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Direct and Large-Eddy Simulation XI

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Volume 25

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Preface

The DLES Workshop series, which started in 1994, focuses on modern techniques to simulate turbulent flows based on the partial or full resolution of the instantaneous turbulent flow structures, as Direct Numerical Simulation (DNS), Large-Eddy Simulation (LES), or hybrid models based on a combination of LES and RANS approaches.

With the growing capacities of modern computers, these approaches have been gaining more and more interest over the years. Significant progress has been made in computational techniques as well as in subgrid scale (SGS) modeling. In parallel, these approaches are applied to more and more complex flow problems and configurations, both in academic and industrial contexts, and they will undoubtedly be further enhanced and applied in the future. Nonetheless, open problems and challenges still remain. The increasing complexity of the simulated problems and the use of turbulence resolving approaches in an engineering context require the development of numerical methods being accurate but at the same time able to deal with complex geometries and/or with physical phenomena interacting with turbulence, e.g., particle/droplet dispersion, combustion, or heat transfer. At the same time, physical models must be developed, improved, and validated for the increasing complexity and variety of applications. Validation is indeed a crucial issue for LES and hybrid simulations, since different sources of errors may be present (numerics, boundary conditions, closure models) and these errors may interact in a complicated way. Moreover, systematic sensitivity studies to computational or modeling parameters are difficult to be carried out because of the large cost of each single simulation. On the other hand, the availability of more and more DNS data sets provides a detailed and accurate reference to validate the other approaches and to guide in the development of physical models.

The goal of the workshop series is to establish a state-of-the-art of DNS, LES, and related techniques for the computation and modeling of turbulent and transitional flows and to provide an opportunity for discussions about recent advances and applications.

The 11th edition of the bi-annual Workshop series on Direct and Large-Eddy Simulation (DLES11) was held in Pisa, Italy on May 29–31, 2017. A record number of 140 participants from 17 different countries attended this 3-day workshop. The majority of participants was from academia and research institutes, but several companies were also represented. Eight keynote lectures were given by experts in different scientific fields: extreme scale direct numerical simulations of turbulent combustion (Jacqueline Chen, Sandia National Laboratories, USA), modulation and control of jets and flames (Arthur Tyliszczak, University of Czestochowa, Poland), ocean modeling and idealized DNS applied to rotating and stratified flows (Beth Wingate, University of Exeter, UK), direct numerical simulations of fluid–structure interaction in biological flows (Marco De Tullio, Politecnico di Bari, Italy), simulation and control of wind farms by means of large-eddy simulation (Johan Meyers, Katholieke Universiteit Leuven, Belgium), new insight on how roughness affects the dynamics of turbulence (Ugo Piomelli, Queen's University, Kingston, Canada), applications of DNS and LES to multiphase flows of industrial interest (Djamel Lakehal, ASCOMP, Switzerland), and direct numerical simulations of particulate flows (Markus Uhlmann, Karlsruhe Institute of Technology, Germany).

Next to the invited lectures, 114 oral and poster presentations were selected by a Scientific Committee of 28 experts. This volume contains most of the contributed papers, which were submitted and further reviewed for publication. They cover advances in computational techniques, SGS modeling, boundary conditions, post-processing and data analysis, and applications in several fields, namely, multiphase and reactive flows, convection and heat transfer, compressible flows, aerodynamics of airfoils and wings, bluff-body and separated flows, internal flows and wall turbulence, and other complex flows.

The organization of DLES11 and the preparation of these proceedings would not have been possible without the help of many. Funding from ERCOFTAC (SIG1) enabled the participation of Ph.D. students to DLES11 to be supported. J. M. Burgerscentrum and University of Pisa are also gratefully acknowledged for their support. Finally, thanks go to the members of the Scientific Committee for their help in reviewing the submitted abstracts and the contributions to the proceedings.

Pisa, Italy
March 2018

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Part I
Numerical Methods

Adaptive Direct Numerical Simulation with Spatially-Anisotropic Wavelet-Based Refinement

G. De Stefano, E. Brown-Dymkoski and O. V. Vasilyev

1 Methodology

In the wavelet-based adaptive multi-resolution approach to the numerical simulation of turbulent flows, the separation between resolved energetic structures and unresolved flow motions is achieved through the application of a wavelet thresholding filter. For very small threshold values, the effect of residual motions upon the resolved flow dynamics can be completely neglected, which leads to the adaptive Wavelet-based Direct Numerical Simulation (W-DNS) approach. The method allows for the direct solution of the organized flow motions, which consist of both large-scale and small-scale coherent structures with non-negligible energy, e.g. [6, 8].

