Large-eddy simulations of 3D Taylor-Green vortex: comparison of Smoothed Particle Hydrodynamics, Lattice Boltzmann and Finite Volume methods

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Abstract. In the paper we present Large-eddy simulation (LES) results of 3D Taylor-Green vortex obtained by the three different computational approaches: Smoothed Particle Hydrodynamics (SPH), Lattice Boltzmann Method (LBM) and Finite Volume Method (FVM). The Smagorinsky model was chosen as a subgrid-scale closure in LES for all considered methods and a selection of spatial resolutions have been investigated. The SPH and LBM computations have been carried out with the use of the in-house codes executed on GPU and compared, for validation purposes, with the FVM results obtained using the open-source CFD software OpenFOAM. A comparative study in terms of one-point statistics and turbulent energy spectra shows a good agreement of LES results for all methods. An analysis of the GPU code efficiency and implementation difficulties has been made. It is shown that both SPH and LBM may offer a significant advantage over mesh-based CFD methods.

1. Introduction
In recent years, Smoothed Particle Hydrodynamics (SPH) [7] and the Lattice Boltzmann Method (LBM) [9] become more and more popular approaches for incompressible flow simulations. One of the advantages of SPH is its meshless character and suitability to solve multiphase flows with interfaces [11]. The LBM offers easy implementation, computational efficiency and ability to treat complex geometries on regular grids [5]. Another reason for the growing use of both approaches is their adaptivity for massively parallel computations on Graphics Processing Units (GPU). Thus, it is worth making research on turbulence models that would widen the field of applicability of SPH and LBM for high-Re and multiphase flows.

2. Smoothed Particle Hydrodynamics
SPH is a meshfree method [7] that solves the Navier-Stokes equations in the Lagrangian setting of notional fluid particles identified by their locations \( \mathbf{r}(t) \) and velocities \( \mathbf{u}(t) \):

\[
\frac{d\mathbf{r}}{dt} = \mathbf{u}, \quad (1)
\]

\[
\frac{d\mathbf{u}}{dt} = -\frac{1}{\rho} \nabla p + \nu \nabla^2 \mathbf{u} + \mathbf{g}, \quad (2)
\]

\[
\frac{d\rho}{dt} = -\rho \nabla \cdot \mathbf{u}. \quad (3)
\]
It consists in a spatial discretisation in terms of moving fluid volumes (particles) and associates with them some special interpolating functions (further called kernel functions or, shortly, kernels). A scalar field $A$ is interpolated at position $r$ as follows:

$$\hat{A}(r) = \int_{\Omega} A(r') W(r - r', h) \, dr',$$

where $\Omega$ is the simulation domain, $h$ is the smoothing length and $W(r, h)$ is the kernel function.

Function $W$ should have the following features:

- $W(r, h) = W(-r, h)$,
- $\lim_{h \to 0} W(r, h) = \delta(r)$, where $\delta(r)$ is the Dirac delta function,
- $\int_{\Omega} W(r, h) \, dr = 1$.

The flow field gradients can be easily obtained from integration by parts using the kernel symmetry:

$$\hat{\nabla} A(r) = \int_{\Omega} A(r') \nabla W(r - r', h) \, dr'.$$

In the discretised form, the integrals are expressed as sums within the kernel range (kernels of compact support are used to decrease the computational effort):

$$\hat{A}(r_a) \approx \langle A \rangle_a = \langle A \rangle_a(r_a) = \sum_b A(r_a) W(r_a - r_b, h) \Omega_b,$$

$$\hat{\nabla} A(r_a) \approx \langle \nabla A \rangle_a = \langle \nabla A \rangle_a(r_a) = \sum_b A(r_a) \nabla W(r_a - r_b, h) \Omega_b,$$

where $a$ and $b$ are particles indexes and $\Omega_b$ is the volume of particle $b$. In this paper we present results of weakly compressible SPH (WCSPH) [10] where the pressure field is related to density according to the following equation of state:

