
This version is available at https://strathprints.strath.ac.uk/63146/

Strathprints is designed to allow users to access the research output of the University of Strathclyde. Unless otherwise explicitly stated on the manuscript, Copyright © and Moral Rights for the papers on this site are retained by the individual authors and/or other copyright owners. Please check the manuscript for details of any other licences that may have been applied. You may not engage in further distribution of the material for any profitmaking activities or any commercial gain. You may freely distribute both the url (https://strathprints.strath.ac.uk/) and the content of this paper for research or private study, educational, or not-for-profit purposes without prior permission or charge.

Any correspondence concerning this service should be sent to the Strathprints administrator: strathprints@strath.ac.uk
Performance of high-order implicit large eddy simulations

Konstantinos Ritos*, Ioannis W. Kokkinakis, Dimitris Drikakis*

University of Strathclyde, Glasgow, G1 1Xj, UK

ARTICLE INFO

Article history:
Received 24 January 2017
Revised 30 October 2017
Accepted 23 January 2018
Available online 31 January 2018

Keywords:
ILES
High-Order methods
Turbulent flows
Parallel computing

ABSTRACT

The performance of parallel implicit Large Eddy Simulations (iLES) is investigated in conjunction with high-order weighted essentially non-oscillatory schemes up to 11th-order of accuracy. Simulations were performed for the Taylor Green Vortex and supersonic turbulent boundary layer flows on High Performance Computing (HPC) facilities. The present iLES are highly scalable achieving performance of approximately 93% and 68% on 1536 and 6144 cores, respectively, for simulations on a mesh of approximately 1.07 billion cells. The study also shows that high-order iLES attain accuracy similar to strict Direct Numerical Simulation (DNS) but at a reduced computational cost.

© 2018 The Authors. Published by Elsevier Ltd. This is an open access article under the CC BY license. (http://creativecommons.org/licenses/by/4.0/)

1. Introduction

Implicit Large Eddy Simulations (iLES) originated from the observations made in [1] that the embedded dissipation of a certain class of numerical methods can be used in lieu of the explicit Sub-Grid Scale (SGS) models. Modified Equation Analysis (MEA) was developed [2] aiming at determining the stability of a difference equation by examining the truncation errors. Such an analysis was performed for the truncation error of certain schemes, e.g., [3–9]) leading to a better understanding of the implicit sub-grid dissipation. In iLES, the Navier–Stokes Equations (NSE) are discretised using high-resolution methods without involving a low-pass filtering operation, which leads to SGS terms that require additional modelling. Instead, only the (implicit) de facto filtering introduced through the finite volume integration of the NSE over the mesh cells is utilised in conjunction with non-linear numerical schemes that adhere to a number of principles; see [10,11], and reviews [9,12,13]. It has been shown [7] that iLES methods need to be carefully designed, optimised, and validated for the particular differential equation to be solved. Direct MEA of high-resolution schemes for NSE is difficult to be performed, thus understanding of the numerical properties of these methods to date still relies on performing computational experiments.

The use of iLES in free and wall-bounded flows has been justified by several authors [14,15], while a validation of the approach through theoretical analysis has been presented by Margolin et al. [8]. In incompressible flows, it is possible to develop an optimised stencil with regards to numerical dissipation [16], however, in the case of compressible flows the numerical method should be monotonic with respect to the thermodynamic quantities. Poggie et al. [17] and Ritos et al. [18] applied compressible iLES to study Turbulent Boundary Layer (TBL) flows and showed that iLES can achieve close to strict DNS (see page 4 for definition of strict DNS) accuracy on significantly coarser meshes. Despite iLES (and similarly classical LES) being computationally less demanding than DNS, it still requires significant computational resources for simulating near-wall turbulence at high Reynolds numbers.

To date, there has been no systematic attempt to investigate the parallel scalability of different high-order compressible iLES methods in free and wall-bounded flows. The aim of this study is to present results regarding the accuracy, efficiency and parallel scalability of high-order iLES with reference to the Taylor Green Vortex (TGV) and supersonic TBL flows.

2. Numerical methods and flow cases

We have employed iLES in the framework of the CFD code CNS3D [12,15]. The Navier–Stokes equations are solved by using a finite volume Godunov-type method for the convective terms, which comprises the HLLE approximate Riemann solver [13,19] and two high-resolution schemes. The Monotone Upstream-centered Scheme for Conservation Laws (MUSCL) with second-order piece-wise linear monotонised central limiter [20] (labelled as M2), and the Weighted-Essentially Non-Oscillatory (WENO) ninth-order scheme [21] (labelled as W9). Furthermore, in order to examine the parallel scalability of high-order iLES, simulations were also performed using an eleventh-order WENO scheme (labelled as W11).
The viscous terms are discretised using a second-order central scheme. The solution is advanced in time using a five-stage (fourth-order accurate) optimal strong-stability-preserving Runge-Kutta method [22]. Further numerical details are provided in [15] and references therein.

