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A Comparative Study Between a Lattice Boltzmann Method and a Finite Volume Method in Resolving Turbulent Heat Transfer in a Low Porosity Face-Centered Cubic Unit

Mona Al-Mqbas ^{1,†}, Tony Rosemann ^{2,*}, Nico Jurtz ¹ , Harald Kruggel-Emden ² and Matthias Kraume ¹ 

¹ Chair of Chemical and Process Engineering, Technische Universität Berlin, Ackerstraße 76, 13355 Berlin, Germany

² Chair of Mechanical Process Engineering and Solids Processing, Technische Universität Berlin, Ernst-Reuter-Platz 1, 10587 Berlin, Germany

* Correspondence: t.rosemann@tu-berlin.de

† These authors contributed equally to this work.

Abstract

Direct Numerical Simulations (DNS) are widely employed to simulate thermo-fluid dynamics in packed bed reactors, offering high-fidelity insights into complex flow and heat transfer phenomena. However, recent studies have revealed notable differences in isothermal turbulent flow results across different DNS frameworks, leaving open the question of how conjugate heat transfer is affected. This study presents a comparison between DNS based on a finite volume method (FVM) and a lattice Boltzmann method (LBM) for predicting turbulent heat transfer in a low porosity face-centered cubic (FCC) packed unit. First, the methods are compared with respect to the required resolution and computational cost. Subsequently, global parameters for drag, heat transfer, and spatial as well as temporal variances are evaluated. The flow topology is further analyzed by examining the mean and fluctuating components of hydrodynamic and thermal fields. While good agreement between the methods is shown regarding time-averaged velocity and temperature profiles, more pronounced differences are observed when comparing the respective temporal variances between the two methods. Additionally, the FVM, which relies on a surface-fitted mesh, requires more degrees of freedom to obtain a grid-converged solution but delivers results of higher certainty than the LBM. These findings highlight important methodological considerations when selecting DNS approaches for resolving turbulent heat transfer in complex porous geometries.

Keywords: lattice Boltzmann method (LBM); finite volume method (FVM); direct numerical simulation (DNS); computational fluid dynamics (CFD); packed bed; turbulent flow; heat transfer



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1. Introduction

The flow through arrangements of spherical particles is a phenomenon exhibited in various environmental and industrial processes, e.g., fluidized and packed bed reactors. These reactors play an important role in applications such as thermal energy storage and catalytic reactions [1]. The popularity of packed bed reactors can be attributed to their high surface area and good heat and mass transfer capabilities between the solid particles and the surrounding fluid [2]. The packed bed configuration, consisting of a complex matrix of solid particles, influences the flow topology when it interacts with the fluid medium.

This flow topology encompasses regions of acceleration and deceleration, the formation of vortices, and the appearance of jet flow patterns [3]. In situations characterized by moderately high Prandtl numbers (Pr), approximately $Pr \leq 10$ as is common in industrial packed bed applications [4], the specific flow topology plays an essential role in governing heat and mass transfer dynamics.

Despite recent advances in measurement techniques and numerical methods, the characteristics of turbulent flow within porous media, of which the packed bed is considered a representative example, remain inadequately understood [5]. Computational modelling plays an important role in improving our understanding of these systems due to the inherent difficulty of making detailed measurements in packed beds [6]. Early research on the characteristics of packed beds focused on developing empirical correlations for global parameters such as pressure drop and drag forces. These correlations, proposed by Zhaivoronkov et al. [7–10], Reichelt [8,10,11], Einfeld and Schnitzlein [12–15], and Ergun [16–18], and further extended to heat transfer correlations by Gnielinski [19] and Wakao et al. [20], continue to serve as essential tools for validation and closure modeling in numerical studies of macroscale behavior [21,22]. However, while these correlations effectively describe global trends, they provide limited insight into the underlying flow and thermal patterns which govern transport phenomena in such systems.

The complex flow topology created by the bed particles induces areas of separation and reattachment in the flow field, which represents a challenge for the computationally efficient Reynolds-Averaged Navier-Stokes (RANS)-based turbulence models that are used by most available Computational Fluid Dynamics (CFD) codes [23]. Moreover, there is a lack of comprehensive experimental data for validating RANS-based analysis, due to the challenge in experimentally identifying the complex fluid dynamics within packed bed configurations [24]. Scale-resolving modeling approaches, such as Large Eddy Simulation (LES) and Direct Numerical Simulation (DNS), are better suited for accurately simulating the flow in packed bed domains. DNS provides a complete resolution of all scales of motion, while LES captures large-scale turbulent motions and models the unresolved subgrid scales. As a result, these methods are less reliant on modeling assumptions, which are inherent in RANS-based simulations. Nevertheless, the computational demands of LES and DNS are prohibitively high, rendering them impractical for routine engineering design applications. A promising approach is to use highly resolved particle-resolved DNS simulations as basis to gain a mechanistic understanding of the turbulent flow in packed beds, and to use this knowledge and data to enhance RANS models, which, due to their efficiency, will still be state-of-the-art for most industrial applications. Although LES produces more accurate results compared to RANS models, it still involves some degree of subgrid-scale modeling. Consequently, DNS stands out as the sole method that completely obviates the need for modeling, making it the preferred tool for detailed analyses. Furthermore the obviation of modelling allows results obtained by DNS to be used as pseudo-experimental data to validate results obtained through RANS methods [25].

The finite volume method (FVM) and lattice Boltzmann method (LBM) have been most used for modeling the fluid flow in packed beds [26]. A particle-resolved DNS (pr-DNS) investigation of turbulence characteristics in a low porosity domain consisting of few spheres in a face-centered cubic (FCC) arrangement was conducted with an FVM-based solver by Hill and Koch [27] and later with an LBM-based solver by He et al. [3,28]. DNS were also used to identify possible deficiencies of existing turbulence models. Shams et al. [29–31] performed a series of investigations using the FVM which started with pr-DNS including heat transfer in a cubic domain composed of spherical particles arranged in FCC configuration [29], followed by a LES of this FCC domain [30] as well as a full-scale packed bed reactor simulation [31]. In the LES of the FCC domain by Shams et al. [30] turbulent

heat flux components showed deviations of 33–50% compared to the DNS while other quantities were in good agreement. On the other hand, Ambekar et al. [2] compared the hydrodynamics predicted by LES and various RANS turbulence closure models with a reference LBM-based DNS case of a full-scale bed. The authors found that inappropriate closure models can lead to an underprediction of Reynolds stress and turbulent kinetic energy by multiple orders of magnitude [2]. A possible deficiency based on a comparison with experimental data was also shown by Yang et al. [32] who performed a computational study of thermo-fluid flow through various ordered sphere packings using the RNG k - ϵ turbulence model and found that computed Nusselt numbers are notably lower compared to the widely used heat transfer correlation of Wakao et al. [20]. A variety of other DNS studies [4,33–38] performed simulations of heat transfer in random assemblies of spheres with the aim of deriving Nusselt number correlations as a function of porosity and Reynolds number, but were limited to flow regimes that are not fully turbulent and limited to high to medium porosities.

The FVM and LBM are both widely used in modeling and simulating flows, including heat transfer, in packed beds. Nevertheless, the extent to which the solutions obtained by these methods diverge from one another, as well as the relative sensitivity of mean and turbulent flows and thermal fields to the applied methods, remain unresolved. Authors such as Manelil et al. [39], Geller et al. [40], Breuer et al. [41], and Adeeb et al. [42] conducted comparisons between FVM and LBM for isothermal flow over single and multiple spheres and cylinders where the influence of the confining walls and the complex flow pattern, which are characteristic for flow through porous media, are not considered. He et al. [3,28] reported good agreement in terms of drag forces and spatial variances of velocity between their FVM-based DNS of isothermal flow through a FCC packing with the LBM-based DNS study of Hill and Koch [27]. No further detailed investigation of the efficiency and accuracy of both methods are presented in the literature to the knowledge of the authors in the context of turbulent flow through low voidage particle beds with coupled heat transfer.

This investigation aims to quantify the effects of applying either an FVM-based or an LBM-based solver in predicting turbulent heat transfer in packed units composed of spherical particles at the lowest possible voidage. To be specific, an FVM with an unstructured body-fitted mesh is compared to an LBM with a non-body-fitted Cartesian mesh consisting of equal-sized cubes. These two solvers and their associated mesh types were deliberately chosen since the inherent characteristics of both methods make them highly efficient at handling their respective meshes [43,44]. Therefore, previous comparative DNS studies [43–45] also involved these solver/mesh combinations. Comparing these two mesh types is also of relevance due to the findings of Finn and Apte [46] who have shown that a fictitious-domain-method-based FVM with a body non-conforming mesh may yield higher turbulent kinetic energy in iso-thermal turbulent flows when being compared to an FVM with a body conforming mesh. It remains unclear whether this behavior is specifically tied to the fictitious domain method employed by Finn and Apte [46]—particularly since their approach exhibited a strong deviation in the grid convergence study, which was not observed in other FVM-based body conforming implementations such as the one used in the work of Shams et al. [29]. Furthermore, the impact of such effects on turbulent heat transfer in coupled thermo-fluid simulations has yet to be established.

To achieve the present work's objectives, a comparative study of turbulent heat transfer in a low porosity FCC configuration (as seen in Figure 1) is conducted. Section 2 introduces the governing equations used for each method, the numerical solvers and schemes, as well as the numerical set up, including the boundary conditions and fluid physical properties and the depiction of flow properties. In Section 3.1, the numerical quality of the generated pr-DNS cases is investigated through temporal and spatial convergence, and it is looked at

computational efficiency. Section 3.2 focuses on global parameters, including spatial and temporal variances, drag force, and Nusselt number, while Sections 3.3 and 3.4 discuss the influence of the methods in predicting local flow and thermal patterns qualitatively and quantitatively. Finally, conclusions are drawn in Section 4 based on the performance analysis of the methods.

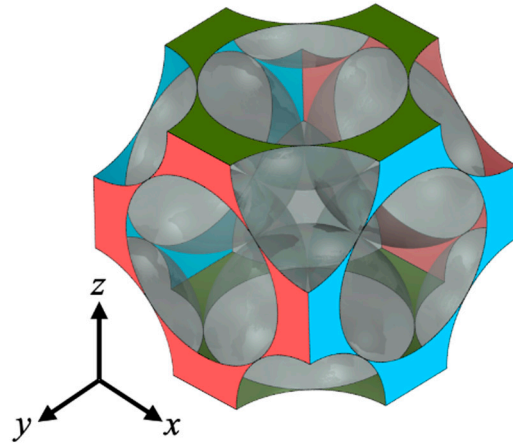


Figure 1. Schematic of used simulation domain with colored surfaces indicating periodic boundaries.

2. Numerical and Computational Details

2.1. Finite Volume Solver

The finite volume method (FVM) is a numerical approach that relies on the integral form of the conservation laws as its starting point [47]. The computational domain is subdivided into a finite number of contiguous control volumes (CVs), and the conservation equations are applied to each CV. The variables of interest are evaluated at the centroid of each control volume, while interpolation schemes are used to approximate their values at the CV surfaces. Surface and volume integrals are then approximated using suitable quadrature rules, resulting in a set of algebraic equations for the nodal values. An important property of the FVM is that it is conservative by construction, since fluxes through a shared face are equal and opposite for the two adjacent CVs.

Within the context of this work, the FVM was employed to resolve the incompressible continuity, momentum, and energy equations, as given in Equations (1)–(3):

$$\frac{\partial u_i}{\partial x_i} = 0, \quad (1)$$

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{1}{\rho} \frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 u_i}{\partial x_j \partial x_j} + F_i^b, \quad (2)$$

$$\frac{\partial T}{\partial t} + u_j \frac{\partial T}{\partial x_j} = \frac{\kappa}{\rho c_p} \frac{\partial^2 T}{\partial x_j \partial x_j}, \quad (3)$$

where ν , κ , c_p , and ρ are the kinematic viscosity, thermal conductivity, specific heat capacity, and density, respectively. A body force F_i^b was used to initiate the flow and adjust the desired Reynolds number. Equations (1)–(3) are solved with fully periodic boundary conditions in all directions for both velocity and temperature. For the temperature field, this introduces a temporal evolution of the domain-averaged mean temperature, as there is no fixed reference point in the periodic domain. To analyze local heat transfer fluctuations, the temperature field is normalized relative to its instantaneous domain-averaged mean. This ensures that Equation (3) describes the physically meaningful spatial temperature deviations and allows consistent comparison with velocity fluctuations, while fully respecting

the periodicity of the domain. Further discussion of the boundary conditions is provided in Section 2.3.

