Direct Numerical Simulations of Incompressible Flow through Porous Packs over a wide Range of Reynolds Numbers

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Direct numerical simulations of incompressible flow through periodic square/rectangular (two-dimensional; 2-D) and cubic (three-dimensional; 3-D) arrays of particles and periodic random packs of polydisperse spheres over a wide range of Reynolds numbers and at various porosities are performed. The unsteady Navier-Stokes equations are solved with either a 3-D parallel finite-difference (FD) in-house research code on a collocated Cartesian grid and with an immersed boundary method (IBM) to treat the internal boundaries, or with the finite-volume (FV) solver OpenFOAM® on an unstructured grid and with an explicit treatment of the boundaries. The FD explicit solver is used for 2-D flows and 3-D laminar flows while the FV implicit solver is preferred for 3-D transitional and turbulent flows for the consideration of computational cost.

Macroscopic friction factors for periodic arrays of cylinders and ellipses and periodic cubic arrays of spheres with a porosity range of $0.30 \leq \sigma \leq 0.70$ and $0.55 \leq \sigma \leq 0.85$, respectively, and varying Reynolds numbers ranging from the creeping to (pseudo-)turbulent flow regimes are calculated; we reserve “turbulent flow” for 3-D cases and refer to 2-D turbulent flow as “pseudo-turbulent flow”. The effects of Reynolds number and porosity on friction factor and permeability are investigated; the for-
mer is in good agreement with the modified Forchheimer friction factor and a modified curve fit based on the Gebart relation is proposed for the latter. A similar study was conducted for periodic random packs of spheres in the creeping and inertial flow regimes with varying distributions of particle diameters, and modified curve fits are proposed.

The onset of unsteady flow, identified through the critical Reynolds number and defined as the Hopf bifurcation, is found to be particle shape and porosity dependent. It is also found that transition to turbulence occurs when significant vertical cross flow starts to emerge, causing an imprint on statistics such as vorticity budget and two-point double correlation field. The transitional and pseudo-turbulent flow features are then analyzed for square array of particles in 2-D with peculiar and normal transitional behaviors. Peculiar transitional behavior refers to mixed steady-unsteady flows at different Reynolds numbers in the transitional regime and was discovered by our numerical simulations for certain porosities. Time histories and statistics of probe data and flow fields are used to analyze the time and length scales, respectively. For transitional flows, the length scales of instantaneous vorticities decrease with increasing Reynolds number while the temporal signals experience wider power distributions as the Reynolds number increases. For pseudo-turbulent flows, the instantaneous length scales and the length scales identified by two-point double correlations are similar for the range of pseudo-turbulent flow Reynolds numbers considered, specific to 2-D pseudo-turbulence. High frequency in probe data is identified with periodic flows as the flow pass-through resonance of the “tail”, high $u$-velocity stream originated from the left boundary. For transitional and pseudo-turbulent flows, this high frequency resonance is superimposed on distributed “tail” flapping. Interesting intermittent
behavior of the “tail” tilting is observed and discussed for transitional and pseudo-turbulent flows. Pseudo-turbulent flows also display similar Gaussian PDFs of probe data as a result of a variety of vortex and “tail” motions. The effect of the size of the representative elementary volume (REV) on the instantaneous, mean, and \( \text{rms} \) flow fields for packs with peculiar transitional behavior is also studied. Finally, initial results of 3-D DNS of turbulent flow are presented, and similar to the 2-D cases, the association of transition with flow perpendicular to the stream-wise direction is observed.
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List of Abbreviations

1-D One-dimensional
2-D Two-dimensional
3-D Three-dimensional
AMR Adaptive mesh refinement
BI Boundary intercept
cPBICCG Coupled preconditioned bi-conjugated gradient
DILU Diagonal incomplete lower upper
DNS Direct numerical simulation
DVM Dynamic Vreman model
FFT Fast Fourier transform
GAMG Generalized geometric-algebraic multi-grid
GC Ghost cell
GIBM Ghost cell immersed boundary method
GS Gauss-Seidel
GUC Geometric unit cell
IP Imaginary point
IBM Immersed boundary method
LBM Lattice Boltzmann method
LDDRK Low-dissipation and low-dispersion Runge-Kutta
LES Large eddy simulation
MPI Message Passing Interface
NS Navier-Stokes
OF OpenFOAM®
PDF Probability density function
PIMPLE Merged PISO-SIMPLE
PISO Pressure implicit split operator
REV Representative elementary volume
SIMPLE Semi-implicit method for pressure-linked equations
SRT Single-relaxation time

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<td>(U)RANS</td>
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<td>WENO</td>
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$U_i^*$ Intermediate face centered velocity
$u, v, w$ Velocity in $x, y, \text{and} z$ direction
$u_i$ Cell centered velocity
$\bar{u}_i$ Averaged cell centered velocity
$\bar{u}_{\text{max}}$ Time averaged of the maximum $u$-velocity at $x_{\text{min}}$
$u_i^*$ Intermediate cell centered velocity
$[V]$ Vandermonde matrix
$V$ Total volume of the domain
$V_f$ Total volume of the fluid
$w_k$ Non-linear weights
$x_i$ Location
$x_{\text{quarter}}, x_{\text{mid}}$ Quarter and mid length in the $x$ direction
$x_{\text{min}}, x_{\text{max}}$ Minimum and maximum location in the $x$ direction
$y_{\text{min}}, y_{\text{max}}$ Minimum and maximum location in the $x$ direction
$\beta$ Empirical material-dependent inertial flow coefficient
$\beta_l$ Smoothness indicators
$\Gamma_b$ Immersed boundary
$\gamma_l$ Averaging weights
$\gamma_{W,S,B}$ Linear interpolation weight for west, south, and back face velocities
$\Delta l$ Length of the line segment
$\Delta m$ Filter width
$\hat{\Delta} m$ Test filter width
$\Delta p$ Pressure difference
$\Delta t$ Time step
$\Delta x$ Grid spacing
$\Delta^+, \Delta^-$ Operator
$\epsilon$ Poisson solver tolerance
$\mu$ Viscosity
$\nu$ Kinematic viscosity
$\nu_T$ SGS eddy viscosity
$\rho$ Fluid density
$\sigma, \sigma_{\text{min}}$ Porosity and minimum porosity
$\sigma_s$ Scaled porosity
$\sigma_c$ Critical porosity
$\tau_{ij}$ Subgrid-scale stress tensor
$\phi$ Scalar field
$\tilde{\phi}$ General filtered of a scalar field
$\hat{\phi}$ General test filtered of a scalar field
$\bar{\phi}$ Time averaged of a scalar field
$\phi_p$ Momentum source term
\(|\omega|\)  Vorticity magnitude
\(\Omega_f\)  Fluid domain
\(\omega_i\)  Vorticity in \(i\) direction
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Chapter 1

Introduction

1.1 Motivation

A detailed macroscopic and microscopic understanding of flow passing through porous material has been pursued since the 19th century [1] as understanding of this flow is especially important due to its abundance in nature (e.g. sand, mammal hair, etc.) [2] and its numerous engineering applications. The increased computing power attained in the last decades has provided the required resources to increase our understanding of porous material through detailed microscopic analyses not attainable through experimental investigations [2]. This has also resulted in an increased interest in the irregular flow fields encountered when fully resolving the underlying structures of the porous material (e.g. grains of sand, hair fibers, wood fibers, etc.). Though flows at a wide range of Reynolds numbers and porosities have been extensively studied for numerous configurations, recent publications in this field [3, 4, 5] have shown that further research is required to properly characterize the temporal and spatial structures, and to develop more accurate macroscopic
relations and models. This dissertation tackles all three tasks by investigating the flow fields for a wide range of Reynolds numbers and porosities encountered in canonical and random porous packs.

1.2 Flow through Porous Media

Present in many science and technology systems, flow through porous media is ubiquitous in the natural physical world [2, 6, 7, 8]. Applications of porous media include but are not limited to hydrology, geological, agriculture, civil engineering, petroleum engineering, chemical engineering, biomedical engineering, and extraction industries (mining) [8, 9, 10, 11, 12]. Chemical engineering is particularly dependent on porous media flow for packed fluidized bed and packed fluidized bed reactors, fluid contacting filtration, and separation and purification processes [13]. Porous media flows are also important for environment (subsurface flow of oil and groundwater - fracking - and underground percolation of chemical waste) and renewable energy studies (fuel cell) [14, 15]. As such, a good understanding of flow through porous media for a wide range of Reynolds numbers and microstructural geometries is paramount and not yet achieved [16].

Since Darcy’s [1] seminal paper on flow through porous media, macroscopic correlations to characterize porous media, such as its friction factor and permeability, have been sought after. Through experiments on steady state unidirectional flow in a uniform medium, Darcy [1] proposed the correlation

\[ \langle U \rangle = \frac{1}{\mu} K \frac{\Delta p}{L}, \]  

(1.1)

where \( \Delta p \) is the pressure difference across the porous medium, \( L \) is the length
of the porous medium, \( \mu \) is the viscosity, \( K \) is the specific permeability of the medium, and \( <U> \) is the superficial velocity; the permeability computed from (1.1) at \( Re>0 \) is called “apparent” permeability. The linear relationship between the superficial velocity and the pressure difference is only valid in the Stokes limit [12, 17] as at higher Reynolds numbers the increasing role of the inertial forces results in deviations from Darcy’s law [12]. The inclusion of the inertial effects results in a non-linear relationship [12, 18].

Forchheimer proposed that flow through a porous pack may be best described through the use of a higher order empirical relationship [12, 17] of the form

\[
\frac{\Delta p}{L} = \frac{<U>}{K} \mu + \beta \rho <U>^2,
\]

(1.2)

where \( \rho \) is the fluid density and \( \beta \) (or \( k_f \)) is an empirical material-dependent inertial flow coefficient. In the Stokes limit, the linear term dominates and at higher \( Re \)'s the quadratic term leads to a deviation from the linear relationship.

Though valid for a wider range of Reynolds numbers, the Forchheimer relation depends on experimental or numerically determined parameters. To overcome this limitation and after a series of experiments determining the effects of flow and microstructural properties, Ergun proposed a generalized Forchheimer equation [17] of the form

\[
\frac{\Delta p}{L} = A \frac{(1 - \sigma)^2}{\sigma^3} \mu <U> + B \frac{1 - \sigma \rho <U>^2}{D},
\]

(1.3)

where \( \sigma \) is the porosity of the medium, \( D \) is the particle diameter, and \( A=150 \) and \( B=1.75 \) are the curve fitting parameters.

Further studies on flows through porous media have found that the curve fitting
parameters vary considerably and are subject to the effects of particle microstructure, particle shape, particle roughness, size distribution, orientation, etc. [10]. Though modifications and new correlations attempting to address these drawbacks have been proposed [10, 19], the complex nature of flow through porous media poses a daunting task in determining a generalized correlation.

The resistance of a particular packed bed may also be expressed through a friction factor

\[
f_p = \frac{\Delta p}{L} \frac{D}{\rho \langle U \rangle^2},
\]

where \( f_p \) is the Darcy friction factor. The Ergun and Forchheimer relations may also be recast in the form presented above [10, 19].

As many attempts at obtaining a general empirical relation to describe the fluid flow as a function of the properties of porous medium have been well documented [17, 20], this discussion is focused on more recent numerical studies. Through the use of steady state experiment and numerical results using FLUENT [21], for a range of porosities \( (0.35 < \sigma < 0.95) \), Reynolds numbers \( (0.001 < Re_p < 200) \), and fiber orientations (among other parameters), Tamayol et al. [22] showed that the pack’s permeability and Forchheimer coefficient are functions of porosity and fiber orientation. Tamayol et al. [22] used the numerical results to propose a compact accurate correlation to determine the Forchheimer coefficient for one-, two-, and three-dimensional (1-D, 2-D, and 3-D, respectively) porous structures and to show the limited applicability of the Ergun equation.

Yazdchi and Luding [10] conducted an in-depth analysis of published correlations of friction factors and highlighted their limitations for a range of porosities, Reynolds numbers, and/or pack configurations. Through the use of the steady
state Navier-Stokes (NS) solver in ANSYS®, Yazdchi and Luding [10] considered both ordered and random fiber arrays to relate macroscopic flow properties to their microstructures (arrangements) and porosities, and obtained an analytical closure relation based on the gap Reynolds number $Re_g$ that agrees well with numerical results for $Re<30$.

Other numerical investigations in determining a general curve fit for friction factor include those by Teruel and Rizwan-uddin [23] and Kuwahara et al. [24]; both studies encountered a limited application of the Ergun equation and provided a curve fit with better comparison with their numerical results. Teruel and Rizwan-uddin [23] proposed a power law as a function of $(1−\sigma)/\sigma$ which produces predicted friction factors with errors below 20%. Kuwahara et al. [24] proposed a correlation based on Ergun’s and Forchheimer’s friction factor relations with modifications to their coefficients.

Despite numerous limitations of the Ergun relation, it remains the most popular relationship to describe the dependence of the friction factor on fluid velocity and pack properties. This is due to the intrinsic inclusion of the Blake-Kozeny equation and Burke-Plummer equation for low and high fluid velocities, respectively [17].

Permeability is another macroscopic property and may be defined as the measure of flow conductance in a solid matrix (ability of a fluid to flow) [23, 25, 26]. It was first introduced by Darcy [1] during his experiments of steady state unidirectional flow in uniform media. Correlating the pore-scale parameters to macroscopic bulk media is complex and highly dependent on the complicated flow pattern in the porous media. This makes permeability highly medium dependent and limits the possibility of a general permeability model as a function of the bulk medium properties. Since it’s understandably harder to study pore-scale flow features through
experiments, early experimental attempts were mainly focused on macroscale properties. The alternative analytical approaches pursued are dominated by those for simplified well defined porous structures, such as ordered packs of cylinders and two-dimensional obstacles. The majority of the existing correlations are based on numerical and/or experimental curve fitting and analytical models for limited applications (significant assumptions restrict the correlations to a small range of porosities and Reynolds numbers) [27].

Using lubrication theory, Gebart [28] was able to derive a permeability relation in terms of porosity for creeping flow perpendicular to the long axis of the fibers, which is more valid in the limit of close-packed fibers with a maximum discrepancy of less than 1%.

Recent works on permeability include those of Yazdchi [8], Nabovati et al. [15], Yazdchi et al. [27], and Matsumura et al. [29, 30, 31]. Yazdchi et al. [8] used the steady state NS solver in ANSYS® to determine the effect transverse permeability of random porous packs for a range of porosities. Using neighbor distance statistics, pair distribution functions, and the lubrication effect, Yazdchi et al. [8] determined a universal power law between the permeability and the mean values of the shortest Delaunay triangulation edge. This semi-empirical relation is valid for ordered and disordered porous arrays for all porosities and accounts for microstructural changes. A maximum error of 10% was observed for very dense porous packs with $\sigma<0.30$.

Nabovati et al. [15] used single-relaxation-time (SRT) lattice Boltzmann method (LBM) to conduct three-dimensional flow simulations of randomly generated porous packs. They proposed a semi-empirical relation for permeability as a function of porosity and fiber diameter; the constitutive model was based on Gebart [28] per-
meability relation. They obtained excellent agreement for the porosity range of $0.08 < \sigma < 0.99$.

Yazdchi et al. [27] numerically investigated the microstructural effects on permeability for ordered arrays. The numerous permeability correlations currently used and their limitations were also presented. Using the steady state NS solver in ANSYS®, Yazdchi et al. [27] performed investigations complementary to those by Hill et al. [32, 33] and Van der Hoef et al. [34] to determine the effects that fiber (particle) shape, aspect ratio, orientation, and staggered unit cell have on permeability for creeping flow. A merged function attempting to address the drawbacks of analytical correlations at high and low porosities was proposed with a deviation of 2% from the numerical results.

Matsumura and Jackson [29, 30, 31] numerically investigated the macroscopic properties of two-dimensional periodic random packs of cylinders and ellipses with various types of size distributions including monomodal, bimodal, bidisperse, and polydisperse. An in-house research code using the immersed boundary method to treat the internal flow boundaries and a 3rd-order weighted essentially non-oscillatory (WENO) scheme was used to solve the unsteady Navier-Stokes equations. Matsumura and Jackson [29, 30, 31] showed that the permeability is correlated with the microstructure by means of the shortest Delaunay edge, and through appropriate scaling the monodisperse and polydisperse results collapse onto a universal curve. Tortuosity was also determined to be highly dependent on the aspect ratio of the ellipses.

Other investigations in determining a general curve fit for permeability include those of Chai et al. [18], Van der Hoef et al. [34], Tamayol and Bahrami [35], Kuwahara et al. [36], and Chen and Papathanasiou [37] (and references there-in).
Most of these studies have been devoted to models for drag law [10] and using steady state solutions to the Navier-Stokes equations. Few studies were on transient and statistical features of the flow, mainly due to the focus on “creeping” flow or mildly inertial flow [8, 15, 22, 27, 30, 31]. The very recent works by Agnaou et al. [3], Jin et al. [4, 38], and Uth et al. [5] highlighted the limited understanding of transitional and turbulent flows in ordered and mildly disordered periodic arrays of particles of regular shape (e.g. square, cylinders, spheres, etc.). Agnaou et al. [3] presented some new flow features in transitional flow through 2-D packs. Jin et al. [4, 38] and Uth et al. [5] are amongst the first to address fundamental turbulence questions for flow through ordered periodic porous packs. Turbulence research for porous packs is dominated by turbulence models (primarily U/RANS) that are based on length scale assumptions which were recently verified for simple ordered periodic packs in [4]. This recent understanding on the length scales involved in flow through porous packs needs to be supplemented with further studies focused on turbulence.

1.3 Immersed Boundary Method

The immersed boundary method (IBM) was first developed by Peskin [39] in 1972. The term immersed boundary method refers to any method that solves the Navier-Stokes equations with embedded boundaries on grids that do not conform to the shapes of these boundaries [39].

Based on the treatment of the boundary conditions of the embedded geometries, IBMs are divided into continuous forcing and discrete forcing [39]. The
incompressible Navier-Stokes equations may be written as,

\[ \mathcal{L}(U) = 0, \quad \text{in } \Omega_f, \]

with \( U = U_{\Gamma_b} \), on \( \Gamma_b \),

\[ (1.5) \]

where \( U=(u,p) \) and \( \mathcal{L} \) is the operator.

Continuous forcing implements the boundary conditions through a source term in the governing equations (1.5) [39]; the source term is defined as the forcing function \( f_b \) and is composed of a momentum \( f_m \) and a pressure \( f_p \) term. The forcing function is application specific and different formulations have been proposed for rigid and moving bodies [39]. The modified governing equations are subsequently solved over the entire domain making the continuous forcing method independent of the spatial discretization scheme. This approach is best suited for elastic boundaries where it has a strong physical basis and its application is straightforward. For rigid bodies the forcing functions are not well suited and have difficulties in attaining sharp representations of the immersed boundary resulting in numerical accuracy and stability concerns. As the Reynolds number increases, the need to solve the discretized equations over the entire domain may pose computational difficulties as the number of grid points inside the immersed boundary increases [39].

Discrete forcing implements the discretized boundary conditions on the cells near the embedded geometry. Discrete forcing methods are further divided into indirect (implicit) and direct (explicit) boundary condition imposition. In indirect boundary condition imposition, a forcing function applies a predetermined condition on the immersed boundary. With an \textit{a prior} estimate, the forcing function
may be determined and this approach may be extended to complex 3-D problems [39]. In direct boundary condition imposition, the boundary conditions are explicitly imposed on the immersed boundary. In this approach the local accuracy near the immersed boundary is critical. The effect of the immersed boundary must not be spread, as in continuous forcing, and therefore the method needs a “sharp” interface. “Ghost cells” or splicing of cells (“cut-cell”) near the immersed boundary may be used to impose the boundary conditions. Discrete forcing, though dependent on the spatial discretization scheme, does not have a forcing function that has user dependent parameters [39]; the stability constraints with user inputs are therefore not encountered.

1.4 Objectives

Detailed understanding of the spatial and temporal flow features and macroscopic properties such as friction factor and permeability associated with flow through porous media encountered for a wide range of Reynolds numbers and porosities is pursued in the current work. The behavior of the flow from laminar to (pseudo-)turbulent flow is studied with a focus on that encountered at transitional and (pseudo-)turbulent Reynolds numbers. Flow fields and discrete probe data are examined. The turbulent flow statistics previously pursued in [4, 5] will be presented and extended to include statistics such as probability density functions and vorticity budget plots. The macroscopic scale analysis focuses on the behavior and trends of friction factors and permeability for transitional and (pseudo-)turbulent Reynolds numbers.
1.5 Structure/Approach

The structure of this dissertation is as follows. This chapter, Chapter 1, introduces the background information and objectives of the current research. In Chapter 2, we present the governing equations and numerical methods. Chapter 3 presents several verification cases and the grid resolution studies. Results are presented in Chapter 4. The established and proposed empirical relations for friction factors for Reynolds numbers ranging from the creeping to (pseudo-)turbulent flow regime are followed by the analysis of the permeability correlations. Transitional and (pseudo-)turbulent flows are further discussed in great detail through a variety of analyses focusing on length and temporal scales of flow features. Finally, in Chapter 5 we present the conclusions and suggested future work.
Chapter 2

Governing Equations and Numerical Methods

This chapter presents the governing equations for the direct numerical simulation and immersed boundary method for the in-house research code. The numerical schemes supported by the current research code are also discussed. The research code was developed during this research and relies on open-source research packages. Additional developments currently supported by the in-house research code but not used for the current research may be found in Appendix A.

An overview of OpenFOAM’s® (OF’s) computational model is also presented. The governing equations and numerical schemes supported by OF are not discussed and the reader is encouraged to refer to [40] and [41] for more detailed discussions.
2.1 Navier-Stokes Equations and Numerical Methods

The nondimensionalised continuity and Navier-Stokes (NS) equations to be solved for direct numerical simulations (DNS) of incompressible viscous flows are

\[
\frac{\partial u_j}{\partial x_j} = 0, \quad \text{(2.1)}
\]

\[
\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{1}{Re} \frac{\partial^2 u_i}{\partial x_j \partial x_j}, \quad \text{(2.2)}
\]

where \(i, j = 1, 2, 3\), \((u_1, u_2, u_3) = (u, v, w)\) are the velocity components in the \(x, y, z\)-directions, respectively, \(p\) is the pressure, and \(Re = \rho U_0 d / \mu\) is the Reynolds number. The reference length scale is \(d\) (e.g. diameter of a cylinder), velocity scale \(U_0\) (e.g. inlet velocity), and pressure scale \(\rho U_0^2\). The reference scales for the different geometries considered are noted in each relevant section.

The incompressible Navier-Stokes equations are integrated numerically using a modified numerical method presented by Mittal et al. [42]. As shown in Figure 2.1(a), the primary variables, \(u_i\) and \(p\), are defined at the cell-centers of the collocated mesh and an additional face-centered velocity \(U_i\) is also tracked. This arrangement is chosen to take advantage of the cell-centered structure of the linear solver and adaptive mesh refinement (AMR) package in Boxlib [43], discussed in Appendix A. The temporal scheme is based on a modified three sub-step fractional-step scheme of Van Kan [44] combined with the optimized two step 4-6 alternating low-dissipation and low-dispersion Runge-Kutta (LDDRK) scheme of Hu et al. [45]. The equation solved during the first sub-step is given by
Figure 2.1: Sketches of (a) the grid and (b) the classification of cells in the immersed boundary method. GC=ghost cell; IP=image point; BI=boundary intercept. The solid line in (b) shows the immersed boundary. The collocated variables \((u_1, u_2, u_3), p, p'\) are defined at the cell-center.

\[
\frac{u_i^* - u_i^n}{\Delta t} = -H_i^n - \frac{\partial p^n}{\partial x_i} + \frac{1}{Re} \left( \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial x_3^2} \right) u_i^n, \tag{2.3}
\]

where \(H^n_i = u_j \partial u_i / \partial x_j\) are the convective terms. To eliminate the large pressure variations of collocated grids, the edge (2-D)/face (3-D) velocities are obtained through the averaging procedure presented by Mittal et al. [42] shown below

\[
\tilde{u}_i = u_i^* + \Delta t \left( \frac{\partial p^n}{\partial x_i} \right)_{cc}, \tag{2.4}
\]

\[
\tilde{U}_1 = \gamma_W \tilde{u}_1 + (1 - \gamma_W) \tilde{u}_{1W}, \tag{2.5}
\]

\[
\tilde{U}_2 = \gamma_S \tilde{u}_2 + (1 - \gamma_S) \tilde{u}_{2S}, \tag{2.6}
\]
\[ \tilde{U}_3 = \gamma_B \tilde{u}_3 + (1 - \gamma_B)\tilde{u}_{3B}, \quad (2.7) \]

\[ U_i^* = \tilde{U}_i - \Delta t \left( \frac{\partial p^n}{\partial x_i} \right)_{fc}, \quad (2.8) \]

where \( p' \) is the pressure correction, discussed below, and \( \tilde{u}_i \) and \( \tilde{U}_i \) are the velocities in the subsequent LDDRK intermediate time step. Also, \( \gamma_W, \gamma_S \) and \( \gamma_B \) are the linear interpolation weights for the west, south, and back face velocities as shown in Figure 2.1(a) and the subscripts \( cc \) and \( fc \) represent cell-centered and face-centered discrete finite difference operators, respectively. For a uniform Cartesian grid the linear interpolation weights are all equal to 0.50. The spatial discretization of the convective terms \( H^n_i \) is the 5th-order weighted essentially non-oscillatory (WENO) scheme presented by Jiang and Shu [46] and the spatial discretization of the viscous terms is the 4th-order central difference. The application of the 5th-order WENO scheme to the convective terms was presented and verified by Zhang and Jackson [47].