$$p = \frac{c_s^2 \rho_0}{\gamma} \left( \left( \frac{\rho}{\rho_0} \right) \gamma - 1 \right),$$

where $\rho_0$ is the density of fluid, $\gamma$ is a constant (here equal to 7) and $c_s$ denotes the speed of sound. In the SPH formalism eqs. (2) and (3) can take different forms. For eq. (3), due to good stability properties, we decided to choose the form proposed by Hu and Adams [6]:

$$\rho_a = m_a \Theta_a = m_a \sum_b W(r_a - r_b, h),$$

where $\Theta_a$ denotes the inverse of particle $a$ volume. In eq. (2) the terms corresponding to pressure forces and viscous forces are approximated respectively as follows:

$$\langle \nabla p \rangle_a = \frac{1}{m_a} \sum_b \left( \frac{p_a}{\Theta_a^2} + \frac{p_b}{\Theta_b^2} \right) \nabla W(r_{ab}, h),$$

$$\langle \mu \Delta u \rangle_a = \frac{1}{m_a} \sum_b \left( \frac{\mu}{\Theta_a^2} + \frac{\mu}{\Theta_b^2} \right) \frac{r_{ab} \cdot \nabla W(r_{ab}, h)}{r_{ab}^2 + \eta^2} u_{ab},$$

where:

- $r_{ab} = r_a - r_b$ - the distance between particles $a$ and $b$,
- $u_{ab} = u_a - u_b$ - the relative velocity of particles $a$ and $b$,
- $\mu$ - the dynamic viscosity,
- $\eta = 0.01h$ - a coefficient preventing from singularity.
3. Lattice Boltzmann Method

The LBM is based on the kinetic theory of gases. The discretised Boltzmann equation is solved (instead of the Navier-Stokes equations) for the probability density function of fluid particles moving at specified speeds in specified directions. The spatial discretisation is done on a regular square grid; moreover, only a finite number of directions are allowed for particle velocity [9].

In this paper we present results obtained with a code implementing the D3Q15 lattice, i.e., 3 dimensions and 15 allowed directions. The discretised Boltzmann equation takes the following form:

\[
\mathcal{f}_\alpha(x + e_\alpha \Delta t, t + \Delta t) - \mathcal{f}_\alpha(x, t) = -\frac{1}{\tau} (\mathcal{f}_\alpha(x, t) - \mathcal{f}^{eq}_\alpha(x, t)),
\]

(12)

where:

- \( \alpha \) - the index of velocity direction \((\alpha = 0, 1, ..., 14)\),
- \( \tau \) - the nondimensional relaxation time,
- \( x \) - position in space,
- \( e_\alpha \) - the lattice velocity in direction \( \alpha \),
- \( \Delta t \) - the time step.

The equilibrium distribution \( \mathcal{f}^{eq} \) is calculated as follows:

\[
\mathcal{f}^{eq}_\alpha = w_\alpha \rho \left[ 1 + 3 c_s^2 e_\alpha \cdot u + \frac{9}{2c^2}(e_\alpha \cdot u)^2 + \frac{3}{2c^2} u \cdot u \right],
\]

(13)

where:

- \( \rho = \sum_\alpha \mathcal{f}_\alpha \) - the fluid density,
- \( u = \rho^{-1} \sum_\alpha e_\alpha \mathcal{f}_\alpha \) - the macroscopic velocity,
- \( w_\alpha \) - a weighting coefficient (depending on direction \( \alpha \)),
- \( c = \Delta x/\Delta t \) - the lattice speed.

The discretised Boltzmann equation is solved in two steps, called respectively the collision step and the propagation step:

\[
\mathcal{f}_\alpha(x + e_\alpha \Delta t, t + \Delta t) = \mathcal{f}_\alpha(x, t) - \frac{1}{\tau} (\mathcal{f}_\alpha(x, t) - \mathcal{f}^{eq}_\alpha(x, t)),
\]

(14)

\[
\mathcal{f}_\alpha(x + e_\alpha \Delta t, t + \Delta t) = \mathcal{f}_\alpha(x, t).
\]

(15)

In our implementation \( \Delta x = \Delta t = 1 \), what results in \( c = 1 \). The speed of sound \( c_s = 1/\sqrt{3} \).