The FVM-based Segregated solver which uses the Semi-Implicit Method for Pressure Linked Equations (SIMPLE) algorithm to resolve the coupling between pressure p , velocity vector $\mathbf{u} = (u, v, w)^T$, and temperature T was used for the simulation. A central differencing scheme was used for the spatial discretization while a second order scheme was used for temporal discretizing of the unsteady terms. The simulations were performed using Simcenter STAR-CCM+ (version 2020.1.1, build 15.02.009). Simulations were conducted in parallel using HLRN supercomputing cluster hardware. The FVM implementation within the STAR-CCM+ software is widely used in the literature for resolving the flow within packed beds composed of spherical [13] and non-spherical particles [14] and has also been heavily utilized for modelling turbulent heat transfer including RANS [1,23], LES [30,31], and DNS [1,29] simulations.

2.2. Lattice Boltzmann Solver

The flow solver used to obtain the DNS results using LBM in the present study has been applied to simulate the flow through particulate systems considering both momentum and heat transfer in previous works [37,48–50] which also include validation. During the simulation, the collision and streaming of velocity distribution functions f_l and temperature distribution functions g_l are performed for each fluid node on a structured uniform Cartesian mesh exemplarily shown in Figure 2.

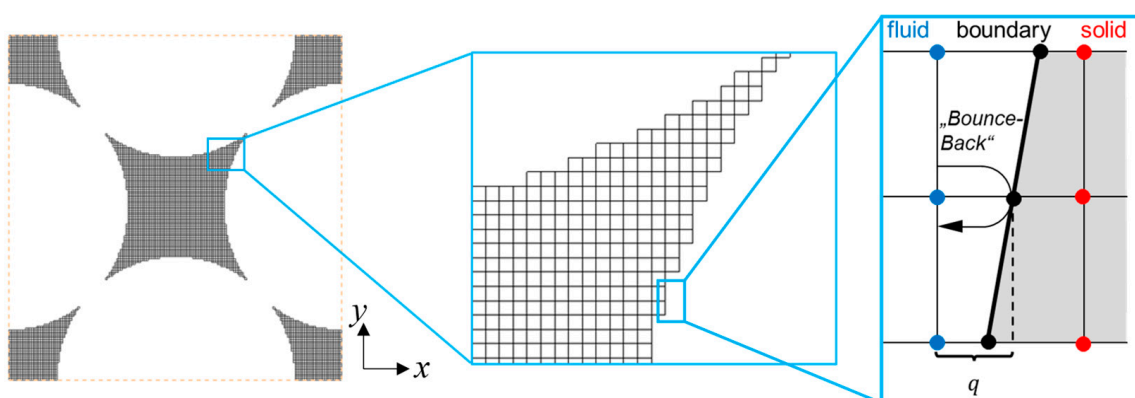


Figure 2. Cross-sectional view of numerical grid used to conduct LBM DNS simulation. Shown is the mesh that consists of the fluid nodes in which the collision of distribution functions takes place before these distribution functions are streamed to neighboring fluid nodes. Distribution functions that are streamed from a fluid node towards the particle surface are treated with interpolated bounce-back methods [51,52] to account for the exact distance q between fluid node and the curved particle boundary in order to fulfill the no-slip and isothermal boundary conditions.

For each of the fluid nodes $\mathbf{r}$ separated by Δx , the collision and streaming in the direction of the discrete lattice velocities $\mathbf{e}_l$ to the neighbour fluid node $\mathbf{r} + \mathbf{e}_l \Delta t$ during one time step Δt can be written as

$$f_l(\mathbf{r} + \mathbf{e}_l \Delta t, t + \Delta t) = f_l(\mathbf{r}, t) - \Omega_l(f) + F_l^b \Delta t, \quad l = 1, 2, \dots, 19 \quad (4)$$

$$g_l(\mathbf{r} + \mathbf{e}_l \Delta t, t + \Delta t) = g_l(\mathbf{r}, t) - \Omega_l(g), \quad l = 1, 2, \dots, 7 \quad (5)$$

where Ω denotes the collision operator and F^b an external body force which was adjusted in the present study to achieve the desired Reynolds numbers. The D3Q19 lattice featuring 19 lattice velocities was used for the velocity distribution functions and the D3Q7 lattice featuring 7 lattice velocities for the temperature distribution functions. Unless stated other-

wise, all LBM results shown in this work were obtained with the Multiple-Relaxation-Time (MRT) collision operator by d’Humières et al. [53], including the therein defined parameters when considering the velocity distribution functions. For selected cases, however, simulations with the Bhatnagar–Gross–Krook (BGK) collision operator were performed to analyze the influence of the collision operator on the results. Considering the temperature distribution functions, the MRT collision operator by Yoshida and Nagaoka [54] was used. Although the mesh shown in Figure 2 gives the impression of a staggered approximation of the sphere surfaces, we used interpolated bounce-back boundary conditions that take into account the exact distance between the boundary fluid nodes and the particle surface on each boundary link, where the boundary link denotes a lattice velocity that intersects the surface of a particle. The no-slip boundary condition was established using the linearly interpolated bounce-back method by Bouzidi et al. [52] and the isothermal boundary condition was realized with the linearly interpolated bounce-back method by Li et al. [51]. The momentum exchange between fluid and particle was computed with the momentum exchange method by Wen et al. [55] and the heat transfer between particle and fluid was calculated by the heat exchange method described in Rosemann et al. [50]. A more detailed description of the methods used in the LBM implementation can be also found in Rosemann et al. [50].

2.3. Simulation Setup and Depiction of Flow Properties

The simulation domain consists of 14 spherical particles with diameter $d_p = 0.03$ m arranged in FCC configuration with a low porosity of 0.26. The domain used for this study is geometrically periodic in all three directions as shown already in Figure 1 and, therefore, contains only the total solid volume of 4 spherical particles. It should be noted that different thermal boundary conditions have been used in the literature to simulate thermal flows through assemblies of spheres for a specified void fraction. First, there are inlet/outlet boundary conditions [56,57] that impose a constant temperature and velocity at the inlet and require sufficiently large inlet and outlet regions that are disregarded from the analysis, because flow conditions in these regions are not representative for the fully developed flow inside the actual considered porous structure. Second, there are fully periodic boundary conditions for momentum transfer in all directions combined with fully periodic boundary conditions for heat transfer in lateral directions and a thermal similarity condition for the temperature field in the driving flow direction [4,23,35]. The thermal similarity condition copies the temperature field at the downstream boundary face to the corresponding upstream boundary face but scales it by a factor that accounts for the amount of heat exchanged by fluid and particle phase. Third, there are fully periodic boundary conditions for both momentum and heat transfer in all directions, which have been recently successfully applied by Chen and Müller [36] for a DNS of gas–solid heat transfer in random assemblies of spheres under laminar flow conditions. The difficulty that arises from both inlet/outlet and thermal similarity boundary conditions is that an underlying spatial temperature gradient along the driving flow direction is present, since the temperature difference between fluid and particle phase is decreasing along the driving flow direction due to the fluid’s ability to exchange heat with the commonly assumed isothermal particles. Therefore, local heat transfer phenomena can only be analyzed slice-wise for slices perpendicular to the driving flow direction. However, in the context of turbulent heat transfer in the considered pore geometry it is desirable to define quantities such as spatial deviations of temperature with respect to a domain-averaged mean temperature in order to be consistent with the definition of the spatial deviations of velocity which are also defined with respect to a domain-averaged mean velocity. The fully periodic boundary conditions for heat transfer introduce a temporal gradient in the temperature field since there is no fixed temperature

anchor for the fluid and the temperature difference between particle and fluid phase is decreasing over time. However, this effect can be easily eliminated using the normalized temperature field as defined below. Therefore, these boundary conditions are used in the current study. A more rigorous comparison of the boundary conditions discussed above and elaboration on the advantages of the herein used fully periodic thermal boundary conditions can be found in Chen and Müller et al. [36].

Based on the particle diameter d_p and the double averaged (in time and space) streamwise velocity $\langle \bar{u} \rangle$, the Reynolds number was estimated to be

$$Re = \frac{\langle \bar{u} \rangle d_p}{\nu} = 1000, \quad (6)$$

representing a fully turbulent regime as classified by Chu et al. [58]. The flow was induced by a body force in both the FVM and the LBM, pointing in positive x-direction (see Figure 1 or Figure 2 for comparison). The fluid had a dimensionless initial temperature $T_f = 1$. A constant temperature boundary condition $T_w = 0$ was applied to the walls of the particles. Physical and thermal properties such as density, viscosity, and thermal diffusivity were adjusted to obtain a Prandtl number of

$$Pr = \frac{\mu c_p}{\kappa} = 0.7, \quad (7)$$

where μ , c_p , and κ are fluid dynamic viscosity, specific heat capacity, and thermal conductivity, respectively. Within the context of this work, dimensionless thermal and flow fields are used. All the relevant flow and thermal field quantities are expressed as dimensionless values by dividing them by either the double-averaged (in time and space) streamwise velocity, $\langle \bar{u} \rangle$, or the volume-averaged instantaneous temperature $\langle T \rangle$, as shown in Table 1. The fluctuating quantities such as u_i' (or T') were computed by subtracting the temporal mean velocity from the instantaneous field as $u_i' = u_i - \bar{u}_i$. The star superscript denotes a dimensionless quantity while the overbar sign indicates a time averaging operation in this work. The dimensionless turbulent kinetic energy $\bar{k}^*$ is computed as $\bar{k}^* = 0.5 \left(\overline{u'u'^*} + \overline{v'v'^*} + \overline{w'w'^*} \right)$.

Table 1. Definitions of relevant dimensionless quantities: $\bar{U}^*$ is velocity magnitude computed as $U = \sqrt{u^2 + v^2 + w^2}$, $\bar{u}_i'^*$ is a velocity component, $\overline{u_i' u_i'^*}$ is a velocity variance component, $\bar{T}^*$ is temperature, $\overline{T' T'^*}$ is temperature variance and $\overline{u_i' T'^*}$ is a turbulent heat flux component.

Quantity	Definition
$\bar{U}^*$	$\bar{U} / \langle \bar{u} \rangle$
$\bar{u}_i'^*$	$\bar{u}_i / \langle \bar{u} \rangle$
$\overline{u_i' u_i'^*}$	$\overline{u_i' u_i'} / \langle \bar{u} \rangle^2$
$\bar{T}^*$	$\bar{T} / \langle T \rangle$
$\overline{T' T'^*}$	$\overline{T' T'} / \langle T \rangle^2$
$\overline{u_i' T'^*}$	$\overline{u_i' T'} / \langle \bar{u} \rangle \langle T \rangle$

3. Results

The results obtained from the FVM and LBM simulations are structured into four sections. First, the numerical quality of high-resolution DNS cases was examined with regards to statistical convergence and spatial resolution as well as computational efficiency (Section 3.1). Second, a comparison between the performance of the methods in predicting global parameters of interest such as spatial and temporal variances, particle drag force, and Nusselt number was performed and, if possible, parameters were compared

against available data from the literature (Section 3.2). Third, local flow topology, including the turbulence and thermal fields as well as the thermal-hydrodynamics coupling represented by the turbulent heat flux, is discussed qualitatively (Section 3.3) and quantitatively (Section 3.4).

