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1 **On the Effect of Flow Regime and Pore Structure on the Flow Signatures**
 2 **in Porous Media**

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7
 8 **Abstract**

9 In this study, lattice Boltzmann method (LBM) is utilised for three-dimensional simulation of fluid
 10 flow through two porous structures, consisting of grains with the same diameter: (i) a homogeneous
 11 porous domain, in which the grains are placed with a simple cubic packing configuration, and (ii) a
 12 randomly-packed porous domain. An ultra-fine mesh size is considered to perform the simulations in
 13 three orders of magnitude of Reynolds number (Re), covering laminar to turbulent flow regimes, and
 14 capture different flow signatures. Pore velocity fields are derived, and their sample probability density
 15 functions (PDF) are analysed versus time to investigate the dynamics of the flow. The analysis of the
 16 PDFs clearly shows that stagnant zones play a significant role in the formation of the pore flow fields,
 17 manifested by multimodal PDFs, and the distribution of the velocities in porous media at various Re
 18 cannot be characterised by a single PDF model regardless of the pore structure. While the velocities
 19 at the stagnant regions and in the vicinity of the solid boundaries are primarily affected by the viscous
 20 forces and exhibit a power-law PDF at different Re , the velocities in the main (preferential) flow
 21 pathways away from the boundaries are shown to be influenced by the inertial forces, hence having
 22 an exponential PDF when Re is low. At high Re , however, depending on the tortuosity of the porous
 23 structure, the velocities may exhibit an exponential or even Laplace PDF.

24

25 **Keywords:** Pore-scale modelling, Lattice Boltzmann Method, Probability density function.

26

27 **1. Introduction**

28 Porous systems are found in various scientific fields and engineering applications such as oil and
 29 gas recovery, geological storage of CO₂ and H₂, geothermal energy storage, groundwater
 30 remediation, chromatography, exploitation of unconventional reservoirs, and fuel cells¹⁻⁵. Such a
 31 wide array of applications necessitates a profound understanding of heat and mass transfer
 32 phenomena occurring in pore space, which are associated with single or multiphase fluid flow. Given
 33 the flow in porous media is substantially influenced by its complex disordered nature, the physics of
 34 flow is essential to be characterised to achieve a desired flow rate-pressure drop response. This is of
 35 particular importance when the flow is required to be tailored for a given application⁶.

36 Despite its micro-scale characteristics, fluid flow in porous media has been typically described
 37 using Darcy's law in various scientific and industrial applications, a macro-scale approach with several
 38 simplifying assumptions, which neglects local aspects such as pore-scale flow variations within the
 39 interstitial regions and may even fail to accurately predict the transport properties under the high-flow
 40 conditions within intricate pore space⁷⁻⁹. On the other side of the coin, several experimental and
 41 modelling studies substantiated that the local flow dynamics can significantly influence transport
 42 phenomena such as solute transport, mixing, and heat transfer in pore space at different flow regimes
 43¹⁰⁻¹⁴, necessitating the incorporation of the pore-scale characteristics into the effective transport
 44 properties. Therefore, it is of utmost priority to investigate fluid flow and the evolution of the velocity
 45 fields at pore level¹⁵. These investigations are essential to be conducted in correlation with the inertia
 46 effect, i.e. Reynolds number (Re), and geometric heterogeneity of porous media as they directly
 47 control the flow signatures within pores and also the local deviations from Darcy's law^{16,17}. The pore-
 48 scale insights are of particular importance at high-velocity conditions, where the local level of
 49 turbulence impacts the transport of scalar properties and improves heat and mass transfer^{18,19}. This
 50 enhancement is welcomed in many industrial applications and widely investigated by scholars, a
 51 comprehensive review in this regard can be found elsewhere²⁰.