Due to the ability to identify and efficiently represent energetic dynamically important turbulent eddies, the method has been proven reliable and effective for the simulation of unsteady external flows [7, 9]. However, when dealing with flow around obstacles, one of the main challenges of the traditional W-DNS approach is the requirement of high spatial grid resolution in both the near-wall and the wake regions. Furthermore, when the presence of the obstacle is mimicked by means of the volume-penalization technique, e.g. [5, 12], for the accurate estimation of the wall stresses, and thus the aerodynamic loads, the thin boundary layer inside of

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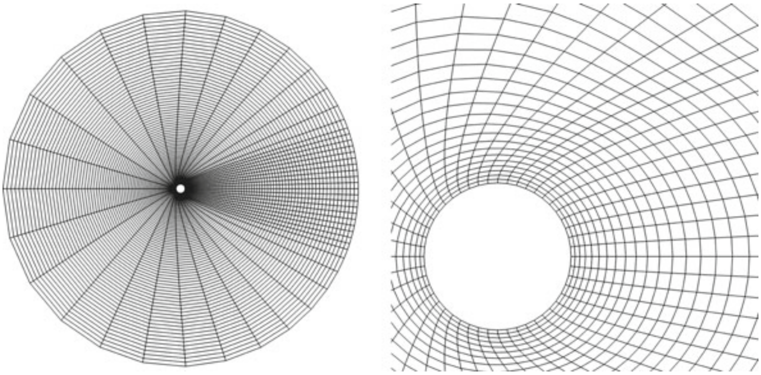

Fig. 1 Example of spatially non-adaptive anisotropic two-dimensional mesh: (left) global and (right) close-up views of the near wake zone

the porous region representing the obstacle also needs to be accurately resolved. The isotropic mesh refinement, which is characteristic of classical wavelet-based methods, results in the simultaneous grid refinement in all directions, irrespective of the actual requirement, even in situations where just one particular direction is involved. This represents a strong constraint of realizability and limits the application of W-DNS to moderate Reynolds number flows. In this study, a novel approach that overcomes this limitation is exploited.

The new W-DNS methodology is developed by making use of the adaptive wavelet transform on curvilinear grids recently introduced in [3]. The traditional wavelet methods suffer from the "curse of anisotropy," due to the isotropic wavelet refinement procedure and the inability to deal with mesh elements with spatially varying aspect ratio and orientation. The new approach utilizes a spatially anisotropic wavelet-based refinement, which takes advantage of coordinate mapping between the physical space, where the curvilinear numerical mesh is defined, and the computational space, where the adaptive rectilinear wavelet collocation grid is used. The new approach permits to construct dynamically adaptive body-fitted meshes, thus avoiding the use of the volume penalization technique. The anisotropic wavelet-based mesh refinement has been recently employed also to develop adaptive unsteady Reynolds-averaged turbulence models of external flows [4].

2 Numerical Experiments

In this work, the flow around a circular cylinder is considered as a prototype for wall-bounded external flows. The curvilinear approach makes it possible to construct stretched body-fitted O-meshes, differently from [2], where the same flow was simulated by exploiting uniform rectilinear meshes in conjunction with a volume penalization approach. Moreover, the introduction of a suitable mapping between computational and physical spaces allows for a particular arrangement of the grid

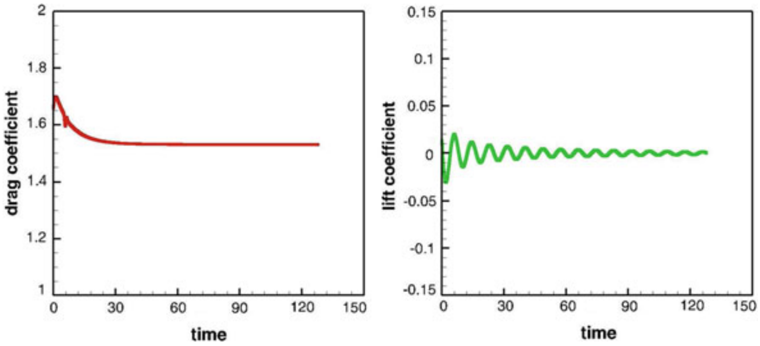

Fig. 2 Two-dimensional cylinder flow at $Re_D = 40$: time histories of (left) the drag and (right) the lift force coefficients

points that permits a more efficient representation of both the wall and the wake regions. In the current work, a more favorable mesh anisotropy is imposed using the wake envelope mapping proposed in [1]. For example, a non-adaptive spatially anisotropic two-dimensional mesh is illustrated in Fig. 1, along with the close-up view of the grid in the near wake region.