3.1. Numerical Quality: Temporal and Spatial Convergence as Well as Computational Efficiency

The numerical quality of the DNS cases is essential for accurately capturing the diverse length and time scales observed in the flow field. Figure 3 presents exemplary snapshots of the vortical flow structures exhibited in the domain as calculated by the FVM and LBM solvers. Using the commonly applied Q-criterion [59,60], the vortex boundaries are shown as iso-surfaces for a dimensionless value of $Q(d_p/\langle\bar{u}\rangle)^2 = 488$, which corresponds to the ratio $Q/Q_{\max} = 0.05$ considering the maximum value $Q_{\max}$ in the flow field. The iso-surface coloring is based on the normalized velocity magnitude $\bar{U}^*$. Both methods result in a similar pattern of vortices with a diverse range of spatial scales, highlighting the importance of examining the influence of grid resolution on the performance of each method.

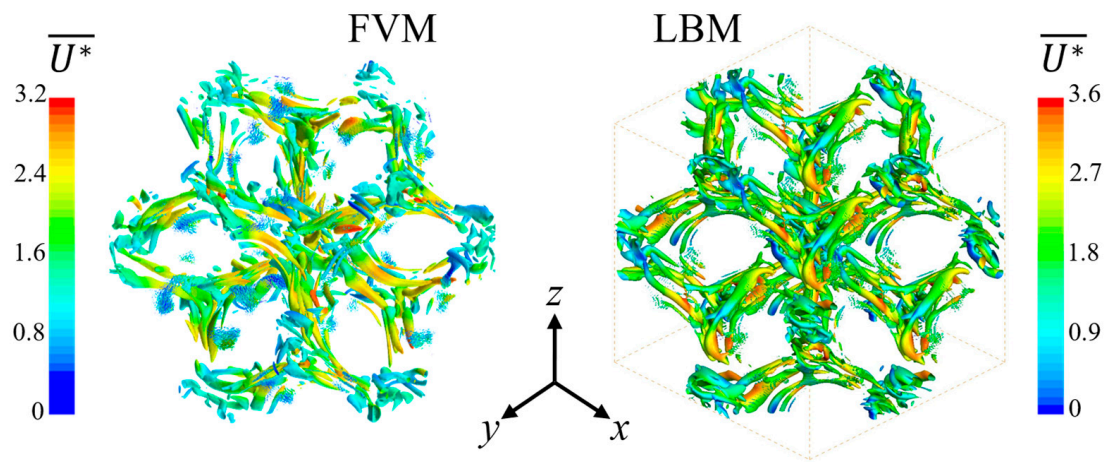


Figure 3. Exemplary snapshot with iso-surfaces using Q-criterion with $Q/Q_{\max} = 0.05$ colored in velocity magnitude $\bar{U}^*$.

The simulations reported here were performed over a sufficiently long integration period to achieve statistical convergence for mean and fluctuating quantities (see Table 1). The integration time is represented by the Flow Through Time, which is denoted as FTT, defined as domain length over mean interstitial velocity: $FTT = L/\langle\bar{u}\rangle$. The FVM and LBM results showed statistical convergence after 22 FTT. The results presented in this work consist of 1000 samples with a sampling frequency of 0.025 FTT for both FVM and LBM.

Based on this, the reliability of the obtained results from the DNS of the two methods is investigated with regard to the spatial resolutions. Given the nature of the FVM and LBM, different grid requirements apply to each method (see Section 3.1.1 for the FVM and Section 3.1.2 for the LBM). Additionally, the solvers' computational efficiency is investigated (Section 3.1.3).

3.1.1. Finite Volume Method

For the FVM, the local grid scaling $\Delta = \sqrt[3]{\Delta_i\Delta_j\Delta_k}$ is compared with the local Kolmogorov length scale η , which is computed as

$$\eta = \left(\frac{\nu^3}{\varepsilon}\right)^{\frac{1}{4}} \quad (8)$$

where ν is the kinetic viscosity and ε is the dissipation of the turbulent kinetic energy and is defined as

$$\varepsilon = \nu \frac{\partial u'_i}{\partial x_j} \frac{\partial u'_i}{\partial x_j} \quad (9)$$

The average and maximum values of the ratio of local grid spacing to the Kolmogorov length scale of $(\Delta/\eta)_{\text{avg}} = 0.82$ and $(\Delta/\eta)_{\text{max}} = 4.6$ were found comparable to the recommendations of Chu et al. [58] for modeling turbulent flows in porous structures. This grid spacing resulted in a cell count of 21 million polyhedral cells (Figure 4a) and a near wall resolution of $y^+ = 0.138$ across the domain.

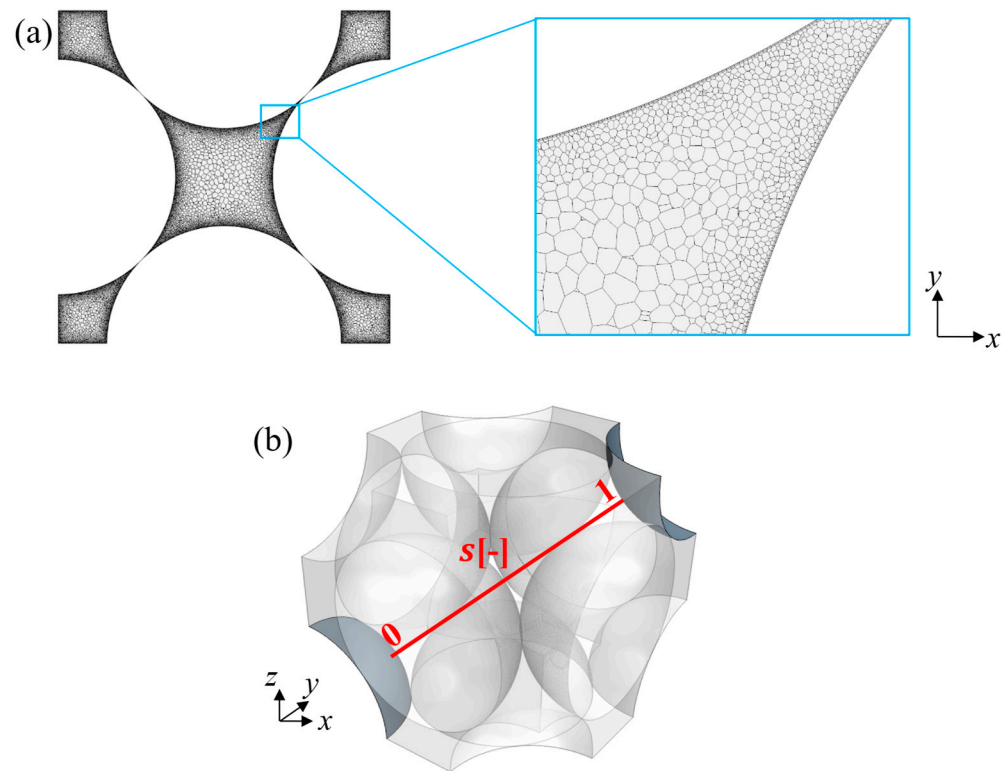


Figure 4. (a) Cross-sectional view of numerical grid used to conduct FVM DNS simulation with a close-up of near wall resolution for a cell count of 21 million cells. (b) Along line s shown as a projection diagonally crossing the domain, mean velocity, mean temperature, turbulent kinetic energy, fluctuating temperature, and heat flux are evaluated (see Figure 5).

To ensure mesh quality and minimize skewness near particle contact points, the local caps approach was employed. In this method, particles are locally flattened at the contact region, thereby reducing high skewness that could otherwise compromise numerical stability and accuracy—an issue frequently reported in unstructured grids generated for similar porous geometries [5]. This approach and the corresponding mesh settings have been presented in detail by Eppinger et al. [13]. A grid convergence study was performed using five grids, consisting of approximately 4.98, 10.2, 12.8, 16.2, and 21.1 M cells, respectively, to verify the independence of the pr-DNS FVM solution regarding spatial resolution. It should be noted that the lowest grid resolution of 4.98 M had yielded the values of $(\Delta/\eta)_{\text{avg}} = 1.6$ and $(\Delta/\eta)_{\text{max}} = 6.7$, which do not meet the resolution criteria suggested by Chu et al. [58]. Nevertheless, this lowest-resolution mesh is included because its size is comparable to that of the LBM grid, allowing for direct comparison. A time step of $\Delta t = 0.00005$ s was identified as being sufficiently small to enable the resolution of the Kolmogorov time scale, which is of the magnitude of 0.000145 s.

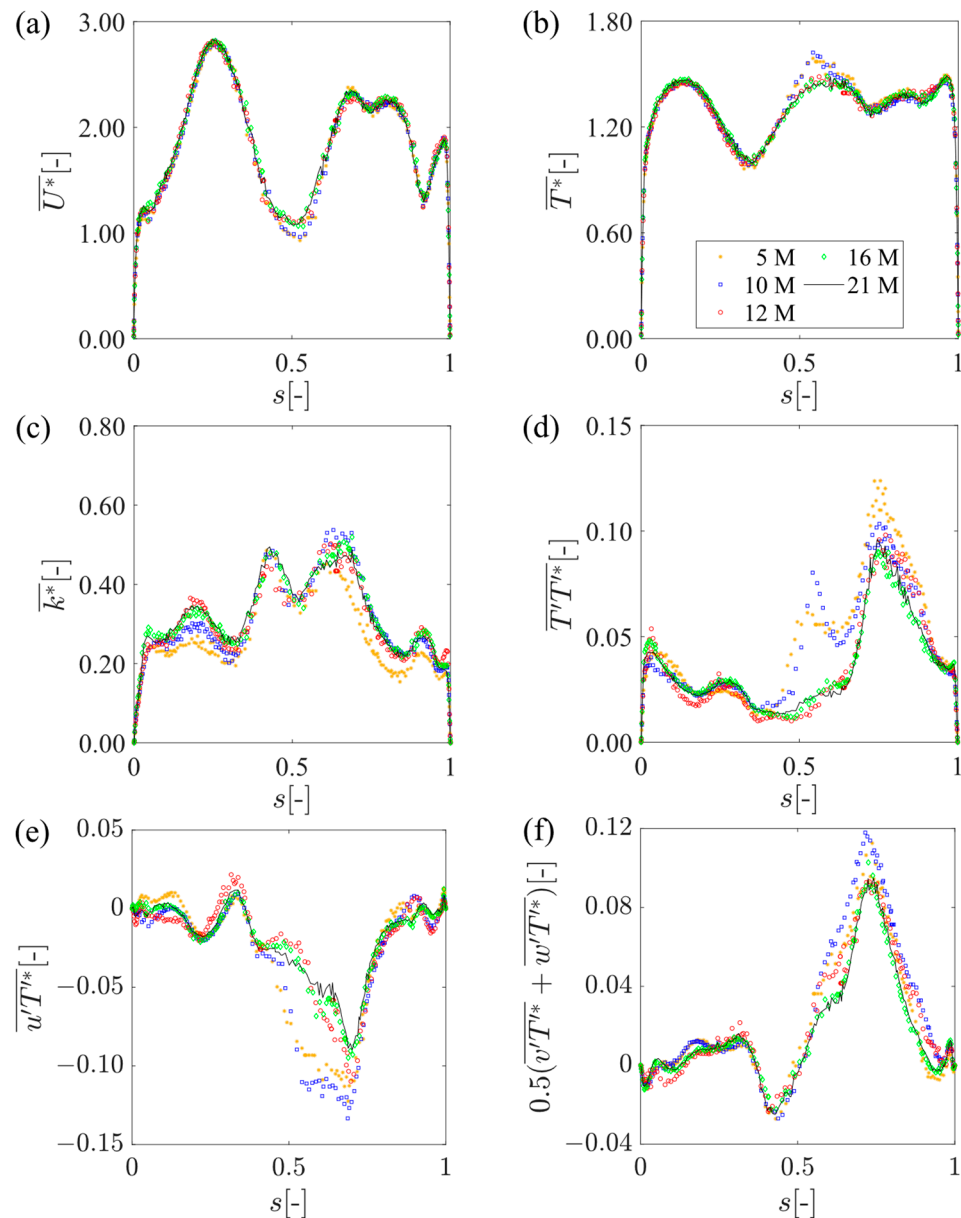


Figure 5. Time-averaged and normalized quantities for FVM grid convergence study: (a) velocity magnitude $\overline{U}^*$, (b) temperature $\overline{T}^*$, (c) turbulent kinetic energy $\overline{k}^*$, (d) temperature variance $\overline{T'T'}$, (e) streamwise turbulent heat flux $\overline{u'T'}$, and (f) spanwise turbulent heat flux given by $\frac{1}{2}(\overline{v'T'} + \overline{w'T'})$, sampled along diagonal line, as depicted in Figure 4b for different resolutions.