For completeness, the 5th-order WENO scheme [47] is repeated below, where the reconstruction of \( f \) along the \( j \)-direction follows

\[ \hat{f}_{j+1/2} = \sum_{k=1}^{3} \omega_k \hat{f}^k_{j+1/2}, \quad (2.9) \]

where \( \hat{f}^k_{j+1/2} \) are the second order polynomial reconstructions on the \( k \)th set of stencils and \( \omega_k \) are the nonlinear weights [47] given by

\[ \omega_k = \tilde{\omega}_k / \sum_{l=1}^{3} \tilde{\omega}_l, \quad \tilde{\omega}_l = \frac{\gamma_l}{(\epsilon + \beta_l)^2}, \quad (2.10) \]
where $\beta_l$ are the smoothness indicators, $\gamma_l$ are the averaging weights, and $\epsilon$ is set to $10^{-6}$ to avoid divisions by zero in the calculations of the nonlinear weights.

Upwinding is naturally implemented through the sign of $u_j$ in $u_j \partial u_i / \partial x_j$; to calculate $\hat{f}_j^{k+1/2}$ we use $u_{j+1/2}$ which is averaged from its neighbors to determine upwinding. For example, for $u_{j+1/2} > 0$, $\gamma_1 = 0.3$, $\gamma_2 = 0.6$, $\gamma_3 = 0.1$, and $\hat{f}_j^{k}$ follows

\[
\begin{align*}
\hat{f}_j^{1/2} & = \frac{1}{3} f_j + \frac{5}{6} f_{j+1} - \frac{1}{6} f_{j+2}, \\
\hat{f}_j^{2/2} & = -\frac{1}{6} f_{j-1} + \frac{5}{6} f_j + \frac{1}{3} f_{j+1}, \\
\hat{f}_j^{3/2} & = \frac{1}{3} f_{j-2} - \frac{7}{6} f_{j-1} + \frac{11}{6} f_j,
\end{align*}
\]

where the smoothness indicators $\beta_l$ follow

\[
\begin{align*}
\beta_1 & = \frac{13}{12} (f_j - 2f_{j+1} + f_{j+2})^2 + \frac{1}{4} (3f_j - 4f_{j+1} + f_{j+2})^2, \\
\beta_2 & = \frac{13}{12} (f_{j-1} - 2f_j + f_{j+1})^2 + \frac{1}{4} (f_{j-1} - f_{j+1})^2, \\
\beta_3 & = \frac{13}{12} (f_{j-2} - 2f_{j-1} + f_j)^2 + \frac{1}{4} (f_{j-2} - 4f_{j-1} + 3f_j)^2.
\end{align*}
\]

For $u_{j+1/2} < 0$, $\gamma_1 = 0.1$, $\gamma_2 = 0.6$, $\gamma_3 = 0.3$, and $\hat{f}_j^{k}$ follows

\[
\begin{align*}
\hat{f}_j^{1/2} & = \frac{11}{6} f_{j+1} - \frac{7}{6} f_{j+2} + \frac{1}{3} f_{j+3}, \\
\hat{f}_j^{2/2} & = \frac{1}{3} f_j + \frac{5}{6} f_{j+1} - \frac{1}{6} f_{j+2}, \\
\hat{f}_j^{3/2} & = -\frac{1}{6} f_{j-1} + \frac{5}{6} f_j + \frac{1}{3} f_{j+1},
\end{align*}
\]
and the smoothness indicators follow

\begin{align*}
\beta_1 &= \frac{13}{12} (f_{j+1} - 2f_{j+2} + f_{j+3})^2 + \frac{1}{4} (3f_{j+1} - 4f_{j+2} + f_{j+3})^2, \\
\beta_2 &= \frac{13}{12} (f_j - 2f_{j+1} + f_{j+2})^2 + \frac{1}{4} (f_j - f_{j+2})^2, \\
\beta_3 &= \frac{13}{12} (f_{j-1} - 2f_j + f_{j+1})^2 + \frac{1}{4} (f_{j-1} - 4f_j + 3f_{j+1})^2.
\end{align*}

The discretization of \((\partial f / \partial x)_j\) follows

\[
\left( \frac{\partial f}{\partial x} \right)_j \approx \frac{\hat{f}_{j+1/2} - \hat{f}_{j-1/2}}{\Delta x_j}.
\] (2.11)

To avoid the large stencil size required for the 5th-order WENO scheme, at the fluid cells adjacent to ghost cells local modifications to the spatial discretization schemes are needed for the two fluid layers closest to the immersed boundary. For the first fluid layer, the viscous terms are discretized with the canonical 2nd-order central difference and the convective terms are discretized with the canonical 1st-order upwinding one-sided difference. The second layer of fluid cells adjacent to the ghost cells have their convective terms discretized with a 3rd-order upwinding WENO scheme [46, 48] and the viscous terms follow the default 4th-order central differencing scheme. This approach resembles that presented by Matsumura and Jackson [29].

The 3rd-order upwinding WENO scheme [46, 48, 49] for a general flow variable \(f\) is presented for completeness. The left-sided stencil given by the WENO scheme
and using the operators $\Delta^+ f_i = f_{i+1} - f_i$ and $\Delta^- f_i = f_i - f_{i-1}$ follows

\[
\left( \frac{\partial f^-}{\partial x} \right)_i = \frac{1}{2\Delta x_i} (\Delta^+ f_{i-1} + \Delta^+ f_i) - \frac{\omega_-}{2\Delta x_i} (\Delta^+ f_{i-2} - 2\Delta^+ f_{i-1} + \Delta^+ f_i), \quad (2.12)
\]

where $\Delta x_i$ is the mesh size in the $i$-direction and

\[
\omega_- = \frac{1}{1 + 2r_-^2}, \quad r_- = \frac{\epsilon + (\Delta^- \Delta^+ f_{i-1})^2}{\epsilon + (\Delta^- \Delta^+ f_i)^2},
\]

(2.13)

where $\epsilon$ is again inserted to avoid divisions by zero and is now set to $10^{-8}$. The right-sided stencil follows

\[
\left( \frac{\partial f^+}{\partial x} \right)_i = \frac{1}{2\Delta x_i} (\Delta^+ f_{i-1} + \Delta^+ f_i) - \frac{\omega_+}{2\Delta x_i} (\Delta^+ f_{i+1} - 2\Delta^+ f_i + \Delta^+ f_{i-1}), \quad (2.14)
\]

where

\[
\omega_+ = \frac{1}{1 + 2r_+^2}, \quad r_+ = \frac{\epsilon + (\Delta^- \Delta^+ f_{i+1})^2}{\epsilon + (\Delta^- \Delta^+ f_i)^2}. \quad (2.15)
\]

The partial derivative of $f$ then follows

\[
\left( \frac{\partial f}{\partial x} \right)_i = c_{upwind} \left( \frac{\partial f^-}{\partial x} \right)_i + (1 - c_{upwind}) \left( \frac{\partial f^+}{\partial x} \right)_i, \quad (2.16)
\]

where $c_{upwind}$ is the upwinding coefficient and takes the value of zero or one based on the sign of $u_j$ in $u_j \partial u_i / \partial x_j$.

The second sub-step of the temporal scheme solves the pressure correction
\[
\frac{u_{i}^{n+1} - u_{i}^{*}}{\Delta t} = -G(p'),
\]

(2.17)

with

\[
D(u^{n+1}) = 0,
\]

(2.18)

where \(G\) and \(D\) are the discrete gradient and divergence operators, respectively. The resulting Poisson equation for the pressure correction \(p'\) is

\[
\frac{\partial}{\partial x_i} \left( \frac{\partial p'}{\partial x_i} \right) = \frac{1}{\Delta t} \frac{\partial U_{i}^{*}}{\partial x_i},
\]

(2.19)

where the cell-centered velocities \(u_{i}^{*}\) are substituted with the edge (2-D)/face (3-D) velocities \(U_{i}^{*}\) to avoid the odd-even de-coupling of collocated grids. The Poisson equation is solved with Boxlib’s multigrid V-cycle biconjugate gradient stabilized linear solver with red-black Gauss-Seidel (GS) smoothing [50].

During the final sub-step, the pressure and velocity variables are updated with the pressure correction as follows

\[
p^{n+1} = p^{n} + p',
\]

(2.20)

\[
u_{i}^{n+1} = u_{i}^{*} - \Delta t \left( \frac{\partial p'}{\partial x_i} \right)_{cc},
\]

(2.21)

\[
U_{i}^{n+1} = U_{i}^{*} - \Delta t \left( \frac{\partial p'}{\partial x_i} \right)_{fc}.
\]

(2.22)
As further discussed in Appendix A, through Boxlib the current in-house research code uses MPI for parallel computing.

2.2 Immersed Boundary Method

The immersed bodies in the flow field are treated using the discrete direct forcing ghost cell immersed boundary method (GIBM) [39, 42]. Implementation of the ghost cell method begins with identifying the fluid, solid, and ghost cells. Figure 2.1(b) shows the different cells in the GIBM. The fluid cells are those cells with their cell-centers in the fluid domain. The solid cells are those cells whose cell-centers lie inside the solid with no neighboring fluid cells. In two-dimensions, a ghost cell (GC) is then defined as a cell whose cell-center is inside the solid but has at least one north, south, east or west neighbor cell in the fluid. An image point (IP) is defined on a line segment extended from each ghost cell normal to the surface of the body and is the image of the GC about the boundary of the immersed body. The cross point of this line segment and the surface is defined as a boundary intercept (BI), and is located midway between the IP and GC. In two-dimensions, a flow variable at the image point is calculated using a bi-linear interpolation from the values at the surrounding four cell-centers. A linear extrapolation is then applied to determine the value at the ghost cell from that at the image point and the boundary intercept for a given set of boundary conditions. In this way the flow domain is extended throughout the entire computational domain, and standard Cartesian-based numerical methods can be employed. That is, at each sub-step of the temporal integration, the variables on the fluid cells are updated by solving the governing equations, and those on the image cells are
then updated by the bi-linear (2-D)/tri-linear (3-D) interpolation scheme where the boundary conditions are applied. Extension to 3-D is straightforward and has been implemented.

The bi-linear interpolation scheme for a general flow variable $\phi$ is presented for completeness and follows

$$\phi(x, y) = C_1 x y + C_2 x + C_3 y + C_4,$$  \hspace{1cm} (2.23)

where $C_1, C_2, C_3,$ and $C_4$ are unknown coefficients which depend on the values of the variable and the locations $(x, y)$ of the surrounding cells. The coefficient vector $\{C\}$ follows

$$\{C\} = \{V\}^{-1}\{\phi\},$$ \hspace{1cm} (2.24)

where

$$\{C\}^T = \{C_1, C_2, C_3, C_4\},$$ \hspace{1cm} (2.25)

$$\{\phi\}^T = \{\phi_1, \phi_2, \phi_3, \phi_4\},$$ \hspace{1cm} (2.26)

are the vectors of the unknown coefficients and values of the variable, respectively, of the surrounding cells. $[V]$ is the Vandermonde matrix for bi-linear interpolation and has the form

$$[V] = \begin{pmatrix} xy|_1 & x|_1 & y|_1 & 1 \\ \vdots \\ xy|_4 & x|_4 & y|_4 & 1 \end{pmatrix},$$

21
where the subscripts after “|” are identifiers for the surrounding cells. The value of the variable at the image point is then calculated from

\[ \phi_{IP} = \sum_{i=1}^{4} \beta_i \phi_i + T.E., \quad (2.27) \]

where \( \beta_i \) depend on the coefficients \( C_i \) and coordinates of the image point; T.E. is the truncation error and is on the order \( O(\Delta x^2) \), where \( \Delta x \) is the grid spacing.

The ghost cell value is obtained from the image point value through linear extrapolation along the normal line segment connecting these two points and the required boundary condition. For Dirichlet boundary conditions, the linear profile leads to

\[ \phi_{BI} = \frac{1}{2}(\phi_{IP} + \phi_{GC}) + O(\Delta l^2), \quad (2.28) \]

where \( \Delta l \) is the length of the line segment. Substituting (2.27) in the above equation leads to

\[ \phi_{GC} + \sum_{i=1}^{4} \beta_i \phi_i = 2\phi_{BI}. \quad (2.29) \]

For von Neumann boundary conditions, a 2nd-order central difference is used and follows

\[ \left( \frac{\partial \phi}{\partial n} \right)_{BI} = \frac{\phi_{IP} - \phi_{GC}}{\Delta l} + O(\Delta l^2), \quad (2.30) \]

and upon substituting (2.27) in the above equation, the ghost cell value can be
obtained from

\[ \phi_{GC} - \sum_{i=1}^{4} \beta_i \phi_i = \Delta l \left( \frac{\partial \phi}{\partial n} \right)_{BI}. \]  

(2.31)

No-slip Dirichlet and von Neumann boundary conditions are imposed on the velocity and pressure variables, respectively.

To extend the applicability of the fluid solver, the ghost cell scheme preprocessing algorithm (determination of fluid, solid, and ghost cells) is designed to either accept the boundary points of the immersed geometry or a scalar \( \phi \) field, similar to a level set or signed distance function. If the boundary of the immersed geometry is provided, a procedure similar to that presented in Mittal et al. [42] is used. The dot product of the distance \( d \) between the surface node/element closest to a given domain cell-center and the surface’s node/element normal \( n \), \( (d \cdot n) \), is used to determine if a cell is a fluid or solid cell. If a scalar \( \phi \) field is provided, differentiation between fluid and solid cells is based on the values of \( \phi \).

The use of a Cartesian grid significantly simplifies grid generation. Unlike body-fitted grids, IBM is not prone to grid quality deterioration. Regardless of the geometry, the grid quality is preserved. IBM has the potential of greater grid resolution control. The computational cost of solving the Navier-Stokes equations on a Cartesian-based grid is also less than traditional body-fitted methods as there are no additional grid transformation terms. Cartesian-based grids have the potential of lower per-grid-point operation count for line-iterative techniques and multigrid methods. Cartesian-based grids also facilitate straightforward implementation of high order schemes, such as those used in the current research.
2.3 OpenFOAM® Computational Setup

A brief overview of OF’s computational setup and framework is presented and is supplemented by the detailed documentation in [40] and [41]. The implicit scheme of OF is pursued to address the computational cost placed by the explicit temporal scheme of the current version of the in-house NS-GIBM research code, especially for 3-D turbulent flow simulations, and is used for Section 4.2 and 4.3.

OF’s grid generator *snappyHexMesh* is used to generate all grids used with the OF fluid solver. *snappyHexMesh* is a parallel automatic 3-D hexahedral and split-hexahedral mesh generator that requires triangulated surface geometries and a background rectilinear mesh. The former may be generated through various codes (e.g. MATLAB®) and/or softwares (e.g. CAD software) while the latter must be generated through OF’s structured mesh generator *blockMesh*.

OF’s mature implicit Navier-Stokes solver allows for the large time step necessary to simulate 3-D transitional and turbulent flows. The *pimpleFoam* solver, developed for large time step transient incompressible turbulent flow, is used. This solver is based on the PIMPLE algorithm and is the combination of the pressure implicit split operator (PISO) algorithm and semi-implicit method for pressure-linked equations (SIMPLE) algorithm.

OF’s flexibility is highlighted by the numerous numerical schemes available for the spatial and temporal discretizations. The time derivatives ($\partial/\partial t$) are discretized with the bounded 2nd-order implicit Crank-Nicolson scheme while the surface normal gradients and gradient terms ($\nabla U$) are discretized with an unbounded 4th-order scheme. The interpolation follows a 2nd-order unbounded scheme and the Laplacian ($\nabla^2 U$) and divergence terms ($\nabla \cdot U$) are all discretized with a 2nd-
order unbounded scheme.

The iterative nature of the PIMPLE algorithm is the result of the iterative PISO and SIMPLE algorithms. The system of linear velocity equations is solved using a coupled preconditioned bi-conjugated gradient (cPBICCG) solver with a diagonal incomplete lower-upper (DILU) preconditioner. The linear pressure equation is solved using the generalized geometric-algebraic multigrid (GAMG) solver with a Gauss-Seidel smoother. The tolerances for all linear system solvers are set to $10^{-5}$ which has been deemed appropriate for flow through porous packs [3, 51].
Chapter 3

Validation and Verification

In this chapter the validation and verification of the flow solver will be discussed. To verify the NS-GIBM solver, standard verification cases such as flow past blunt objects and flow through periodic arrays of particles are considered and the current results are compared with those in reported literature. It should be noted that the chosen NS-GIBM verification cases are also successfully performed with the OF fluid solver (not shown).

3.1 Taylor-Green Vortex

The Taylor-Green (TG) test problem is a standard verification case for incompressible viscous flow solvers and is used to establish the order of accuracy of the fluid
The exact solution for the unsteady 2-D problem follows

\[ u(x, y, t) = -\cos(kx)\sin(ky)\exp(-2k^2t/Re), \]
\[ v(x, y, t) = \sin(kx)\cos(ky)\exp(-2k^2t/Re), \]
\[ p(x, y, t) = -\frac{1}{4}(\cos(kx) + \cos(ky))\exp(-4k^2t/Re), \]  

(3.1)

where \( Re \) is the Reynolds number and \( t \) is the time. The numerical solutions are computed on a square domain of side \( 2\pi \) with periodic boundary conditions for \( u \), \( v \), and \( p \) in the \( x \) and \( y \)-direction. A Reynolds number of \( Re=100 \), \( k=4 \), and a time step \( \Delta t=0.01 \) are used. Table 3.1 shows the convergence rates of the fluid solver for grid sizes of \( 32^2 \), \( 64^2 \), and \( 128^2 \). The velocity variables \( u \) and \( v \) have convergence rates better than 2nd-order and pressure \( p \) has a 2nd-order convergence rate. Note that if pure cell-centered variables are used, 4th-order convergence rates for the velocity variables can be achieved. As presented by Zhang and Jackson [47], a full 2nd-order accuracy for the elliptic operator in the pressure Poison solver is remarkable and expected as the temporal discretization is explicit. The larger infinity norm \( L_{\infty}=\max(\|\psi_{ij}\|) \), where \( \psi_{ij}=\psi_{ij}\text{analytical} - \psi_{ij}\text{numerical} \), of the current solver is due to the averaging procedure (2.4) to (2.8) required to eliminate the odd-even de-coupling of collocated grids. Figure 3.1 shows the instantaneous \( u \)-velocity field for the parallel NS (MPI-NS) solver at \( t=1.0 \).

<table>
<thead>
<tr>
<th>Variables</th>
<th>32</th>
<th>Rate</th>
<th>64</th>
<th>Rate</th>
<th>128</th>
</tr>
</thead>
<tbody>
<tr>
<td>( u )</td>
<td>9.28e-3</td>
<td>3.85</td>
<td>6.45e-4</td>
<td>2.54</td>
<td>1.11e-4</td>
</tr>
<tr>
<td>( v )</td>
<td>9.28e-3</td>
<td>3.85</td>
<td>6.45e-4</td>
<td>2.55</td>
<td>1.11e-4</td>
</tr>
<tr>
<td>( p )</td>
<td>2.05e-1</td>
<td>2.09</td>
<td>4.81e-2</td>
<td>1.98</td>
<td>1.22e-2</td>
</tr>
</tbody>
</table>

Table 3.1: \( L_{\infty} \)-norms and convergence rates after 100 time steps for the TG test problem with \( \Delta t=0.01 \).
Figure 3.1: Instantaneous $u$-velocity field for the TG test problem at $Re=100$ and with $k=4$.

The 3-D unsteady Taylor-Green test problem does not have an exact solution and thus the verification relies on the comparison between the current and previously published results. For a more accurate verification procedure and to further exercise the current research code, semi 3-D simulations are conducted for the three possible coordinate combinations (i.e. (1) $n_x>1$, $n_y>1$, $n_z=1$; (2) $n_x>1$, $n_y=1$, $n_z>1$; (3) $n_x=1$, $n_y>1$, $n_z>1$; $n_x$, $n_y$, and $n_z$ are the number of grid points in the $x$, $y$, and $z$-direction, respectively.). The simulation conditions (initial conditions, boundary conditions, etc.) follow those previously presented for the 2-D unsteady Taylor-Green test problem and the analytical solutions are derived from (3.1). The $L_\infty$-norms and convergence rates for the three semi 3-D cases (not shown) considered are similar to those shown in Table 3.1.

For completeness purposes, the 3-D turbulent Taylor-Green verification case is
also performed. The initial flow field follows

\[ u(x, y, z, 0) = V_0 \sin\left(\frac{x}{L}\right) \cos\left(\frac{y}{L}\right) \cos\left(\frac{z}{L}\right), \]

\[ v(x, y, z, 0) = -V_0 \cos\left(\frac{x}{L}\right) \sin\left(\frac{y}{L}\right) \cos\left(\frac{z}{L}\right), \]

\[ w(x, y, z, 0) = 0, \]

\[ p(x, y, z, 0) = p_0 + \frac{\rho_0 V_0^2}{16} \left( \cos\left(\frac{2x}{L}\right) + \cos\left(\frac{2y}{L}\right) \right) \left( \cos\left(\frac{2z}{L}\right) + 2 \right), \]

where the reference values are \( V_0 = 1, L = 1, p_0 = 0, \) and \( \rho_0 = 1. \) The numerical solution is computed on a cubic domain of side length \( 2\pi \) with periodic boundary conditions for all variables in all three directions and at a Reynolds number of \( Re = 800. \) Verification is determined through the dissipation rate which follows

\[ \epsilon = -\frac{d}{dt} E_k(t), \]  

(3.3)

where \( E_k(t) \) is the kinetic energy integrated over the domain \( \Omega \) and is given by

\[ E_k(t) = \frac{1}{\rho_0 \Omega} \int_{\Omega} \rho \frac{u \cdot u}{2} d\Omega, \]  

(3.4)

with \( \rho = \rho_0. \) Figure 3.2(a) shows the good agreement between the current dissipation rate and those published in [52, 53, 54]. It should be noted that the good agreement between the results by the large eddy simulation (LES) models, discussed in Appendix A, and the DNS results can also be seen in Figure 3.2. Figure 3.3 further shows the turbulent structures by the \( \lambda_2 \) iso-surfaces. Here, \( \lambda_2 \) is the middle eigenvalue of \( S^2 + \Omega^2, \) where \( S = (\nabla u + \nabla u^T)/2 \) and \( \Omega = (\nabla u - \nabla u^T)/2. \)
Figure 3.2: (a) Dissipation rate and (b) kinetic energy time histories for 3-D Taylor-Green vortex at $Re=800$; [52] (red); [53] (black); [54] (blue); Current results: DNS (pink), Vreman model (VM) (cyan), dynamic VM (DVM) (green). Note, the profile for DVM is almost identical to the DNS profile.

Figure 3.3: Iso-surface of $\lambda_2=-6$ colored by vorticity magnitude $|\omega|$ for a turbulent Taylor-Green vortex simulation.

### 3.2 Lid Driven Cavity

The lid driven cavity problem in [55] is another standard verification case for incompressible viscous flow solvers [47, 56, 57]. The boundary condition for pressure
is homogeneous von Neumann boundary for all sides. The boundary condition for the velocity variable is no-slip condition. The boundary condition for the cell-centered velocity follows the no-slip boundary condition in [58] while Dirichlet boundary condition is applied to the edge-centered (2-D)/face-centered (3-D) velocity variable. The boundary conditions for cell-centered velocity components for ghost points at a domain edge with a normal in the $y$-direction, for example, follow

\begin{align}
    u(-y) &= -u(y), \\
    v(-y) &= v(y), \\
    w(-y) &= -w(y).
\end{align}

(3.5)

The results at representative Reynolds numbers are compared with the previous results of Ghia et al. [55]. As shown in Figure 3.4, for $Re=100$ and 3200 the $u$ and $v$-velocity profiles along the $y$ and $x$-direction centerline, respectively, have negligible differences with the results presented by Ghia et al. [55].

Similar to Section 3.1, the 3-D lid driven cavity verification cases are comprised of semi 3-D and 3-D simulations. The results for the semi 3-D cases considered are similar to those shown in Figure 3.4. A 3-D lid driven cavity at $Re=1000$ with similar boundary and initial conditions to the 2-D and semi 3-D cases is also considered. As seen from Figure 3.5, there are negligible differences between the current $u$ and $v$-velocity profiles along the $y$ and $x$-direction centerline, respectively, on the $z$-direction midplane and those of Yang et al. [59].
3.3 Flow past Blunt Objects

2-D flows past a circular cylinder, a square rod, and a square rod rotated 45° are considered next. The domain extent is $30.0D \times 30.0D$ with the particle placed at
\( (x, y) = (10.0D, 15.0D) \), where \( D \) is the particle reference length. For the velocity variables \((u, v)\), a uniform inlet with \( \mathbf{U}_0 = (U_{ref}, 0) \) and zero-gradient outlet in the \( x \)-direction are chosen, and the boundary conditions in the \( y \)-direction are periodic. Pressure \( p \) and pressure correction \( p' \) variables have zero normal gradients at the inlet and outlet, and are periodic in the \( y \)-direction. Verification is performed for both steady, \( Re=20 \) and \( 40 \), and unsteady, \( Re=80 \), flows. For steady flows, the non-dimensional wake bubble length \( L_w/D \) and the coefficient of drag \( C_D \) are used to verify the solutions. For unsteady flows, the Strouhal number \( St = f L_{ref}/U_{ref} \) and \( C_D \) are computed. Table 3.2 shows the good agreement for two different resolutions \( D/dx \) of \( \sim 12 \) and \( \sim 25 \). Table 3.3 shows the good agreement for \( C_D \) and \( St \) for unsteady flows past a circular cylinder at \( Re \) of 100, 300, and 1000.