52 Pore-scale insights into the flow characteristics can be obtained by both experimental and
 53 modelling studies. The experimental approaches usually utilise optical techniques such as micro-
 54 particle image velocimetry (PIV) for the visualisation of flow in pore space^{13,21}. X-ray CT imaging and
 55 magnetic resonance imaging (MRI) are the other advanced techniques for the visualisation of fluid
 56 flow in porous media^{22,23}. The experimental studies are crucial for not only shedding light on the
 57 dynamics of flow in porous structures but also providing an experimental database to support the
 58 verification and improvement of numerical approaches²¹. However, there are some limiting factors
 59 hindering their extensive application in different disciplines. For instance, the majority of the
 60 experimental methods require advanced high-cost facilities (high-speed cameras, illumination
 61 sources, X-ray micro-CT imaging systems, etc.), which are not readily available. Strict health and
 62 safety regulations must also be taken into consideration in laboratory regarding the reactivity and
 63 hazard level of the fluids and apparatuses²⁴. Apart from these concerns, there are some inherent
 64 technical limitations about the spatiotemporal measurement capabilities of these methods, making
 65 their application merely suitable for the pore-scale studies where the flow is slow and/or the pore sizes
 66 are large enough to be observed. In addition, they often provide access to the velocity data in two-
 67 dimensional (2D) planar sheets which makes it difficult to probe the three-dimensional (3D) flow hence
 68 limited statistics can be extracted⁷. Recent advances in stereo-PIV and synchrotron X-ray micro-CT
 69 imaging enable four-dimensional (4D) visualisation of the laminar flow in porous structures²⁵⁻²⁸;
 70 however, higher measurement frequencies are required for the cases in which both spatial velocity
 71 fluctuations and local turbulence exist in pores.

72 Advances in computing capabilities have made it possible to use different pore-scale modelling
 73 approaches to study the dynamics of flow as well as transport properties at the pore level. The
 74 computational methods have shown a great potential for capturing complex flow signatures as well

75 as local pore-scale variations arising from the navigation of tortuous pore space by the fluid and
 76 successfully applied for studying various pore-scale phenomena associated with fluid flow in both
 77 ideal and real porous media²⁹. Pore-network modelling (PNM), as a less computationally demanding
 78 approach, has been successfully used for studying various transport phenomena in porous media
 79 such as single and multiphase flow, immiscible displacement, and solute transport³⁰. Despite its
 80 extensive applications in digital rock physics, PNM does not account for the irregularities and
 81 geometric details of pore/throats for the sake of simplicity³¹. Thus, it cannot be applied to studies
 82 where detailed solid-fluid interactions and their influences on the transport properties and velocity
 83 variations are essential to be captured. Thanks to recent advances in high-performance computing,
 84 computational fluid dynamics (CFD) approaches have been successfully employed for numerical
 85 simulation of transport phenomena in porous media²⁹. The continuum-scale CFD approaches, such
 86 as finite difference method (FDM), finite element method (FEM), and finite volume method (FVM),
 87 directly solve the governing equations to characterise the pore-scale transport and obtain the
 88 macroscopic transport properties such as absolute/relative permeability^{5,11,32,33}. However, the
 89 application of these methods is fairly challenging in complex geometries, particularly at high Re , due
 90 to their inherent high computational costs and intractability in capturing the fluid-solid interactions³⁴.
 91 Among the CFD approaches, lattice Boltzmann method (LBM) is a well-suited approach for pore-
 92 scale simulations primarily owing to its great strength in treating complex irregular solid boundaries
 93 and its parallel computing advantages over the other continuum-scale methods^{35,36}. With an
 94 acceptable computational cost, LBM can provide accurate spatiotemporally resolved flow properties
 95 at the regions away from solid boundaries hence has a great potential to be applied for studies with
 96 interest in the characterisation of velocity fluctuations in the pores.