The distribution of the mean velocity magnitude $\overline{U}^*$, mean temperature $\overline{T}^*$, turbulent kinetic energy $\overline{k}^*$, fluctuating temperature $\overline{T'T'}$, and heat flux components $\overline{u'T'}$, $\overline{v'T'}$, and $\overline{w'T'}$ over a line diagonally crossing the domain as depicted as projection in Figure 4b is presented in Figure 5. The spanwise turbulent heat flux components were averaged as shown in Figure 5f due to the symmetry of the spanwise turbulent heat flux along this sampling line, i.e., $\overline{v'T'} \approx \overline{w'T'}$. The two coarsest grids (~5 and ~10 M cells) exhibited larger deviations, particularly in the turbulent quantities. This outcome is expected, since these resolutions do not satisfy the pr-DNS requirements introduced earlier, but were nevertheless included for comparison with the LBM grid resolution. In contrast, the mean flow variables (velocity and temperature) were reasonably well captured even on the coarser meshes. The simulations, conducted using high resolution meshes, yielded similar results for the mean fields (velocity and temperature) as well as the turbulent quantities represented by the turbulent kinetic energy, fluctuating temperature, and heat

flux. Consequently, it is evident that the FVM-based DNS results employed for this study are grid independent when utilizing a sufficient cell count of 21 million cells as chosen here.

3.1.2. Lattice Boltzmann Method

A grid refinement study was performed for the LBM using 0.2, 0.6, 1.5, 3.0, and 5.1 million fluid nodes, while maintaining the structured uniform Cartesian mesh structure. This corresponds to a particle diameter of 63.6, 95.5, 127.3, 159.1, and 190.9 nodes, respectively, and domain lengths of 90, 135, 180, 225, and 270 nodes, respectively. The viscosity-linked relaxation times were 0.5075 for the two lowest and 0.515 for the three highest resolutions. Additionally, the simulation for 5.1 M was performed with the BGK instead of the MRT collision operator to compute the velocity field since it was shown by Nathen et al. [61] that the MRT scheme can be unable to deliver mesh convergence, and can produce unphysical results and spurious oscillations in turbulent flows at higher Reynolds numbers. However, an advantage of the MRT scheme is generally that it has superior stability properties at lower resolutions and smaller relaxation times compared to the BGK scheme. While we were able to obtain stable simulation results using the MRT scheme for the analyzed resolutions, the BGK scheme led to a divergence when using 0.2 M, 0.6 M, and 1.5 M fluid nodes.

Figure 6 shows various already for the FVM evaluated time-averaged variables sampled over the diagonal sampling line (see again Figure 4b) stretched out throughout the LBM domain for different resolutions. Except for the lowest depicted resolution (0.6 M), the other resolutions show only little deviation from each other for the depicted variables. This is especially true for the velocity magnitude (Figure 6a) and the temperature (Figure 6b). While the resolution of 1.5 M is sufficient to give reliable results for the turbulent kinetic energy (Figure 6c) and the temperature variance (Figure 6d), the resolution 3.0 M is necessary to achieve mesh convergence for the peak values at $s \approx 0.32$ and $s \approx 0.74$, when considering the streamwise (Figure 6e) and spanwise (Figure 6f) components of the turbulent heat flux. Since we also do not find a significant difference between the 5.1 M results obtained with the MRT and the BGK collision operator in any of the variables shown in Figure 6, we conclude that the resolution 5.1 M is sufficient and the MRT scheme is able to produce reliable simulation results for the turbulent flow through the FCC geometry.

A comparison of the grid convergence studies of the finite volume method (FVM) solver (see Figure 5) and the lattice Boltzmann method (LBM) solver (see Figure 6) reveals that the FVM exhibits a gradual convergence towards a stable solution, with minimal divergence between the two highest resolutions (16 and 21 million cells, respectively). This finding suggests a tendency for errors in dispersion to be absent. In contrast, deviations are observed at the lower resolutions of approximately 5 and 10 million cells. The corresponding grid resolutions to those yielded this mesh sizes do not satisfy the mesh requirements for particle resolved DNS (see Section 3.1.1 for further details) but were nevertheless included for comparison with the LBM resolutions.

The LBM, on the other hand, generally achieves reliable results with fewer fluid nodes. Nevertheless, pronounced deviations between resolutions are observed in the temperature variance (Figure 6d) and the streamwise turbulent heat flux (Figure 6e), particularly in the central region of the pore geometry ($s \approx 0.55$). Although the low- and high-resolution LBM results are relatively close to each other, the discrepancy between the two highest resolutions is larger than in the FVM case, leading to greater uncertainty. It should be noted, however, that a certain level of uncertainty in fluctuating turbulent quantities is commonly observed [46].

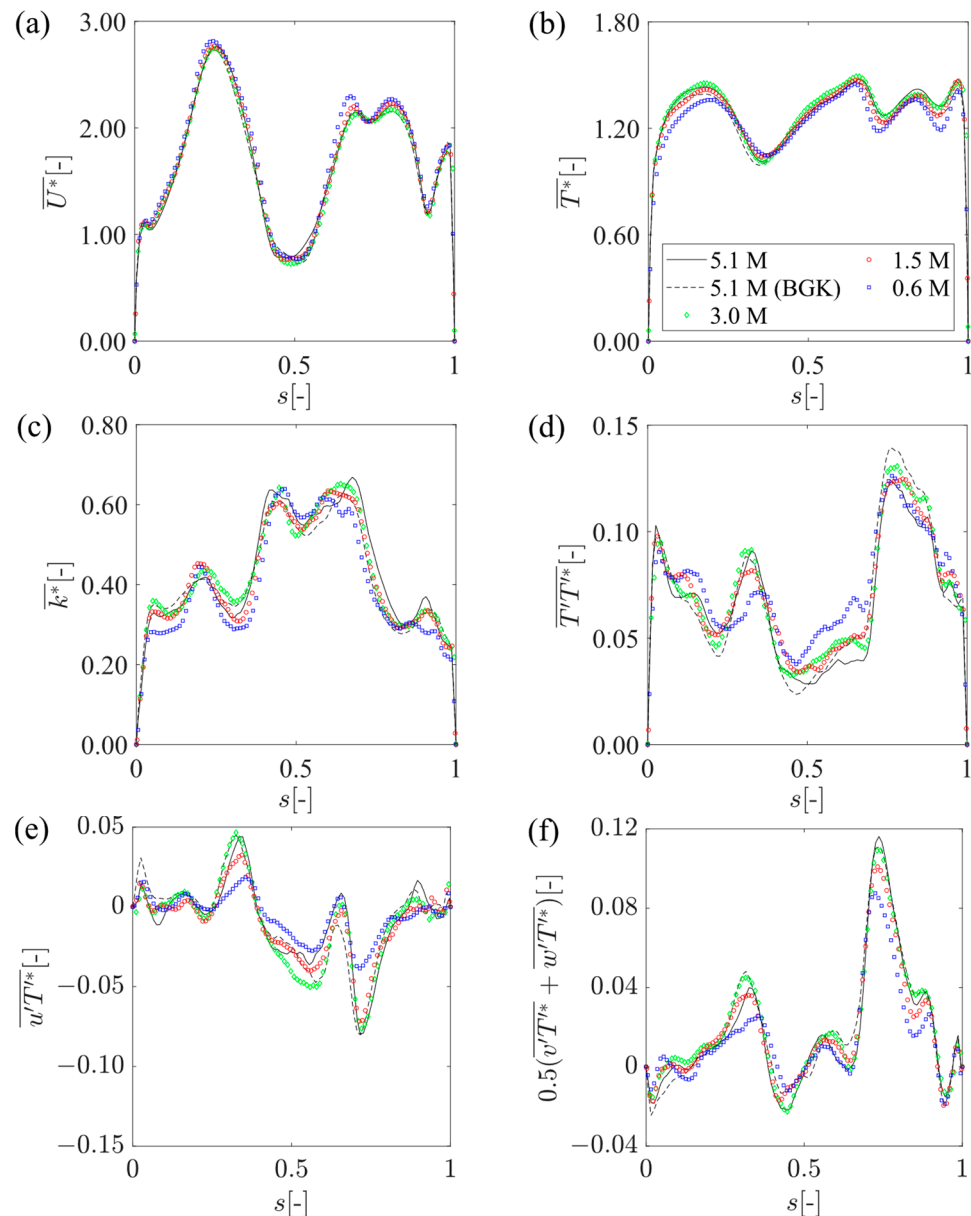


Figure 6. Time-averaged and normalized quantities for the LBM grid convergence study: (a) velocity magnitude $\overline{U^*}$, (b) temperature $\overline{T^*}$, (c) turbulent kinetic energy $\overline{k^*}$, (d) temperature variance $\overline{T'T^*}$, (e) streamwise turbulent heat flux $\overline{u'T^*}$, and (f) spanwise turbulent heat flux $\frac{1}{2}(\overline{v'T^*} + \overline{w'T^*})$, sampled along diagonal line as depicted in Figure 4b for different resolutions.

3.1.3. Solvers Computational Efficiency

It is well established that both the finite volume and the lattice Boltzmann methods have distinct computational requirements. To quantify these differences for the examined porous structure, Table 2 presents a comparative overview of the simulation time and CPU core-hours required to perform one flow through cycle across the domain, which is represented by the FTT. Even though a high-resolution mesh of 21 million cells was employed to compute the actual simulation by FVM, a lower resolution mesh of 4.98 million cells was used to ensure a more equitable computational comparison with the LBM simulation. For the FVM, the 4.98 million cell mesh simulation is typically conducted on 120 cores; nevertheless, it was run on 30 cores to ensure a direct comparison with the LBM case. The core-hour requirements were found to be 118.5 and 54 core-hours for the FVM and LBM, respectively. The resulted core-hours might serve to illustrate the computational efficiency

of the LBM in this context. These observations are consistent with the recent findings of Suss et al. [44], who showed in a detailed runtime comparison that cell updates in a LBM solver are two to three times faster compared to an FVM solver.

Table 2. Computational efficiency of FVM and LBM. Annotations (1P) and (2P) denote number of processors on motherboard.

	FVM	LBM
Mesh cells	4.98 M	5.1 M
Utilized CPU cores	30	30
Simulation time per FTT	3.95 h	1.82 h
Core-hour	118.5	54.0
Node architecture	Epyc 7502 32-core (1P)	Epyc 7443 24-core (2P)

The observed efficiency of the LBM can be attributed to several factors. This method employs a simplified, explicit algorithm based on local stream-and-collide operations (as previously described in Section 2.2), in contrast to the FVM, which involves solving coupled partial differential equations with pressure–velocity correction schemes, often requiring iterative solvers and matrix operations [47]. Furthermore, contemporary hardware is equipped with substantial caches, which have the capacity to efficiently handle the LBM’s elevated memory requirements introduced by the nineteen velocity distribution functions and seven temperature distribution functions being loaded and stored for each updated cell [44]. This high number of the distribution functions induce a higher memory requirement that is further amplified for large domains. Due to this memory limitation, the LBM method is more efficient for small domains, where the memory bandwidth is not being a bottleneck of the method’s performance.