<table>
<thead>
<tr>
<th>Reynolds</th>
<th>20</th>
<th>40</th>
<th>80</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( C_D )</td>
<td>( L_w/D )</td>
<td>( C_D )</td>
</tr>
<tr>
<td><strong>Cylinder</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Dennis and Chang [60]</td>
<td>2.05</td>
<td>0.94</td>
<td>1.25</td>
</tr>
<tr>
<td>Ye <em>et al</em>. [61]</td>
<td>2.03</td>
<td>0.92</td>
<td>1.25</td>
</tr>
<tr>
<td>Wang and Jackson [62]</td>
<td>2.07</td>
<td>0.93</td>
<td>1.25</td>
</tr>
<tr>
<td>Matsumura and Jackson [29]</td>
<td>2.05</td>
<td>0.93</td>
<td>1.25</td>
</tr>
<tr>
<td>current ( dx = dy = 0.078 )</td>
<td>2.04</td>
<td>0.90</td>
<td>1.25</td>
</tr>
<tr>
<td>( dx = dy = 0.039 )</td>
<td>2.06</td>
<td>0.92</td>
<td>1.25</td>
</tr>
<tr>
<td><strong>Square</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Okajima <em>et al</em>. [63]</td>
<td>2.09</td>
<td>-</td>
<td>1.65</td>
</tr>
<tr>
<td>Robichaux <em>et al</em>. [64]</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Sharma and Eswaran [65]</td>
<td>2.43</td>
<td>1.36</td>
<td>1.81</td>
</tr>
<tr>
<td>Matsumura and Jackson [29]</td>
<td>2.33</td>
<td>1.32</td>
<td>1.73</td>
</tr>
<tr>
<td>current ( dx = dy = 0.078 )</td>
<td>2.25</td>
<td>1.28</td>
<td>1.64</td>
</tr>
<tr>
<td>( dx = dy = 0.039 )</td>
<td>2.34</td>
<td>1.34</td>
<td>1.73</td>
</tr>
<tr>
<td><strong>Square rotated 45°</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Yoon <em>et al</em>. [66]</td>
<td>1.99</td>
<td>0.99</td>
<td>1.50</td>
</tr>
<tr>
<td>Matsumura and Jackson [29]</td>
<td>2.02</td>
<td>0.89</td>
<td>1.55</td>
</tr>
<tr>
<td>current ( dx = dy = 0.078 )</td>
<td>1.98</td>
<td>0.82</td>
<td>1.49</td>
</tr>
<tr>
<td>( dx = dy = 0.039 )</td>
<td>2.01</td>
<td>0.86</td>
<td>1.51</td>
</tr>
</tbody>
</table>

Table 3.2: Drag coefficients, \( C_D \), non-dimensional wake bubble lengths, \( L_w/D \), and Strouhal numbers, \( St \), of flows past a cylinder, square rod, and square rod rotated 45°.
Similar to the approach followed for verification of the 3-D NS solver presented in Section 3.1, verification of the 3-D NS-GIBM solver is comprised of semi 3-D and 3-D simulations. The former consists of repeating the 2-D verification cases for all three possible coordinate combinations; the non-dimensional wake bubble length, drag coefficient, and Strouhal number obtained from these runs have essentially the same values as those in Table 3.2 and 3.3. The 3-D verification cases consist of flow past a sphere at various Reynolds numbers, ranging from steady to unsteady flow. Table 3.4 shows the good agreement between the current results and those presented in [67] and [68], with a maximum percentage difference of ∼3%.

### Table 3.3: $C_D$ and $St$ for unsteady flows past a circular cylinder.

<table>
<thead>
<tr>
<th>$Re$</th>
<th>$C_D$</th>
<th>$St$</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>Mittal et al. [42]</td>
<td>1.35</td>
</tr>
<tr>
<td></td>
<td>Current</td>
<td>1.36</td>
</tr>
<tr>
<td>300</td>
<td>Mittal et al. [42]</td>
<td>1.36</td>
</tr>
<tr>
<td></td>
<td>Current</td>
<td>1.34</td>
</tr>
<tr>
<td>1000</td>
<td>Mittal et al. [42]</td>
<td>1.45</td>
</tr>
<tr>
<td></td>
<td>Current</td>
<td>1.41</td>
</tr>
</tbody>
</table>

### Table 3.4: $C_D$ and $St$ for steady, $Re=100$ and 150, and unsteady, $Re=300$, flows past a sphere.

<table>
<thead>
<tr>
<th>$Re$</th>
<th>$C_D$</th>
<th>$St$</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>Johnson and Pattel [67]</td>
<td>1.102</td>
</tr>
<tr>
<td></td>
<td>Mittal [69]</td>
<td>1.088</td>
</tr>
<tr>
<td></td>
<td>Current</td>
<td>1.060</td>
</tr>
<tr>
<td>150</td>
<td>Johnson and Pattel [67]</td>
<td>0.900</td>
</tr>
<tr>
<td></td>
<td>Marella et al. [68]</td>
<td>0.848</td>
</tr>
<tr>
<td></td>
<td>Current</td>
<td>0.853</td>
</tr>
<tr>
<td>300</td>
<td>Johnson and Pattel [67]</td>
<td>0.658</td>
</tr>
<tr>
<td></td>
<td>Marella et al. [68]</td>
<td>0.620</td>
</tr>
<tr>
<td></td>
<td>Current</td>
<td>0.636</td>
</tr>
</tbody>
</table>
3.4 Flow through Periodic Arrays of Particles

Flow through periodic arrays of cylinders at low Reynolds numbers is chosen for verification of flow through particle packs over a wide range of Reynolds numbers presented in Section 4. Figure 3.6 shows a monodisperse periodic square array of cylinders and a rectangular array of ellipses for a porosity $\sigma$ of 0.65 and 0.30, respectively. The size of the domain $(L_x, L_y)$ is determined by the porosity. The simulations are performed with a resolution of $D/dx_i \approx 83-111$. Pressure $p$, pressure correction $p'$, and velocities $(u, v)$ are periodic in all directions. To induce the pressure difference needed to drive the flow a source term $\phi_p$ is added to the momentum governing equation (2.2),

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{1}{Re} \frac{\partial^2 u_i}{\partial x_j \partial x_j} + \phi_p. \tag{3.6}$$

Here, $\left(\Delta p/L\right)_0$ is the reference scale for $\phi_p$, the velocity variable is scaled by $\sqrt{(\Delta p/L)_0 L_p/\rho}$, pressure is scaled by $\rho U_0^2$, and the length is scaled by the particle length $L_p = 4A/P$, where $A$ is the area and $P$ is the perimeter of the particle.

The Ergun friction factor $f_D$ as a function of the particle Reynolds number $Re_p$.
is calculated and compared with the semi-empirical relation presented by Ergun [70]. The friction factor proposed by Ergun [70] is given by

\[ f_D = \frac{150}{Re_p} + 1.75, \quad Re_p = \frac{\rho <U>L_p}{\mu(1 - \sigma)}, \quad (3.7) \]

where \( f_D \) is the non-dimensional friction factor, \( Re_p \) is the particle Reynolds number, \( \sigma \) is the porosity, \( L_p \) is the particle length, \( \mu \) is the viscosity, and \( \rho \) is the density. \( <U> \) is the superficial velocity [6, 27] and follows

\[ <U> = \frac{1}{V} \int_{V_f} u \, dV = \sigma U_{mean} = \frac{Q}{A}, \quad (3.8) \]

where \( V \) is the total volume, \( V_f \) is the fluid volume, \( U_{mean} \) is the area (2-D)/volume (3-D) averaged bulk velocity, \( Q \) is the volumetric flow rate, and \( A \) is the pack cross sectional area.

The modified Forchheimer friction factor \( f_{\sqrt{K}} \) as a function of the modified Reynolds number \( Re_{\sqrt{K}} \) is also calculated and compared with the semi-empirical relation presented by Papathanasiou et al. [19]. The modified Forchheimer friction factor follows

\[ \frac{\Delta p}{L} = f_{\sqrt{K}} \frac{\rho <U>^2(1 - \sigma)}{\sqrt{K} \sigma}, \quad Re_{\sqrt{K}} = \frac{\rho \sqrt{K} <U>(1 - \sigma)}{\mu \sigma}, \quad f_{\sqrt{K}} = \frac{1}{Re_{\sqrt{K}}} + F, \quad (3.9) \]

where \( f_{\sqrt{K}} \) is the modified friction factor, \( Re_{\sqrt{K}} \) is the modified Reynolds number, \( F=0.08 \) is a curve fit constant, and \( K \) is the permeability obtained from (1.1). Note that \( \Delta p/L \) is \( \phi_p \). Figure 3.7 shows our results agree excellently with the semi-empirical relations (3.7), for \( \sigma \geq 0.45 \), and with (3.9), for all \( \sigma \) considered. This is similar to the results of Matsumura and Jackson [29].
Figure 3.7: (a) Friction factor $f_D$ as a function of particle Reynolds number $Re_p$ and Ergun’s equation (3.7) (solid) and (b) the modified Forchheimer friction factor $f_{\sqrt{K}}$ as a function of modified Reynolds number $Re_{\sqrt{K}}$ and modified Forchheimer equation (3.9) (solid) for flow through 2-D monodisperse periodic packs of cylinders.

The deviation between the Ergun relation and the numerical friction factors for decreasing porosity for square arrays of cylinders follows the observations made by Papathanasiou et al. [19]. The decreasing porosity leads to increasing constriction of the flow with regions of significant contracting/expanding resulting in a breakdown of the capillary flow requirement [19]. Although the breakdown is greatest towards the minimum porosity ($\sigma_{\text{min}}=1-\pi/4$), significant differences are also observable up to $\sigma=0.50$ for creeping flow, consistent with the behavior observed by Skartsis et al. [71].

Figure 3.8 shows the numerical results deviate from the Ergun relation (3.7) for decreasing porosity and agree excellently with the modified Forchheimer relation (3.9) for rectangular arrays of ellipses. The increased deviation between the Ergun relation and the numerical friction factors for decreasing porosity for rectangular arrays of ellipses follows the trend observed for square arrays of cylinders.

The 3-D verification cases consist of steady flow through periodic cubic arrays
Figure 3.8: Flow through rectangular arrays of ellipses with a particle aspect ratio $AR=2:1$. (a) Friction factor $f_D$ as a function of particle Reynolds number $Re_p$ and Ergun’s equation (3.7) (solid). (b) Friction factor $f_{\sqrt{K}}$ as a function of modified Reynolds number $Re_{\sqrt{K}}$ and modified Forchheimer equation (3.9) (solid).

of spheres for porosities $\sigma=0.55, 0.65, 0.75,$ and $0.85$. As shown in Figure 3.9, the deviation from the predicted Ergun friction factor for decreasing porosity, discussed previously, is also observed for 3-D flows. The improved relation between the predicted and numerical $f_{\sqrt{K}}$ is also consistent with previous results.
Figure 3.9: Flow through 3-D monodisperse periodic cubic arrays of spheres. (a) Friction factor $f_D$ as a function of particle Reynolds number $Re_p$ and Ergun’s equation (3.7) (solid). (b) Friction factor $f_{\sqrt{K}}$ as a function of modified Reynolds number $Re_{\sqrt{K}}$ and modified Forchheimer equation (3.9) (solid). $\sigma=0.55$ (square); 0.65 (diamond); 0.75 (hexagon); 0.85 (triangle).
3.5 Grid Resolution Study

In this section we carry out grid resolution studies in the laminar and transitional flow regimes.

3.5.1 2-D Flow

Grid resolution studies for flow through a periodic square array of cylinders for laminar and transitional flows are first considered and provide valuable insight for the subsequent 3-D grid resolution studies.

3.5.1.1 Laminar Flow

A grid resolution study is first conducted for steady laminar flow at $Re_p=53.5$ for a periodic square array of cylinders with $\sigma=0.30$. As seen from Figure 3.10 a resolution of $dx_i=0.0041$ ($D/dx_i\approx243$), where $i=1, 2$, properly resolves the $u$-velocity profile. Table 3.5 shows the error in the superficial velocity for $dx_i=0.0041$ is less than 0.50% compared with $dx_i=0.0021$. A resolution of $dx_i=0.0083$ ($D/dx_i\approx120$) results in a percentage difference of $\sim2.5\%$. This corresponds to a higher resolution than that required for creeping flow through periodic arrays of cylinders discussed in Section 3.4.

<table>
<thead>
<tr>
<th>$dx_i$</th>
<th>$Re_p=53.5$</th>
<th>$Re_p=267.5$</th>
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<tr>
<td>0.0166</td>
<td>0.677</td>
<td>0.850</td>
</tr>
<tr>
<td>0.0083</td>
<td>0.776</td>
<td>1.069</td>
</tr>
<tr>
<td>0.0041</td>
<td>0.794</td>
<td>1.249</td>
</tr>
<tr>
<td>0.0021</td>
<td>0.796</td>
<td>1.240</td>
</tr>
</tbody>
</table>

Table 3.5: Superficial velocities for flow through a periodic square array of cylinders with $\sigma=0.30$ at $Re_p$ of 53.5 and 267.5 at different grid resolutions.
Figure 3.10: The \( u \)-velocity profiles along the vertical slices at (a) \( x_{\text{quarter}} = -0.25L_x \) and (b) \( x_{\text{mid}} = 0.0 \). \( dx_i \approx 0.0021 \) (\( G_1 \)); 0.0041 (\( G_2 \)); 0.0083 (\( G_3 \)); 0.0166 (\( G_4 \)). Note, the profiles of \( G_2 \) are almost identical with the profiles of \( G_1 \).

### 3.5.1.2 Transitional Flow

A resolution study for transitional flow at \( Re_p = 267.57 \) for a square array of cylinders with \( \sigma = 0.30 \) is conducted next. Table 3.5, third column, shows the superficial velocities for different grid resolutions. A resolution of \( dx_i \approx 0.0041 \) resolves the superficial velocity with a percentage difference of less than 1% with respect to the finest grid; this coincides with the laminar flow grid resolution study. A resolution of \( dx_i \approx 0.0083 \) (\( D/dx_i \approx 120 \)) results in a percentage difference of \( \sim 13.8\% \).

Due to the potential impact of transient features in transitional flow, discussed later in Section 4.4, on the resolution study we also examine the adequacy of the resolution in terms of time and length scales identified with the fast Fourier transform (FFT). As seen from Figure 3.11, the dominant length scale, for an example vertical slice of the instantaneous \( u \)-velocity at \( x_{\text{mid}} = 0.0 \), identified by the wavenumber peak at \( k = 2.862 \), is 0.349. The smallest length scales are on the order of \( O(10^{-1}) \) while the resolution is \( dx_i \approx 0.0041 \). Figure 3.12 shows that the dominant temporal scale, for an example probe data at the midpoint of the domain,
is 0.0688 with a frequency $f$ of 14.527. The smallest significant temporal scale with $A^*>0.10$ is $t\approx0.02$ with a frequency $f$ of 49.206, while the temporal resolution is $\Delta t=O(10^{-5})$. The FFTs shown in Figure 3.11 and 3.12 are representative of the length and time scales, respectively, observed for transitional flow. In addition, the spectra and FFT results, presented in the subsequent sections, further show that the chosen spatial and temporal resolutions are able to resolve the smallest length and time scales.

![Graph](image)

Figure 3.11: (a) Instantaneous $u$-velocity profile at $x_{mid}$ and (b) its power spectrum for a square array of cylinders with $\sigma=0.30$ at $Re_p=267.57$. $A^*=A/A_{max}$ is the normalized amplitude and $k=1/y$.

### 3.5.2 3-D Flow

Grid resolution studies, with the NS-GIBM and OF solvers, for flow through periodic cubic arrays of spheres for laminar flow are conducted next. As indicated by Jin et al. [4], low resolution grids ($D/dx_i\approx10$ at the center of the domain; $D/dx_i\approx50$ near the surface of the particles) are appropriate for turbulent flow through periodic arrays of 3-D cylinders. The lower and higher resolutions presented in [4] are pursued here for turbulent flow through cubic arrays of spheres.
Figure 3.12: (a) Time history of vorticity magnitude and (b) its power spectrum for a probe at the midpoint of the domain for a square array of cylinders with $\sigma=0.30$ at $Re_p=267.57$.

The grid resolution study for 3-D turbulent flow through a cubic array of spheres with a porosity $\sigma=0.75$ will be presented in Section 4.3.2.

A grid resolution study is conducted with the NS-GIBM solver for steady flow at $Re_p=0.559$ for a periodic cubic array of spheres with a porosity $\sigma=0.55$. As seen from Table 3.6 a resolution of $dx_i\simeq0.0109$ ($D/dx_i\simeq91$), where $i=1, 2, 3$, properly resolves the superficial velocity with a percentage difference of less than 0.50% compared with $dx_i\simeq0.0073$. A resolution of $dx_i\simeq0.0219$ ($D/dx_i\simeq45$) results in a percentage difference of less than 1.5%. This is consistent with the resolution requirement for creeping flow through square arrays of cylinders.

A grid resolution study is also conducted with the OF solver for a periodic cubic array of spheres for steady flow at $Re_p=175.56$ and with a porosity $\sigma=0.75$. As seen from Table 3.7, a resolution of $dx_i\simeq0.0116$ ($D/dx_i\simeq86$) properly resolves the superficial velocity with a percentage difference of less than 0.50% while a resolution of $dx_i\simeq0.0457$ ($D/dx_i\simeq21$) results in a percentage difference of less than 3.60%. The former resolution is consistent with the resolution requirement for the
NS-GIBM solver. A resolution of $D/dx_i \simeq [16-24]$, resulting in a percentage difference in the superficial velocity of no greater than 5%, is used for 3-D simulations of random packs of polydisperse spheres in Section 4.2.

<table>
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<tr>
<th>$dx_i$</th>
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<tr>
<td>0.0219</td>
<td>0.4974</td>
</tr>
<tr>
<td>0.0109</td>
<td>0.5027</td>
</tr>
<tr>
<td>0.0073</td>
<td>0.5030</td>
</tr>
<tr>
<td>0.0055</td>
<td>0.5028</td>
</tr>
</tbody>
</table>

Table 3.6: Superficial velocities for flow through a cubic array of spheres with $\sigma=0.55$ at $Re_p=0.559$ at different grid resolutions and for the NS-GIBM solver.

<table>
<thead>
<tr>
<th>$dx_i$</th>
<th>$\langle U \rangle$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0457</td>
<td>14.524</td>
</tr>
<tr>
<td>0.0233</td>
<td>14.141</td>
</tr>
<tr>
<td>0.0116</td>
<td>14.045</td>
</tr>
<tr>
<td>0.0058</td>
<td>14.020</td>
</tr>
</tbody>
</table>

Table 3.7: Superficial velocities for flow through a cubic array of spheres with $\sigma=0.75$ at $Re_p=175.56$ at different grid resolutions and for the OF solver.
Chapter 4

Results & Discussion

In this section we present the results for 2-D flow through periodic arrays of cylinders and ellipses, and then 3-D flow through random packs of polydisperse spheres and cubic arrays of monodisperse spheres. The macroscopic properties (e.g. friction factor) and microscopic characteristics, such as time and length scales of flow features, are presented.

4.1 2-D Periodic Arrays of Particles

In this section we present the new results for the critical Reynolds number and permeability curve fits for periodic arrays of cylinders and ellipses for a range of porosities. The Ergun and modified Forchheimer friction factors will be presented. Detailed analyses of the temporal and spatial structures in periodic, transitional, and pseudo-turbulent flows will also be conducted and discussed.
4.1.1 Critical Reynolds Number

To characterize the different flow regimes we first determine the first instance of unsteady flow. Agnaou et al. [3] and Kumar and Mittal [72] characterized Hopf bifurcation as the first bifurcation of the steady flow solution for which a time-periodic solution with vortices and oscillations arises. First Hopf bifurcation, identified through the critical Reynolds number $Re_{p,cr}$, corresponds to a breakdown in flow symmetry, defined as a non-zero spatial averaging of the velocity component perpendicular to the pressure source term [3, 73]; here zero spatial averaging is defined as a value smaller than the Poisson solver tolerance $\epsilon=1\times10^{-4}$. This methodology is verified by determining the critical Reynolds number for flow through a square array of cylinders with $\sigma=0.60$. The critical Reynolds number $Re'=Re_{p,cr}\times(1-\sigma)$ obtained in the current work, between steady flow at $Re'\approx149.8$ and periodic flow at $Re'\approx161.8$, is in good agreement with the results obtained by Koch and Ladd [74] where transition occurs between steady flow at $Re'\approx133.3$ and simple periodic oscillation at $Re'\approx154.7$. The critical Reynolds numbers for flow through periodic arrays of cylinders and ellipses at different porosities are implied in Figure 4.1 as the boundary between steady (diamonds) and unsteady flows (squares). It should be noted that the aspect ratio of $AR=2:1$ for the rectangular arrays of ellipses is held fixed. Although transition between steady and unsteady flow through periodic arrays of aligned cylinders was examined by Koch and Ladd [74], to the author’s knowledge the critical Reynolds numbers for flow through periodic arrays of cylinders and ellipses for a relatively wide range of porosities have not been previously documented. Agnaou et al. [3] first documented the critical Reynolds numbers for periodic packs of rectangles. As seen from Figure 4.1(b), the profile of $Re_{p,cr}$ as a function of porosity $\sigma$ is particle shape dependent.
Figure 4.1: Critical Reynolds numbers as a function of porosity $\sigma$ for flow through periodic arrays of (a) cylinders and (b) ellipses. Black symbols (diamonds) represent steady flow cases while red symbols (squares) unsteady flow. The blue line is midway between the last steady and the first unsteady case for each porosity. For comparison purposes the blue line in (a) is plotted as a green line in (b).

### 4.1.2 Friction Factor

The excellent agreement between the numerical results and the Ergun equation (3.7) for creeping flow through square arrays of cylinders was discussed in Section 3.4. Figure 4.2(a) shows the numerical friction factors for $O(10^0) \leq Re_p \leq O(10^4)$ (flows in the non-creeping, transitional, and pseudo-turbulent flow regimes) for square arrays of cylinders. Unlike creeping flow, for $Re_p > \sim 10$ the numerical $f_D$ deviates from the Ergun relation for all porosities $\sigma$ considered. As seen by comparing the $f_D$ values for $\sigma$ between 0.40 and 0.70 with those shown in Figure 3.7(a), the difference between the theoretical and numerical friction factors increases with $Re_p$.

This increase in the deviation with $Re_p$ was also encountered by Papathanasiou et al. [19]. The over-prediction of $f_D$ observed for $\sigma > \sim 0.40$ was also described by Papathanasiou et al. [19] and Tamayol et al. [22]. Figure 4.2(b) shows the Ergun relation also breaks down for rectangular arrays of ellipses for $Re_p>10$ with
increasing $Re_p$.

Figure 4.2: Friction factors for periodic arrays of (a,c) cylinders and (b,d) ellipses. Black line in (a) is the Ergun relation (3.7) and in (b) is the modified Forchheimer relation (3.9). Blue line in (c) and (d) are the proposed curve fit (4.1) for the pseudo-turbulent flow regime.

For friction factor $f_{\sqrt{K}}$, it can be seen from Figures 4.2(c) and 4.2(d) that the numerical friction factors agree with the modified Forchheimer relation (3.9) significantly better than with the Ergun relation but start to deviate from the modified Forchheimer relation (3.9) at the non-laminar flow regime. Slightly over- and under-predicted $f_{\sqrt{K}}$ values were also observed by Papathanasiou et al. [19], Tamayol et al. [22], and Ghaddar [51]. It can also be seen from Figures 4.2(c)
and 4.2(d) that the data points for transitional and pseudo-turbulent flows seem to closely follow another curve fit. Thus, similar to [19, 20], a new curve fit, shown as the blue line in Figures 4.2(c) and 4.2(d), is proposed and follows

\[ f_{\sqrt{K}} = mRe_{\sqrt{K}}^n + l, \]  

(4.1)

where \( Re_{\sqrt{K}} \) follows (3.9), and \( m, n, \) and \( l \) are constants taking the values shown in Table 4.1 and depend on the shape of the particle. It should be noted that the new curve fit for rectangular arrays of ellipses merges with (3.9) at \( Re_{\sqrt{K}} \) above \( \sim 60. \)

<table>
<thead>
<tr>
<th></th>
<th>( m )</th>
<th>( n )</th>
<th>( l )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cylinders</td>
<td>1.478</td>
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<td>0.1559</td>
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<td>Ellipses</td>
<td>1.075</td>
<td>-0.5906</td>
<td>0.01572</td>
</tr>
</tbody>
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Table 4.1: Proposed parameter values for coefficients \( m, n, \) and \( l \) of the modified curve fit (4.1).

### 4.1.3 Permeability

We next examine the permeability of flow through periodic arrays of cylinders and ellipses. A unified permeability relation derived from microscopic numerical results to better characterize macroscopic porous packs is sought after. Figure 4.3(a) shows that for creeping flow the normalized numerical permeability \( K^* \equiv K/L_p^2 \) agrees excellently with the canonical Gebart permeability relation [28]

\[ K^* = C_1 \left( \sqrt{\frac{1 - \sigma_{min}}{1 - \sigma}} - 1 \right)^{C_2}, \]  

(4.2)
where \( C_1 = 4/9\pi \sqrt{2} \) and \( C_2 = 5/2 \), for low porosities \( (\sigma < \sim 0.60) \) and with the Lee and Yang [75] permeability relation

\[
K^* = \frac{\sigma^3(\sigma - 0.2146)}{31(1 - \sigma)^{1.3}},
\]

(4.3)

for higher porosities for square arrays of cylinders. This dependence of validity on porosity was also observed by Nabovati et al. [15] and Yazdchi et al. [27]; both studies had excellent agreement with the Gebart relation [28] for \( \sigma < 0.60 \). Figure 4.3(b) shows that for creeping flow through rectangular arrays of ellipses the normalized permeability follows the same trend as the Gebart relation [28] but deviates slightly.

![Figure 4.3: Normalized permeability for periodic arrays of (a) cylinders with 0.25 \( \leq \sigma \leq 0.70 \) and (b) ellipses with 0.30 \( \leq \sigma \leq 0.70 \) in the creeping flow regime. Blue line: Gebart relation [28]; Black line: Lee and Yang relation [75]; Red Symbols: Current results.](image)

We next examine the effect of Reynolds number on the permeability of flow through periodic arrays of cylinders and ellipses. Figure 4.4(a) shows that the Gebart relation [28] over-predicts the permeability \( K^* \) at higher \( Re_p \)’s, and the deviation increases with \( Re_p \). Decreasing \( K^* \) with increasing \( Re_p \) was also observed.
by Nagelhout et al. [76] and Edwards et al. [77], and is a trend independent of particle shape and pack configuration.