97 It is a given that pore-scale transport is markedly influenced by the geometric characteristics of
 98 porous structures³⁷. However, a common approach for the simulation of flow and investigation of
 99 transport mechanisms in porous media is to adopt regular geometries such as Simple Cubic (SC) and
 100 Body-Centred Cubic (BCC) packing structures^{38–40}. Although these regular geometries help with
 101 incorporating the fluid-solid interactions and can be considered as alternatives to real pore structures
 102 when they are not available, there is still a big concern about their capability to account for the
 103 complexities arising from the heterogeneous and tortuous nature of real porous media and the effect
 104 of the solid-fluid interactions on the flow signatures. Therefore, it is essential to understand the
 105 differences of the flow properties in ordered ideal structures with those of disordered real porous
 106 media. These insights are necessary when studying dispersion and mixing in different porous
 107 structures due to the fact that the transport of the scalar properties is fundamentally controlled by the
 108 distribution of the pore velocities⁴¹. In other words, modelling mixing in porous media requires a
 109 profound understanding of the probability density function (PDF) of the velocities in correlation with
 110 the structural heterogeneity⁴², particularly at the low-velocity range as it governs the possible
 111 anomalous nature of transport in porous media. This makes it necessary to investigate the velocity
 112 distribution in two physically distinct regimes: small and high velocities⁴¹. The previous experimental
 113 and numerical studies show that the small velocities – found in dead-end pores and the volumes in
 114 the proximity of the fluid-solid interfaces – should be described by a power-law PDF model while the
 115 high velocities – found in the main pathways – exhibit an exponential PDF⁴³. However, there are still
 116 uncertainties about the velocity PDFs. For instance, some studies reported increasing power-law
 117 PDFs in the low-velocity regions^{44,45}, contradicting the flat or even decreasing behaviours found in
 118 the other works^{42,46–48}. Such inconsistencies indicate that active debate still remains about the nature
 119 of the velocity PDFs in porous media.

120 In this work, we utilise LBM for 3D simulation of single-phase fluid flow through both regularly-
 121 and irregularly-packed porous media. The main objective of this study is to shed light on the
 122 dependency of the flow signatures on Re and tortuosity of the pore structure at both local and global
 123 scales. Given the low and high Re flows in porous media occur in various environmental, geoscience,

124 and industrial applications^{49,20,50}, the simulations are carried out at three orders of magnitude of Re ,
 125 covering Stokes, laminar, and turbulent flow regimes. The statistical analysis of the simulation results
 126 will also help with providing fundamental insights regarding the effect of the pore structure and
 127 geometric characteristics on the flow features at various flow regimes.

128 2. Method

129 In this section, a detailed description is provided regarding the geometry of the porous structures
 130 as well as the governing flow equations, boundary conditions, and the numerical method employed
 131 to solve the equations for obtaining the evolution of the pore-scale velocity fields.

132 2.1 Governing equations

133 Fluid flow in the pore space can be described by the incompressible continuity and Navier-Stokes
 134 equations:

$$\nabla \cdot \vec{u} = 0 \quad (1)$$

$$\frac{\partial \vec{u}}{\partial t} + (\vec{u} \cdot \nabla) \vec{u} = -\frac{1}{\rho} \nabla p + \nu \nabla^2 \vec{u} \quad (2)$$

135 where $\vec{u} = (u_x, u_y, u_z)$ is the fluid velocity, p is the pressure, and ν is its dynamic viscosity. In this
 136 work, LBM is employed to conduct the fluid flow simulations. LBM is a discrete form of the continuous
 137 kinetic Boltzmann equation with discretised time and space coordinates³⁵. The solution algorithm
 138 assumes the fluid as a large number of randomly moving fictive particles that exchange momentum
 139 (and energy for the non-isothermal problems) through collision and streaming processes, evolving
 140 the density of the fluid $\rho(\vec{x}, t)$, for \vec{x} the position and t the time⁵¹. A finite set of vectors are used to
 141 limit the space coordinate and construct a lattice to denote the directions where the fluid particles can
 142 move. It is common to classify the lattice models as “DnQm” where “Dn” and “Qm” are “n space
 143 dimensions” and “m discrete velocity vectors” in the model⁵². In this study, we use D3Q19 lattice
 144 model, in which each lattice node is surrounded by 18 neighbouring nodes.