LBM operations facilitate excellent parallel scalability, as each node update depends only on neighboring nodes, thus minimizing communication overhead. In the case of the FVM, the pressure correction loop gives rise to global dependencies, which can hinder parallel efficiency at scale. It should also be noted that there is a certain effort associated with creating a high-quality unstructured mesh as used in the FVM, which has to satisfy certain quality criteria such as a low skewness of cells. A structured uniform Cartesian mesh as used in the LBM can be more efficiently handled and is automatically created during the start of the simulation in the LBM implementation of the present work. It is also worth noting that in STAR-CCM+ memory usage and I/O demands associated with post-processing can contribute significantly to the overall computational cost, particularly in high-resolution FVM simulations. Operations such as transient data export and visualization increase memory pressure and I/O time, potentially extending the wall-clock duration of simulations and, hence, the total core-hours consumed. These effects were considered during the evaluation and may have contributed to the higher resource usage observed for the FVM.

3.2. Prediction of Global Quantities

In the following, we consider domain-averaged spatial fluctuations extracted from the fluid’s instantaneous velocity and temperature field as well as interphase momentum and heat transfer to compare the FVM and LBM results against each other and against available data from the literature.

The spatial velocity fluctuation

$$\tilde{\mathbf{u}} = \mathbf{u} - \langle \mathbf{u} \rangle \quad (10)$$

represents the deviation of the instantaneous velocity $\mathbf{u}$ from the domain-averaged velocity $\langle \mathbf{u} \rangle$. Following the definitions in Hill and Koch [27] and He et al. [28], the spatial variance of the streamwise velocity normalized with the interstitial velocity $\langle \bar{u} \rangle$ is given by

$$R_{u,\parallel}^{s*} = \langle \tilde{u}\tilde{u} \rangle / \langle \bar{u} \rangle^2 \quad (11)$$

and of the spanwise velocity by

$$R_{u,\perp}^{s*} = 0.5 \left(\langle \tilde{v}\tilde{v} \rangle + \langle \tilde{w}\tilde{w} \rangle \right) / \langle \bar{u} \rangle^2. \quad (12)$$

In a similar way, the spatial variance of temperature is defined as

$$R_T^{s*} = \langle \tilde{T}^* \tilde{T}^* \rangle \quad (13)$$

by considering the instantaneous normalized temperature field $T^* = T / \langle T \rangle$. Temporal variances $R_{u,\parallel}^{t*}$, $R_{u,\perp}^{t*}$ and R_T^{t*} are defined using the temporal fluctuations introduced in Section 2.3 instead of the spatial fluctuations.

Momentum exchange between particle and fluid phase is analyzed in terms of the total force F that includes both the drag force and pressure-gradient force contribution, and is normalized by the Stokes drag as

$$F^* = \frac{F}{3\pi d_p \nu \rho (1 - \phi) \langle \bar{u} \rangle} \quad (14)$$

where the term $(1 - \phi) \langle \bar{u} \rangle$ represents the streamwise superficial velocity by taking into account the solids volume fraction ϕ .

The interphase heat transfer with the FVM is evaluated in terms of the Nusselt number Nu that can be obtained by integrating the fluid temperature gradient in normal direction $\mathbf{n}$ to the sphere surface over the whole sphere surface S_p with surface area A_p as

$$Nu = \frac{d_p}{A_p \kappa (T_p - T_{\text{ref}})} \oint_{S_p} -\kappa \frac{\partial T}{\partial \mathbf{n}} dS \quad (15)$$

where the temperature difference $\Delta T = T_p - T_{\text{ref}}$ between particle and fluid requires a specification of a suitable reference temperature T_{ref} in the fluid. In the LBM framework the heat exchange method as described in Rosemann et al. [50] is used, which calculates the Nusselt number as

$$Nu = \frac{d_p \dot{Q}}{\rho c_p \alpha A_p (T_p - T_{\text{ref}})} \quad (16)$$

with thermal diffusivity α and normalized heat transfer rate $\dot{Q}$. Herein, the heat transfer rate is efficiently calculated by the following sum:

$$\frac{\dot{Q}}{\rho c_p} = \frac{\Delta x^3}{\Delta t} \sum_{\mathbf{r}_f} \sum_{l_{bl}} \left[\tilde{g}_l(\mathbf{r}_f, t) - \tilde{g}_{\bar{l}}(\mathbf{r}_f, t + \Delta t) \right], \quad (17)$$

meaning that for each boundary fluid node $\mathbf{r}_f$ that is connected to solid nodes via boundary links l_{bl} the difference between post-collision temperature distribution functions ($\tilde{g}_l$) streamed towards the particle surface and pre-collision temperature distribution functions ($\tilde{g}_{\bar{l}}$) bounced back from the surface in opposite direction ($\bar{l}$) are accumulated. In this work, we used the domain-averaged fluid temperature $T_{\text{avg}} = \langle T \rangle$ as reference temperature, which is not constant since the fluid temperature is adapting to the constant particle

temperature T_p over time in the fully periodic setup. The integral in Equation (15) represents the heat exchange between particle and fluid phase and is also decreasing over time due to the decreasing temperature difference between the phases. However, during the simulation we observed that the Nusselt number reaches a constant time-averaged value, which is consistent with the findings of Chen and Müller [36] for laminar flow conditions.

The time-averaged values for the quantities defined in Equations (11)–(15) were computed for each resolution of the FVM and LBM simulations. Figure 7 shows the relative deviation δ_{HR} of the values obtained from lower resolutions with respect to the corresponding value obtained for the highest simulated resolution being the reference solution. Since we focus on the convergence behavior of each method here and an analytical reference solution does not exist, the reference solution is therefore method-dependent. The resolution is given in terms of the approximate number of degrees of freedom $N^{1/3}$, where N is the number of fluid nodes/cells in the simulation. The deviation drops below 2% for each of the quantities at the highest shown $N^{1/3}$ value (second highest simulated resolution) for both FVM (Figure 7a) and LBM (Figure 7b). This indicates that the highest resolution is sufficient in both methods. Due to the fluctuating nature of the flow and limitation of the sampling size, the time-averaging process leads to unavoidable errors, which is why a further convergence towards zero deviation is not feasible. A remarkable difference in the convergence behavior of the total force and the Nusselt number exists between FVM and LBM. While the total force converges slowly in the LBM, a reliable value is achieved at low resolutions in the FVM. Regarding the Nusselt number, the LBM value does not vary significantly with the used resolution, which is not the case for the FVM, where the Nusselt number converges slowly to a reliable value. The data presented in Figure 7 further confirms that the LBM requires a lower number of degrees of freedom to achieve grid independent results in this benchmark case.

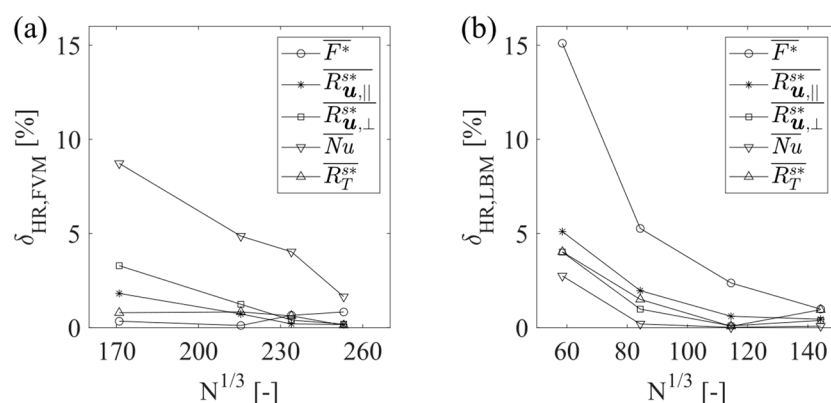


Figure 7. Relative deviation from value for highest resolution δ_{HR} against degrees of freedom in one dimension $N^{1/3}$ for time-averaged quantities total force F^* , Nusselt number Nu , streamwise and spanwise components of velocity's spatial variance $R_{u,\parallel}^{S*}$ and $R_{u,\perp}^{S*}$, and spatial variance of temperature R_T^{S*} , computed from (a) FVM and (b) LBM results.

In Table 3, the values for the quantities defined in Equations (11)–(15) obtained at the highest resolution in the FVM and LBM simulation are listed. For comparison, reference values from the studies by He et al. [28] and Hill and Koch [27] are also included. Although these authors did not consider exactly the same Reynolds number, their data allow for interpolation and extrapolation to obtain values for $Re = 1000$. Regarding hydrodynamics related variables for the total force F^* and the spatial variances $R_{u,\parallel}^{S*}$ and $R_{u,\perp}^{S*}$, the deviations among all simulation frameworks remain below 10%. While the spatial velocity variances from the LBM are close to those reported by He et al. [28], the FVM results lie between He et al. [28] and Hill and Koch [27]. Regarding heat transfer related variables and

temporal velocity variances, the deviations between FVM and LBM are larger. In the FVM simulation, the Nusselt number $\overline{Nu}$ is 11.6% lower and the spatial temperature variance $\overline{R_T^{s*}}$ is 12.2% lower compared to the LBM simulation. The temporal velocity variances $\overline{R_{u,\parallel}^{t*}}$ and $\overline{R_{u,\perp}^{t*}}$ are up to 13.9% lower in the FVM compared to the LBM which delivers values that are more in line with the results of He et al. [28]. The temporal temperature variance $\overline{R_T^{t*}}$ is 39.8% lower in the FVM simulation than in the LBM simulation. Although this percentage appears much larger than the differences observed for other quantiles, the absolute difference remains relatively small. Note that we consider the normalized variances here and, therefore, the data shows that the temporal temperature variance is significantly smaller than the temporal velocity variances. This deviation does also not translate into a substantially different turbulent heat flux. The magnitude of the turbulent heat flux vector $\|u'T^*\| = \sqrt{(u'T^*)^2 + (v'T^*)^2 + (w'T^*)^2}$ is only 8.2% lower in the FVM simulation. Finally, we note that we could not detect a significant difference in the values when the BGK instead of the MRT model was used in the LBM framework.

Table 3. Time-averaged values for total force $\overline{F^*}$, Nusselt number $\overline{Nu}$, and spatial variances $\overline{R^{s*}}$, as well as temporal variances $\overline{R^{t*}}$ of velocity and temperature and turbulent heat flux magnitude $\langle \|u'T^*\| \rangle$ obtained for Reynolds number 1000 at highest simulated resolution. Reference values shown for study of He et al. [28] were interpolated and values shown for Hill and Koch [27] were extrapolated using data from available Reynolds numbers. Relative deviations are provided in brackets with respect to values of LBM simulation.

Simulation	$\overline{F^*}$ [-]	$\overline{Nu}$ [-]	$\overline{R_{u,\parallel}^{s*}}$ [-]	$\overline{R_{u,\perp}^{s*}}$ [-]	$\overline{R_T^{s*}}$ [-]	$\overline{R_{u,\parallel}^{t*}}$ [-]	$\overline{R_{u,\perp}^{t*}}$ [-]	$\overline{R_T^{t*}}$ [-]	$\langle \ u'T^*\ \rangle$ [-]
LBM (baseline)	1728	61.17	0.5801	0.7325	0.2733	0.1721	0.2267	0.05842	0.05225
LBM (BGK)	1728 (+0.0%)	61.33 (+0.3%)	0.5805 (+0.1%)	0.7304 (−0.3%)	0.2728 (−0.2%)	0.1734 (+0.8%)	0.2229 (−1.7%)	0.05780 (−1.1%)	0.05246 (+0.4%)
FVM	1696 (−1.9%)	54.1 (−11.6%)	0.5506 (−5.1%)	0.7017 (−4.2%)	0.2399 (−12.2%)	0.1481 (−13.9%)	0.2005 (−11.6%)	0.03517 (−39.8%)	0.04799 (−8.2%)
He et al. [28]	1816 (+5.1%)	-	0.5752 (−0.8%)	0.7223 (−1.4%)	-	0.1721 (+0.0%)	0.2289 (+1.0%)	-	-
Hill and Koch [27]	1774 (+2.7%)	-	0.5360 (−7.6%)	0.6660 (−9.1%)	-	-	-	-	-

In Figure 8, we present a more thorough comparison of our data with available data from the literature for the Nusselt number and total force. For this purpose, two additional Reynolds numbers ($Re = 2000$ and $Re = 3000$) were simulated with the LBM flow solver omitting simulations with the FVM. All presented data from the literature in Figure 8 was carefully adjusted to match the Reynolds number definition used in the present work. Figure 8a shows that the total force $\overline{F^*}$ closely follows the correlation of Hill and Koch [27] and the data of He et al. [28] who have obtained their data by performing DNS in a FCC unit cell with fully periodic boundaries as used in the present study. The two empirical correlations fitted to experimental data by Ergun [16] and Fand et al. [62] also exhibit low deviations to the DNS results when the voidage of the FCC packing is used in the respective formulas. This should not be taken for granted since the correlations are based on experimental data for particle beds with solids volume fractions ranging from 0.46 to 0.57 [16] and 0.64 to 0.66 [62]. However, such correlations are generally applicable to a wider range of bed voidages and are applicable to the low voidage FCC particle bed as well for the considered Reynolds number range.