![Figure 4.4](image)

Figure 4.4: Normalized permeability for periodic arrays of (a) cylinders and (b) ellipses at various porosities $\sigma$‘s and $Re_p$‘s. The arrows show the direction of increasing $Re_p$. The $Re_p$ ranges are $\sim$80 to $\sim$2000 and $\sim$80 to $\sim$4300 for (a) and (b), respectively.

The apparent similarity between the Gebart relation [28] and numerical $K^*$ for a range of $\sigma$‘s and $Re_p$‘s favors modifying the semi-empirical relation. This approach was also pursued, partially, by Yazdehi et al. [8] and Nabovati et al. [15]. In our modified curve fit relation, coefficient $C_1$ in (4.2) now depends on $Re_p$, and is given by the two-term exponential equation

$$\ln(C_1/Re_p) = ae^{bRe_p} + ce^{dRe_p},$$

(4.4)

where $a$, $b$, $c$, and $d$ are constants taking the values shown in Table 4.2. These parameters depend on the shape of the particle. A double exponential equation is pursued for its compact form whereas the non-double exponential curve fits currently explored resulted in expressions with many terms and lower coefficients of determination $R^2$. Figure 4.5 shows the dependence of coefficient $C_1$ on $Re_p$. 

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The particle geometry has a large effect on the packs’ permeability. The effect of microstructural changes on $K^\ast$ was also observed by Yazdchi et al. [27] and Tamayol and Bahrami [35]. Figure 4.6 shows good agreement between the proposed modified curve fit and the numerical modified normalized permeability $K^{**} = K^\ast / C_1$ for various $\sigma$’s for periodic arrays of cylinders and ellipses. The predicted $K^{**}$ is located within $\sim 20\%$ of the midpoint value of the $K^{**}$ range for each $\sigma$. It should be noted that the dependence of $K^\ast$ on $Re_p$ is accounted for by the curve fit of $C_1(Re_p)$ and once it is determine, $K^{**}$ follows

\[ K^{**} = \left( \sqrt{\frac{1 - \sigma_{\min}}{1 - \sigma}} - 1 \right) C_2 \]  

by (4.2) and becomes independent of $Re_p$.

<table>
<thead>
<tr>
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<th>$c$</th>
<th>$d$</th>
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<tr>
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<td>5.032</td>
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<td>-0.001703</td>
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</table>

Table 4.2: Proposed parameter values for coefficient $C_1$ in (4.4) for the modified curve fit.
Figure 4.5: Modified Gebart relation coefficient $\ln(C_1/Re_p)$ for various $Re_p$’s: Numerical (symbols); Lines: Proposed curve fits for $\ln(C_1/Re_p)$ as a function of $Re_p$; cylinder (black); ellipse (red). The $Re_p$ ranges are the same as those in Figure 4.4.

Figure 4.6: Modified normalized permeability $K^{**}$ for various porosities $\sigma$’s and $Re_p$’s for periodic arrays of (a) cylinders and (b) ellipses: Line: (4.5); Symbols and data are the same as in Figure 4.4. Blue triangles in (a) are nearly superimposed on each other.
4.1.4 Packs with Peculiar Transition Behavior

Taking advantage of the wide range of $Re_p$'s afforded by 2-D simulations, it is also of interest to systematically examine the microscopic properties of transitional/pseudo-turbulent flows in particle packs. The effects of Reynolds number and porosity on the spatial and temporal features, and the corresponding statistics, are presented. The basic analyses such as FFTs and PDFs for probe data, and two-point correlations and energy spectra for the flow fields will be established first. After the highlights of the peculiar and unusual yet interesting behavior such as the mixed steady-unsteady flows in the transitional flow regime discovered for $\sigma$ of 0.30 in this section, the microscopic properties for fully pseudo-turbulent flow through square arrays of particles with normal transitional behavior for a selected porosity of $\sigma=0.50$ will examined in Section 4.1.5.

4.1.4.1 Effect of Reynolds Numbers on Temporal Behavior

As seen in Figure 4.7, the existence of coherent structures in two-dimensions is apparent; the regions of significant vortex motion are populated by well defined large scale vortices. As will be discussed in detail later, transition to pseudo-turbulent flow occurs when significant vertical cross flow starts to emerge. The vertical cross flow causes intense vorticities along the surface of the cylinders as shown in Figures 4.7(c)-4.7(g). It should also be noted that mixed steady-unsteady flows occur at different Reynolds numbers in the transitional flow regime for this particular $\sigma$ of 0.30. For this reason, the regime is referred to as the peculiar regime. It is however not a general case as we will discuss later.

Probe data is used to further characterize the flow behavior at various Reynolds numbers. Figure 4.8 shows the probe locations. Figure 4.9 shows the $v$-velocity...
Figure 4.7: Instantaneous $z$-vorticity fields for flow through a periodic array of cylinders with $\sigma=0.30$ and at various $Re_p$’s: (a) 102.18 (steady), (b) 210.87 (periodic), (c) 267.57 (transitional/intermittent), (d) 274.14 (steady), (e) 377.08 (periodic), (f) 545.53 (transitional/pseudo-turbulent), and (g) 1079.08 (transitional/pseudo-turbulent).
time histories and the corresponding power spectra at probe 1 (near the inlet along $y=0.0$) at increasing $Re_p$. At $Re_p$ of 102.18 and below, the flow is steady after an initial transient period. As $Re_p$ is increased to the values of 159.28 and 210.87, the $v$-velocity signals exhibit an initial transient phase followed by periodic oscillations of increasing amplitude until fully periodic behaviors with constant amplitude are reached. The time required to attain a periodic behavior decreases with $Re_p$ and is consistent with Agnaou et al. [3]. At $Re_p=159.28$, the quasi-steady signal is truly periodic and there is only one frequency in the spectrum, whereas at $Re_p=210.87$, higher and lower frequencies start to emerge. As $Re_p$ is further increased to 267.57, the velocity signal becomes transitional/intermittent. The signal is now characterized by high frequency modes with $f^*=1/t^*\approx 1$ superimposed on low frequency modes $f^*\approx 10^{-2}$ as demonstrated by the power spectrum. Here, the scaled time $t^*$ follows

$$ t^* = \frac{t}{t_{ref}}, \quad (4.6) $$

where

$$ t_{ref} = \frac{L_p}{\bar{u}_{max}}, \quad (4.7) $$

where $\bar{u}_{max}$ is the maximum time averaged $u$-velocity at $x_{min}$. At $Re_p=274.14$, after an initial transient period, the $v$-velocity probe signal becomes steady again. When $Re_p$ is increased further to 377.08, the flow re-transitions to periodic flow with small amplitude periodic oscillations. As $Re_p$ is increased above 377.08, the flow remains unsteady for the $Re_p$’s examined. At $Re_p=545.53$, the velocity time history resembles a transitional/turbulent flow probe signal. The spectrum becomes broad with peak low frequencies around $\sim 10^{-2}$ and traces of high frequency peaks of $f^*\approx 1$. 

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Figure 4.8: Locations of the probes for flow through a square array of cylinders with $\sigma=0.30$.

Figure 4.9: (a,b) The time histories of $v$-velocity and (c) the corresponding power spectra at probe 1 at various $Re_p$'s: 102.18 (Black-dashed, steady); 159.28 (Cyan, periodic); 210.87 (Blue, periodic); 267.57 (Red, transitional/intermittent); 274.14 (Magenta, steady); 377.08 (Green, periodic); 545.53 (Black, transitional/pseudoturbulent). $t^*$ is given by (4.6); $A^*=A/A_{\text{max}}$; $f^*=1/t^*$. Note, only the time dependent behavior and frequency features are focused on so the $v$-velocity signals are vertically shifted and are not plotted with the same scale.

4.1.4.2 Temporal Flow Features

The physical processes responsible for the frequencies observed in Figure 4.9 at different $Re_p$'s are further analyzed through instantaneous flow fields and probe data. Figure 4.10 shows the periodic vorticity magnitude $|\omega|=\sqrt{\omega_1\omega_i}$ oscillation at probe 1 with selected instances labeled $t_i^*$ for a square array of cylinders with
σ=0.30 and \( Re_p=210.87 \). The corresponding flow fields and close up views (about probe 1) are plotted in Figure 4.11. The dominant high frequency identified by the power spectrum for \( v \)-velocity corresponds to the periodic oscillation of the flow feature referred to as the “tail” about the \( y=0.0 \) line; this periodic oscillation can be seen from the probe data and close up flow fields in Figures 4.10 and 4.11(e) to 4.11(h), respectively. Note that the high frequency oscillation period \( t^*=1/f^*=1.131 \), where \( f^*=0.88417 \) as shown in Figure 4.9, is close to the flow pass-through time \( t_p^*=1.0592 \). The pass-through time is defined as

\[
    t_p^* = \frac{L_x}{u_{\max}} t_{ref},
\]

(4.8)

where \( t_{ref} \) follows (4.7) and \( L_x \) is the length of the flow domain. Therefore, the high frequency oscillation seems to be the result of the resonance of the “tail” motion with the flow pass-through. The “tail” is defined as the coherent region emanating from \( x_{\min} \) and is characterized by a negligible vorticity region, \( tail_{mid} \), separating two regions of intense vorticity, \( tail_{up} \) and \( tail_{down} \), originating from the boundary layer. These three sections experience in-phase motion. This resonance is expected to exist for all unsteady \( Re_p \)'s.

As seen from Figure 4.12, the “tail” feature also manifests itself in the \( u \)-velocity field. As seen from Figure 4.12(b), the streamline passing through the midpoint between the particles centered at \( x_{\min} \) corresponds to \( tail_{mid} \), while \( tail_{up} \) and \( tail_{down} \) are the upper and lower, respectively, boundaries of the “tail”.

Figure 4.13 shows the unsteady vorticity magnitude time history at probe 1 with selected instances labeled \( t_i^* \) for \( Re_p=267.57 \) in the transitional/intermittent flow regime. The broad low frequencies in Figure 4.13(c), approximately centered
Figure 4.10: Vorticity magnitude $|\omega|$ at probe 1 for flow through a square array of cylinders with $\sigma=0.30$ at $Re_p=210.87$. (b) Close up view with time instances labeled. The time instances labeled correspond to the flow fields shown in Figure 4.11.

Figure 4.11: Instantaneous vorticity magnitude fields at different instances of “tail” resonant oscillation for flow through a square array of cylinders with $\sigma=0.30$ at $Re_p=210.87$ (periodic). Black dot shows probe 1. (a,e): $t^*_1 \approx 805.7$; (b,f): $t^*_2 \approx 806.3$; (c,g): $t^*_3 \approx 806.8$; (d,h): $t^*_4 \approx 807.4$.  

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Figure 4.12: Instantaneous $u$-velocity fields and streamlines for flow through a square array of cylinders with $\sigma=0.30$ at $Re_p=210.87$ (periodic). (b) Close up view about probe 1 with $tail_{down}$, $tail_{mid}$, and $tail_{up}$ labeled. Black dot shows probe 1.

about the dominant low frequency of $\sim 10^{-2}$ correspond to “tail” flapping and $t^*_1-t^*_5$ is roughly one flapping period as explained next. This is best seen by relating the annotated time instances in the vorticity magnitude time histories of the selected probes in Figure 4.13 to their corresponding flow fields in Figure 4.14. As seen from Figure 4.14 at $t^*_1 \approx 874.5$, probe 1 is at approximately the mid point of $tail_{mid}$; this region has negligible vorticity consistent with Figure 4.13. At $t^*_2$, the “tail” exhibits a clear tilting towards $y_{min}$, resulting in the intersection between probe 1 and the upper high vorticity magnitude region of $tail_{up}$; probe 1 records a higher vorticity magnitude value. Between $t^*_3$ and $t^*_5$ the “tail” reverses its tilting and at $t^*_5$ it has a clear tilting towards $y_{max}$; the location of probe 1 progresses from $tail_{up}$ at $t^*_2$ to $tail_{mid}$ at $t^*_3$ to $tail_{down}$ at $t^*_5$. The broad range of low frequencies $f^*<\sim 10^{-1}$ recorded at probe 1, shown in Figure 4.13(c), is thus the result of “tail” flapping. Note that the difference between $t^*_2$ and $t^*_5$ is $\sim 23.1$ which corresponds to
a frequency $f^*$ of 0.043; as seen in Figure 4.13(c), this frequency is approximately between the second and third most dominant frequencies at probe 1. For probes away from the centerline, like probe 5, significant vorticity magnitudes correspond to the moment when the probe is in the region of vortex shed from the surface as seen in Figures 4.14(c) and 4.14(d), while negligible vorticity magnitudes during an extended time interval, like from $t^*\sim900$ to 980, occur when probe 5 is outside the region of significant vorticity as seen in Figure 4.14(e), causing intermittency as seen in Figure 4.13(b). On the other hand, the high frequency peaks discernible in Figures 4.13(c) and 4.13(d) correspond to the resonance oscillations previously discussed for $\sigma=0.30$ at $Re_p=210.87$. The oscillation frequencies are superimposed on the flapping frequencies. Also, as seen from Figure 4.13, the “intermittent”-like behavior tends to be more apparent at probe 5, near the edge of the region with significant “tail” and vortex activity. In summary, periodic flow is solely characterized by “tail” oscillations due to resonance and unsteady non-periodic flow has a range of frequencies with significant low frequencies corresponding to “tail” flapping and high frequencies corresponding to “tail” oscillations.

It should be noted that “tail” flapping and oscillations are not limited to the region about $y=0.0$ line, the “tail” can also flap at a tilted location at the transitional flow regime as seen in Figure 4.7(f) for $Re_p=545.53$.

### 4.1.4.3 Probability Density Function

One of the important turbulent statistics is the probability density function (PDF). Consider the evolution of, say the vorticity magnitude $|\omega|$, at a single point in space. It is possible to estimate the PDF of $|\omega|$ by taking the temporal average over the
Figure 4.13: (a,b) Vorticity magnitude time histories and (c,d) the corresponding normalized power spectra for flow through a square array of cylinders with $\sigma=0.30$ at $Re_p=267.57$ (transitional/intermittent) at probe 1 (a,c) and probe 5 (b,d). Note the “intermittent” behavior of $|\omega|$ especially at probe 5. The high frequency ($f^*>0.5$) peak is the resonance frequency. The time instances labeled in (a,b) correspond to the flow fields shown in Figure 4.14.

The time instance $T$

\[
f(|\omega(t)|) = \frac{1}{T} \int_{0}^{T} \delta(|\omega(t)| - g) dt = <\delta(|\omega(t)| - g)>,
\]

where $g$ denotes the sample space variable and $|\omega(t)|$ denotes the actual realization of this fluctuating quantity; this formula generates the histogram $f(|\omega(t)|)$ from
Figure 4.14: Instantaneous vorticity magnitude fields at different “tail” flapping phase and attendant re-circulation instances, (a) $t^*_1 \simeq 874.5$, (b) $t^*_2 \simeq 886.1$, (c) $t^*_3 \simeq 891.9$, (d) $t^*_4 \simeq 897.7$, and (e) $t^*_5 \simeq 909.2$, for flow through a square array of cylinders with $\sigma = 0.30$ at $Re_p = 267.57$ (transitional/intermittent). Probes 1 and 5 are shown. Note, $t^*_1 - t^*_5$ is approximately one period of the “tail” flapping.

which a PDF is obtained. As shown in Figure 4.15, the PDFs of vorticity magnitude at probe 1 are plotted for various $Re_p$’s. For steady flow at $Re_p = 102.18$, the PDF is a delta function while at higher $Re_p$’s, corresponding to periodic or “intermittent”-like/pseudo-turbulent flow, the PDFs have increasingly broader distributions. Note that for periodic flow at $Re_p = 210.87$, the PDF has the expected shape of that for a sine/cosine wave, two peaks of increasing density separated by a range of insignificant probability. For “intermittent”-like flow at $Re_p = 267.57$, the PDF becomes increasingly more distributed without apparent isolate peaks. There is also a larger vorticity magnitude range indicating the emergence of strong
vortices. At $Re_p=545.53$ (transitional/pseudo-turbulent flow), the emergence of a dominant peak with non-symmetric decay rates is observed. Note the peak is at $|\omega|_{\text{peak}}=12.671$. The decay rate for $|\omega|<|\omega|_{\text{peak}}$ is significantly larger than that for $|\omega|>|\omega|_{\text{peak}}$. It should be noted that the decay rate for $|\omega|>|\omega|_{\text{peak}}$ is Gaussian-like as seen from Figure 4.15(d), where a one-term Gaussian curve fit is plotted. It should also be noted that as the $Re_p$ increases the vorticity magnitude range increases too; for $Re_p$ of 545.53, the upper limit of the vorticity magnitude $|\omega|$ is $\sim 600$ while it is $\sim 300$ for $Re_p$ of 210.87. This increase in vorticity magnitude with $Re_p$ in the transitional/pseudo-turbulent flow regime is also highlighted by the nearly doubling of the vorticity magnitude range as $Re_p$ is increased from 545.53 to 1079.08. At $Re_p$ of 1079.08 vorticities with $|\omega|>\sim 400$ have significantly greater probability densities than at lower particle Reynolds numbers. It should be noted that flow at $Re_p$ of 1079.08 is not in the fully pseudo-turbulent flow regime. Fully pseudo-turbulent flow will be discussed in Section 4.1.5 for a square array of cylinders with $\sigma=0.50$.

PDFs of vorticity magnitude are expected to be space-dependent. As shown by Figure 4.16, for “intermittent”-like flow at $Re_p$ of 267.57, the PDFs are space-dependent due to the dominance of large scale coherent structures. As shown in Figure 4.8, probe 1 and probe 3 are located along the $y=0.0$ line and have different distributions, see Figure 4.15(c) and Figure 4.16(b) respectively; the latter has a more distinguishable peak at $|\omega|=257.59$ with two different decay rates at each side. Figures 4.16(a) and 4.16(c) for probe 2 and probe 4, respectively, on the other hand show similar Gaussian-like PDF distributions due to “tail” flapping and the smearing of the “tail” edge as seen in Figure 4.14. Figure 4.16 shows that space-dependent PDFs are also present for transitional/pseudo-turbulent flow at $Re_p$ of
Figure 4.15: PDFs of vorticity magnitude $|\omega|$ at probe 1 for (a) $Re_p=102.18$ (steady), (b) 210.87 (periodic), (c) 267.57 (transitional), (d) 545.53 (transitional/pseudo-turbulent), and (e) 1079.08 (transitional/pseudo-turbulent) for a square array of cylinders with $\sigma=0.30$. Red line: Gaussian curve fit.
545.53. Probe 1 and probe 3 have different distributions, see Figures 4.15(d) and 4.16(e); the latter has a peak at $|\omega|=122.05$ with two different decay rates. Probe 2, Figure 4.16(d), has a Gaussian-like PDF with a peak at $|\omega|=156.24$. Probe 4, Figure 4.16(f), on the other hand has a distinguishable peak at $|\omega|=68.45$ and also has two different decay rates on either side of $|\omega|=68.45$.

The increasing breakdown of instantaneous flow symmetry with increasing Reynolds number has a larger effect on the PDF distributions of probe data. At $Re_p$ of 267.57, probes 2 and 4 experience similar flow features as they are located symmetrically below and above, respectively, the “tail” flapping centerline, leading to similar Gaussian-like vorticity magnitude PDF distributions as seen in Figures 4.16(a) and 4.16(c). Probes 2 and 4 at $Re_p$ of 545.53 on the other hand do not exhibit similar PDF distributions as a result of the significant upwards tilting of the “tail”, as seen in Figure 4.7(f). As seen from Figure 4.7(f), at $Re_p$ of 545.53, probe 2 primarily records the vortex behavior below the “tail”; its location relative to the vertical cross flow path more closely resembles that of probe 2 for $Re_p$ of 267.57 so both have a Gaussian-like PDF. On the contrary, probe 4 is located in a region with increasingly complex flow structures and behaviors; it is located in the primary path of the upwards tilting “tail” and predominantly records the vortex behavior originating from the “tail” and the interaction of the “tail” with the vertical cross flow.

4.1.4.4 Vorticity Budget

To better characterize the behavior of $z$-vorticity, the vorticity budgets for periodic and steady flows in the supercritical flow regime are considered. The 2-D time
averaged vorticity equation follows

\[ \frac{\partial \bar{\omega}}{\partial t} + \bar{u}_j \frac{\partial \bar{\omega}}{\partial x_j} + \frac{\partial}{\partial x_j} \bar{u}_j' \omega' = \nu \nabla^2 \bar{\omega}, \tag{4.10} \]

where, \( \bar{\psi} \) is the time averaged value and \( \psi' \) is the fluctuation. For the non-dimensional time averaged vorticity budget equation \( \nu \) is taken as \( 1/Re \). For steady flow \( \bar{\psi} = \psi \), and the term \( \partial(\bar{u}_j' \omega')/\partial x_j \) is zero. \( \bar{u}_j \partial \bar{\omega}/\partial x_j \) represents the convection of the mean vorticity, \( \partial(\bar{u}_j' \omega')/\partial x_j \) is the turbulent vorticity diffusion, and \( \nu \nabla^2 \bar{\omega} \) is the viscous vorticity diffusion [78].

Figure 4.17 shows the viscous vorticity diffusion \( (\nu \nabla^2 \bar{\omega}) \) along a vertical slice at \( x_{mid} \) at various \( Re_p \)'s. Flows at different \( Re_p \)’s but in similar flow sub-regimes (determined by the “tail” behavior) exhibit similar vorticity budget profiles.

The budgets for periodic flow at \( Re_p = 159.28 \) and 210.87 exhibit similar locations of maximum viscous vorticity diffusion and are adequately symmetric about \( y = 0.0 \) with a gradual decrease for increasing \( |y| \). The limited region of significant viscous vorticity diffusion for both \( Re_p \)’s is indicative of the size and limited motion of the “tail” as seen in Figure 4.7 and Figure 4.18. In particular, for \( Re_p = 159.28 \) the region influenced by the time averaged “tail” is located at \( |y| \leq \sim 0.08 \) and corresponds to the region of significant viscous vorticity diffusion. The regions of \( \omega_{z,\text{max}} \) and \( \omega_{z,\text{min}} \) are located at approximately the inner boundaries of the \( \text{tail}_{up} \) and \( \text{tail}_{down} \) regions, respectively, while the second largest \( |\omega_z| \) peaks are located near the outer boundaries of these regions. The attenuating non-monotonic viscous vorticity diffusion at \( |y| \sim 0.15 \) is due to the re-circulation resulting from “tail” impinging. Figure 4.18 shows the wall jet flows originating from the imping-
ing zones on the surface of particles centered $x_{max}$. It should be noted that the impinging zone is analogous to the stagnation point for flow past a blunt object.

For periodic flow at $Re_p=210.87$ the peaks of maximum and minimum viscous vorticity diffusion are symmetric about $|y|≈0.0105$ and have lower magnitudes compared to $Re_p=159.28$. The appreciable differences in the profiles of the two $Re_p$’s are due to the differences in the locations of the standing vortices. As seen from Figure 4.18, as $Re_p$ is increased from 159.28 to 210.87 the standing vortices adjacent to the “tail” become closer to the particles downstream as the smaller standing vortices located near the $y$-direction domain edges move closer to $y=0.0$ line.

For the peculiar regime, there can be steady flows above $Re_{p,cr}$, such as, steady flow at $Re_p=323.51$. Steady flow at $Re_p=323.51$ and periodic flow at 377.08 also exhibit similar vorticity budget profiles at $x_{mid}$. Significant vorticity generation throughout the domain is the result of a prominent flow in the vertical direction as mentioned in Section 4.1.4.1; Figure 4.19 shows this vertical cross flow with the $v$-velocity field. This vertical flow intensifies with the contracting area between the particles at $y_{min}$ and $y_{max}$. The viscous vorticity diffusion peaks for $-0.3≤y≤-0.1$ are due to the “tail”; those in $-0.1≤y≤0.0$ and $y≤-0.3$ are the results of the vortex generated by “tail” impinging and its wall jets headed towards $y=0.0$ and $y=y_{min}$, respectively, as seen in Figure 4.19. The viscous vorticity diffusion peaks for $-0.25≤y≤y_{max}$ correspond to the previously mentioned vertical cross flow while those for $0≤y≤0.25$ result from a significant standing vortex as seen in Figure 4.19.

Figure 4.20 shows the complete vorticity budget along a vertical slice at $x_{mid}$ for $Re_p=210.87$ (periodic). For $-0.064≤y≤-0.072$ the $\bar{u}\partial\bar{\nu}/\partial x$ and $\partial(\bar{v}\bar{\omega})/\partial y$ terms
are the most significant; this region comprises the majority - \(\sim 90\%\) - of the “tail” width. This can be understood through the time averaged and \(rms\) of the velocity fields shown in Figure 4.21. The appreciable \(\overline{u}\partial \overline{\omega}/\partial x\) term results from the large \(\overline{u}\)-velocity in the well defined “tail” as seen from Figure 4.21(a). The significant \(\partial (\overline{v}'\overline{\omega}')/\partial x\) term on the other hand results from the periodic oscillation of the \(v\)-velocity due to the “tail” resonance oscillation while negligible \(\partial (\overline{u}'\overline{\omega}')/\partial x\) term stems from the notably smaller fluctuation in \(u\)-velocity seen in Figures 4.21(c) and 4.21(d), respectively. Finally, the \(\overline{v}\partial \overline{\omega}/\partial y\) term is small due to the negligible \(v\)-velocity along \(x_{mid}\) seen in Figure 4.21(b).