The first flow case considered here is the TGV in a triple-periodic cubic domain of length $2\pi$ (m). A series of meshes was used: $32^3, 64^3, 128^3, 256^3$, and $512^3$ evenly-spaced computational cells. The flow is initialised by solenoidal velocity profile,

$$u_0 = U_0 \sin(kx) \cos(ky) \cos(kz),$$

$$v_0 = -U_0 \cos(kx) \sin(ky) \cos(kz),$$

$$w_0 = 0,$$

and the pressure is obtained by solving the Poisson equation:

$$P_0 = P_\infty + \frac{1}{16} \mu u_0^2 [2 + \cos(2kz)] \cdot [\cos(2kx) + \cos(2ky)],$$

(2)

where the wavenumber $k = 1$. An ideal gas equation of state is used and the Mach number, $U_0/\sqrt{\gamma} P_0/\rho_0$, is 0.08. The results are presented in terms of non-dimensional units; distance $\lambda' = kx$ and time $t' = k\mu t$.

The second flow case considered here is a supersonic turbulent flow over a flat plate at Mach number $M = 2.25$ and Reynolds number of $1.5 \times 10^6$ based on the freestream properties for air and the length of the plate, $L$; see also Table 1.

Periodic boundary conditions are used in the spanwise direction (z). In the wall-normal direction (y) a no-slip isothermal wall at temperature $T_w = 323K$ is imposed. Supersonic outflow conditions are applied at the outlet, while far-field conditions are applied on the upper boundary opposite to the wall.

A synthetic turbulent inflow boundary condition is used to produce a freestream flow with a superimposed random turbulence. The synthetic turbulent inflow boundary condition is based on the digital filter (DF) method [18–25]. According to DF, instead of using a white-noise random perturbation at the inlet, energy modes within the Kolmogorov inertial range scaling with $k^{-5/3}$, where $k$ is the wavenumber, are introduced into the turbulent boundary layer. A cutoff at the maximum frequency of 50 MHz is applied since the finest mesh would under-resolve higher frequency values. The turbulence intensity at the inlet (I) is set as $\pm 3\%$ of the intensity of the freestream velocity. This perturbation has been found to be sufficient to trigger bypass transition and turbulence downstream (see Fig. 1).

iLES have been performed on fine meshes but still coarser than DNS [17,26]. We employed four meshes with the coarsest and finest meshes containing ~4.5 million and ~100 million cells, respectively. For the calculation of the mesh spacing $\Delta y$ the conventional inner variable scaling method $\Delta y^+ = u_1 \Delta y/\nu$ is used, where $u_1 = \sqrt{\nu u_0^2/\rho_0}$ is the friction velocity; $\nu_0, \tau_w$ and $\rho_0$ are the wall viscosity, shear stress and density, respectively. Typical mesh resolution recommendations for LES lie in the range of 50 $< \Delta x^+ < 150$ and 15 $< \Delta z^+ < 40$, and for DNS in the range of 10 $< \Delta x^+ < 20$ and 5 $< \Delta z^+ < 10$ [17,27,28]. For wall-resolved LES and DNS the near-wall spacing should be $\Delta y^+ < 1$. A strict definition for DNS mesh spacing requires $\Delta x^+ \leq 1$ and $\Delta y^+ \leq 1$. The mesh spacing used in this study is in the range of $9.06 < \Delta x^+ < 27.14$, $0.497 < \Delta y^+ < 1.22$ and $8.53 < \Delta z^+ < 24.95$, where the smallest values correspond to the finest mesh. Based on the above analysis, the present iLES on the finest mesh can be considered as an under-resolved DNS.

The TBL properties are presented in Table 2. To enable the comparison of the present results with other publications, various definitions of the Reynolds number have been employed based on the momentum thickness, the friction velocity, and the near-wall viscosity. The flow statistics are computed by averaging in time over three flow cycles and, spatially, in the spanwise direction. The statistical convergence of the simulations based on the standard error of the mean is less than 2%.

3. Results

3.1. TGV

Instantaneous visualisations of the TGV at $t^* = 15$ (Fig. 2) show the dominance of disorganised vortices in the decaying worm-vortex flow regime. The results were obtained using the ninth-order WENO scheme on $64^3$, $128^3$, $256^3$ and $512^3$ meshes. The snapshots of the flow are based on the Q-criterion, which defines a vortex as a continuous fluid region with a positive second invariant of the velocity gradient [30], i.e. $Q > 0$. All renderings are performed at the same level ($Q = 1$) and are coloured with the velocity magnitude.