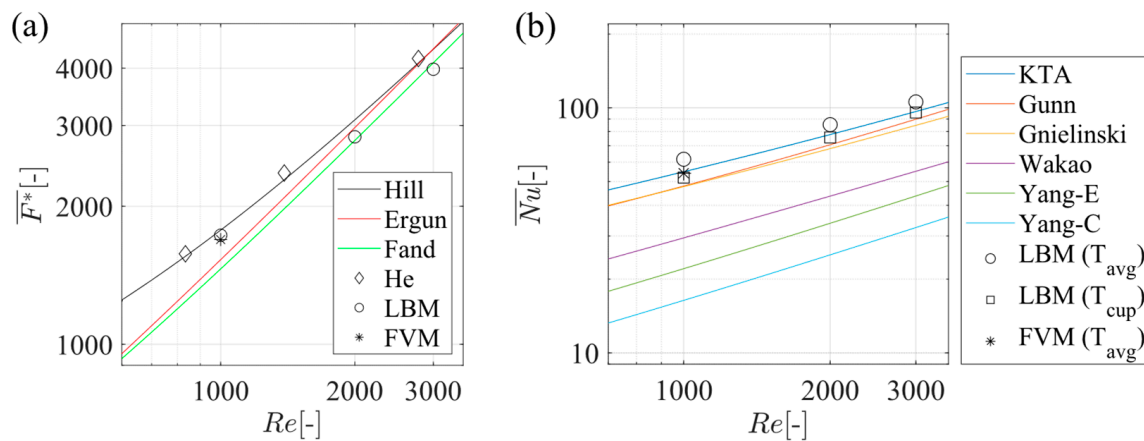


Figure 8. (a) Time-averaged and normalized total force $\overline{F}^*$ acting on particle in FVM and LBM simulations compared to results of Hill and Koch [27], Ergun [16], Fand et al. [62], and He et al. [28]. (b) Time-averaged Nusselt number $\overline{Nu}$ obtained by LBM and FVM simulations compared to data obtained by KTA [63], Gunn [64], Gnielinski [19], Wakao et al. [20], the experimental (“E”) study of Yang et al. [56], and the computational (“C”) study of Yang et al. [32].

When it comes to the available data for the Nusselt number $\overline{Nu}$, however, we find that there is a large discrepancy between the depicted studies [19,20,32,56,63,64], five of which are experimental [19,20,56,63,64] and one of which is computational [32]. In the computational study [32], periodic boundaries were only used in the spanwise directions and inlet/outlet boundaries were applied in streamwise direction such that the FCC cells are placed between particle-free inlet and outlet regions. Furthermore, the CFD simulations [32] relied on turbulence models and the particle diameter was artificially decreased to allow for easier mesh generation resulting in a slightly higher voidage. A final remark needs to be made with respect to the reference temperature that is used in computational studies to calculate the Nusselt number as defined in Equation (15). The Nusselt number values presented in Table 3 were obtained using the fluid domain averaged temperature T_{avg} as reference temperature. Yang et al. [32] used the cup mixing temperature T_{cup} as reference temperature that is based on the energy heat flux. Figure 8b shows that the use of the cup mixing temperature leads to lower Nusselt numbers, but the effect is too small to explain the deviation of our data with the data of Yang et al. [32].

Regarding the experimental correlations [19,20,56,63,64], the Nusselt numbers reported by Yang et al. [56] for the flow through the FCC packing ($\phi = 0.74$) are below the values obtained by the correlation of Wakao et al. [20] for randomly packed beds ($\phi \approx 0.6$). This is unexpected considering that various previous studies (see e.g., Kravets et al. [37] for an overview) predicted that the Nusselt numbers generally increase with decreasing bed voidage. However, it has to be noted that bed voidages as low as the one in the FCC geometry are usually outside the analyzed parameter space of previous studies. The correlations of KTA [63] and Gunn [64] were derived based on experimental data for particle beds with solids volume fractions up to 0.64 and 0.65, respectively. In Figure 8b, we show the values of these two correlations [63,64] when the solids volume fraction of the FCC packing is used and find that it agrees well with the DNS data. The widely used correlation of Gnielinski et al. [19] was derived for a bed voidage as low as in the FCC geometry and also shows only minor deviation to our data.

3.3. Qualitative Comparison of the Methods Performance

The flow within the corresponding packed units exhibits a variable and complex behavior that is strongly influenced by the confining walls, hence presenting a challenge for particle-resolving computations. In the light of this, the performance of FVM with an

unstructured body fitted mesh and LBM relying on interpolated bounce-back methods on a structured uniform Cartesian mesh in capturing local features in the flow and thermal fields is qualitatively investigated in this section.

3.3.1. Mean and Fluctuating Velocity Fields

Figure 9 presents a cross-sectional view of the computational domain, perpendicular to the flow direction, used to compare the performance of the methods. The first components of the mean $\bar{u}^*$ and fluctuating velocities $u'u'^*$, as well as the turbulent kinetic energy $\bar{k}^*$, are selected for the qualitative comparison of the methods. The iso-contours of the represented quantities have been time-averaged and non-dimensionalized following procedures outlined in Table 1. The left column of Figure 9 displays the FVM predictions, the center column shows the LBM solution, and the right column depicts the relative difference. Local relative differences δ between the two methods are computed in this section as

$$\delta(\bar{u}^*) = \frac{(\bar{u}^*)_{\text{FVM}} - (\bar{u}^*)_{\text{LBM}}}{\max(|(\bar{u}^*)_{\text{FVM}}|, |(\bar{u}^*)_{\text{LBM}}|) + 0.01} \quad (18)$$

for the variable $\bar{u}^*$ and analogously computed for all other considered variables. As can be seen in the plots of Figure 9, the flow patterns are similar in 8 sub-areas of the sampled area due to the geometric symmetry. Four of these sub-areas are defined by the isolated areas in the plot corners and four sub-areas form the connected center. Variables were averaged over these eight sub-areas to remove noise and the relative differences were calculated based on these averaged fields to obtain more reliable values.

It is observed by Figure 9a,b that the mean flow field computed by both methods exhibits a symmetrical topological distribution. Acceleration patterns represented by high streamwise velocities at the four corners of the central pore region can be seen while a deceleration is exhibited in the middle of the central pore region. This prediction of the mean flow distribution confirms the observations of the work of He et al. [3] who concluded that regardless of the Reynolds number, an identical flow pattern emerges in the considered geometrical particle configuration. Elevated deviations are limited to areas near the particle surfaces where velocities are low (see Figure 9c). Hence, one can conclude that both methods (FVM and LBM) converged to the same solution and had not much impact on resolving the mean flow field qualitatively.

A merely complex pattern emerges in the spatial distribution of the streamwise fluctuating velocity $u'u'^*$. The variable u' is computed by subtracting the temporal mean velocity from the instantaneous field as $u' = u - \bar{u}$. The overbar sign indicates time averaging operation in this work. As can be observed in Figure 9d,e, a pair of flow structures with maximum magnitude across the domain appear on both corners across the contact points between the spheres. Similar to the mean velocity, the variance exhibits a deceleration in the central region of the pore, indicating that the instantaneous velocity has a stronger variance in the regions near corners than in the center of the pore. It can be observed that even though both methods (FVM and LBM) compute a symmetrical semi-identical spatial distribution of $\bar{u'u'^*}$, deviance is exhibited in the magnitude and occurs predominantly in the low variance area near the pore center (see Figure 9f).

To further incorporate how the methods (FVM and LBM) are predicting the variation from the mean velocity components, the performance in predicting the turbulent kinetic energy $\bar{k}^*$, which is computed as $\frac{1}{2}(\overline{u'u'^*} + \overline{v'v'^*} + \overline{w'w'^*})$, is investigated. Figure 9g,h show the distribution of $\bar{k}^*$. Both methods predict the same topological distribution consisting of an increase of $\bar{k}^*$ magnitude away from the wall but with a sharp decrease when reaching the central region of the pore. This observation is aligned with the conclusions of

He et al. [3] as well. Only minor differences can be observed in Figure 9i due to the slightly lower level of turbulent kinetic energy in the FVM.

Hence, it can be concluded that both methods do not report distinct disparities when it comes to computing the mean velocity field and its variance represented by the turbulent kinetic energy.

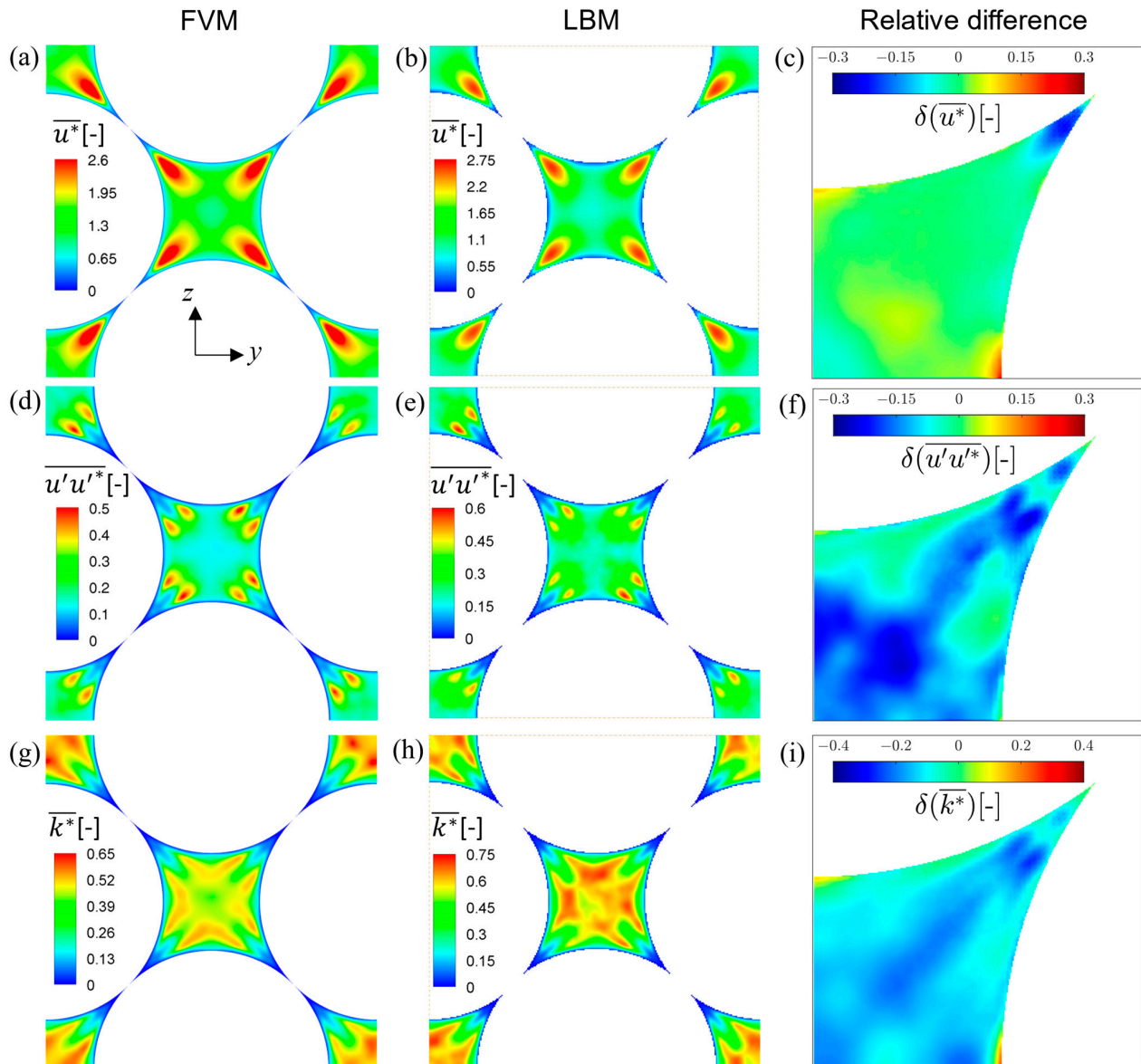


Figure 9. Left column shows flow contours from FVM while center column shows results from LBM. Relative differences δ as defined in Equation (18) are depicted in right column. Flow direction is going through page in positive x-direction. Presented quantities are streamwise mean velocity $\bar{u}^*$ (a–c), streamwise velocity variance of $\bar{u}'u'^*$ (d–f), and turbulent kinetic energy $\bar{k}^*$ (g–i), corresponding to first, second, and third rows, respectively.