### 4.1.4.5 Effect of Reynolds Number on Length Scales of Spatial Structures

We next examine the effect of Reynolds number on spatial structures and length scales for flow through a square array of cylinders. Figure 4.22 shows the instantaneous \(z\)-vorticity profiles and their FFTs along a vertical slice at \(x_{mid}\) at different \(Re_p\)'s for periodic and fluctuating flows. For periodic flow at \(Re_p=210.87\), the \(z\)-vorticity profile is characterized by symmetric \(|\omega_z|\) spikes close to \(y=0.0\) with a gradual decrease for increasing \(|y|\) as seen from Figures 4.7(b) and 4.22(a). The power spectrum is smooth with a gradual decrease in amplitude for \(k>k_{max}\) and \(k<k_{max}\), where \(k_{max}=4.76\) and corresponds to approximately the width of \(\sim 0.2\) of the symmetric \(|\omega_z|\) spikes. For periodic flow at a higher \(Re_p\) of 377.08, the \(\omega_z\) profile is dominated by the asymmetric “tail” with a clear tilting towards \(y_{min}\), as seen from Figure 4.7(e). The power spectrum is “rough” with highly non-monotonic amplitude variations for \(k>k_{max}\), where \(k_{max}\approx 0.95\) corresponds to a wavelength of \(1.0526\), similar to the domain length. For the transitional/pseudo-turbulent flow at
$Re_p=545.53$, the $z$-vorticity profile has a wider range of length scales as seen from the power spectrum; the FFT shows that there are increasingly larger wavenumber powers than at lower $Re_p$’s, as seen by comparing Figures 4.22(d) and 4.22(f). The increasing power of small length scales with increasing particle Reynolds number can also be seen with the FFT for $Re_p=1079.08$; there is a power shift towards higher wavenumbers, smaller length scales. The increase in the amount of flow features with smaller length scales can also be seen from the $z$-vorticity fields shown in Figure 4.7.

The energy spectrum is often used for the analysis of turbulent structures. The energy spectrum tensor $E_{ij}(x_0, k_2)$ [79] for a vertical slice at $x_{mid}$ is calculated for this analysis. $E_{ij}(x_0, k_2)$ is obtained by performing the FFT of the two-point double correlation tensor $R_{ij}(r, x_0)$, given by

$$R_{ij}(r, x_0) = u'_i(x_0, t) u'_j(x_0 + r, t), \quad (4.11)$$

where $\psi'$ is the unsteady fluctuation, $x_0=(x_{mid}, y_{mid})=(0, 0)$ (middle of the domain), and $r$ is the distance vector covering the whole domain. $E_{ij}(x_0, k_2)$ then follows

$$E_{ij}(x_0, k_2) = (\pi)^{-1} \int_{-\infty}^{\infty} e^{-ir_2k_2} R_{ij}(e_2 r_2, x_0) dr_2, \quad (4.12)$$

where $i=\sqrt{-1}$, $r_2=y$, and $k_2=1/y$ is the wavenumber. Hereafter, we will simply use $R_{ij}$ and $E_{ij}(k_2)$ as our notation without causing confusion. Note in the current work, two-point double correlations $R_{ii}$ are used to detect turbulent structures and analyze their scales. $R_{ij}$ with $i \neq j$ will be examined in the future when a turbulent model is to be developed.
Figure 4.23 shows the two-point double correlation $R_{11}$ and $R_{22}$ fields for a point located at the center $\mathbf{x}_0 = (x_{mid}, y_{mid})$ of the domain for periodic and transitional/intermittent flows. For $Re_p = 210.87$ (periodic), by comparing the time averaged and instantaneous flow fields, non-zero correlation is related to the “tail” resonant oscillation. This is best seen from the high positive and negative correlations shown in Figures 4.23(a) and (e) located near the end of the “tail” and near the “tail” impinging zones as shown in Figure 4.11 with instantaneous flow fields and Figure 4.18(b) with time averaged flow fields. Correlations in the transitional/intermittent flow regime at $Re_p = 267.57$ shown in Figures 4.23(b) and (f) are induced by the “tail” flapping and “tail” oscillations as seen from the significant $R_{11}$ and $R_{22}$ inside the “tail” flapping zone shown in Figure 4.14. For transitional/pseudo-turbulent flow at $Re_p = 545.53$ and 1079.08, due to the significant vertical cross flow that starts to emerge at transitional/pseudo-turbulent Reynolds numbers as shown in Figure 4.19 in Section 4.1.4.4, strong correlations emerge near the vertical boundaries especially for $R_{22}$ as seen in Figures 4.23(g) and (h). Overall, as seen in Section 4.1.4.4 vorticity activities concentrate in an elongated region near the $y=0.0$ line at low $Re_p$’s due to the limited oscillatory motion of the “tail”. The active region is widened at higher $Re_p$’s when the “tail” starts to flap and a vertical cross flow eventually appears at transitional Reynolds numbers. This transition leads to the qualitative differences in the vorticity budgets in Figure 4.17 and in the correlation flow fields in Figure 4.23 between low and high Reynolds numbers.

We next examine the energy spectra extracted from these correlation flow fields. As seen in Figure 4.23, the energy spectra $E_{11}(k_2)$ and $E_{22}(k_2)$ are generally qualitatively different due to the different profiles of $R_{11}$ and $R_{22}$ along the vertical slice. The $E_{11}(k_2)$ spectra have broader distributions than $E_{22}(k_2)$ due to the
more complex profiles and multiple peaks in $R_{11}$ along the vertical direction. The widening of the active region of the “tail” and increase in vorticity with Reynolds number discussed above also cause the $E_{11}(k_2)$ spectra to become more concentrated towards lower $k_2$ and larger length scales at higher Reynolds numbers. The $E_{22}(k_2)$ spectra on the other hand are dominated by a single peak at $k_2 \approx 0.959$ for the three lower $Re_p$ ’s, which corresponds to a length scale $l_y = 1.043$ close to the domain width of 1.0592. This is consistent with the simple one wavelength profiles of $R_{22}$ along the vertical slice. At transitional/pseudo-turbulent $Re_p$ of 1079.08, due to the emergence of strong correlations at the vertical boundaries, the vertical slice of $R_{22}$ now has two wavelengths and the peak shifts to $k_2 \approx 1.918$ with a length scale $l_y = 0.521$, half of those at lower $Re_p$’s. Note that $E_{22}(k_1)$ is expected to be qualitatively similar to $E_{11}(k_2)$. Also, note that unlike the spectra for instantaneous profiles in Figure 4.22, the energy spectra tend to identify large scales as small scale instantaneous structures are likely smoothed out by the averaging during the calculation of the two-point double correlation tensors. This can also be appreciated by comparing the instantaneous and the mean flow fields for $Re_p$ of 1079.08 in Figures 4.7(g) and 4.24, respectively.
Figure 4.16: PDFs of the vorticity magnitude for a square array of cylinders with $\sigma=0.30$ at $Re_p=267.57$ (a-c) and $Re_p=545.53$ (d-f) at different locations for probe 2 (a,d), probe 3 (b,e), and probe 4 (c,f). Red line: Gaussian curve fit.
Figure 4.17: Time averaged $z$-vorticity $\bar{\omega}_z$ diffusion ($\nu \nabla^2 \bar{\omega}$) budgets for a square array of cylinders with $\sigma=0.30$ at various $Re_p$’s. $Re_p=159.28$ (pink; periodic); $Re_p=210.87$ (red; periodic); $Re_p=274.14$ (green; steady); $Re_p=323.51$ (blue; steady); $Re_p=377.08$ (black; periodic).

Figure 4.18: Time averaged $z$-vorticity $\bar{\omega}_z$ fields for a square array of cylinders with $\sigma=0.30$ at (a) $Re_p=159.28$ and (b) $Re_p=210.87$. Dashed green line: $x_{mid}$; Grey lines: streamlines. White arrows show the “tail” impinging zones. Colored arrows show the directions of the similarly colored wall jets.
Figure 4.19: Steady $v$-velocity field for a square array of cylinders with $\sigma=0.30$ at $Re_p=323.51$. Dashed pink line: $x_{mid}$. White arrow shows the “tail” impinging zone. Colored arrows show the directions of the similarly colored wall jets. Bold white streamline is within the $tail_{mid}$ region. Grey lines: streamlines.

Figure 4.20: Terms in the time averaged vorticity equation (4.10) for flow through a square array of cylinders with $\sigma=0.30$ at $Re_p=210.87$ (periodic). $\nu\nabla^2\omega$ (pink); $\bar{u}\partial\omega/\partial x$ (red); $\bar{v}\partial\omega/\partial y$ (green); $\partial(\bar{u}\omega)/\partial x$ (blue); $\partial(\bar{v}\omega)/\partial y$ (black).
Figure 4.21: Time averaged (a) $u$ and (b) $v$-velocity and $rms$ of (c) $u$ and (d) $v$-velocity fields for flow through a square array of cylinders with $\sigma=0.30$ at $Re_p=210.87$. Dashed pink line: $x_{mid}$. 
Figure 4.22: Instantaneous $z$-vorticity profiles (left column) along a vertical slice at $x_{mid}$ and their power spectra (right column) for a square array of cylinders with $\sigma=0.30$ at various $Re_p$’s. $Re_p=210.87$ (row 1); $Re_p=377.08$ (row 2); $Re_p=545.53$ (row 3); $Re_p=1079.08$ (row 4).
Figure 4.23: $R_{11}(r, x_0)$ (a-d), $R_{22}(r, x_0)$ (e-h), $E_{11}(x_0, k_2)$ (i-l), and $E_{22}(x_0, k_2)$ (m-p) for a square array of cylinders with $\sigma=0.30$ at $Re_p = 210.87$ (1st column), 267.57 (2nd column), 545.53 (3rd column), and 1079.08 (4th column). The two-point correlation ranges from maximum positive correlation (yellow) to maximum negative correlation (cyan) with zero correlation being white. $k$ in (i)-(p) is $k_2$; $k_2$ is the wavenumber defined as $1/y$. 

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Figure 4.24: Time averaged $z$-vorticity $\mathcal{Q}_z$ field for a square array of cylinders with $\sigma=0.30$ at $Re_p=1079.08$. Green lines with arrows: streamlines.
4.1.4.6 Representative Elementary Volumes

As large macroscale simulations of porous media are computationally expensive, representative elementary volumes (REVs) are extensively used [80]. An REV is the smallest sub-volume that exhibits the same behavior as a complete porous medium matrix. REVs permit a comprehensive characterization of the microscale physics and macroscale parameters that can be subsequently used to treat porous columns as homogenized porous media [80]. Though it has been widely accepted and assumed that for a geometrically regular matrix the REV is on the order of the pore scale [4, 5] - one geometric unit cell (GUC) - recent DNS investigations of porous media have challenged this assumption for the critical Reynolds number regime [3]. To enhance our understanding of the effect of the size of REV at transitional Reynolds numbers especially for the peculiar mixed steady-unsteady regime for $\sigma=0.30$, referred to as the peculiar regime below, shown in Figure 4.1(a), flows through a square array of cylinders with $\sigma=0.30$ and with various REV sizes are simulated and investigated. Figure 4.25 shows the schematic for a general REV where an $l \times m$ REV means there are $l$ GUCs in the $x$-direction and $m$ GUCs in the $y$-direction.

We first examine the case of $Re_p = 267.57$ that exhibits significant intermittency as seen in Figure 4.13. Figures 4.26(a) and 4.26(c) plot the time averaged velocity fields for a $2 \times 2$ REV. It is seen that for GUC$_1$ and GUC$_3$ the time averaged “tail” tilts upwards and has a significant vertical cross flow while for GUC$_2$ and GUC$_4$ the “tail” tilts only slightly downwards. The time averaged flow fields are more periodic in the $y$-direction. A similar difference is observed for the flow fields of $rms$ of velocity seen in Figures 4.26(b) and 4.26(d).

Increasing the size of the REV further to $3 \times 3$ reveals an interesting change
from unsteady to steady flow. The flow fields are also perfectly periodic as seen in Figure 4.27. The steady “tail” tilts upwards with a significant upwards vertical cross flow in all GUCs. This perfect periodicity might seem expected because of the absence of the complications due to intermittency associated with unsteady flow. However, when the same REV is used for another $Re_p$ of 323.51, also in the peculiar regime, the flow is only periodic in the $y$ but not the $x$-direction, as shown in Figure 4.28. In addition, the change between steady and unsteady flow when the size of the REV is changed also occurs for $Re_p$ of 323.51. In particular, the flow is steady for $1 \times 1$ but becomes unsteady for $2 \times 2$, and is steady again for $3 \times 3$. This change certainly reminds one of the mixed steady-unsteady flow in the peculiar regime as the Reynolds number is changed.
Figure 4.26: Time averaged (a) $u$-velocity and (c) $v$-velocity, and $rms$ of (b) $u$-velocity and (d) $v$-velocity fields for flow through a $2 \times 2$ REV square array of cylinders with $\sigma=0.30$ for $Re_p=267.57$.

In all the cases examined above, the flow is periodic in the $y$-direction, consistent with the behavior observed in the instantaneous flow fields of [3]. Taking this into account, an REV with three GUCs in the $x$-direction is considered next. As seen from Figure 4.29, the non-periodic behaviors observed in each GUC comprising the $1 \times 3$ REV are the same as those seen for flow through a $3 \times 3$ REV at $Re_p=323.51$. 

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Figure 4.27: Steady (a) $u$-velocity and (b) $v$-velocity fields for flow through a $3\times3$ REV square array of cylinders with $\sigma=0.30$ for $Re_p=267.57$.

Figure 4.28: Steady (a) $u$-velocity and (b) $v$-velocity fields for flow through a $3\times3$ REV square array of cylinders with $\sigma=0.30$ for $Re_p=323.51$.

For nearly pseudo-turbulent flow at $Re_p=545.53$, as seen from Figure 4.30, the flow is less susceptible to the effect of the size of the REV than at lower transitional flow Reynolds numbers. The time averaged and $rms$ of velocity fields for all GUCs exhibit essentially the same behavior.
Finally in this section, the effect of the size of the REV is examined in terms of the macroscopic properties, such as friction factor and permeability, that are dependent on the superficial velocity. As seen from Table 4.3, the size of the REV only has an effect on the superficial velocity when there is a change between steady and unsteady flow. When the steadiness or unsteadiness of the flow is the same, the superficial velocity remains the same. It should also be noted that as the $Re_p$ increases from the transitional flow regime at $Re_p=267.57$ to the nearly pseudo-turbulent flow regime at $Re_p=545.53$, the effect of the size of the REV diminishes. Hence, for pseudo-turbulent flow, the canonical $1\times1$ REV seems appropriate while for transitional flow, larger REV sizes must be considered. The effect of the size of the REV for other porosities and for flow in the fully pseudo-turbulent flow regime will be examined in the future.

<table>
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<td>323.51</td>
<td>545.53</td>
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<td>1.249 (US)</td>
<td>1.132 (S)</td>
<td>1.273 (US)</td>
</tr>
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<td>1.262 (US)</td>
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<td>1×3</td>
<td>1.075 (S)</td>
<td>1.146 (S)</td>
<td>1.268 (US)</td>
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Table 4.3: Superficial velocities for flow through a square array of cylinders with $\sigma=0.30$ and at $Re_p=267.57$, 323.51, and 545.53 and with various REV sizes. S: steady flow; US: unsteady flow.
Figure 4.30: Time averaged (a) $u$-velocity and (c) $v$-velocity, and $rms$ of (b) $u$-velocity and (d) $v$-velocity fields for flow through a $2 \times 2$ REV square array of cylinders with $\sigma=0.30$ for $Re_p=545.53$. 

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4.1.5 Packs with Normal Transition Behavior

After the highlights of the peculiar and unusual yet interesting behavior such as the mixed steady-unsteady flows in the transitional flow regime discovered for \( \sigma \) of 0.30 in the previous section, we will now return to the normal regime with a selected porosity of \( \sigma=0.50 \). The basic analyses such as FFTs and PDFs for probe data, and two-point correlations and energy spectra for the flow fields have been established in the previous section and will also be conducted for \( \sigma=0.50 \); appropriate comparisons will be made with the results for \( \sigma=0.30 \). The analysis of flows in the fully pseudo-turbulent flow regime is also focused on the similarities in PDFs, two-point correlations, etc., specific to 2-D pseudo-turbulent flow between various Reynolds numbers. In addition, intermittent change in the direction of titling of the “tail” is observed for \( \sigma=0.50 \). This behavior was not observed for the cases and flow fields explored for a square array of cylinders with \( \sigma=0.30 \).

4.1.5.1 Effect of Reynolds Numbers on Temporal Behavior

Instantaneous \( z \)-vorticity fields are plotted in Figure 4.31 for flow through a square array of cylinders with \( \sigma=0.50 \) for a wide range of Reynolds numbers. Coherent structures in two-dimensions still exist as in the cases with \( \sigma=0.30 \). Transition to pseudo-turbulent flow is associated with significant vertical cross flow resulting in intense vorticities along the surface of the cylinders near the top and bottom in addition to the left and right boundaries. It should be noted that the increased fluid volume for \( \sigma=0.50 \) results in a wider “tail”, as defined in Section 4.1.4.2. The flow fields, vertical flows, and the “tail” behavior will be further analyzed in the sections that follow.

Like for \( \sigma=0.30 \), FFTs of probe data for flows through a square array of cylin-
Figure 4.31: Instantaneous $z$-vorticity fields for flow through a square array of cylinders with $\sigma=0.50$ and at various $Re_p$'s: (a) 137.48 (steady), (b) 369.98 (periodic), (c) 399.30 (periodic), (d) 429.54 (periodic), (e) 769.12 (transitional/intermittent), (f) 3139.96 (pseudo-turbulent), (g) 4345.62 (pseudo-turbulent), (h) 6279.77 (pseudo-turbulent), (i) 9915.60 (pseudo-turbulent).
ders with $\sigma=0.50$ at various Reynolds numbers are obtained and analyzed. As we shall see, a main frequency corresponding to the “tail” resonance with flow pass-through, similar to that observed for $\sigma=0.30$, is again identified for periodic flows.

The probe locations are shown in Figure 4.32. Note the relative locations of the probes are the same as those for $\sigma=0.30$, e.g. probe 1 is at $d_{\text{probe}}/L=0.25$, with $d_{\text{probe}}$ being the distance of the probe to $x_{\text{min}}$. Figure 4.33 shows the $v$-velocity time histories and the corresponding power spectra at probe 1 at increasing $Re_p$.

As seen from the dashed black line in Figure 4.33, for $Re_p$ of 137.48 and below, the flow remains steady after an initial transient period. As $Re_p$ is increased to values between 369.98 and 429.54, the $v$-velocity exhibits an initial transient phase followed by periodic oscillations. The time required to attain a periodic behavior decreases with $Re_p$, as more clearly seen in Figure 4.33(a) for $Re_p$ of 369.98 to 429.54, and this behavior is consistent with the results for $\sigma=0.30$ and Agnaou et al. [3]. As seen from the FFTs in Figure 4.33(d), at $Re_p=369.98$, the periodic signal has a single frequency in the spectrum, while at $Re_p=399.30$, higher and lower frequencies start to appear. Furthermore, as seen from Figure 4.33(c), the periodic oscillation initially consists of a single mode and later transitions to multiple mode periodic oscillations. In particular, for $t^*<\sim500$, the FFT of the $v$-velocity signal displays a single frequency/mode at $f^*$ of 0.705 (not shown) while for $t^*>\sim700$ the signal is composed of the superposition of multiple modes as seen from the blue line in Figure 4.33(d), i.e., the FFT has three distinguishable frequencies with significant power. The main frequency $f^*$ is 0.709. As shown in the next section, this main frequency is again associated with the resonance of the “tail” with the flow pass-through, like for $\sigma=0.30$.

As $Re_p$ is further increased to 769.12, the velocity probe signal indicates the
flow is now transitional with significant fluctuations, caused by the onset of apparent vortex shedding shown in Figure 4.31. The flow remains unsteady for higher $Re_p$’s which is more intuitive and normal compared to the peculiar and unusual mixed steady-unsteady behavior previously discussed for $\sigma=0.30$. The signal is now characterized by more distributed power and a shift of the dominant frequencies to lower frequencies. This is presumably due to the variety of motions in the pseudo-turbulent flow regime including vortex shedding, increasing advection of the vortices by the vertical flow and “tail” tilting.

Figure 4.32: Locations of the probes for flow through a square array of cylinders with $\sigma=0.50$.

4.1.5.2 Intermittent Change in the Direction of “Tail” Tilting

In this section, we will demonstrate the intermittent change in the direction of the titling of the “tail” observed for flow through a square array of cylinders with $\sigma=0.50$; this pack configuration has a relatively large fluid domain between its constituent particles. As this behavior was not observed for the cases and flow fields for $\sigma=0.30$ currently explored, it seems to be associated with the larger fluid domain afforded by larger porosities.
Figure 4.33: (a,b,c) The time histories of $v$-velocity and (d) the corresponding power spectra at probe 1 at various $Re_p$‘s: 137.48 (Black-dashed, steady); 369.98 (Green, periodic); 399.30 (Blue, periodic); 429.54 (Red, periodic); 769.12 (Magenta, transitional/intermittent); 1271.80 (Cyan, pseudo-turbulent); 3139.96 (Black, pseudo-turbulent). (c) Close up view of the transition between the two periodic behaviors at $Re_p=399.30$. $t^*$ is given by (4.6); $A^*=A/A_{max}$; $f^*=1/t^*$.

We first, however, demonstrate the main frequency of 0.709 obtained in the section above, shown in Figure 4.33(d), is again the result of the resonance of the “tail” with the flow pass-through. To this end, Figure 4.34 shows the periodic $z$-vorticity, $\omega_z$, oscillation at probe 1 with selected instances labeled $t^*_i$, for which the corresponding flow fields and close up views (about probe 1) are plotted in Figure 4.35 for $Re_p=399.30$. The dominant high frequency identified by the power
spectrum for \( v \)-velocity corresponds to the periodic oscillation about the \( y=0.0 \) line seen from the probe data in Figure 4.34 and the close up views of the flow fields in Figures 4.35(f) to 4.35(h). The period of \( \sim t_1^* - t_5^* = 1.420 \) of the oscillation inferred from these figures is consistent with the period of \( t^* = 1/f^* = 1.411 \), corresponding to \( f^* = 0.709 \), identified by the FFT shown in Figure 4.33(d). This period is close to the flow pass-through time \( t_p^* = 1.2533 \). Therefore, the high frequency oscillation seems again to be the result of the resonance of the “tail” motion with the flow pass-through and is consistent with the result for \( \sigma = 0.30 \).

We now demonstrate the intermittent change in the direction of the titling of the “tail” in the transitional and pseudo-turbulent flow regimes. Figure 4.36 shows the unsteady \( z \)-vorticity time histories at probe 1, with selected instances labeled \( t_i^* \), and at probes 2 to 4, for \( Re_p = 769.12 \) in the transitional flow regime. This intermittent behavior is best understood by relating the labeled time instances in the \( z \)-vorticity time history of probe 1 to their corresponding flow fields in

Figure 4.34: Evolution of \( z \)-vorticity \( \omega_z \) at probe 1 for flow through a square array of cylinders with \( \sigma = 0.50 \) at \( Re_p = 399.30 \). (b) Close up view with time instances labeled. The time instances labeled correspond to the flow fields shown in Figure 4.35.
Figure 4.35: Instantaneous $z$-vorticity fields at different instances of the “tail” resonant oscillation for flow through a square array of cylinders with $\sigma=0.50$ at $Re_p=399.307$ (periodic). Black dot shows probe 1. (a,f): $t^*_1 \simeq 1687.45$; (b): $t^*_2 \simeq 1687.60$; (c,g): $t^*_3 \simeq 1688.02$; (d,h): $t^*_4 \simeq 1688.44$; (e): $t^*_5 \simeq 1688.87$.

Figure 4.37. As seen from Figure 4.37(a) at $t^*_1 \simeq 1348.0$, the “tail” tilts downwards induced by the downward cross flow shown by the streamlines. At $t^*_2 \simeq 1351.8$, the “tail” starts to rise. This rising continues for $t^*_3$ to $t^*_5$ and is accompanied by the
weakening of the downward cross flow and the onset of an upward cross flow. The vertical flow also induces an upward tilting of the “tail”, which starts at $t^*_6$ as shown by the streamlines in Figure 4.37(f). The upward cross flow and tilting of the “tail” are fully achieved by $t^*_8$ as seen in Figures 4.37(g) and 4.37(h). Note advection of the vortices in the vertical direction is also induced by the vertical cross flow. The upward cross flow and tilting of the “tail” then remain for the rest of the probe signal, up to $t^*$ of 2500, examined. The sign/value of the mean $z$-vorticity recorded by the probe also changes accordingly with the changes in the direction of the cross flow and tilting of the “tail”.

We now comment that as seen from the time histories of $z$-vorticity at probes 1 to 4, the intermittent behavior of the transitional flow at $Re_p=769.12$ for $\sigma=0.50$ is different from those for $\sigma=0.30$ at $Re_p=267.57$, shown in Figure 4.13. For $\sigma=0.50$, the intermittent behavior is primarily restricted to the time range of $t^* \approx 1348.0$ to 1560 and is associated with the intermittent change in the direction of the tilting of the “tail”, discussed above, whereas for $\sigma=0.30$, the intermittent behavior is due to the limitation of space of the “tail” motion and flapping shown in Figure 4.14. Also, for $\sigma=0.50$, the intermittency occurs during essentially the same time period among the different probes, indicating it is the result of the same large scale global motions discussed above for Figure 4.37.