The results on $256^3$ and $512^3$ meshes are very similar with respect to the turbulent structures resolved. The kinetic energy rate of dissipation, $\varepsilon_1$, and pressure dilation-based dissipation rate, $\varepsilon_2$, are shown in Fig. 3. The kinetic energy rate of dissipation is calculated by $\varepsilon_1 = -\frac{1}{\rho_0} \int \frac{1}{2} \rho u \cdot u \, dV$, where

$$\varepsilon_1 = \frac{1}{\rho_0} \int \frac{1}{2} \rho u \cdot u \, dV$$

(3)

is the volumetric-averaged kinetic energy. The simulations are nearly grid converged with respect to $\varepsilon_1$ and agree with other published results [31,32] (not shown here). The pressure dilatation-based dissipation rate is defined by

$$\varepsilon_2 = -\frac{1}{\rho_0} \int \Delta p \cdot u \, dV$$

(4)

$\varepsilon_2$ measures the effect of compressibility on the dissipation of turbulent energy and takes small values for low Mach flows.

A widely used performance metric for assessing parallel computations is the speedup:

$$S_n = \frac{T_n}{T_{ref}}$$

(5)

where $T_n$ is the execution time on $n$ cores and $T_{ref}$ is the execution time on a reference number of processors, usually equal to a single
core or to the number of cores in a computational node of the HPC facility used. For the TGV simulations on meshes up to $512^3$ cells, 12 cores were used as reference; one HPC node has two Intel Xeon X5650 processors with 6 cores each. The ideal speedup of parallel computations would be equal to $n/n_{ref}$, but this efficiency is not possible due the communication overhead between the computational cores and the idle time of computational nodes associated with load balancing. Fig. 4a shows the parallel speedup for the TGV case using the ninth-order iLES, achieving 77% speed-up using 480 cores. Furthermore, for scalability purposes the parallel performance of the eleventh-order WENO iLES on 6144 cores for the $1024^3$ simulation is shown; a Cray HPC facility compromising two Intel E5-2697v2 processors with 12 cores each was used. The reference execution time was obtained on 192 cores. The parallel performance of the $1024^3$ simulation is approximately 93% and 68% on 1536 and 6144 cores, respectively. The parallel performance of the second-order iLES is not shown because it involves less calculations for the same mesh size and as a consequence the scalability will always be worse when comparing to higher order iLES.

### 3.2. TBL

The second flow case is a supersonic TBL for which DNS results and experimental data at similar Mach numbers are available.

---

Fig. 1. Iso-surfaces of Q-criterion, coloured by Mach number, for (a) M2 and (b) W9 iLES simulations; the computational domain has been truncated. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article).

Fig. 2. Iso-surfaces of Q-criterion ($Q = 1$) coloured by velocity magnitude at $t^* = 15$. The $32^3$ mesh is not shown as no structure is visible at this level of $Q$. All shown TGV simulations are with W9. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article).
Comparisons with DNS and/or experiments are presented for the van Driest velocity profile, $u_{DV}$, and normal Reynolds stress, $\tau_{uu}$ (Fig. 5). The van Driest velocity profile is given by

$$u_{DV} = \int_0^u \sqrt{\frac{\rho}{\rho_w}} du^+,$$

(6)

where the superscript ‘+’ denotes wall scaling, $u^+ = u/\nu$. Previous publications [26,33] have shown that for adiabatic walls a satisfactory agreement of the velocity data is expected in near-wall region. Small variations are expected for different Reynolds number and the present iLES are in agreement with the DNS of Pirozzoli et al. [26]. The ninth-order iLES is also in excellent agreement with the experimental data [29]. The second-order iLES, conducted on the same mesh resolution, shows significant deviation from the reference DNS and experiments. Performing the ninth-order iLES on 1/3 mesh resolution shows that mesh convergence is achieved, hence the high-order iLES reliably attain high accuracy on a relatively coarse mesh.

In respect of $\tau_{uu}$, the second-order iLES significantly overestimate the Reynolds normal stress, especially in the peak region of the buffer zone. The ninth-order iLES show very good agreement with the DNS results up to about $y^+ \approx 20$, where the Reynolds similarity holds [34]. Further away from the wall it is typical to observe a strong dependence on Reynolds number for results presented in inner scaling coordinates. This explains the differences in the results in the logarithmic region due to the differences in the local Reynolds number.
more pragmatic approach than using a second order method on a significantly finer mesh.

Acknowledgements

Results were obtained using the EPSRC funded ARCHIE-WeSt High Performance Computer (www.archie-west.ac.uk) under EPSRC grant no. EP/K000586/1. The authors would also like to thank EPSRC for providing access to computational resources on the National HPC facility ARCHIE through the UK Applied Aerodynamics Consortium Leadership Project “e529”.

References