3.3.2. Mean and Fluctuating Thermal Fields

Figure 10 illustrates how the temporally averaged mean temperature field and its variance as well as the turbulent heat flux are predicted by the FVM and the LBM approaches. Disparities are exhibited in the prediction of the thermal field computed by the two methods. Even though both methods predict a symmetrical pattern in the spatial distribution of $\bar{T}^*$ (see Figure 10a,b), moderate deviations are present in the areas of the higher velocities as shown in Figure 10c. FVM predicts a more homogenous temperature

distribution while LBM computes the maximum temperatures at the high velocity spots. The temperate variance $\overline{T'T'^*}$ distribution exhibits the strongest dependence on the applied numerical method. As seen in Figure 10d,e, different patterns emerge based on the methods. The computed distribution by the FVM exhibits the maximum magnitude in the area near the walls of the spheres. However, the LBM computes a profile that is similar to $\overline{u'u'^*}$ in Figure 9e with maximum magnitudes appearing as pair of regions in the four corners of the pore. Although absolute differences between the methods in temperature variance are small due to the low absolute level of these fluctuations, the respective relative differences reach high values as can be seen in Figure 10f. The lower level of temperature variances in the FVM compared to the LBM has already been discussed in the context of the domain-averaged data in Table 3 in Section 3.2.

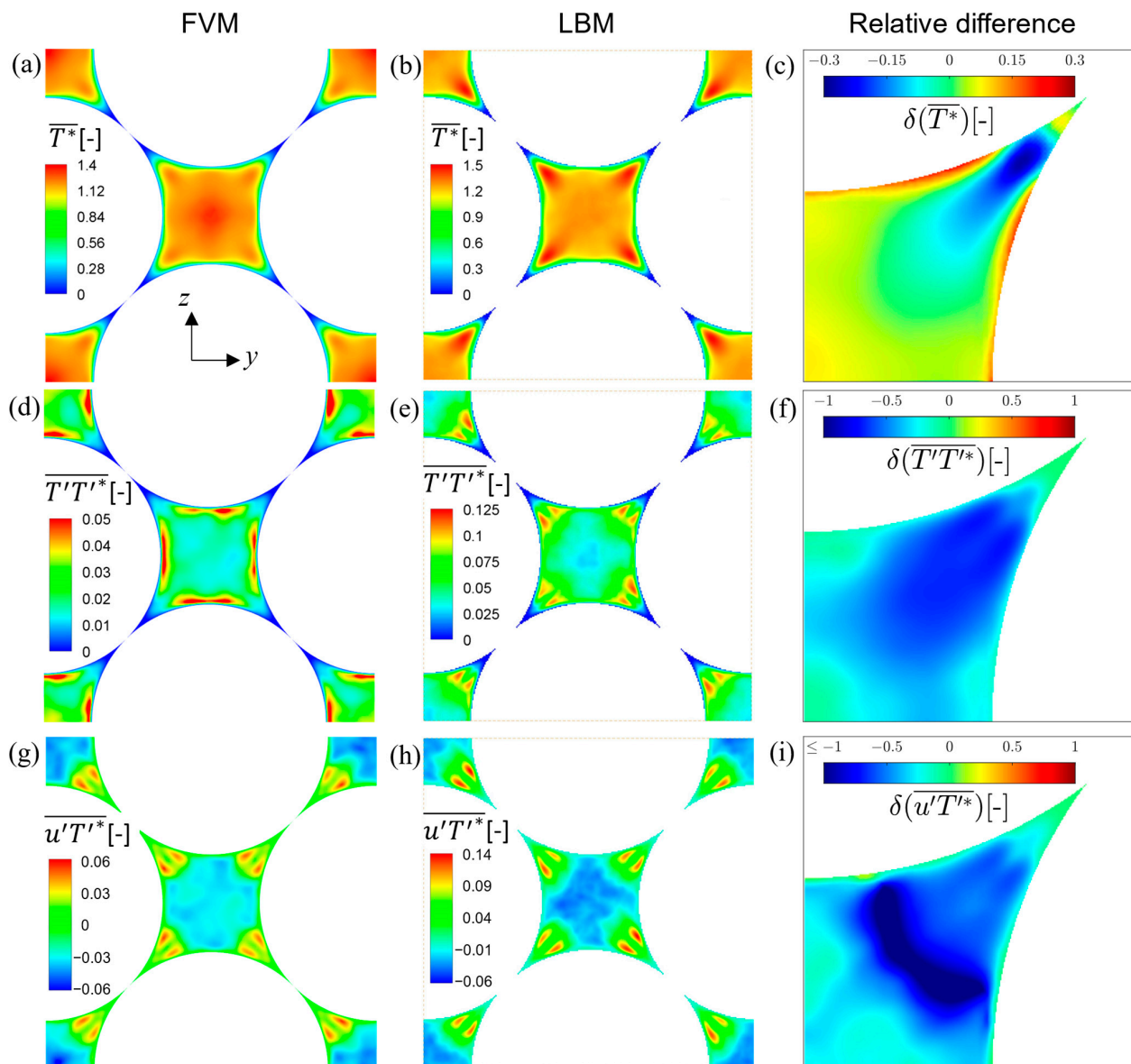


Figure 10. Left column shows flow contours from FVM while center column shows results from LBM. Relative differences δ as defined in Equation (18) are depicted in right column. Flow direction is going through page in positive x-direction. Presented quantities are mean temperature $\overline{T^*}$ (a–c), temperature variance $\overline{T'T'^*}$ (d–f), and first component of turbulent heat flux $\overline{u'T'^*}$ (g–i), corresponding to first, second, and third rows, respectively.

The turbulent heat flux vector $\overline{u'T'^*}$ is computed as the temporal mean of the product of multiplying the fluctuating velocity components (u' , v' , and w') by the fluctuating temperature T' . This quantity has the potential to offer insight into the mechanism of heat transfer and aid in confirming the accuracy of sophisticated temperature closure models [30]. In this analysis, only the first component of $\overline{u'T'^*}$ is included due to the minor impact of the second and third component when compared to the principal streamwise velocity component.

The iso-contour of the $\overline{u'T'^*}$ distribution is shown in Figure 10g,h. As a consequence of $\overline{u'u'^*}$ having a higher order of magnitude in comparison to $\overline{T'T'^*}$, both methods compute a spatial distribution that is dominated by the emerged patterns in $\overline{u'u'^*}$ (see Figures 9d,e and 10g,h). The previously observed symmetrical profiles, the maxima pairs at the pore region corners and the decrement in the central region, are consequently exhibited by both methods' solutions. The better match of the turbulent heat flux profiles translates into a smaller magnitude of relative difference in the pore corner (see Figure 10i) when compared to the relative difference in temperature variances (see Figure 10f). The peak values ($\delta(\overline{u'T'^*}) \leq -1$) are observed in the transition area between pore corner and pore center where the turbulent heat flux is close to zero and changes sign.

3.4. Quantitative Comparison of the Methods

As evidenced by the comparison presented in the preceding sections, both methods demonstrated efficacy in predicting global parameters such as drag force, Nusselt number, and spatial variances (see Section 3.2). Additionally, they were able to capture the complex topological distribution of the flow field, as reported by He et al. [3] for the FCC geometrical configuration (see qualitative comparison in Section 3.3). Upon examination of the local spatial distributions of the mean and fluctuating quantities, a variety of flow patterns were observed in the central pore region. This raises the question of how the numerical methods are capturing the acceleration, deceleration, stagnation, and reattachment areas with regard to flow and thermal fields, which is quantitatively investigated in this section.

3.4.1. Mean and Fluctuating Velocity

Accordingly, a central cut aligned with the flow direction is employed, as illustrated in Figure 11a. The flow enters the domain from the left side into the central pore in positive x-direction, subsequently exiting through the pore region corners on the right side. Two symmetrical structures with the highest magnitude of mean streamwise velocity are exhibited in combination with a low-velocity stagnation zone behind the sphere and a reattachment pattern ahead of the sphere on the right.

The mean velocity components were extracted over a sampling line (illustrated in black in Figure 11a) are presented in Figure 11b. The alignment of the profiles captured by the LBM and FVM reflects the agreement between the methods in predicting the mean velocity distribution observed in the previous sections. The anticipated flow pattern of stagnation behind the sphere on the left side (in terms of both magnitude and distribution) is illustrated by the negative velocity. As the flow progresses towards the center of the channel, a maximum is reached, which is represented by the two methods. However, there is a discrepancy in how both methods resolve the reattachment areas, with the FVM predicting a larger area where the streamwise velocity is almost equal to zero.

It is evident that the numerical methods are more sensitive to the influence of spatial resolution when calculating turbulent quantities such as velocity field variances and turbulent kinetic energy. This is illustrated in Figure 11c,d, which shows that the LBM DNS case exhibits a magnitude approximately 25% higher value of $\overline{k^*}$ than the predicted

value by FVM. It is nevertheless noteworthy that both methods yielded comparable results regarding the general trends observed for these quantities.

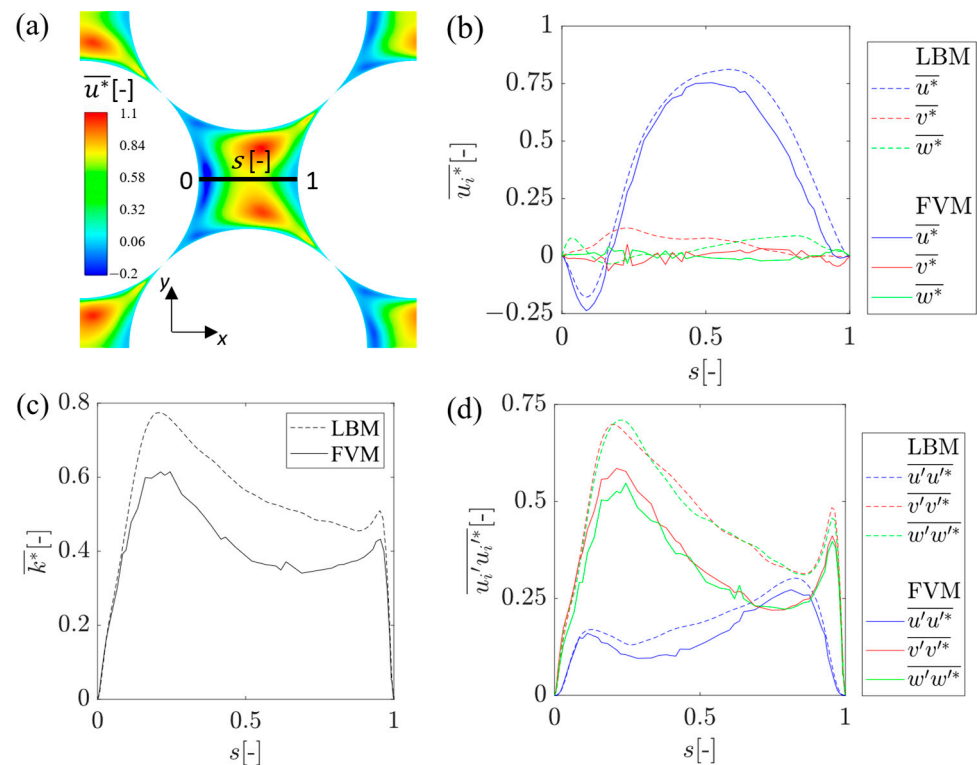


Figure 11. (a) Cross-sectional visualization of steam-wise mean velocity $\overline{u^*}$ with black line indicating location of data sampling, (b) mean velocity components ($\overline{u^*}$, $\overline{v^*}$, $\overline{w^*}$), (c) turbulent kinetic energy $\overline{k^*}$, and (d) velocity variances ($\overline{u' u'^*}$, $\overline{v' v'^*}$, $\overline{w' w'^*}$).