For pseudo-turbulent flow at $Re_p=3139.96$, as highlighted by the sectional averaging shown by the dashed white lines in Figure 4.38, the intermittent behavior observed for transitional flow at $Re_p=769.12$ is also present. Moreover, at higher $Re_p$’s the intermittency becomes more frequent. Similar to the behavior observed for $Re_p$ of 769.12 and for flow through a rectangular array of ellipses with $\sigma=0.40$ at $Re_p=1015.3$ (discussed later in Section 4.4.2), the intermittent $z$-vorticity signal
Figure 4.36: Evolutions of $z$-vorticity $\omega_z$ at probe (a) 1, (c) 2, (d) 3, and (e) 4 for flow through a square array of cylinders with $\sigma=0.50$ at $Re_p=769.12$. (b) Close up view of (a) with time instances labeled. The time instances labeled correspond to the flow fields shown in Figure 4.37.

at probe 1 is the result of the intermittent change in the direction of the tilting of the “tail”. Here, as seen from Figure 4.39(a), at $t^*_1\approx208.11$, the cross flow and the tilting of the “tail” are downwards while at $t^*_2\approx416.23$ the “tail” tilts upwards as seen in Figure 4.39(b). The sign of the mean vorticity recorded by probe 1 also changes accordingly, positive at $t^*_1$ and negative at $t^*_2$ as seen in Figure 4.39.

Finally, we comment that turbulent flow statistics need to be collected with care due to the intermittency shown above. In the current work, the statistics are collected without distinction of the up- or downward tilting period. More meaningful turbulent flow statistics may be collected for individual up- or downwards
Figure 4.37: Instantaneous \( z \)-vorticity fields at different “tail” tilting phase and the attendant re-circulation, (a) \( t^*_1 \approx 1348.0 \), (b) \( t^*_2 \approx 1351.8 \), (c) \( t^*_3 \approx 1359.4 \), (d) \( t^*_4 \approx 1363.2 \), (e) \( t^*_5 \approx 1367.0 \), (f) \( t^*_6 \approx 1370.8 \), (g) \( t^*_7 \approx 1384.6 \), and (h) \( t^*_8 \approx 1378.4 \) for flow through a square array of cylinders with \( \sigma = 0.50 \) at \( Re_p = 769.12 \) (transitional/intermittent). Black dot shows probe 1. Green lines with arrows: streamlines.
tilting periods yet this may not be practical or necessary when the intermittency is relatively frequent. We do show the effect of this distinction on the mean flow fields in Section 4.1.5.4 for $Re_p$ of 769.12, where up- or downward tilting periods are distinct and can be identified.

Figure 4.38: (a) Evolution of $z$-vorticity $\omega_z$ at probe 1 for flow through a square array of cylinders with $\sigma=0.50$ at $Re_p=3139.96$. (b,c) Close up views with time instances labeled. The time instances labeled correspond to the flow fields shown in Figure 4.39. Dashed white line: sectional averaging.
Figure 4.39: Instantaneous $z$-vorticity fields at different “tail” tilting phase and the attendant re-circulation, at (a) $t^*_1\simeq208.11$, and (b) $t^*_2\simeq416.23$ for flow through a square array of cylinders with $\sigma=0.50$ at $Re_p=3139.96$ (pseudo-turbulent). Black dot shows probe 1. Grey lines with arrows: streamlines.

4.1.5.3 Probability Density Function

As shown earlier with Figure 4.33, the behavior of the onset of unsteady flow and then transition to pseudo-turbulent flow as the Reynolds number increases for a square array of cylinders with $\sigma=0.50$ is quite normal compared to that for the peculiar case for a square array of cylinders with $\sigma=0.30$. The onset of unsteady flow also seems to be standard as a similar behavior was observed by Agnaou et al. [3] for square cylinders, which is different in geometry compared to the current work. In both works, the onset of unsteady flow is associated with the excitation of increasingly more modes of different amplitudes in the periodic evolution of flow variables, such as $v$-velocity shown in Figure 4.33 for $Re_p$ of 369.98 to 429.54. The corresponding variation of the PDFs of vorticity magnitude evolution as the Reynolds number increases is examined in this section for $\sigma=0.50$.

As shown in Figure 4.40, the PDFs of vorticity magnitude are plotted for
different values of $Re_p$'s; recall Figure 4.31 for the corresponding instantaneous flow fields and Figure 4.33 for the temporal behavior of the probe signals. We first note that for steady flow at $Re_p=137.48$, the PDF is a delta function. At $Re_p$ of 346.27, even though the flow is periodic, the PDF shown in Figure 4.40(b) does not resemble that for a single mode/frequency periodic signal where the range of vorticity magnitude in the PDF is bounded by the two spikes at the value of the peak and valley in the evolution as seen, for example, in Figures 4.10 and 4.15(b) for $|\omega|$. To understand the difference, we show in Figure 4.41 the actual signal and the FFT of it. It is seen that there are multiple modes identified by the FFT. The effect of these multiple modes on the PDF is the deviation from the PDF for a single mode periodic evolution. The non-zero probability density to the left of the spike at $|\omega|\approx 25.32$ in the PDF is due to the extension of the range of $|\omega|$ towards lower values for some modes in the evolution, as seen in Figure 4.41(a). This behavior is also present for periodic flow at $Re_p=369.98$, as seen in Figure 4.40(c). Note this behavior has not been observed for $\sigma=0.30$ within the data range examined in Section 4.1.4.3. Thus, this seems to be the result of the increased fluid volume and the associated wider “tail” and more diffused $tail_{mid}$ region for larger porosities as seen by comparing Figures 4.31(b) and 4.7(b). The more space afforded by larger porosities allows for the excitation of more modes in the flow.

For $Re_p=399.30$, even though the flow is still periodic, the PDF shown in Figure 4.40(d) is seen to start to deviate from those for $Re_p=346.27$ and 369.98. Despite the traces of spikes at, for example, $|\omega|\approx 35.67$ and 48.77, increases in probability at other values cause the profile of the PDF to approach that of transitional flow at $Re_p$ of 769.12, shown in Figure 4.40(f). The signal for the vorticity magnitude itself for $Re_p=399.30$ was shown in Figure 4.34 and it is seen that the
signal becomes increasingly random compared to that for $Re_p=346.27$, indicating the approaching of transition Reynolds number as indeed seen for $Re_p$ of 769.12 shown in Figure 4.40(f). At $Re_p=429.54$, shown in Figure 4.40(e), the trend of approaching transition Reynolds number with less discernible individual spikes in the PDF profile continues. We also note that the increase in the vorticity magnitude range with increasing $Re_p$ is also observed in the laminar and transitional flow regimes discussed so far and indicates the increasing strength of the standing vortices with Reynolds number. This is similar to the results for $\sigma=0.30$.

At $Re_p$ of 769.12, transition to pseudo-turbulent flow starts to occur. Transition, seen earlier in Figure 4.31(e), is associated with the onset of vortex shedding/advection and with significant vertical cross flow, shown in Figure 4.37 and discussed in more detail later in Section 4.1.5.4. The PDF shows there is a significant increase in the vorticity magnitude range compared to the laminar flow regime. This is in part due to the stronger vortices at higher Reynolds numbers and in part the result of the vertical flow shown in Figure 4.37. These motions expose probe 1 to both different parts of the “tail” and to the advected vortices. As a result, the PDF starts to look similar to those at pseudo-turbulent flow for higher $Re_p$'s, shown next in Figures 4.40(g)-4.40(j).

The PDFs for pseudo-turbulent flow shown in Figures 4.40(g)-4.40(j) are in fact Gaussian distributions. As seen in Figures 4.31(f)-4.31(i), the vortices become smaller and stronger in pseudo-turbulent flow than in transitional flow, and there are many vortices in pseudo-turbulent flow. The vertical cross flow is also stronger. As a result of the exposure to the strong sweeping of the “tail” and the many strong vortices shed from the surface, advected from upstream or vertically by the vertical flow, the Gaussian distributions of the PDFs for pseudo-turbulent flow
indicate a complete randomness. To appreciate this randomness, the signal for the 
z-vorticity itself was shown in Figure 4.38 for $Re_p$ of 3139.96. The similarity of the 
PDFs for pseudo-turbulent flow at different Reynolds numbers is demonstrated in 
Figure 4.40(k) and they are all shown to be Gaussian distribution. In addition, it is 
interesting to note that the ranges of vorticity magnitude in 2-D pseudo-turbulent 
flow are also essentially identical for different Reynolds numbers, as may also be 
appreciated from the flow field plots in Figures 4.31(f)-4.31(i). The ranges of length 
scales of the vortices are also similar, as will be discussed in more detail later in 
Section 4.1.5.5. This is different from 3-D turbulent flow where the length scales 
of the smallest eddies are expected to decrease with Reynolds number.

We next examine the PDFs at other locations in the flow to analyze their 
spatial dependence. The probe locations were shown in Figure 4.32. Probe 1 and 
probe 3 are located along the $y=0.0$ line while probe 2 and probe 4 are symmetric 
about the $y=0.0$ line. Therefore, the PDFs are expected to be qualitatively similar 
between probes 1 and 3, and between probes 2 and 4. The qualitative similarity 
can be seen by comparing Figure 4.40(b) for probe 1 and Figure 4.42(b) for probe 
3 for periodic flow at $Re_p$ of 346.27. Also, the similar PDFs for probe 2 and probe 
4 are shown in Figures 4.42(a) and 4.42(c), respectively. When comparing the 
PDFs of, for example, probe 1 and probe 2 we find that unlike probe 1 which 
records a signal composed of multiple significant modes, as discussed above, the 
PDF for probe 2 implies a single mode periodic signal as shown to be indeed 
the case in Figure 4.42(a). This difference is due to the difference in the relative 
locations of the probes with respect to the “tail”. While probes 1 and 3 are located 
in, approximately, the $tail_{mid}$ region, probes 2 and 4 are at the edge of $tail_{down}$ 
and $tail_{up}$, respectively, subjecting them to an intense, yet, single mode vorticity
Figure 4.40: PDFs of vorticity magnitude $|\omega|$ at probe 1 for (a) $Re_p=137.48$ (steady), (b) 346.27 (periodic), (c) 369.98 (periodic), (d) 399.30 (periodic), (e) 429.54 (periodic), (f) 769.12 (transitional/intermittent), (g) 3139.96 (pseudo-turbulent), (h) 4345.62 (pseudo-turbulent), (i) 6279.77 (pseudo-turbulent), and (j) 9915.60 (pseudo-turbulent) for a square array of cylinders with $\sigma=0.50$. Red dashed line: Gaussian curve fit. (k) Normalized PDF (by maximum PDF) for various pseudo-turbulent $Re_p$’s.
Figure 4.41: (a) Time history and (b) FFT of vorticity magnitude $|\omega|$ at probe 1 for $Re_p = 346.27$ (periodic) for a square array of cylinders with $\sigma = 0.50$.

oscillation, as seen from the $z$-vorticity field plots in Figures 4.31(b)-4.31(d).

On the other hand, for pseudo-turbulent flow in Figures 4.42(d) to 4.42(f), along with Figure 4.40(g), the PDFs of vorticity magnitude at probes 1 to 4 are all Gaussian distributions even though probes 2 and 4 experience a wider range of strength of vortices than probes 1 and 3. Therefore, the PDFs show less dependence on location than at laminar flow, discussed above. This can again be understood by examining the turbulent flow features shown in Figure 4.31. As discussed earlier, the full randomness induced by advection of vortices and change in direction of the “tail” tilting makes the PDFs Gaussian and removes the dependence of the shape of the PDFs on the probes’ locations.

4.1.5.4 Pseudo-Turbulent Flow Fields and Vorticity Transport

The discussion of vorticity budgets in Section 4.1.4.4 for $\sigma = 0.30$ was mainly for laminar flow. Here in this section, to better and further characterize the behavior of transition and pseudo-turbulent flows, we expand that discussion by focusing on transition and pseudo-turbulence for $\sigma = 0.50$.

We begin by first noting that the distributions of various terms in (4.10) along
the vertical slice in the laminar flow regime have similar general characteristics to those for $\sigma=0.30$ discussed in Section 4.1.4.4 and shown in Figures 4.17(a) and 4.20. The only difference is the more diffused and wider “tail” because of the larger porosity as shown in Figure 4.43. Thus, we will not repeat that discussion here.

We, however, show in Figure 4.44 that as the flow transitions to pseudo-turbulent flow, the turbulent terms such as the turbulent vorticity diffusion ($\partial(u'\omega')/\partial x$ and $\partial(v'\omega')/\partial x$) become significant as can be seen by comparing their profiles for laminar periodic flow at $Re_p=346.27$, shown in Figure 4.44(a), and pseudo-turbulent flow at $Re_p=3139.96$, shown in Figure 4.44(c). Note as discussed in Section 4.1.4.4 for $\sigma=0.30$, the appreciable $\partial(v'\omega')/\partial x$ term in the laminar flow regime is due to the periodic oscillation of the $v$-velocity induced by the “tail” oscillation. There are essentially no oscillations in $u$-velocity leading to an essentially zero $\partial(u'\omega')/\partial x$
Figure 4.43: The time averaged $z$-vorticity $\omega_z$ field for flow through a square array of cylinders with $\sigma=0.50$ and $Re_p=346.27$.

term seen in Figure 4.44(a). Once transition to pseudo-turbulence starts to occur, pseudo-turbulent flow fluctuations in both $u$ and $v$-velocity lead to significant increases of the $\partial (u'\omega')/\partial x$ and $\partial (v'\omega')/\partial x$ terms. This is accompanied by the decrease in the viscous vorticity diffusion ($\nu \nabla^2 \omega$) as seen by comparing Figures 4.44(a) and 4.44(b). As seen in Figure 4.45(a) below, in the pseudo-turbulent flow regime, the “tail” is not as extended in the $x$-direction as in the laminar flow regime, shown in Figure 4.43. Thus, the gradient of mean vorticity along the slice at $x_{mid}$ becomes much smaller in the pseudo-turbulent flow regime, resulting in the decrease in the viscous vorticity diffusion.

In the fully pseudo-turbulent flow regime, we choose the flow at $Re_p$ of 4345.62 for the discussion of the general characteristics. As such, Figure 4.45 first shows the time averaged flow fields. It can be seen in Figure 4.45(a) that the $tail_{up}$ and $tail_{down}$ regions defined in Section 4.1.4.2 are quite thin and close to the wall due to the higher Reynolds number. The time averaged “tail” tilts, slightly, down as can be seen in Figure 4.45(b), and this is caused by the downward mean flow at
Figure 4.44: Terms in the time averaged vorticity equation (4.10) for flow through a square array of cylinders with $\sigma = 0.50$ at $Re_p = 346.27$ (a, periodic), 769.12 (b, transitional/intermittent), and 3139.96 (c, pseudo-turbulent). The terms are $\nu \nabla^2 \omega$ (red), $u \partial \omega / \partial x$ (black), $v \partial \omega / \partial y$ (blue), $\partial (\overline{u' \omega'}) / \partial x$ (green), and $\partial (\overline{v' \omega'}) / \partial y$ (magenta).
Figure 4.45: Time averaged (a) $z$-vorticity, (b) $u$-velocity, and (c) $v$-velocity fields for flow through a square array of cylinders with $\sigma=0.50$ at $Re_p$ of 4345.62. White lines with arrows: streamlines.
both the top and bottom boundaries shown in Figure 4.45(c) and by the mean streamlines.

We next examine vorticity transport in the flow. Figure 4.46 shows the time averaged flow fields for the viscous ($\partial \omega / \partial y$) and turbulent ($\overline{v' \omega'}$ and $\overline{u' \omega'}$) vorticity flux terms in (4.10) along with the $rms$ of $v$-velocity. Vertical slices at successive streamwise locations are extracted and shown in Figure 4.47. Even though the current simulation is 2-D, it is remarkable that the distribution of vorticity fluxes at $x_{min}$ and $0.10D$ downstream (with $D$ being the diameter of the particle), shown in Figures 4.47(a) and 4.47(b), are similar to those for a turbulent channel flow [81]. In particular, the viscous vorticity flux $\partial \omega / \partial y$ increases then decreases with the distance from the wall (see also Figure 4.46(a)). There is a countergradient in the turbulent flux $\overline{v' \omega'}$ near the wall (see also Figure 4.46(b)), making a turbulent diffusivity model untenable [81]; for $\overline{u' \omega'}$, there is also a countergradient near the wall but the trend is opposite to that of $\overline{v' \omega'}$ (see also Figure 4.46(c)). The similarity is expected because of the nearly parallel surfaces of the top and bottom particle close to $x_{min}$. Further downstream at $\sim 0.15D$ from $x_{min}$, flow separation and vortex shedding occurs, as may be seen from Figure 4.31(g). The flow separation manifests itself in the time averaged $\partial \omega / \partial y$ field as the point where $\partial \omega / \partial y$ changes sign from positive to negative at $\sim x_{min}+0.15D$ along the surface of the particle as seen in Figure 4.46(a). As such, the viscous vorticity flux distribution deviates from the channel flow-like profile as seen in Figure 4.47(c). The turbulent fluxes still resemble those for a channel flow since the turbulent eddy motions are expected to be similar, relatively unaffected by flow separation. Finally, moving away from the region between the particles and to the vertical slice at $x_{mid}$, the turbulent characteristics are no longer similar to those of a turbulent channel flow.
and become significantly different. The turbulent flux due to \( v \)-velocity fluctuations dominates near the top and bottom boundaries as seen in both the field plots in Figures 4.46(a)-4.46(c) and the slice plot Figure 4.47(d). This dominance is caused by the significant \( v \)-velocity fluctuations shown in Figure 4.46(d) by the \( \text{rms} \) of \( v \)-velocity. These high fluctuations are induced by the vertical flow present in pseudo-turbulent flow, shown previously in Figure 4.45(c), and it is worthwhile to point out that the fluctuations are a factor of 2-3 times larger than the mean. Note also that the “tail” is the main contributor to the viscous vorticity flux \( \partial \vec{\omega} / \partial y \), yet as noted earlier it is not as extended in the \( x \)-direction as in the laminar case. Therefore, the viscous vorticity flux is quite small around the \( x_{\text{mid}} \) slice as seen in Figure 4.46(a) and Figure 4.47(d).

The profiles of vorticity transport for laminar and pseudo-turbulent flow are next compared in Figure 4.48 to show the effect of transition. A clear trend of the shifting of dominance from viscous to turbulent vorticity flux is demonstrated as the \( R_{\text{ep}} \) is increased from 346.27 for laminar periodic flow to 769.12 for transitional flow to 4345.62 for pseudo-turbulent flow. Again, the main contribution to the viscous vorticity flux \( \partial \vec{\omega} / \partial y \) in laminar flow shown in Figure 4.48(a) is from the “tail”, seen in Figure 4.43, whereas the turbulent flux is the result of pseudo-turbulent fluctuations, shown in Figure 4.46(d).

To further demonstrate the effect of transition on flow characteristics, we next show time averaged velocity fields at Reynolds numbers from laminar to pseudo-turbulent flow regime. Figure 4.49(a) shows that in the laminar flow regime, the “tail” is bounded by two standing vortices at the top and bottom, with no mean vertical flow like in the pseudo-turbulent flow regime shown in Figure 4.45(c) for \( R_{\text{ep}}=4345.62 \). As touched on in Section 4.1.4.1 for \( \sigma=0.30 \), this mean vertical flow
Figure 4.46: Time averaged (a) $\frac{\partial \omega}{\partial y}$, (b) $\overline{v' \omega'}$, (c) $\overline{u' \omega'}$, and (d) $v_{rms}$ fields for flow through a square array of cylinders at $Re_p=4345.62$. 

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Figure 4.47: Vorticity fluxes along slices at (a) $x_{\min}$, (b) $x_{\min}+0.10D$, (c) $x_{\min}+0.25D$, and (d) $x_{mid}$ for a square array of cylinders with $\sigma=0.50$ at $Re_p=4345.62$. The terms are $\partial \omega / \partial y$ (red), $\overline{u' \omega'}$ (blue), and $\overline{v' \omega'}$ (green).
starts to emerge at transitional Reynolds numbers. This is also true for $\sigma=0.50$ as seen in Figure 4.49(b) for the transitional $Re_p$ of 769.12. This mean vertical flow causes the tilting of the time averaged “tail” as illustrated for $Re_p=4345.62$ with Figure 4.45. Interestingly, this tilting is not always in a fixed direction and can be different for different $Re_p$'s, or more interestingly, different during different periods of time. For example, Figure 4.50 shows the variation of the direction, i.e., up or down determined by the sign of the mean $v$-velocity, of the mean vertical flow with Reynolds number. It can be seen that at $Re_p=6279.77$, the mean vertical flow is in the upward direction while it is downwards for the other pseudo-turbulent $Re_p$'s. The time averaged flow fields are plotted in Figure 4.51 for comparison with the flow fields for other Reynolds numbers shown earlier and to show the slight upward tilting of the “tail” caused by the upward mean flow. As also mentioned above, the tilting of the time averaged “tail” can also be different during different periods of time. As discussed for transitional $Re_p$ of 769.12 in Figure 4.36, the
Figure 4.49: Time averaged $v$-velocity fields for flow through a square array of cylinders with $\sigma=0.50$ at $Re_p$ of (a) 346.27 and (b) 769.12. White lines with arrows: streamlines.

“tail” has intermittent changes in the direction of the tilting with a downwards and upwards tilting during the positive and negative periods, respectively. As a result, if the time averaged flow field is obtained for the negative period between $t^*$ of $\sim1367.00$ and $\sim1518.90$, we obtain Figure 4.52 where the vertical flow is now upwards as opposed to downwards in Figure 4.49(b) obtained with the positive period. Due to this intermittent change in the direction of “tail” tilting, time averaging needs to be done in a careful fashion. It seems that the intermittency is more frequent in the fully pseudo-turbulent flow regime as shown in Figure 4.38, so time averaging without the distinction of positive and negative periods is expected to be nominally sensible and this is what we do for the fully pseudo-turbulent flow regime. For the transitional flow regime, the distinction between positive and negative periods becomes more necessary.
Figure 4.50: Time averaged $v$-velocity profiles along a vertical slice at $x_{mid}$ at various $Re_p$’s. $Re_p = 346.27$ (green), 769.12 (red), 3139.96 (cyan), 4345.62 (blue), 6279.77 (black), and 9915.60 (brown).

Figure 4.51: Time averaged (a) $u$-velocity and (b) $v$-velocity fields for flow through a square array of cylinders with $\sigma=0.50$ at $Re_p$ of 6279.77. White lines with arrows: streamlines.
4.1.5.5 Effect of Reynolds Number on Length Scales of Spatial Structures

We next examine the effect of Reynolds number on the length scales of the spatial structures. Again, we will focus on the discussion of pseudo-turbulent flows like in the previous section, and the discussion on turbulent characteristics there facilitates the analysis in this section. Figure 4.53 shows the instantaneous $z$-vorticity profiles along the vertical slice at $x_{mid}$ and the FFTs of the profiles at different $Re_p$'s for periodic and transitional flows while Figure 4.54 is for fully pseudo-turbulent flows. For periodic flow at $Re_p=346.27$, the $z$-vorticity profile is characterized by essentially symmetric $|\omega_z|$ peaks close to $y=0.0$ with a gradual decrease for increasing $|y|$ as seen from Figure 4.53(a). As seen from Figures 4.31(b) to 4.31(d) for the laminar periodic flow regime, these symmetric peaks correspond to the tail$_{down}$ and tail$_{up}$ that stem from the surface of the particles centered at $x_{min}$. The power spectrum is smooth with a gradual decrease in amplitude for $k>k_{max}$.
being the wavenumber corresponding to the maximum power and equal to 1.63 here. This wavenumber corresponds to approximately the width of \( \sim 0.614 \) of the symmetric \( \omega_z \) profile. This width is also close to the width of the “tail” that is identified by the FFT. Since the widths of the “tail”s are almost identical for all the periodic flows considered here, as seen in Figure 4.31 and Figure 4.53(a), \( k_{max} \) is the same. As the \( Re_p \) is increased to 429.54, the \( z \)-vorticity profile has a wider range of length scales as seen from the power spectrum where there is increasingly larger power for \( k>10 \).

For transitional flow at \( Re_p=769.12 \), the \( z \)-vorticity profile starts to have a wider range of length scales than for the laminar periodic cases. There are also increasingly larger powers at higher wavenumbers as can be seen by comparing Figures 4.53(b) and 4.53(d). The increasing power at larger wavenumbers, or small length scales, with increasing Reynolds number becomes apparent with the FFT for \( Re_p=3139.96 \). The increase in the number of vortices and structures with smaller length scales can also be appreciated from the \( z \)-vorticity fields shown in Figure 4.31. The increasing power at larger wavenumbers is accompanied by the increase in the range of the strength of the vortices discussed with the PDFs of vorticity evolution in the previous section.

In the fully pseudo-turbulent flow regime, analogous to the similarity in PDFs of the probe signals discussed in Section 4.1.5.3, the FFTs at different Reynolds numbers are also remarkably similar as seen in Figure 4.54. The dominant length scale identified by \( k_{max} \) of \( \sim 5 \) is \( \sim 0.2 \), consistent with the similar sizes of the vortices seen in Figures 4.31(g)-4.31(i) for the fully pseudo-turbulent flow regime. The strengths of the vortices are also similar as indicated by the similar PDFs of the probe signals discussed in Section 4.1.5.3. Again, these are specific to 2-D
Figure 4.53: Instantaneous $z$-vorticity profiles (left column) along a vertical slice at $x_{mid}$ and their power spectra (right column) for square arrays of cylinders with $\sigma=0.50$ at various $Re_p$'s. $Re_p=346.27$ (row 1; black solid line); $Re_p=429.54$ (row 1; red dashed line); $Re_p=769.12$ (row 2); $Re_p=3139.96$ (row 3).
pseudo-turbulence.

Correlation flow fields and energy spectra are examined next. Figure 4.55 shows the two-point double correlation $R_{11}$ and $R_{22}$ fields defined by (4.11) for a point located at the center $x_0=(x_{mid}, y_{mid})$ of the domain. For $Re_p=346.27$ (periodic), the flow features are dominated by standing vortices as seen in Figure 4.49(a) and the “tail” resonant oscillations discussed in Section 4.1.5.1. As a result, the flow is dominated by fluctuations in the vertical direction in the middle of the domain and near the end of the “tail” yet the fluctuations in $u$-velocity in the middle of the domain are quite small as seen in Figure 4.56. This directional difference in fluctuations leads to the very different $R_{11}$ and $R_{22}$ fields as seen by comparing Figures 4.55(a) and 4.55(e). In particular, $R_{11}$ looks essentially featureless yet $R_{22}$ shows the footprint of the “tail” and its oscillations in the vertical direction.