The newly proposed W-DNS method is demonstrated for both the laminar steady separated two-dimensional flow at a low Reynolds number, which is $Re_D = 40$, and the three-dimensional turbulent flow at a sub-critical Reynolds number, which is $Re_D = 1000$, where the Reynolds number is based on the cylinder diameter D. For the low Reynolds number simulation, five levels of resolution are used to simulate the vortex shedding flow, which corresponds to employing five nested wavelet collocation grids in the computational space ($J = 5$). Based on previous experience, the wavelet thresholding level is prescribed at the value of $\varepsilon = 5 \times 10^{-4}$.

Looking at the aerodynamic loads on the cylinder, the time histories of the drag and the lift force coefficients are reported in Fig. 2. After the transient period, during which the regular shedding flow develops starting from initial conditions, the drag coefficient achieves the constant value of $C_D = 1.52$, which is very close to the reference value of 1.51 provided in [11]. As to the lift coefficient, predictably, it tends towards zero, with oscillations of decreasing amplitude. The present method allows for the exact enforcement of the no-slip condition at the body surface, whereas, with the volume penalization approach, the same condition could be only approximated. In that case, the inexact nature of the wall boundary condition manifested itself in higher resolution requirement to compensate for the velocity slip error at the body surface [2]. Due to the adaptivity of the method, the number of retained wavelets, and thus the computational cost, nearly follow the flow evolution. After the initial increase caused by the evolution of the wake region, the number of grid points remains practically constant for fully developed flow.

The key characteristic of the proposed W-DNS method stands in the possibility to effectively control the accuracy of the numerical solution. On the one hand, the spatial resolution can be increased by adding further levels of resolution. On the

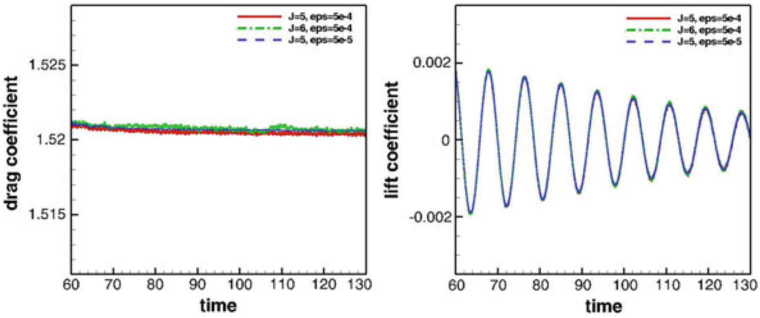

Fig. 3 Two-dimensional cylinder flow at $Re_D = 40$: time histories of (left) the drag and (right) the lift coefficients for three different resolutions that are ($J = 5$; $\varepsilon = 5 \times 10^{-4}$) (solid line), ($J = 6$; $\varepsilon = 5 \times 10^{-4}$) (dash-dotted line) and ($J = 5$; $\varepsilon = 5 \times 10^{-5}$) (dashed line)

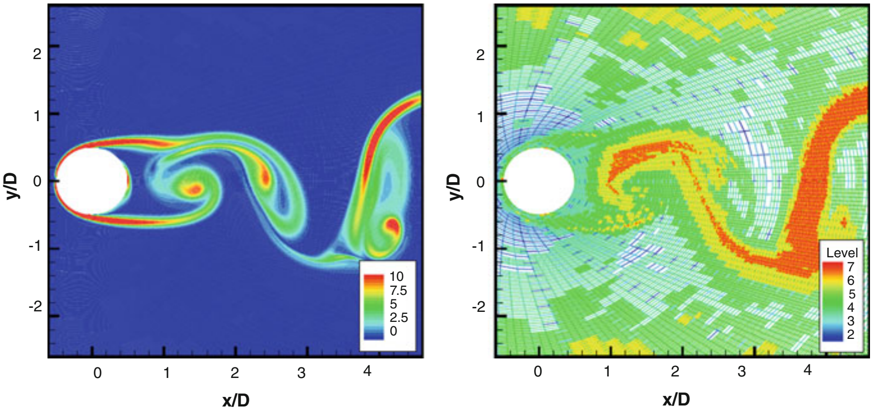

Fig. 4 Three-dimensional cylinder flow at $Re_D = 1000$: (left) instantaneous vorticity contours and (right) adaptive mesh in the mid plane, colored by the level of resolution

