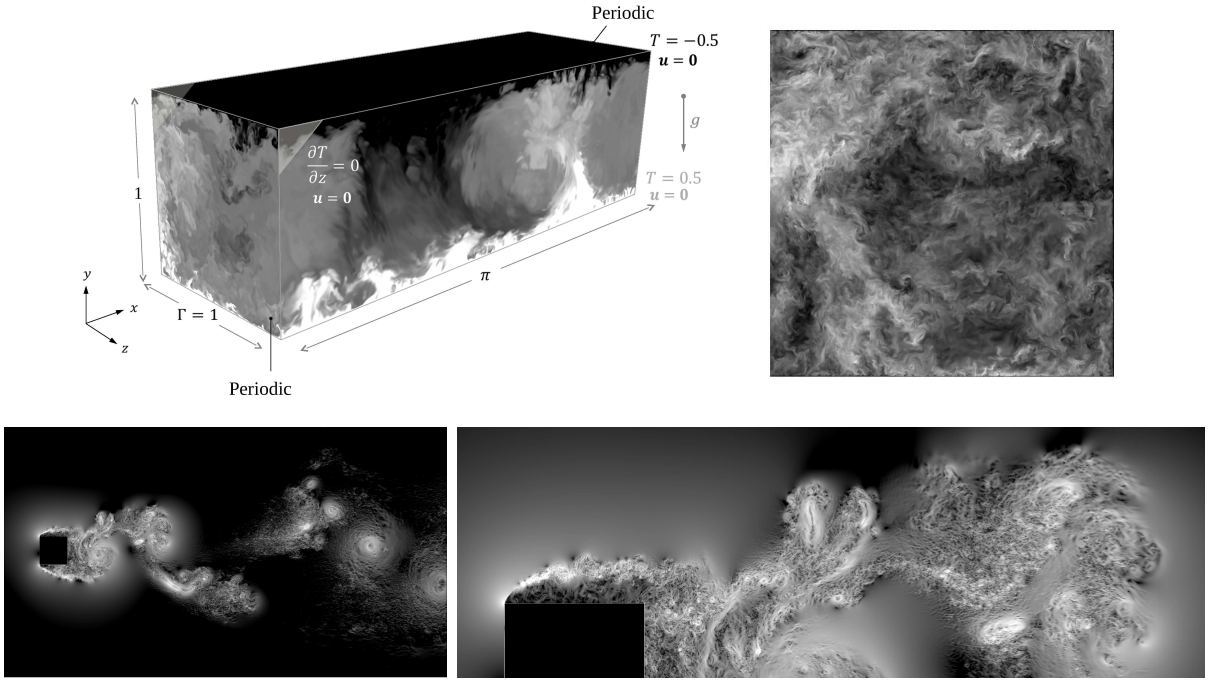

Figure 1: Examples of DNSs computed using symmetry-preserving discretizations. Top: air-filled ($Pr = 0.7$) Rayleigh–Bénard configuration studied in Ref. [1]. Instantaneous temperature field at $Ra = 10^{10}$ (left) and instantaneous velocity magnitude at $Ra = 10^{11}$ (right) for a spanwise cross section are shown. The latter was computed on 8192 CPU cores of the MareNostrum 4 supercomputer on a mesh of 5.7 billion grid points. Bottom: DNS of the turbulent flow around a square cylinder at $Re = 55000$ computed on 3136 CPU cores of the MareNostrum 5-GPP supercomputer on a mesh of 2.6 billion grid points [2].

For portability and maintainability, a very useful strategy is to express the numerical method in terms of sparse discrete operators and a reduced set of algebraic kernels, such as sparse matrix-vector products (`SpMV`), dot products and vector updates. This algebra-based representation separates the mathematical formulation from the hardware-dependent implementation; then, efficient performance of the code depends on the design and optimization of a reduce set of underlying kernels. This strategy was previously proposed for scale-resolving simulations using a minimal set of algebraic kernels [3, 4]. The DNS and LES solvers considered here are based on symmetry-preserving discretizations of the incompressible Navier–Stokes equations. This family of methods was originally developed for Cartesian staggered grids [5], was later on extended to collocated unstructured grids [6]. Some representative examples are shown in Figure 1.

This algebraic representation also makes a central bottleneck explicit: `SpMV`'s have low arithmetic intensity and, therefore, are typically memory-bandwidth limited [7, 8]. Therefore, increasing data reuse becomes essential for efficient implementations on modern CPU- and GPU-based systems. In this work, we revisit algebra-based CFD from this point-of-view and discuss how repeated applications of the same sparse operators to multiple fields, vector components or time blocks arising in parallel-in-time formulations can

be rearranged to increase arithmetic intensity without changing the underlying numerical formulation.

2 CHALLENGES AND OPPORTUNITIES

The algebra-based point-of-view reduces many CFD operations to sparse matrix kernels, but practical DNS and LES solvers require more than an efficient implementation of `SpMV`. Boundary conditions, nonlinear terms, time-step restrictions and Poisson solvers, among others, must also be expressed in a form compatible with the same operator-based framework. Boundary conditions introduce local and often irregular operations that must be incorporated without compromising portability. Stable explicit time advancement requires efficient estimates of CFL constraints; algebraic eigenvalue bounds provide a natural strategy for this purpose [9]. Projection methods, in turn, require scalable Poisson solvers, for which spatial symmetries can be exploited to reduce the computational cost and improve solver convergence [10, 11].

The main opportunity here is to identify repeated applications of the same sparse operator and process them simultaneously. Whenever the same sparse operator acts on multiple fields, vector components or time blocks arising in parallel-in-time formulations, repeated `SpMV` can be rearranged as a sparse matrix–matrix product (`SpMM`). That is, in any situation where a matrix, $\hat{\mathsf{A}} \in \mathbb{R}^{N\times N}$, can be viewed as a Kronecker product between a diagonal matrix $\mathsf{C} \equiv diag(\boldsymbol{c}) \in \mathbb{R}^{K\times K}$ and a sparse matrix, $\mathsf{A} \in \mathbb{R}^{N/K\times N/K}$, *i.e.*

$$\boldsymbol{y} = \hat{\mathsf{A}}\boldsymbol{x} \text{ (with } \texttt{SpMV}) \qquad \{\boldsymbol{y}_1, \ldots, \boldsymbol{y}_K\} = \mathsf{A}\,\{c_1\boldsymbol{x}_1, \ldots, c_K\boldsymbol{x}_K\} \text{ (with } \texttt{SpMM}), \tag{1}$$

where $\hat{\mathsf{A}} = \mathsf{C} \otimes \mathsf{A}$ and $\boldsymbol{x}_i, \boldsymbol{y}_i \in \mathbb{R}^{N/K}$. In this way, the sparse matrix coefficients are reused for several right-hand sides, leading to higher data reuse and arithmetic intensity without changing the underlying numerical formulation [8, 12].

3 CONCLUSIONS AND OUTLOOK

We have outlined an algebra-based strategy to increase the arithmetic intensity of scale-resolving CFD solvers while preserving portability across heterogeneous HPC architectures. The key idea is to identify repeated sparse-operator applications and reorganize them as block operations or `SpMM`'s, together with algebraic treatments of boundary conditions, time-step estimation and Poisson solvers.

Representative DNS and LES results, together with performance analyses on contemporary HPC systems, will be presented at the conference. Furthermore, a companion contribution [13] focuses on structure-preserving multiphysics discretizations based on exact energy exchanges, providing a complementary numerical framework for portable algebra-based CFD.

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