The pressure field is obtained from the following equation of state:

\[
p = c_s^2 \rho.
\]

It can be shown that \( u \) and \( p \) satisfy the Navier-Stokes equations with the kinematic viscosity \( \nu = (\tau - 0.5)c_s^2 \) with error \( \mathcal{O}(Ma^2) \).

4. Large-eddy simulation in SPH and LBM

LES is a method of turbulence modelling that consists in spatial filtering of flow fields [8] that can be implemented as a local increase of kinematic viscosity \( \nu \):

\[
\nu_{\text{eff}} = \nu + \nu_{\text{turb}},
\]

(16)

where \( \nu_{\text{eff}} \) is the effective local viscosity and \( \nu_{\text{turb}} \) denotes a turbulent (or sub-grid scale, SGS) viscosity that in the Smagorinsky model is computed as

\[
\nu_{\text{turb}} = (C_S \Delta)^2 |S|,
\]

(17)

where:
• $\Delta$ - the filter size,
• $|S| = \sqrt{2S_{ij}S_{ij}}$, where $S_{ij} = \frac{1}{2}(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i})$ is the strain rate tensor,
• $C_S$ - a constant, most often equal to 0.17.

4.1. LES implementation in LBM

We present now the application of the Smagorinsky SGS model to LBM [4, 12]. In the lattice Boltzmann method, the kinematic viscosity of fluid $\nu$ is uniquely linked with the relaxation time $\tau$. The effective relaxation time is determined as:

$$\tau_{\text{eff}} = 3(\nu + \nu_{\text{turb}}) + \frac{1}{2}. \quad (18)$$

It can be shown that

$$\nu_{\text{turb}} = (C_S\Delta)^2|S| = \frac{1}{6} \left( \sqrt{\tau^2 + \frac{18(C_S\Delta)^2 P}{\rho}} - \tau \right), \quad (19)$$

where $P = (2P_{ij}P_{ij})^{\frac{1}{2}}$ with $P_{ij} = \sum_\alpha e_{\alpha i}e_{\alpha j}(f_{\alpha} - f^e_{\alpha})$ being the stress tensor. Combining eqs. (18) and (19), we obtain:

$$\tau_{\text{eff}} = \frac{\tau}{2} \left( 1 + \sqrt{1 + \frac{18(C_S\Delta)^2 P}{\rho \tau^2}} \right). \quad (20)$$

In our implementation of LES in the LBM we set $\Delta = \Delta_x$.

4.2. LES implementation in SPH

In SPH the strain rate tensor needed in eq. (17) is approximated in the same way as other flow fields, i.e., with the use of kernel functions:

$$\langle S_{ij}\rangle_a = \frac{1}{2m_a} \left( \sum_b u_{ab,i} \nabla_j W(u_{ab}, h) \rho_b + \sum_b u_{ab,j} \nabla_i W(u_{ab}, h) \rho_b \right). \quad (21)$$

Consequently, eq. (11) will now take the following form:

$$\langle \nu \Delta \mathbf{u} \rangle_a = \frac{1}{m_a} \sum_b \left( \frac{\rho_{\text{eff},a}}{\Theta_a^2} \frac{\rho_{\text{eff},b}}{\Theta_b^2} + \frac{\rho_{\text{eff},b}}{\Theta_a^2} \frac{\rho_{\text{eff},h}}{\Theta_b^2} \right) \mathbf{r}_{ab} \cdot \nabla W(\mathbf{r}_{ab}, h) \mathbf{u}_{ab}. \quad (22)$$

The LES filter size is taken equal to the kernel smoothing length in SPH, i.e. $\Delta = h$.