other hand, for a given number of wavelet collocation grids, the thresholding level can be properly reduced. In this work, two additional simulations are carried out, starting form the previous baseline solution at the non-dimensional time $tU/D = 60$, where U stands for the freestream velocity, by either using a further level of resolution ($J = 6$) or choosing a lower wavelet threshold that is $\varepsilon = 5 \times 10^{-5}$. The time histories of the drag and the lift force coefficients for three different simulations with different resolutions are reported in Fig. 3. While the use of an extra level of resolution, without changing ε, results in a more noisy solution, the use of a lower threshold undoubtedly results in a more accurate solution. This demonstrates that the direct numerical solution is actually achieved for a sufficiently low level of thresholding.

The present method has been developed for the accurate and efficient simulation of wall-bounded turbulent flows. Some preliminary experiments for the unsteady

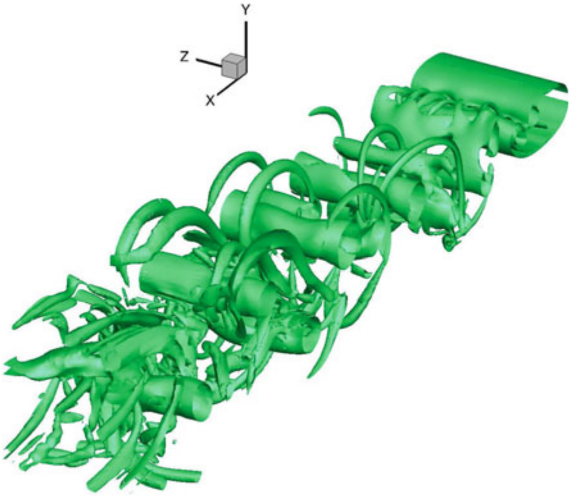

Fig. 5 Three-dimensional cylinder flow at $Re_D = 1000$: main vortical structures in the near wake of the cylinder identified by the iso-surfaces of Q

three-dimensional W-DNS solution of the turbulent flow past a circular cylinder are conducted for the sub-critical flow regime, where the boundary layer exhibits laminar separation and the transition to turbulence occurs in the shear layers developing on the cylinder side, e.g. [10]. The calculation is performed at $Re_D = 1000$, by using seven nested rectilinear wavelet collocation grids in the computational space. The associated anisotropic O-meshes in the physical space are constructed following the same approach of the previous two-dimensional solution in the cross-section planes, while no mapping is used in the third spanwise homogeneous direction, where uniform grid spacing is used. The adaptive method provides a non-uniform spatial resolution, which is actually varying in time following the dynamic evolution of the turbulent flow structures in the three spatial dimensions. This is illustrated in Fig. 4, where the contours of the vorticity magnitude and the numerical mesh, colored by the level of resolution, in the mid-plane, are reported at a given time instant. The anisotropic refinement results in a more efficient representation of the flow field at the wall region, which, in turn, translates into the decrease of the number of active wavelet collocation points and, ultimately, into the reduction of the computational cost. In fact, the use of anisotropically stretched mesh elements close to the surface reduces the number of wavelet levels that are actually needed to resolve the local flow structures. In particular, the maximum level of resolution ($J = 7$) is only involved in very limited zones, compared to excessively high resolution requirement in the near-wall region for the volume penalization approach [3]. Finally, in order to demonstrate how the complex three-dimensional vortex structures in the wake behind the cylinder are well represented by the W-DNS solution, the instantaneous iso-surfaces of the second invariant of the velocity gradient tensor, $Q = 0.4U^2/D^2$, are shown in Fig. 5.