For transitional/pseudo-turbulent flows at $Re_p=769.12$ and 3139.96, due to the significant vertical cross flow that starts to emerge, strong correlations emerge near the top and bottom boundaries especially for $R_{22}$ as seen in Figures 4.55(g) and 4.55(h). Due to the vertical cross flow, the region with significant vorticity activities is widened at transitional and pseudo-turbulent Reynolds numbers, where the “tail” starts to flap as illustrated with Figure 4.14. This widening continues with increasing $Re_p$ as seen by comparing Figures 4.55(c) and 4.55(d). Unlike for the periodic flow discussed above, $R_{11}$ now becomes much more organized with recognizable features similar to $R_{22}$. This is the result of the fact that the flows in the transitional and pseudo-turbulent flow regimes are characterized by vortex shedding and advection with less directional difference. Note the appreciable asymmetric $R_{11}$ and $R_{22}$ fields for $Re_p=769.12$ and 3139.96, especially for the former, are the result of the downward tilting of the “tail”, as discussed previously.
Figure 4.54: Instantaneous $z$-vorticity profiles (left column) along a vertical slice at $x_{mid}$ and their power spectra (right column) for square arrays of cylinders with $\sigma=0.50$ at various $Re_p$'s. $Re_p=4345.62$ (row 1); $Re_p=6279.77$ (row 2); $Re_p=9915.60$ (row 3).
We next examine the energy spectra extracted from these correlation flow fields. As seen in Figure 4.55, the energy spectra $E_{11}(k_2)$ and $E_{22}(k_2)$ are qualitatively different for laminar periodic flow due to directional difference of the fluctuation discussed above which in turn leads to the different profiles of $R_{11}$ and $R_{22}$ along the vertical slice at $x_{\text{mid}}$. The $E_{11}(k_2)$ spectra have broader distributions than $E_{22}(k_2)$ due to the more random-looking profiles in $R_{11}$ along the vertical direction. The $E_{22}(k_2)$ spectra on the other hand are dominated by a single peak at $k_2 \approx 0.814$, which corresponds to a length scale $l_y = 1.229$ close to the domain width of 1.2533. This is consistent with the simple one wavelength profiles of $R_{22}$ along the vertical slice. At pseudo-turbulent $Re_p$ of 3139.96, due to the emergence of strong correlations at the vertical boundaries, $E_{22}(k_2)$ has a peak shift to $k_2 \approx 1.628$ with a length scale $l_y = 0.614$, half of those at lower $Re_p$'s, consistent with the two wavelengths seen in the vertical middle slice through the $R_{22}$ fields. The $E_{11}(k_2)$ spectra on the other hand start to look qualitatively more like $E_{22}(k_2)$ due to the more organized $R_{11}$ fields discussed above. Note that $E_{22}(k_1)$ is expected to be qualitatively similar to $E_{11}(k_2)$ as well due to the directional similarity as seen by comparing Figure 4.55(l) and Figure 4.57.

For fully pseudo-turbulent flow, similarity was observed for the PDFs of the probe signals discussed in Section 4.1.5.3 and the FFTs of the instantaneous z-vorticity slices previously discussed. Figure 4.58 shows that the similarity in vorticity strengths and sizes in 2-D pseudo-turbulence also leads to almost identical two-point correlations and energy spectra at different Reynolds numbers. The similarity can be best demonstrated by Figure 4.59 which shows the comparison of the energy spectra at different Reynolds numbers in the same plot. The spec-
Figure 4.55: $R_{11}(r, x_0)$ (a-d), $R_{22}(r, x_0)$ (e-h), $E_{11}(x_0, k_2)$ (i-l), and $E_{22}(x_0, k_2)$ (m-p) for a square array of cylinders with $\sigma=0.50$ at $Re=346.27$ (1st column), 429.54 (2nd column), 769.12 (3rd column), and 3139.96 (4th column). The two-point correlation ranges from maximum positive correlation (yellow) to maximum negative correlation (cyan) with zero correlation being white. $k$ in (i)-(p) is $k_2$; $k_2$ is the wavenumber defined as $1/y$. 
Figure 4.56: (a,c) Time averaged and (b,d) \( \text{rms} \) of (a,b) \( u \) and (c,d) \( v \)-velocity fields for flow through a square array of cylinders with \( \sigma=0.50 \) at \( Re_p=346.27 \).
Figure 4.57: $E_{22}(x_0, k_1)$ for a square array of cylinders with $\sigma=0.50$ at $Re_p=3139.96$. $k=k_1$ and is the wavenumber defined as $1/x$.

tra are remarkably similar and almost overlap, especially for $E_{11}(k_2)$. Note the slight differences in $R_{11}$ and $R_{22}$ at different Reynolds numbers are caused by the different directions of the tilting of the “tail” discussed in Section 4.1.5.4. As a result, there is an increased negative correlations towards $y_{min}$ in Figures 4.58(a) and 4.58(c). The “tail” tilts downwards for $Re_p=4345.62$ and $9915.60$, while the “tail” tilts upwards for $Re_p=6279.77$ as shown previously in Figures 4.50 and 4.51.

4.1.5.6 Effect of Particle Shape

In this section for $\sigma$ of 0.50, we finally examine the effect of particle shape on the temporal and spatial scales of transitional and pseudo-turbulent flows. Figure 4.60 shows the instantaneous $\tau$-vorticity fields for flow through a rectangular array of ellipses with $\sigma=0.50$. The smaller surface curvature of the ellipses and the smaller vertical distance between the particles result in the generation and subsequent shedding of stronger vortices than the cylinder counterpart. This may be appreciated by comparing Figure 4.60 and the PDFs in Figure 4.61 with their cylinder counterparts shown in Figures 4.31 and 4.40 for cases in the pseudo-turbulent flow.
regime. In particular, the maximum vorticity magnitude for the rectangular array of ellipses is \( \sim 1000 \) whereas it is \( \sim 500 \) in the square array of cylinders. As a result of the stronger vortices for the rectangular array of ellipses, the ranges of vorticity magnitude in the PDFs are also greater for ellipses. Note the transition of the PDFs from a non-Gaussian distribution at \( Re_p \) of 2629.31 to a Gaussian distribution at \( Re_p \) of 4263.67 indicates the transition to fully pseudo-turbulent flow at \( Re_p \) of 4263.67, similar to the behavior observed earlier for square arrays of cylinders in Section 4.1.5.3.

As seen from Figure 4.62 the particle shape also affects the spatial length scales. Despite a similar range in length scales as the cylinder case, flow through a rectangular array of ellipses at similar Reynolds numbers tends to have more smaller scale flow features as seen by comparing Figure 4.62(b) with 4.62(d) and Figure 4.62(f) with 4.62(h). For the ellipse case, there are appreciably more powers at \( k \sim 10 \) than the cylinder case, partly due to the smaller vertical domain size, resulting in the smaller and stronger vortices seen in Figure 4.60. In fact, there is a significant spike near \( k \approx 10 \) shown in Figures 4.62(d) and 4.62(h) for the ellipse case whereas the significant spikes are concentrated at \( k < 5 \) for the cylinder case.

We are now also at the position to make some further comments on transition. As discussed earlier for square arrays of cylinders, transition occurs when a strong vertical cross flow starts to emerge at transitional Reynolds numbers. This is also true for rectangular arrays of ellipses. Thus, this behavior seems to be general.

We also note that the higher critical Reynolds numbers of periodic arrays of ellipses compared to their cylinder counterpart seen in Figure 4.1 may be traced to the increased tendency of the “tail” remaining attached due to the smaller surface curvature.
Figure 4.58: \( R_{11}(r, x_0) \) (a-c), \( R_{22}(r, x_0) \) (d-f), \( E_{11}(x_0, k_2) \) (g-i), and \( E_{22}(x_0, k_2) \) (j-l) for a square array of cylinders with \( \sigma = 0.50 \) at \( Re_p = 4345.62 \) (1st column), 6279.77 (2nd column), and 9915.60 (3rd column). The two-point correlation ranges from maximum positive correlation (yellow) to maximum negative correlation (cyan) with zero correlation being white. \( k \) in (g)-(l) is \( k_2 \); \( k_2 \) is the wavenumber defined as \( 1/y \).
Figure 4.59: (a) $E_{11}(x_0, k_2)$ and (b) $E_{22}(x_0, k_2)$ for a square array of cylinders with $\sigma=0.50$ at $Re_p=3139.96$ (solid blue line), 4345.62 (black circle), 6279.77 (green diamond), and 9915.60 (red square). For $Re_p \geq 4345.62$ only peaks with amplitude greater than $A^* > 0.003$ are plotted. $k=k_2$ and is the wavenumber defined as $1/y$.

Figure 4.60: Instantaneous $z$-vorticity fields ($-750 \leq \omega_z \leq 750$) for flow through a rectangular array of ellipses at $Re_p$ of (a) 2629.31 and (b) 4263.67 with $\sigma=0.50$. Black dot shows probe 1.
Figure 4.61: PDFs of the vorticity magnitude for a rectangular array of ellipses at $Re_p$ of (a) 2629.31 and (b) 4263.67 with $\sigma=0.50$ at probe 1.
Figure 4.62: Instantaneous $z$-vorticity profiles (left column) along a (a,c) vertical slice at $x_{mid}$ and (e,g) horizontal slice at $y_{mid}$ and their power spectra (right column) for a periodic array of (a,b,e,f) cylinders at $Re_p=2082.22$ and (c,d,g,h) ellipses at $Re_p=2629.31$ with $\sigma=0.50$. $k$ is defined as $1/x$ in (f) and (h).

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4.2 Random Packs of Polydisperse Spheres

In this section we present the new results for the permeability and modified Forchheimer friction factor curve fits for periodic random packs of polydisperse spheres for a range of porosities and log-normal distributions. In recent years, a packing algorithm that can generate packs of polydisperse convex particles, such as spheres, cylinders, ellipsoids, and polyhedra has been developed by Jackson et al. [82, 83, 84, 85, 86, 87]. We use this packing code to generate random packs of polydisperse spheres for the present section. We consider three different log-normal distributions of \( N=5000 \) spheres: Narrow: \([75, 125] \ \mu m\); Medium: \([50, 150] \ \mu m\); Board: \([25, 175] \ \mu m\). We consider porosities of \( \sigma=0.40, 0.60, \) and \(0.70 \) (the corresponding packing fractions are \( \phi=0.60, 0.40, \) and \(0.30, \) respectively). In the non-dimensional results discussed below, the random packs are scaled such that the mean diameter \( \bar{D}=1 \). Figure 4.63 shows two representative packs and Figure 4.64 and Figure 4.65 show the steady \( u \)-velocity and pressure fields for 2-D slices for flow through a random pack of polydisperse spheres with \( \sigma=0.60 \) and a narrow distribution at \( Re_p=0.40 \) and \( 98.93 \).

4.2.1 Friction Factor

Figure 4.66 shows the numerical friction factors for \( O(10^{-4}) \leq Re_p \leq O(10^2) \) (flows in the creeping and inertial flow regimes) for random packs of polydisperse spheres. For the narrow particle size distribution with \( D_\sigma=0.11 \), the numerical friction factors follow the Ergun relation (3.7) in the creeping flow regime. The numerical friction factor \( f_D \) is seen to be dependent on the particle size distribution and shows a slight dependence on \( \sigma \) for all \( Re_p \)'s considered. As seen from the close up view...
Figure 4.63: Plots of 3-D random packs of polydisperse spheres with porosity $\sigma=0.40$ for (a) narrow distribution ([75, 125] µm) and (b) broad distribution ([25, 175] µm). Courtesy of Dr. T.L. Jackson.

In Figure 4.66(b), the difference between the empirical relation and the numerical friction factors increases as the standard deviation of the particle size distribution $D_\sigma$ increases. However, the numerical friction factors for all the distributions seem to follow a same trend indicating the need for parameter fine-tuning. A new and generalized curve fit for each distribution, shown in Figures 4.66(a) and 4.66(b), is proposed and follows

$$f_D = m_D Re_p^{-1} + l_D,$$

(4.13)

where $m_D$ and $l_D$ take the values shown in Table 4.4 and depend on the standard deviation $D_\sigma$. The curve fit may also depend on the particle shape and pack configuration (ordered vs. random) and is subject to future studies.

For friction factor $f_{\sqrt{\kappa}}$, it can be seen from Figure 4.66(c) that the numerical friction factors agree with the modified Forchheimer relation (3.9) significantly better than with the Ergun relation (3.7) for the creeping flow regime, for all
porosities and polydispersities (variations in diameter) currently considered. In the creeping flow regime, the modified Forchheimer relation (3.9) is in fact exact due to the definition of the modified Reynolds number $Re_{\sqrt{K}}$. At $Re_{\sqrt{K}} \sim 0.20$, the numerical friction factors $f_{\sqrt{K}}$ at various $\sigma$’s and $D_\sigma$’s seem to follow a single curve, albeit different from (3.9). Thus, similar to [19, 20], a new curve fit shown
Figure 4.65: Steady (a,c) $u$-velocity and (b,d) pressure fields for a slice at $z=0.50L_z$ of a random pack of polydisperse spheres with $\sigma=0.60$ and a narrow distribution at $Re_p=0.40$ (a,b) and 98.93 (c,d).

as the red dashed line in Figures 4.66(c) and 4.66(d) is proposed and follows

$$f_{\sqrt{K}} = m_{\sqrt{K}}Re^{-1}_{\sqrt{K}} + l_{\sqrt{K}},$$  \hspace{1cm} (4.14)
Table 4.4: Proposed parameter values for the coefficients $m_D$ and $l_D$ of the modified curve fit (4.13) for various polydispersities (variations in diameter).

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<th>$D_\sigma$</th>
<th>$m_D$</th>
<th>$l_D$</th>
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<tr>
<td>0.24 (Medium)</td>
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<tr>
<td>0.43 (Broad)</td>
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where $m_{\sqrt{K}}=0.9807$ and $l_{\sqrt{K}}=0.2912$ are the modified constants and are independent of porosity and particle size distribution.

4.2.2 Permeability

Before examining the permeability of random packs, the effect of porosity on the permeability of cubic arrays of monodisperse spheres for the creeping flow regime is considered first. As shown in Figure 4.67, a universal scaling proposed by [88] collapses the numerical permeability $K$ onto a single linear curve fit ($\log_{10}(K')=m\log_{10}(\sigma_s)+b$). The scaled numerical permeability follows

$$K' = \frac{K}{K_0}, \quad (4.15)$$

where $K_0=2<S>R^2/(9<S>R^2\phi)$, $<R^n>$ is the $n$th moment of the sphere size distribution (e.g. $<R^2>$=variance) and takes the values shown in Table 4.5, $\phi=1-\sigma$, and the scaled porosity follows $\sigma_s=\sigma - \sigma_c$, where $\sigma_c$ is the critical porosity and $\sigma_c \approx 0.03$ [88]. The proposed linear curve fit has a slope $m=3.715$ and is consistent with the slope of $m \approx 4.00$ proposed by [88].

We next examine the effects of porosity and polydispersity on permeability for creeping and inertial flows through random packs of polydisperse spheres. As seen from Figure 4.68, the universal scaling proposed by Martys [88] does not collapse
Figure 4.66: (a,b) Friction factor $f_D$ as a function of particle Reynolds number $Re_p$ and Ergun’s equation (3.7) (blue solid line) and (c,d) friction factor $f_{\sqrt{K}}$ as a function of modified particle Reynolds number $Re_{\sqrt{K}}$ and modified Forchheimer equation (3.9) (blue solid line) for flow through 3-D random packs of polydisperse spheres. Green symbols: $D_\sigma=0.43$ (broad distribution); Black symbols: $D_\sigma=0.24$ (medium distribution); Magenta symbols: $D_\sigma=0.11$ (narrow distribution); Square symbols: $\sigma=0.40$; Diamond symbols: $\sigma=0.60$; O symbols: $\sigma=0.70$; Green dashed line: proposed curve fit (4.13) for $D_\sigma=0.43$; Black dashed line: proposed curve fit (4.13) for $D_\sigma=0.24$; Magenta dashed line: proposed curve fit (4.13) for $D_\sigma=0.11$; Red dashed line: proposed curve fit (4.14).

the data onto a single linear curve as previously seen with the cubic arrays of monodisperse spheres. The limited applicability of the universal scaling proposed by [88] is mainly due to the relatively wide range of the standard deviation $D_\sigma$ of
Figure 4.67: Scaled permeability proposed by [88] for cubic arrays of monodisperse spheres at various porosities $\sigma$ and Reynolds numbers. Black symbols: current results; Blue dashed line: Martys’ universal scaling [88] curve fit; Red dashed line: Proposed curve fit.

<table>
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<th>$D_\sigma$</th>
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<th>$&lt;R^3&gt;$</th>
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</tbody>
</table>

Table 4.5: The 2nd and 3rd moment, $<R^2>$ and $<R^3>$ respectively, of the sphere size distribution for various polydispersities (variations in diameter).

the particle size distribution. Though the proposed scaling in [30] does not collapse the data onto a seemingly single curve either, using a similar approach a multi-step scaling is currently proposed. The intermediate scaling follows

$$K_s^* = D_\sigma K^*, \quad (4.16)$$

where $K^* \equiv K/L_p^2$ and as shown in Figure 4.69(a), the scaled normalized permeability $K_s^*$ displays a linear behavior with curve fits that follow

$$\log_{10}(K_s^*) = m_{K_s} \sigma + b_{K_s}, \quad (4.17)$$

where the constants $m_{K_s}$ and $b_{K_s}$ take the values shown in Table 4.6. As seen from
Table 4.6, with the proposed scaling the standard deviation of the slope $m_{K_s}$ of the scaled values $K_s^*$ also decreases compared to the slope $m_{K_{us}}$ of the unscaled values $K^*$. Figure 4.69(a) shows that the permeability $K_s^*$ depends on both the porosity and particle size distribution. This is consistent with the behavior observed for 2-D random polydisperse packs [30]. Using the average of the scaled $m_{K_s}$ values for the three particle size distributions in Table 4.6, the dependence of $b_{K_s}$ on $D_\sigma$ is given by the linear curve fit that follows

$$b_{K_s} = aD_\sigma + c,$$  \hspace{2cm} (4.18)

where $a=2.559$ and $c=-5.769$. The final scaling follows

$$K_{s}^{**} = \frac{K_s^*}{10^{b_{K_s}}},$$  \hspace{2cm} (4.19)

and as shown in Figure 4.69(b), with this scaling the data essentially collapses onto a single linear curve. The linear curve fit of the normalized scaled permeability
$K_{s}^{**}$ follows

$$\log_{10}(K_{s}^{**}) = 4.147\sigma. \quad (4.20)$$

![Figure 4.69: (a) Normalized intermediate scaled permeability (4.16) and (b) proposed normalized scaled permeability (4.19) for random packs of polydisperse spheres for various $D_\sigma$ and Reynolds numbers. Green symbols: broad distribution; Black symbols: medium distribution; Magenta symbols: narrow distribution; Square symbols: $\sigma=0.40$; Diamond symbols: $\sigma=0.60$; O symbols: $\sigma=0.70$; Red dashed line: proposed curve fit (4.20).](image)

<table>
<thead>
<tr>
<th>$D_\sigma$</th>
<th>$m_{Kus}$</th>
<th>$b_{Kus}$</th>
<th>$m_{Ks}$</th>
<th>$b_{Ks}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Narrow (0.11)</td>
<td>4.174</td>
<td>-4.579</td>
<td>4.154</td>
<td>-5.513</td>
</tr>
<tr>
<td>Medium (0.24)</td>
<td>4.157</td>
<td>-4.500</td>
<td>4.157</td>
<td>-5.112</td>
</tr>
<tr>
<td>Broad (0.43)</td>
<td>4.148</td>
<td>-4.315</td>
<td>4.153</td>
<td>-4.686</td>
</tr>
</tbody>
</table>

Table 4.6: Proposed parameter values for coefficients $m_{Kus}$, $b_{Kus}$, $m_{Ks}$, and $b_{Ks}$ of the modified curve fit (4.17).
4.3 Initial Results of 3-D DNS of Turbulent Flow through a Periodic Array of Spheres

In this section, we discuss the initial results for DNS of turbulent flow through a periodic cubic array of spheres for $Re_p$ of 4988.98. For the purpose of comparison and highlighting of the turbulent flow features, we also present the results for a steady laminar flow at $Re_p$ of 590.06. Both have a porosity of $\sigma=0.75$. For the convenience of reference, Figure 4.70 shows the monodisperse periodic array of spheres with porosity $\sigma=0.75$ used in the simulations.

As an initial comparison, Figure 4.71 shows the instantaneous $Q$ iso-surfaces of vorticity magnitude for half of the domain in the $z$-direction for both the laminar and turbulent case. Obviously, the flow features and structures for turbulent flow are much more complex than the laminar case and require extensive analysis.
Figure 4.71: Instantaneous Q iso-surfaces of vorticity magnitude for $z \leq 0.50L_z$ for flow through a cubic array of spheres with $\sigma=0.75$ at $Re_p$ of (a) 590.06 (steady) and (b) 4988.98 (turbulent).

Further comparisons and analyses are presented below.

### 4.3.1 Laminar Flow

As highlighted in Figure 4.71(a), steady laminar flow displays relatively simple flow features and will be considered first.

A non-uniform grid with dedicated grid clustering and stretching at the surface of the spheres with a coarser resolution at the center of the domain is used. The stretched grid has a wall normal resolution of $dx_i \approx 0.00116$ ($D/dx_i \approx 860$) near the wall and $0.0116$ ($D/dx_i \approx 86$) near the center of the domain. This grid is intended for the turbulent case and is more than adequate for the laminar case as can be seen in Figure 4.72. The dominant length scale, identified by the FFT of the instantaneous $z$-vorticity profile along a vertical slice at $x_{mid}$ for the $z$-direction slice (the $xy$-plane with a normal in the $z$-direction, and similarly below when referring to a 2-D slice through the 3-D field) at $L_z$ is $\sim 1.267$ ($k \approx 0.789$) with the
smallest length scales greater than \( \sim 0.20 \).

As seen from Figure 4.73, the steady flow has a well defined “tail”, referring to the high \( u \)-velocity stripe most clearly seen in Figures 4.73(a) and 4.73(d) for the \( z \)-direction slice at 0.50\( L_z \) and a \( y \)-direction slice at 0.50\( L_y \), respectively. This behavior is expected and is similar to that observed for 2-D flow previously discussed except that the “tail” is now 3-D and becomes thinner between the particles as can be seen by comparing, for example, the \( z \)-direction slices at various locations. As seen from the \( u \)-velocity fields at \( z_{\text{max}} \) and \( y_{\text{max}} \) slices shown in Figures 4.73(a) and 4.73(d), respectively, the flow also tends to be symmetric about the \( y \) and \( z \)-direction centerplane. Figure 4.74 further shows that there are standing vortices between the particles. The imprints of these standing vortices on the extracted 2-D slices may be best demonstrated by the re-circulations shown by the streamlines in Figure 4.75 for the \( L_z \) slice shown in Figure 4.73(b) and the \( L_y \) slice shown in Figure 4.73(f). The existence of standing (mean or steady) vortices in the laminar

Figure 4.72: (a) Instantaneous \( z \)-vorticity profile along a vertical slice at \( x_{\text{mid}} \) for the \( z \)-direction slice at \( L_z \) and (b) its FFT power spectrum for a cubic array of spheres with \( \sigma=0.75 \) at \( Re_p \) of 590.06 (steady). The profile in (a) is shifted by \(-L_y/2\).
The breakdown of symmetry of time averaged flow fields for transitional and pseudo-turbulent flows observed in 2-D has been an intriguing phenomenon that was paid quite some attention to throughout this work. In 3-D, in addition to the intuitive top-bottom symmetry for, e.g., the $z$-direction slice, there is also intuitive $y$-$z$ symmetry, i.e., the flow should intuitively be the same when observed in the $y$- or $z$-direction. This is indeed nominally the case for the steady laminar case here as may be appreciated by the similarity between Figures 4.73(b) and 4.73(f), or Figures 4.73(c) and 4.73(e). The nominal similarity and thus $y$-$z$ symmetry can also be more clearly seen in Figure 4.75. As will be shown below, this symmetry is broken in the turbulent case, where the symmetry in the $z$-slices is broken by the vertical cross flow and “tail” tilting, similar to the 2-D pseudo-turbulent case.

4.3.2 Turbulent Flow

We now present the results for 3-D turbulent flow through a cubic array of spheres with a porosity $\sigma=0.75$ at $Re_p=4988.98$, shown previously in Figure 4.71(b).

We begin the discussion by assessing the grid resolution. To properly capture the turbulent boundary layer, a dedicated boundary layer stretching is implemented to resolve the large gradients found near the wall and especially at the location with the smallest distance between the spheres (i.e. the domain edges). Figure 4.76 shows the time averaged and $rms$ of $u$-velocity profiles along a vertical 1-D slice at $x_{min}$ for the $z$-direction slice at $L_z$. Note first the asymmetry in the time averaged $u$-velocity is the result of the tilting of the “tail” discussed below. A non-uniform grid with a wall-normal resolution for the first grid point of $dy=0.00116$ and a $y^+\simeq 0.0224$ with a stretching ratio of 1.1 is used for a boundary
Figure 4.73: Steady (a,d) $u$-velocity, (b,e) $v$-velocity, and (c,f) $w$-velocity fields for slices at (a,b,c) $z=[0.50, 0.75, 1.00]L_z$ and (d,e,f) $y=[0.50, 0.75, 1.00]L_y$ for flow through a cubic array of spheres with $\sigma=0.75$ at $Re_p=590.06$. 

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Figure 4.74: Streamlines colored by vorticity magnitude showing standing vortices near $L_z$ for laminar flow through a cubic array of spheres with $\sigma=0.75$ at $Re_p$ of 590.06.