5. Test case and results

As the test case the Taylor-Green Vortex (TGV) was chosen [3]. The computational domain is a periodic cube with edge length $L = 1$ m and the initial velocity amplitude is $U_0 = 1$ m/s. The initial conditions for velocity are defined as follows:

$$u_x(x, y, z, 0) = U_0 \cos(2\pi x) \sin(2\pi y) \sin(2\pi z),$$
$$u_y(x, y, z, 0) = -\frac{U_0}{2} \sin(2\pi x) \cos(2\pi y) \sin(2\pi z),$$
$$u_z(x, y, z, 0) = -\frac{U_0}{2} \sin(2\pi x) \sin(2\pi y) \cos(2\pi z).$$
The TGV flow, due to subsequent nonlinear interactions, develops in time to isotropic turbulence. Recently, the SPH simulation of the 2D TGV at \( Re=100 \) was performed by Adami et al. [2] using a modified WCSPH approach.

For LBM simulation the initial pressure (that uniquely determines density) was obtained by solving the Poisson pressure equation with the right-hand side involving gradients of the initial velocity. This step allowed us to avoid transient density oscillations that would occur when initializing the simulation with a constant pressure distribution. In SPH and FVM approaches the initial density was constant. Each method was tested at the Reynolds numbers \( Re = 3 \times 10^3 \) and \( Re = 10^4 \) \( (Re = U_0L/\nu) \) and at two spatial resolutions: 64\(^3\) and 128\(^3\). Additionally, the LBM simulations at \( Re = 3 \times 10^4 \) and \( Re = 10^5 \) at resolution 128\(^3\) were made.

In order to compare the methods in local, i.e. non-statistical sense, temporal evolution of velocity components at position \( x = (L/3, L/5, L/3) \) was investigated at \( Re = 10^4 \). The results presented in Figure 1 indicate that the TGV flow tends to the isotropic state beyond \( t^+ = 4 \), say. Figure 2 shows the temporal evolution of the total kinetic energy of the decaying TGV flow; a good agreement among the three methods is noticed.

![Figure 1. The temporal evolution of normalized velocity components \( u_i(t^+)/U_0 \) at position \( x = (L/3, L/5, L/3) \). Results for \( Re = 10^4 \) at resolution 128\(^3\).](image1)

![Figure 2. Temporal evolution of total kinetic energy \( k(t^+) \). Results for \( Re = 10^4 \) at resolution 128\(^3\).](image2)

For the assessment of the methods, the kinetic energy density spectra

\[
E(\kappa) = \frac{\kappa}{2} \left( \frac{dF_{11}}{d\kappa} + 2 \frac{dF_{22}}{d\kappa} \right),
\]

were calculated from the 1D longitudinal and transversal spectra, \( F_{11} \) and \( F_{22} \), where in general

\[
F_{ij}(\kappa) = \frac{1}{\pi} \int_{-\infty}^{\infty} Q_{ij}(r) \exp(-i\kappa r) dr
\]

were calculated from the 1D longitudinal and transversal spectra, \( F_{11} \) and \( F_{22} \), where in general
and \( \mathbf{r} = r\mathbf{x}^0 \) with \( \mathbf{x}^0 \) being the \( x \)-axis unit vector. The 1D spectra are computed out of the two-point velocity correlation \( Q_{ij} \). In our problem, the ensemble averaging is replaced by the space integral over all the locations \( \mathbf{x} \in \Omega \) (because of the flow periodicity, also \( (\mathbf{x} + \mathbf{r}) \in \Omega \)):

\[
Q_{ij}(\mathbf{r}) = \frac{1}{|\Omega|} \int_{\Omega} u_i(\mathbf{x})u_j(\mathbf{x} + \mathbf{r})d\Omega.
\] (25)

The TGV flow case is deterministic and such an averaging corresponds to what is usually done in the direct numerical simulation (DNS) of isotropic turbulence. The TGV becomes ultimately isotropic in this sense, as illustrated by the maps of vorticity magnitude (Figure 3). However, there is no large-scale forcing (unlike the DNS), so the flow is unsteady and decaying.