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Towards Adaptive Mesh Refinement for the Spectral Element Solver Nek5000

N. Offermans, A. Peplinski, O. Marin, P. F. Fischer and P. Schlatter

1 Introduction

When performing computational fluid dynamics (CFD) simulations of complex flows, the a priori knowledge of the flow physics and the location of the dominant flow features are usually unknown. For this reason, the development of adaptive remeshing techniques is crucial for large-scale computational problems. Some work has been made recently to provide Nek5000 with adaptive mesh refinement (AMR) capabilities in order to facilitate the generation of the grid and push forward the limit in terms of problem size and complexity [10]. Nek5000 is an open-source, highly scalable and portable code based on the spectral element method (SEM) [4], which offers minimal dissipation and dispersion, high accuracy and exponential convergence. It is aimed at solving direct and large-eddy simulations of turbulent incompressible or low Mach-number flows with heat transfer and species transport. The approach chosen for adapting the mesh is the h-refinement method, where elements are split locally, which requires the relaxation of the conforming grid constraint currently

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imposed by Nek5000. Other challenges include the implementation of an efficient management of the grid as refinement is applied, the development of tools to localize the critical flow regions via error estimators and the extension of the current preconditioning strategy to non-conforming grids. In this paper, we present a new procedure to setup an algebraic multigrid solver used as part of the preconditioner for the pressure equation.

2 Pressure Preconditioning in Nek5000

2.1 *Coarse Grid Solver*

The major source of stiffness when solving the Navier–Stokes equations comes from the pressure equation, which requires an efficient preconditioning strategy. The method chosen for Nek5000 is additive Schwarz [2] and the preconditioner can be expressed as $M_0^{-1} = R_0^T A_0^{-1} R_0 + \sum_{k=1}^{K} R_k^T A_k^{-1} R_k$, where K is the number of spectral elements and R_k and R_0 are restrictions operators. This preconditioner can be seen as the sum of the global coarse grid operator (A_0) and local subdomain operators (A_k). The present work focuses on the solution of the coarse grid operator, A_0, a finite element Laplacian matrix. The so-called "coarse grid" denotes the spectral-element grid, where the inner collocation points are not taken into account. Two choices are available in Nek5000 to solve this problem: using a sparse basis projection method, called XXT [11] or an algebraic multigrid (AMG) method, which is more efficient for massively parallel large simulations (more than 10,000 cores and 100,000 elements) [3]. As usual with AMG methods, a setup step is required for the matrix A_0, which will define the necessary data for solving the problem: a coarsening operation and the definition of the interpolation and smoother operators. In the particular case of Nek5000, the AMG solver performs a single V-cycle, and a fixed number of Chebyshev iterations, computed during the setup, is applied during the smoothing part. This method has the advantage to avoid inner products, thus reducing communication. More information about the theoretical background for the setup can be found in Ref. [7]. While the AMG solver is highly scalable and efficient, the setup phase is currently performed by a serial Matlab code, which can take up to a few hours for the largest current cases on a modern desktop computer. This bottleneck is an obstacle to the use of AMR, where the grid, and thus the operator A_0, is modified regularly, every time requiring a new setup computation. For that reason, an alternative method has been investigated to replace the Matlab setup.

Table 1 Summary of the cases used for testing the Hypre setup. The name of the case, number of spectral elements, polynomial order and total number of degrees of freedom for each velocity component are indicated

Case name	Num. of el.	Pol. order	D.O.F.
Jet in crossflow [9]	47,960	7	16,461,424
Straight pipe [1]	853,632	7	293,870,304
NACA4412 [5]	1,847,664	11	1,847,664,000

2.2 Use of Hypre for the AMG Setup

As an alternative way of performing the setup, the Hypre library for linear algebra is used [6]. Specifically, only the time consuming coarsening and interpolation operations are performed with Hypre, while the computation of the smoother remains unchanged in order to keep the good performance of the AMG solver. The use of Hypre offers the possibility to choose among various algorithms for coarsening and interpolation. For the current tests, we chose the Ruge–Stuben algorithm for the coarsening and the so-called “classical” modified technique for the interpolation. The setup is currently performed by a serial, external C code. The main goal with this new setup is to demonstrate two points: the use of the Hypre library reduces significantly the setup time but does not impact the solver time.

3 Validation of the Hypre Setup

In this section, we experiment with the new setup code on several real test cases. In particular, we verify that the Hypre setup is faster than the Matlab one, while the computational time is not affected. We also show the advantage of AMG over XXT for large parallel simulations.