3.4.2. Mean and Fluctuating Temperature

Figure 12 shows the local spatial distribution of the thermal field quantities, including the mean and variance of the temperature and the turbulent heat flux, as predicted by the FVM and LBM. The cross-sectional cut depicted in Figure 12a is analogous to that illustrated in Figure 11. The mean temperature profile distribution is found to be identical for both methods; however, the FVM results in a higher mean temperature (Figure 12b). This behavior can be related to the emerging pattern in the predicted fluctuating temperature (Figure 12c), which represents the transfer of thermal energy due to fluctuations in temperature caused by turbulence motion [65]. The LBM results in a higher magnitude of the temperature variance, which may indicate that a greater amount of thermal energy is being transferred due to turbulence mixing, resulting in a lower fluid temperature. The impact of the numerical method is also noticeable in the turbulent heat flux vector, as illustrated in Figure 12d. Although an alignment is exhibited in the leading component, $\overline{u' T'^*}$, a deviation emerges in the area corresponding to the highest difference between the mean temperature distributions obtained by the methods, as illustrated in Figure 12b. It is noteworthy that the FVM predicts the maximum negative correlation between the fluctuating temperature and the fluctuating velocity, as represented by the turbulent heat flux. This may indicate that the transfer of thermal energy by turbulence mixing is lower than in the LBM in this region, resulting in a higher mean temperature in the case of the FVM.

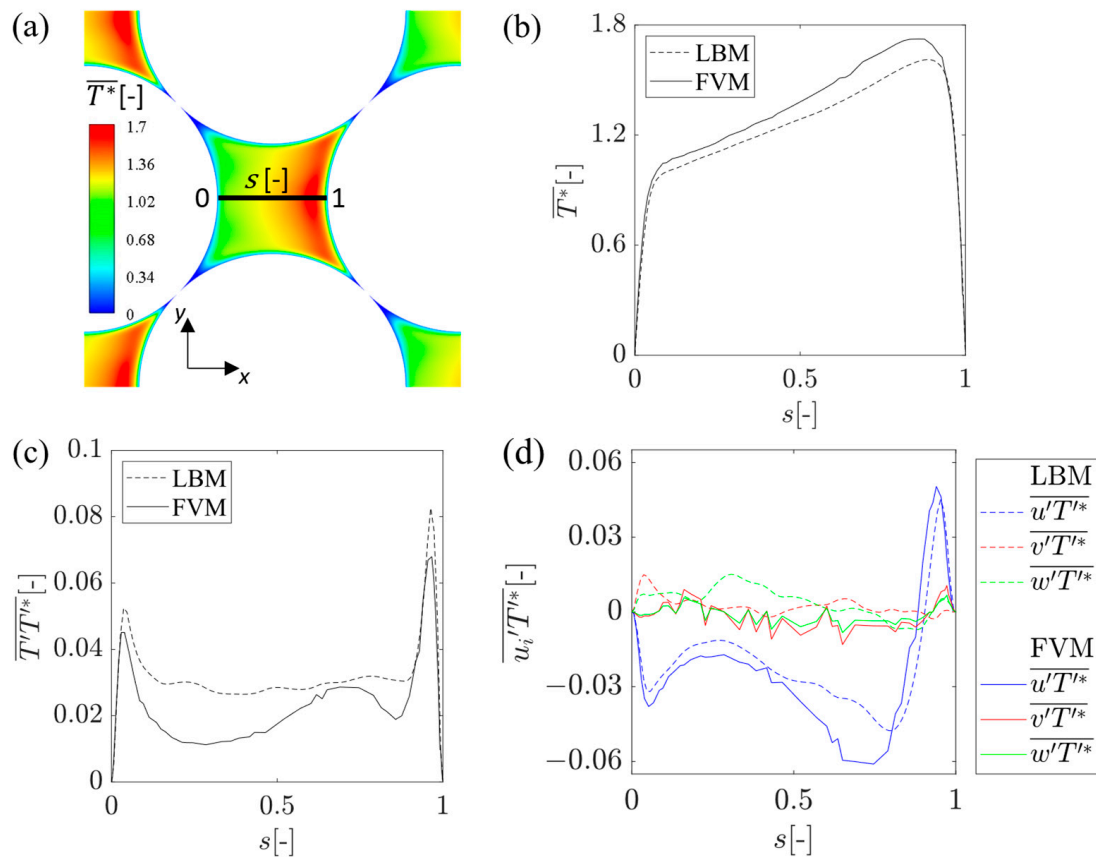


Figure 12. (a) Cross-sectional visualization of mean temperature $\overline{T^*}$ with black line indicating location of data sampling, (b) mean temperature $\overline{T^*}$, (c) temperature variance $\overline{T'T^*}$, and (d) turbulent heat flux $\overline{u_i'T^*}$.

4. Conclusions

Two different DNS frameworks (LBM and FVM) were used in this work to simulate the turbulent flow through the FCC pore geometry under the consideration of heat transfer. A surface-fitted mesh as used in the FVM is especially advantageous when aiming for a high resolution of the confined areas where the particles are close to each other. These areas are only coarsely resolved when relying on a structured uniform Cartesian mesh as used in the LBM (compare Figures 2 and 4a). The fact that the LBM is able to deliver grid-independent results with fewer mesh cells suggests that for the flow through the FCC configuration a high resolution of the particle contact areas is not crucial to achieve mesh independence. While the grid convergence study for an exemplary sampling line through the domain revealed that more accurate results can be obtained with the LBM at much lower resolutions compared to the FVM, the LBM shows a higher level of uncertainty in the streamwise turbulent heat flux and temperature variance at higher resolutions. Therefore, it is not possible to identify a conclusively superior method. The ability of the LBM to achieve satisfactory results at a low computational time favors the LBM when medium error thresholds are sufficient for the desired solution quality, but the FVM may be superior when only very low errors are tolerated [44].

The values for the particle-fluid force and Nusselt number in the two simulation frameworks agree well with each other and commonly used correlations. The discrepancy between the Nusselt numbers calculated in the present work and the values reported in a previous coarsely resolved simulation study [32] relying on turbulence models indicate that special attention has to be paid to the model choice. Existing closure models may not

be sufficiently accurate for heat transfer phenomena in turbulent flows through particle beds with low voidage.

A qualitative and quantitative local analysis of the data revealed that the time-averaged velocity and temperature fields of FVM and LBM match well. Larger deviations occur when comparing fluctuating quantities (Reynolds stresses, turbulent heat flux, temperature variance) where a qualitative match can be shown but notable deviations between the two methods are locally observable. However, averaged spatial and temporal variances are consistently lower in the FVM simulation but the deviations remain limited to 14% with the exception of the temporal variance of temperature being 40% higher due to the low baseline. The values for the hydrodynamic variables (see Table 3) obtained by the FVM and the LBM employed in the present work are also in good agreement with previous isothermal DNS studies by He et al. [28] and Hill and Koch [27]. Given that the LBM and the latter two studies [27,28] used a structured uniform Cartesian mesh opposed to the FVM using a body-fitted mesh, this suggests that, provided sufficient mesh quality, the type of mesh is not a decisive factor in achieving accurate results.

The findings of this study establish a valuable benchmark for flow solvers that incorporate heat transfer under turbulent conditions. Beyond this, both simulation frameworks demonstrate strong potential for validating existing turbulence closure models and guiding the development of new ones. Nevertheless, discrepancies between DNS approaches and mesh types must be acknowledged, as they are primarily linked to the resolution of near-wall turbulence—the dominant region of turbulence production. This indicates that DNS accuracy in low-porosity configurations depends less on solver formulation, and more on adequately resolving the near-wall dynamics governing heat and momentum exchange. The comparison further suggests that both methods capture the same underlying physical mechanisms of turbulence generation and transport, while quantitative deviations mainly arise from differences in local resolution. To advance the field, future comparisons should place greater emphasis on analyzing turbulent kinetic energy (TKE) budget terms, which would provide deeper insight into how different numerical methods capture the mechanisms of production, dissipation, and transport. Furthermore, both methods have already been successfully used for the simulation of turbulent flow through more complex porous structures comprised of non-spherical particles [1,66] and a comparison of the two DNS frameworks for such systems is of high relevance for future investigations.

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Nomenclature

The following nomenclature was used in this manuscript:

Greek letters

Δ	Local grid scaling
δ	Relative deviation
ε	Turbulent kinetic energy dissipation
η	Kolmogorov length scale, m
κ	Thermal conductivity, W/(m · K)
ν	Kinematic viscosity, m ² /s
ρ	Fluid density, kg/m ³
τ_η	Kolmogorov time scale
ϕ	Solids volume fraction
Ω	Collision operator

Mathematical operations

$\langle x \rangle$	Volume averaged quantity
$\bar{x}$	Time averaged quantity
x'	Fluctuating quantity
x^*	Dimensionless quantity

Subscripts

avg	Average
bl	Boundary link
cup	Cup mixing
f	Fluid
HR	Highest resolution
i	Quantity components in the x, y and z directions
l	Lattice direction
p	Particle
ref	Reference
s	Spatial
t	Temporal
w	Wall

Other symbols

A	Surface area, m ²
c_p	Heat capacity, J/(kg · K)
d_p	Particle diameter, m
e_l	Discrete lattice velocity vector
f	Velocity distribution function vector
F	Total particle-fluid force, kg · m/s ²
F^b	Volumetric body force, N/m ³
g	Temperature distribution function vector
h	Convective heat transfer coefficient, W/(m ² · K)
k	Turbulent kinetic energy, m ² /s ²
L	Domain Length, m
n	Normal vector
N	Degrees of Freedom
Nu	Nusselt number ($h \cdot d_p / \kappa$)
p	Pressure, N/m ²
Pr	Prandtl number ($\mu \cdot c_p / \kappa$)
q	Distance between fluid node and particle surface
Q	Q-criterion, 1/s ²
r	Node position vector
$\dot{Q}$	Heat transfer rate, W
R	Variance of specified variable

Re	Reynolds number ($u \cdot d_p / \nu$)
s	Position on sampling line
S	Surface, m^2
Δt	Time step, s
T	Temperature, K
ΔT	Temperature difference, K
u	Velocity in x -direction, m/s
$\mathbf{u}$	Velocity vector, m/s
U	Velocity magnitude, m/s
v	Velocity in y -direction, m/s
w	Velocity in z -direction, m/s
x	Position in first spatial dimension, m
$\mathbf{x}$	Position vector, m
Δx	Spatial discretization, m
y	Position in second spatial dimension, m
z	Position in third spatial dimension, m

Abbreviations

BGK	Bhatnagar–Gross–Krook model
CFD	Computational Fluid Dynamics
FCC	Face-centered cubic
FTT	Flow Through Time
FVM	Finite volume method
LBM	Lattice Boltzmann method
LES	Large Eddy Simulation
MRT	Multiple-Relaxation-Time model
pr-DNS	Particle-resolved Direct Numerical Simulation
RANS	Reynolds-Averaged Navier–Stokes

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