Figure 4.75: Steady (a) $v$-velocity field for the $z$-direction slice at $L_z$ in Figure 4.73(b) and (b) $w$-velocity field for the $y$-direction slice at $L_y$ shown in Figure 4.73(f). White lines with arrows: streamlines.
layer with thickness $\delta \approx 0.0316$. Note, as seen in Figure 4.76, the mean and \textit{rms} profiles of $u$-velocity qualitatively resemble that observed for turbulent channel flow.

To next verify that the smallest scale in the flow is resolved, and therefore the simulation qualifies as DNS, we also examine the adequacy of the resolution with length scales identified with the FFT. Figure 4.77 shows that the dominant length scale is $\sim 0.317$, for an example vertical slice of instantaneous $z$-vorticity at $x_{\text{mid}}$ and on the $z$-direction slice at $L_z$, as identified by the wavenumber peak at $k \approx 3.158$. The smallest length scales are greater than $\sim 0.033$.

The turbulent flow fields are discussed next. The first remarkable feature to note is that, as seen in Figures 4.78(a) and 4.78(d), the time averaged “tail” tilts downward yet does not tilt much in the transverse $z$-direction, showing the breakdown of the $y$-$z$ symmetry. Just as in 2-D pseudo-turbulent flow seen in, for example, Figure 4.45, the tilting is a result of the significant vertical cross flow developed in turbulent flow. The vertical flow is best demonstrated in Figure 4.79(a)
Figure 4.77: (a) Instantaneous $z$-vorticity profile along a vertical slice at $x_{mid}$ for the $z$-direction slice at $L_z$ and (b) its FFT power spectrum for a cubic array of spheres with $\sigma=0.75$ at $Re_p$ of 4988.98 (turbulent). The profile in (a) is shifted by $-L_y/2$.

by the streamlines in the $z$-direction slice at $L_z$ shown in Figure 4.78(b). Therefore, the conclusion drawn in 2-D that transition to pseudo-turbulent flow is associated with the development of significant cross flow perpendicular to the streamwise direction seems also true in 3-D. This cross flow also causes the breakdown of the $y$-$z$ symmetry. Note this vertical flow and the induced “tail” tilting causes the asymmetry in the time averaged profile shown earlier in Figure 4.76. This vertical flow also causes the relatively larger $rms$ of $u$ and $v$-velocity seen in Figures 4.79(b) and 4.79(c) near the tip of the “tail”.

It should be noted that although the time averaged “tail” tilts downward yet not much in the transverse $z$-direction in the current case, the tilting may well be different in a different case and this will be examined in the future. More extensive analyses including those presented for 2-D cases such as FFTs and PDFs of probe data, kinetic energy spectra, etc., along with the Reynolds number effect will also be performed in the future.
Figure 4.78: Time averaged (a,d) $u$-velocity, (b,e) $v$-velocity, and (c,f) $w$-velocity fields for slices at (a,b,c) $z=[0.50, 0.75, 1.00]L_z$ and (d,e,f) $y=[0.50, 0.75, 1.00]L_y$ for flow through a cubic array of spheres with $\sigma=0.75$ at $Re_p$ of 4988.98 (turbulent).

Figure 4.79: (a) Time averaged $v$-velocity, (b) $rms$ of $u$-velocity, and (c) $rms$ of $v$-velocity fields for the $z$-direction slice at $L_z$ for flow through a cubic array of spheres with $\sigma=0.75$ at $Re_p$ of 4988.98 (turbulent). White lines with arrows: streamlines.
4.4 Discussion

Several interesting behaviors have been observed in the numerical simulations, including (1) mixed steady-unsteady flow above $Re_{p,cr}$ at certain porosities $\sigma$ as already seen in Section 4.1.1, (2) lack of statistically steady state for some cases, (3) flow asymmetry in steady flow or time averaged flow field for unsteady flow in the direction perpendicular to the pressure source term when periodic conditions in that direction are imposed, and (4) dependence of the asymmetry in (3) on numerics such as resolution. These behaviors are expected to have important implications on modeling, such as RANS type with time averaging, and how resolution studies should be conducted. Below, we discuss each of these in more detail.

4.4.1 Mixed Steady-Unsteady Flow above $Re_{p,cr}$

Simulations for flows with $Re_p$’s greater than $Re_{p,cr}$, referred to as supercritical flows, show a somewhat unexpected behavior that there can be steady flows in the supercritical flow regime. As seen in Figure 4.1, for certain porosities the Reynolds numbers for steady and unsteady flows are mixed. This can be seen for periodic arrays of cylinders with $\sigma=0.30$ and ellipses with $\sigma=0.50$; the latter displays a very marginal mixed steady-unsteady behavior. To the best of the author’s knowledge this phenomenon has not been previously discovered and requires further investigation through transition theory; this behavior seems analogous to relaminarization.
4.4.2 Lack of Statistically Steady State

For transitional flows like at $Re_p=267.57$ with $\sigma=0.30$ and $Re_p=769.12$ with $\sigma=0.50$, it appears that the velocity and vorticity magnitude signals at some locations can be “intermittent”-like without a statistically steady state as shown in Figure 4.13 and Figure 4.36, respectively. This is also best demonstrated by the probe signals in Figure 4.80 for flow through a rectangular array of ellipses with $\sigma=0.40$ at $Re_p=1015.3$. As can be seen in Figure 4.80, the velocity variables for a particular probe fluctuate either around a positive or negative value at different periods of time, depending on the locations of the “tail” (high $u$-velocity stream originating from the inlet seen in Figure 4.81) at the corresponding periods of time. Thus, Figure 4.81 shows the “intermittent” behavior is related to the switch in the direction (up or down) of the “tail”, i.e., at different periods of time, e.g., around $t^* \approx 95$ and 221, the “tail” tilts upwards and downwards, respectively. This “intermittent” behavior is also present at higher $Re_p$’s explored in the current work (not shown). As shown in Figures 4.80(a) to 4.80(f) and 4.81 this “intermittent”-like behavior is also grid resolution dependent despite the grid independent solution for superficial velocity.

The observable relation between the $v$-velocity at probe 1 and $u$-velocity at probe 2 is further described through the normalized cross-correlation. The normalized cross-correlation is defined as

$$z(t) = \frac{\phi(t) \odot \psi(t)}{\sqrt{E_\phi E_\psi}},$$

(4.21)

where $\phi(t)$ and $\psi(t)$ are discrete signals and $E_\phi = \int_{-\infty}^{\infty} |\phi(t-t_0)|^2 dt$ for some fixed $t_0$ (similarly for $E_\psi$). Figure 4.80(g) shows the correlation between the $v$-velocity at
probe 1 and $u$-velocity at probe 2. The correlation is dominated by a negative peak corresponding to a reversed signal and closely resembles the correlation between $v$ and $-v$ at probe 1 (not shown). The negative correlation observed in Figure 4.80 is the result of the “tail” dynamics. As seen in Figure 4.81, probe 1 is in the way of the “tail” resulting in a positive $v$-velocity when the “tail” tilts upwards and a negative value when the “tail” tilts downwards. Probe 2 is located in the accompanying re-circulation which is clockwise or counter-clockwise when the “tail” tilts up or down, respectively; $u$-velocity is negative and positive for the former and latter re-circulation directions, respectively.

Due to the lack of a statistically steady state, time averaging for the mean flow field becomes difficult. As a result, this “intermittent” behavior also has an impact on the resolution study. It seems to only make sense to pick the “positive” or “negative” periods for convergence checks. Even then, the convergence is only in a nominal sense with possible slightly fluctuating values towards a converged one. Note the lack of a statistically steady state also has an impact on RANS type of modeling.

### 4.4.3 Flow Asymmetry

Supercritical flow is expected to lose its instantaneous flow field symmetry [3, 27, 73]. Unexpectedly, however, asymmetry is also encountered for steady flow in the supercritical flow regime. Figure 4.82(a) shows the loss in symmetry for a supercritical steady flow with $\sigma=0.30$ and $Re_p=323.51$ with a clear “tail” tilting towards $y_{\text{min}}$. The tilting is in fact sensitive to initial perturbations as shown in Figure 4.82(b) for the same conditions as in the simulation shown in Figure 4.82(a) except with small amplitude $O(10^{-15})$ initial perturbations. The “tail” now tilts
upwards. Thus, for different realizations, the direction of the “tail” tilting is random without preference.

This loss in symmetry is also seen for pseudo-turbulent flow through a square array of cylinders with $\sigma = 0.50$ at $Re_p \geq 769.12$, discussed in Section 4.1.5.2, and for turbulent flow through a cubic array of spheres with $\sigma = 0.75$ at $Re_p = 4988.98$, discussed in Section 4.3 and highlighted in Figure 4.79. The tilting of the “tail” is also expected to be sensitive to initial perturbations in these cases.

It is worthwhile to note that the tilting is also observed to be grid resolution dependent as can be seen by comparing Figures 4.82(a) and 4.83. This is similar to the behavior observed for flow through a rectangular array of ellipses with $\sigma = 0.40$ at $Re_p = 1015.3$, discussed above, in that despite achieving a grid independent solution, the “tail” tilting is resolution dependent. Thus, it seems to be only sensible to perform grid resolution studies on integrated quantities such as $<U>$.

### 4.4.4 Turbulent Flow through Packs of Spheres

Spatial and temporal resolution requirements for simulations of turbulent flow through 3-D periodic packs pose difficulties to accurately simulate with the current computational capabilities. Flow through 2-D periodic packs, though pursued extensively, is still not well understood, as highlighted by the recent work in [3], and provides valuable insight into 3-D flow. As discussed in Section 4.3, turbulent flow through a cubic array of spheres with $\sigma = 0.75$ at $Re_p = 4988.98$ displays similar trends as those observed for pseudo-turbulent flow through a square array of cylinders with $\sigma = 0.50$ at $Re_p \geq 3139.96$. Hence, further examination of transitional and pseudo-turbulent flows through 2-D periodic packs should be thoroughly pursued while simultaneously investigating transitional and turbulent flows through 3-D
periodic packs.
Figure 4.80: The $v$-velocity (left column) at probe 1, $u$-velocity (right column) at probe 2, and (g) normalized cross-correlation for flow through a rectangular array of ellipses with $\sigma=0.40$ at $Re_p=1015.3$ at different resolutions; $dx_i=0.0041$ (a,b,g), $dx_i=0.0028$ (c,d), and $dx_i=0.0021$ (e,f). The locations of probe 1 and probe 2 are shown in Figure 4.81.
Figure 4.81: Instantaneous $u$-velocity fields at $t^* \approx 95$ (left column) and $t^* \approx 221$ (right column) for flow through a rectangular array of ellipses with $\sigma = 0.40$ at $Re_p = 1015.3$ at different resolutions; (a,b) $dx_i = 0.0041$, (c,d) $dx_i = 0.0028$, and (e,f) $dx_i = 0.0021$. Probes 1 and 2 are shown. Magenta lines with arrows: streamlines.
Figure 4.82: The $u$-velocity fields for supercritical steady flow through a square array of cylinders with $\sigma=0.30$ at $Re_p=323.51$ for $dx_i=0.0041$ with (a) zero and (b) small amplitude $O(10^{-15})$ initial perturbations.

Figure 4.83: The $u$-velocity fields for supercritical steady flow through a square array of cylinders with $\sigma=0.30$ at $Re_p=323.51$ for the same conditions as Figure 4.82(a) but with different resolutions: (a) $dx_i=0.0021$ and (b) $dx_i=0.0010$. 
Chapter 5

Conclusion & Recommendation

5.1 Conclusion

Direct numerical simulations of incompressible flow through periodic (2-D) and cubic (3-D) arrays of particles and periodic random packs of polydisperse spheres over a wide range of Reynolds numbers and at various porosities are performed. The unsteady Navier-Stokes equations are solved on a collocated Cartesian grid and the immersed boundary method is used to treat the internal flow boundaries in 2-D flow and 3-D laminar flow while the implicit solver of OpenFOAM® is used for 3-D transitional and turbulent flows for the consideration of computational cost.

The effects of Reynolds number and porosity on the macroscopic properties of friction factor and permeability for periodic arrays of cylinders and ellipses are investigated. The numerical friction factors agree well with the Ergun relation in the creeping flow regime for moderate porosities as expected. The increased deviation for non-creeping flows and for decreasing porosity are also consistent.
with previous results. On the other hand, the numerical friction factors reasonably agree with the modified Forchheimer friction factor relation in the laminar flow regime and with a proposed relation in the transitional and pseudo-turbulent flow regimes. A modified curve fit based on the Gebart relation to account for the wide range of Reynolds numbers is proposed for permeability. The constant coefficient $C_1=4/9\pi\sqrt{2}$ in the original Gebart relation is modified to depend on $Re_p$. With this modification, the numerical permeability values fall closely to the proposed curve fit for the wide range of Reynolds numbers considered.

A similar study was conducted for random packs of polydisperse spheres. The numerical friction factors deviate from the Ergun relation as the standard deviation of the particle size distribution increases and agree well with the modified Forchheimer friction factor for the creeping flow regime. Modified curve fits based on the Ergun and modified Forchheimer relations are proposed for $f_D$ and $f\sqrt{K}$, respectively. A modified normalized curve fit following [30] is also proposed for permeability.

Taking the advantage of the wide range of Reynolds numbers considered in two-dimensions, the effect of Reynolds number on transitional and pseudo-turbulent flow features are analyzed. For periodic flows, the dominant time scale corresponds to the “tail” oscillation on a time scale similar to the flow pass-through time scale, while for transitional and pseudo-turbulent flows, this high frequency resonance is superimposed on distributed “tail” flapping frequencies. It was found that transition is associated with strong vertical cross flow at transitional Reynolds numbers. In the periodic and transitional flow regimes, the PDFs of vorticity magnitude for the same probe vary with $Re_p$ yet in the fully pseudo-turbulent flow regime, the PDFs are similar and Gaussian due to a variety of fluid motions including
the vertical flow, vortex shedding and advection, and “tail” tilting and flapping. PDFs are also found to be location dependent due to the different “tail” and vortex behaviors at different regions of the flow. Intermittent change of the direction of vertical flow and the induced “tail” tilting was observed for the \( \sigma \) of 0.50 case.

For spatial structures in fully pseudo-turbulent flows in 2-D, the instantaneous length scales and the length scales identified by two-point double correlations are similar for the range of pseudo-turbulent flow Reynolds numbers considered; this behavior is specific to 2-D pseudo-turbulence and future studies in 3-D will be conducted. The effect of particle shape on the spatial length scales was also analyzed. Flow through a rectangular array of ellipses at \( \sigma = 0.50 \) favors smaller scales and stronger vorticities due to the aspect ratio and smaller vertical domain. It was also noted that flow through rectangular arrays of ellipses had larger critical Reynolds numbers because of the stronger tendency of flow remaining attached.

The effect of the representative elementary volume (REV) on the mean, \( rms \), and superficial velocities is investigated for packs with peculiar transition behaviors at \( \sigma = 0.30 \). Increasing the size of the REV had a significant impact on the mean and \( rms \)-velocities as well as on the time dependent behavior of the flow; the flow may change between steady and unsteady flow as the size of the REV changes in the transitional flow regime. The direction of the “tail” tilting may also change. The time averaged flow became increasingly less dependent on the size of the REV with increasing Reynolds number.

Many trends for laminar, transitional, and pseudo-turbulent flows in 2-D were also observed for flow through a cubic array of spheres in 3-D. In particular, transition to turbulence is dominated by the presence of a cross flow perpendicular to the streamwise direction and a breakdown of the symmetry of the flow.
Several interesting behaviors have been observed in the numerical simulations, including mixed steady-unsteady flow above $Re_{p,cr}$ at certain porosities $\sigma$ and a lack of statistically steady state for some cases. Steady flow for Reynolds numbers larger than the critical Reynolds number was also observed for both periodic arrays of cylinders and ellipses. The behavior of the asymmetric “tail” was found to be very sensitive to small perturbations.

5.2 Future Work and Recommendations

Future work based on this research should address the following points:

- Code Development
  - Further developments to the implicit Navier-Stokes in-house research code.
  - Increase the order of accuracy of the GIBM interpolation scheme.
  - Further speed-up optimizations to the MPI NS-GIBM code with a focus on AMR speed-up.
  - GPU acceleration of the NS-GIBM code; the initialize framework has already been established [89].
  - Further developments to the grid stretching/clustering algorithm with a focus on stability.
  - Further developments to the GIBM algorithm with a focus on stability for the touching of numerous immersed boundaries.
• **Flow through Porous Packs**

  - 3-D simulations of turbulent flow through random periodic packs.
  - Derive appropriate correlations between the permeability and some measure of the microstructure.
  - Derive a robust and general dual-scale (microscopic and macroscopic) turbulent LES model.
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Appendix A

Additional Developments

A.1 Large Eddy Simulation

The nondimensionalised equations to be solved for large eddy simulations (LES) of incompressible viscous flows are

\[
\frac{\partial \tilde{u}_j}{\partial x_j} = 0, \quad (A.1)
\]

\[
\frac{\partial \tilde{u}_i}{\partial t} + \tilde{u}_j \frac{\partial \tilde{u}_i}{\partial x_j} = -\frac{\partial \tilde{p}}{\partial x_i} + \frac{1}{Re} \frac{\partial^2 \tilde{u}_i}{\partial x_i \partial x_j} - \frac{\partial \tau_{ij}}{\partial x_j}, \quad (A.2)
\]
where \( \tilde{\phi} \) is the general filtered variable and \( \tau_{ij} = \tilde{u}_i \tilde{u}_j - \tilde{u}_j \tilde{u}_j \) is the subgrid-scale (SGS) stress tensor and is the difference between the filtered product of velocities and the product of filtered velocities. The SGS stress tensor arises from the filtering of the non-linear convective terms and is determined through a closure model. The LES approach presented by Shetty et al. [53] is used for the current in-house research code and currently only supports the static and dynamic Vreman model (VM and DVM, respectively) discussed below. These two models rely on the classic eddy-viscosity model which follows

\[
\tau_{ij} = -2 \nu_T \tilde{S}_{ij}, \tag{A.3}
\]

where \( \nu_T \) is the SGS eddy viscosity and \( \tilde{S}_{ij} = (\partial \tilde{u}_i/\partial x_j + \partial \tilde{u}_j/\partial x_i)/2 \) is the filtered strain-rate tensor.

The recent static Vreman model [90] is based on a global coefficient and is therefore easy to implement, affordable, and can be applied to inhomogeneous flows [53]. The eddy viscosity for the VM follows

\[
\nu_T = C \Pi^g, \tag{A.4}
\]

where

\[
\Pi^g = \sqrt{\frac{B_\beta}{\alpha_{ij} \alpha_{ij}}}, \tag{A.5}
\]

\[
\alpha_{ij} = \frac{\partial \tilde{u}_j}{\partial x_i}, \tag{A.6}
\]

\[
B_\beta = \beta_{11} \beta_{22} - \beta_{12}^2 + \beta_{11} \beta_{33} - \beta_{13}^2 + \beta_{22} \beta_{33} - \beta_{23}^2, \tag{A.7}
\]

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\[ \beta_{ij} = \Delta_m^2 \alpha_{mi} \alpha_{mj}, \]  
(A.8)

where the global coefficient \( C = 0.07 \) and \( \Delta m \) is the filter width.

Park et al. [91] and You et al. [92] demonstrated that the global coefficient \( C \) varies and presented a dynamic procedure to more accurately determine the model coefficient. The currently supported dynamic Vreman model [92] coefficient follows

\[
C = \frac{\nu}{2} \frac{\langle \hat{\alpha}_{ij} \alpha_{ij} - \hat{\alpha}_{ij} \alpha_{ij} \rangle}{\langle \Pi^g \hat{S}_{ij} \hat{S}_{ij} - \Pi^t \hat{S}_{ij} \hat{S}_{ij} \rangle},
\]  
(A.9)

where \( \nu \) is the kinematic viscosity and

\[
\Pi^t = \sqrt{\frac{B^t_{\beta}}{\alpha_{ij} \alpha_{ij}}},
\]  
(A.10)

\[
B^t_{\beta} = \beta^t_{11} \beta^t_{22} - \beta^t_{12} \beta^t_{12} + \beta^t_{11} \beta^t_{33} - \beta^t_{13} \beta^t_{13} + \beta^t_{22} \beta^t_{33} - \beta^t_{23} \beta^t_{23},
\]  
(A.11)

and \( \hat{\phi} \) is the test filtered quantity, \( \langle ... \rangle \) is the volume average over the entire domain, and \( \hat{\Delta}_m \) is the test filter width.

The temporal and spatial discretization schemes presented in Section 2.1 are used to solve the LES governing equations; all additional partial derivatives, such as \( \hat{S}_{ij} \) and \( \alpha_{ij} \), are discretized with the canonical 4th-order central difference. The volume averaging is calculated with the canonical trapezoidal numerical quadrature.
The test filtering width needed for the dynamic Vreman model is determined through the method proposed by Loh et al. [93] and follows

$$\bar{f}(x) = \frac{1}{\Delta(x)} \int_{x-\Delta(x)/2}^{x+\Delta(x)/2} f(x) \, dx,$$

(A.13)

where $\Delta(x)$ is the spatially varying filter width for all directions $x$. Using Simpson’s numerical quadrature method, the one-dimensional discrete version of (A.13) along the $x$-direction for a uniform grid follows

$$\bar{f}(x) = \frac{1}{6}[f(x_{i-1}) + 4f(x_i) + f(x_{i+1})],$$

(A.14)

and for a non-uniform grid follows

$$f(x_{i+1}) = \frac{\Delta^+ - \Delta^-}{\Delta^+ + \Delta^-} f(x_{i-1}) + 2(1 - \frac{\Delta^-}{\Delta^+}) f(x_i) + \frac{\Delta^- \Delta^-}{\Delta^+(\Delta^+ + \Delta^-)} f(x_{i+1}),$$

(A.15)

where $\Delta^- = x_i - x_{i-1}$ and $\Delta^+ = x_{i+1} - x_i$. This filtering procedure is known to produce good results for non-uniform grids for a lid driven cavity [53] and a channel flow [94]. Shetty et al. [53] showed that the current LES approach does not require a homogeneous direction to dynamically adjust the model coefficient and is most suited for complex flow configurations. Good agreement with DNS results reinforces the approach’s ability to simulate inhomogeneous flows. Shetty et al. [53] also reported that the dynamic Vreman model requires up to 40% more wall-clock time compared to the static Vreman model.
A.2 Grid Modifications

The high resolution required for direct numerical and large eddy simulations favors the use of robust grid manipulations and/or adaptive mesh refinement (AMR) to properly manage computationally feasible grid sizes.

A.2.1 Grid Stretching

To extend the applicability of the current solvers, Cartesian grid stretching/clustering is pursued. To reduce the increased computational cost related to the grid transformation matrices, only rectilinear grids are considered. This approach of simple grid transformations is also favored by the treatment of the immersed boundaries. The rectilinear grids may be obtained either through analytical relations, such as interior clustering [95], or through a dedicated grid generation software. The current input/output implementation of the latter only supports ASCII Xpatch® facet file format from Pointwise® [96]. For rectilinear grids, the physical to computational space transformation simplifies to a set of ordinary differential equations that follow

\[
\frac{du_i}{dx_i} = \frac{du_i}{d\eta_i} \frac{d\eta_i}{dx_i},
\]

\[
\frac{d^2u_i}{dx_i^2} = \frac{d^2u_i}{d\eta_i^2} \left( \frac{d\eta_i}{dx_i} \right)^2 + \frac{du_i}{d\eta_i} \frac{d^2\eta_i}{dx_i^2}, \tag{A.16}
\]
where \( i = 1, 2, 3 \), and \( \eta_i \) is the computational space for the \( x, y, z \)-directions. The derivatives \( d\eta_i/dx_i \) and \( d\eta_i^2/dx_i^2 \) are determined either analytically or through finite differences for grid transformations based on analytical relations or grid input, respectively. For the latter case, 2nd-order central and one-sided differencing are used to determine the derivatives. It should be noted that the calculations of the grid transformations are pre-processed and are stored in memory for increased computational efficiency.

### A.2.2 Adaptive Mesh Refinement

To increase the accuracy and geometrical detail of the simulation, a higher resolution is required to properly resolve the large gradients located near the immersed boundary and at regions of complex flow interactions. To avoid the need of an \textit{a priori} knowledge of the immersed boundary and flow features, local mesh refinement based on solid-fluid interface and flow features is used. The adaptive mesh refinement (AMR) is currently handled through the open-source research package Boxlib. Boxlib was developed by the Center for Computational Sciences and Engineering (CCSE) at Lawrence Berkeley National Laboratory (LBNL) and has “massively parallel, block structure AMR” \cite{50} capabilities including hybrid MPI-OpenMP tiling for 3-D simulations. Boxlib provides the AMR data structure framework and a robust linear solver; the availability of the latter is very advantageous and convenient for incompressible flow solvers. The relative simplicity and easy extendability of Boxlib’s data structure also provides future speed-up opportunities through GPU acceleration.
The fundamental data unit of Boxlib is the Fortran box array $Fab$ and its group collection $MultiFab$. These are also the fundamental parallelization concept as the $Fabs$ composing a $MultiFab$ are distributed among the processors. Boundary conditions, cell refinement tagging, multi-level grid creation, etc., are implemented through customized Boxlib modules derived from their default configuration. Boxlib is constantly being developed and improved [43] and is used for cutting edge research [97, 98, 99]. It should also be noted that the Boxlib toolkit was used to develop the block-structured AMR research package CHOMBO [100].
Appendix B

Vita

Antoine Michael Diego Jost was born in Pretoria, South Africa on 24 April 1991, is the son of Michel Jost and Elisa Belmonte Nieto, and the younger sibling of Taïs Eva Amanda Jost Belmonte. He received a Bachelor of Science degree in aerospace engineering (AE) from Florida Institute of Technology, Melbourne, in 2013. He also received a Master in Science degree in AE from FIT in 2014, and started his Ph.D. in AE at FIT in January 2015. His research at FIT has been supported in part by FIT, DOE, and DTRA.