The test cases considered are the simulations of a jet in a crossflow [9], of a turbulent straight pipe ($Re_\tau = 550$) [1] and of the flow around a NACA4412 airfoil ($Re = 400{,}000$) [5]. Some basic information about the cases is summarized in Table 1. All cases are physically relevant, three-dimensional, flagship simulations. The cases of the straight pipe and the NACA4412 are both obtained by extrusion of a 2D grid and are chosen for their large number of elements. The wing case also has elements with large aspect ratios, which makes it more challenging. The grid of the jet in a crossflow is smaller but is chosen because it is not built by extrusion of a 2D grid. Moreover, the complexity of the grid at the junction between the pipe and the channel makes it an interesting case.

Table 2 Comparison between the timings of the Matlab and Hypre codes for the AMG setup

	Time (s.)	I/O	Computation	Total
Jet in crossflow	Matlab	1.17	97.47	**98.64**
	Hypre	0.4	2.02	**2.42**
Straight pipe	Matlab	26.49	2205	**2231**
	Hypre	32.75	44.4	**77.15**
NACA4412	Matlab	93.98	3662	**3756**
	Hypre	90.4	91.7	**182.1**

3.1 Timing of the AMG Setup

The timings for the setup are reported in Table 2 for the Matlab and the Hypre setups. The total setup time is split between I/O time (reading and writing the setup data) and computational time (coarsening and computation of the interpolation operator and smoother at each level). All setups are performed a single time on the same desktop machine (CPU: Intel Core I7 990 Extreme, RAM: 24gb), in serial.

In all cases, the computational and total times for the setup are reduced by more than one order of magnitude. The timings for I/O remain similar on the other hand. Overall, numerical experiments clearly show that Hypre can be used to drastically reduce the setup time, up to levels that can be used for AMR simulations. In addition, so far only the serial version of Hypre has been used; upon inclusion of the setup phase into the main code, even the parallel capabilities will be employed, which might lead to additional reduction of the setup time.

3.2 Timing of the Simulation

The mean total wall clock time per time step during the simulation is presented in Figs. 1 and 2 for the jet in crossflow and the straight pipe, respectively. A straight line showing linear strong scaling is also plot as an indication. Similarly, the time for the coarse grid solver and the total computational time are shown, per time step, in Fig. 3a, b for the NACA4412 airfoil. For all cases, the reported times correspond to averages over 20 time steps and exclude I/O. Each simulation has been run, once, on Beskow, a Cray XC40 supercomputer (1676 nodes, 32 cores per node) based at The Royal Institute of Technology in Stockholm. For the jet in crossflow and the pipe, several number of cores have been considered and the plots show the strong scaling of the code. The NACA4412 simulation has been run on 16,384 cores only.

The results for the jet in crossflow, illustrated in Fig. 1, show that the Hypre setup does not affect the time to solution, as both setups lead to very similar results in terms of computational time. Regarding the comparison between AMG and XXT, the simulation of the jet in crossflow is too small to see a consistent difference between

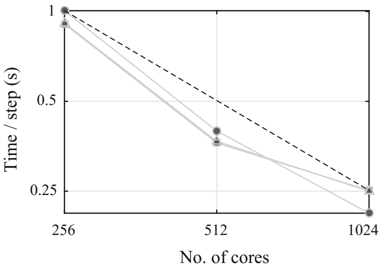

Fig. 1 Jet in crossflow - Total computational time using XXT (circles), AMG with the Matlab setup (squares) and AMG with the Hypre setup (triangles). Dashed line shows linear strong scaling

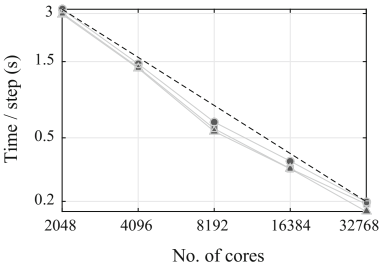

Fig. 2 Straight pipe ($Re_\tau = 550$) - Total computational time using XXT (circles), AMG with the Matlab setup (squares) and AMG with the Hypre setup (triangles). Dashed line shows linear strong scaling

both coarse grid solvers, as can be seen by the fact that the best performing method depends on the number of processes.