**Figure 3.** The vorticity magnitude at \( t^+ = 3.125 \) (left) and \( t^+ = 12.5 \) (right) in \( x-z \) plane at \( y = L/2 \). Results obtained in the LBM approach at \( Re = 10^4 \).

In Figures 4 and 5 we present the energy spectra (normalised by the total kinetic energy \( k \)) at \( Re = 10^4 \) and at a dimensionless time \( t^+ = 6.25 \), where \( t^+ = tU_0/L \). The graphs look noisy because the spectra are obtained by means of numerical differentiation. Nevertheless, the characteristic \( \kappa^{-5/3} \) slope in the inertial range can be clearly distinguished. The minimal size of eddies recovered by the spectra corresponds to approximately \( 2.3\Delta x \) and \( 3.5\Delta x \) for resolutions of \( 64^3 \) and \( 128^3 \), respectively. A similar agreement of results at \( Re = 3 \times 10^3 \) was obtained. A comparison of energy spectra at \( Re = 3 \times 10^3, 10^4, 3 \times 10^4 \) and \( 10^5 \) at resolution \( 128^3 \) obtained by means of LBM is shown in Figure 6. As the Reynolds number grows the inertial range widens and shorter wavelengths occur, what corresponds with theoretical predictions.

**Figure 4.** The comparison of kinetic energy spectra \( E(\kappa)/k \) at \( Re = 10^4 \) and resolution \( 64^3 \) at dimensionless time \( t^+ = 6.25 \).
6. Computational efficiency and GPU implementation

The explicit and local character of both LBM and SPH makes them perfect for parallel implementation. The in-house codes were written in C++ with the use of NVIDIA-CUDA API and executed on NVIDIA GeForce GTX 780 GPU. The LBM is the fastest among the presented methods. It is also well suited for GPU implementation - the code was written without use of any external libraries neither any user-defined structures, only CUDA built-in array pointers have been used. The SPH method is slower than LBM and its implementation is a bit more difficult. To optimise the execution time it is necessary to use the linked-list structure as well as sorting and hashing algorithms that reduce the computational complexity from $O(n^2)$ to $O(n)$. In our code we use the THRUST library that is CUDA implementation of C++ STL (Standard Template Library). The OpenFOAM FVM simulation [1] was executed on 2 cores of Intel Core2Duo CPU and is obviously significantly slower than GPU codes despite the largest timestep used. Figure 7 presents the execution time needed to obtain 1 second of physical time of TGV simulation.

![Figure 5](image5.png)  
**Figure 5.** The comparison of kinetic energy spectra $E(\kappa)/k$ at $Re = 10^4$ and resolution $128^3$ at dimensionless time $t^+ = 6.25$.

![Figure 6](image6.png)  
**Figure 6.** The kinetic energy density spectra at dimensionless time $t^+ = 6.25$ at different Reynolds number values obtained by means of LBM.

![Figure 7](image7.png)  
**Figure 7.** The comparison of the methods efficiency: the wall-clock time (in seconds) needed to obtain 1 s of simulation at resolution $128^3$. Timesteps in LBM, SPH and FVM approaches were 0.0003125 s, 0.0005 s and 0.004 s, respectively.
7. Conclusions and perspectives

In the present work, we have analysed the Taylor-Green vortex as a benchmark to validate different computational approaches. The chosen flow case is of interest because of its affinity to isotropic turbulence and LES studies. We have retrieved the TGV flow properties known from the literature in terms of temporal evolution of local velocity components as well as one-point statistical quantities and the kinetic energy spectra. Results are in good correspondence with theoretical predictions as the Reynolds number varies. It has been shown that spatial resolution has significant influence on the results obtained by means of investigated approaches. From this point of view the great advantage of SPH and LBM is the computational complexity, that scales as $O(n)$ with the problem size.

Promising results presented in this paper and very high efficiency of the codes run on GPU encourage us to further investigation of the LBM and SPH methods. We are planning to test more complex phenomena with these approaches, especially turbulence and two-phase dispersed flows are of interest.

8. References

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