It is observed again in Fig. 2 that both the Hypre and the Matlab setups perform similarly well in the case of the simulation of a turbulent straight pipe. Given the larger size of the case, it also appears that the use of XXT for preconditioning the pressure equation is systematically slower compared to AMG. This difference is a only a few percents but occurs at all numbers of cores considered.

Furthermore, Fig. 3a, b show once more that either setup method can be used without affecting significantly the solver time. The slightly higher time for the coarse grid solver may be partly attributed to a higher number of Chebyshev iterations when using Hypre compared to Matlab (33 vs. 26). Other factors that might explain the difference are the algorithms used for coarsening and interpolation. Both figures also illustrate that the use of AMG should be preferred over XXT for large simulations. In the case of the wing, the gain in coarse grid solver time is about 70%, which translates into a reduction of the total computational time by about 10%.

Finally, we show the effect of the setup method on the number of pressure iterations, i.e. the number of iterations of the iterative solver (GMRES in this case) required to drive the L_2-norm of the residual of the divergence equation to some tolerance (10^{-7} in this case), at the start of the simulation of the straight pipe in Fig. 4.

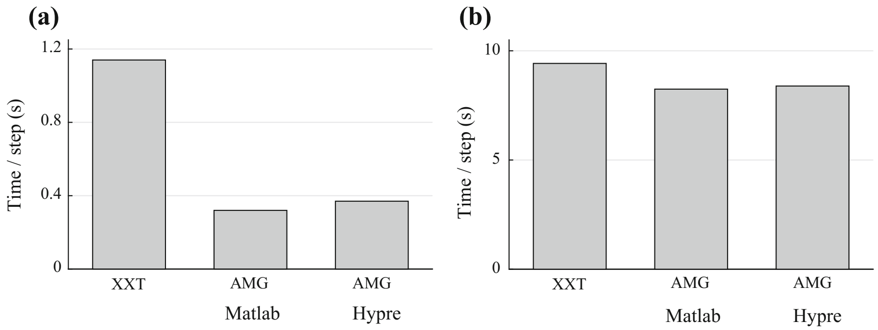

Fig. 3 **a** NACA4412 airfoil - Coarse grid solver time using XXT, AMG with the Matlab setup and AMG with the Hypre setup. **b** NACA4412 airfoil - Total computational time using XXT, AMG with the Matlab setup and AMG with the Hypre setup

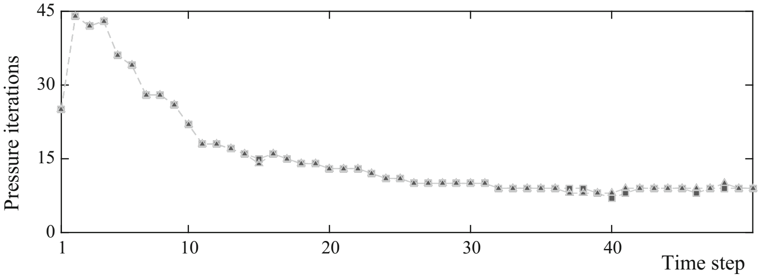

Fig. 4 Comparison of the number of pressure iterations for the AMG setups in the case of the turbulent straight pipe ($Re_\tau = 550$) using Matlab (squares) and Hypre (triangles)

Both plots collapse most of the time, showing once more that both setup methods are equivalent. Similar results have been observed for the two other cases.

4 Conclusion and Outlook

The present work shows numerical results for speeding up the pressure preconditioner with the eventual goal of using adaptive mesh refinement (AMR) with Nek5000 [10].

First, with the help of Hypre, the setup time was reduced by more than one order of magnitude compared to the Matlab code. This improvement will benefit the users of Nek5000 and should facilitate the use of the AMG solver within the framework of AMR. It has been shown that the use of AMG instead of XXT for solving the coarse grid problem in Nek5000 significantly improves the time to solution for large cases (typically more than 100,000 elements on more than 10,000 cores) [8].

Finally, it was shown that replacing the coarsening and interpolation operations of the original Matlab code for the setup by the Hypre routines, while keeping the same strategy for the smoother, does not affect significantly the total solver.

In the future, the setup code using Hypre will be parallelized and included inside Nek5000 such that no interruption in the workflow of a simulation is required. As the result of the AMG setup in Hypre is dependent on the number of parallel processes used, the effect of parallelization on the quality of the coarsening and interpolation operations will also be studied.

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