145 Considering an Eulerian basis $\vec{x} = (x, y, z)$ and assuming i (0, ..., 18) as the direction available
 146 for the fluid movement in the D3Q19 lattice model, the particle distribution function $f_i(\vec{x}, t)$ is defined
 147 as the fraction of the density with the discrete lattice velocity \vec{c}_i at location \vec{x} and time t . The lattice
 148 Boltzmann equation (LBE):

$$f_i(\vec{x} + \vec{c}_i \Delta t, t + \Delta t) = f_i(\vec{x}, t) + \Omega_i \quad (3)$$

149 predicts the space and time evolution of the particle distribution functions that collide and stream along
 150 the direction i ⁵³. The numerical scheme is divided into collision and streaming steps:

$$f_i^*(\vec{x}, t) = f_i(\vec{x}, t) + \Omega_i \quad (4)$$

$$f_i(\vec{x} + \vec{c}_i \Delta t, t + \Delta t) = f_i^*(\vec{x}, t)$$

151 where $f_i^*(\vec{x}, t)$ is the post-collision particle distribution function and Ω_i is the collision operator. Owing
 152 to its computational efficiency and reliability⁵⁴, Bhatnagar–Gross–Krook (BGK) collision operator is
 153 used in this work:

$$\Omega_i = \frac{1}{\tau} \left(f_i^{eq}(\vec{x}, t) - f_i(\vec{x}, t) \right) \quad (5)$$

154 in which τ is the lattice relaxation time and $f_i^{eq}(\vec{x}, t)$ is the equilibrium distribution function:

$$f_i^{eq}(\vec{x}, t) = \omega_i \rho(\vec{x}, t) \left[1 + \frac{\vec{c}_i \cdot \vec{u}}{c_s^2} + \frac{(\vec{c}_i \cdot \vec{u})^2}{2c_s^4} - \frac{\vec{u} \cdot \vec{u}}{2c_s^2} \right] \quad (6)$$

155 In Eq.(6), $c_s = 1/\sqrt{3}$ is the lattice sound speed and ω_i is a fixed weighting factor in the direction i :

$$\omega_i = \begin{cases} 1/3 & i = 0 \\ 1/18 & i = 1 - 3 \text{ and } 10 - 12 \\ 1/36 & i = 4 - 9 \text{ and } 13 - 18 \end{cases} \quad (7)$$

156 The density and velocity could be related to the distribution functions by:

$$\begin{aligned} \rho &= \sum_i f_i \\ \vec{u} &= \frac{1}{\rho} \sum_i f_i \vec{c}_i \end{aligned} \quad (8)$$

157 Through Chapman-Enskog expansion, the governing continuity and Navier–Stokes equations can be
158 recovered from the LBM algorithm and the fluid kinematic viscosity ν can be related to the lattice
159 relaxation time via:

$$\nu = \frac{1}{3} \left(\tau - \frac{1}{2} \right) \quad (9)$$

160 More details regarding LBM can be found elsewhere ³⁵.

161 We adopt D3Q19-BGK-LBM implemented in OpenLB (<https://www.openlb.net/>) to conduct the
162 fluid flow simulations and obtain the flow fields ⁵⁵. Poiseuille flow through a cylindrical tube as a well-
163 known flow problem having exact analytical solution was utilised to validate the developed code; see
164 Appendix A for further details. A constant velocity boundary condition is imposed at the inlet surface
165 and a constant pressure boundary condition is prescribed at the outlet surface. No-slip bounce-back
166 boundary condition is also considered at the outer walls of the domain in the y- and z-directions as
167 well as the fluid-solid interfaces. For a given simulation case, a constant inlet velocity $\vec{u}_{in} = (u_{in}, 0, 0)$
168 is imposed for all the inlet boundary nodes (shown in Yellow in Figure 1) and the evolution of the
169 velocity fields within the pore space is monitored versus time until the flow becomes fully developed
170 and converged. Having u_{in} , Re can be calculated as:

$$Re_p = \frac{(u_{in}/\phi)D_p}{\nu} \quad (10)$$

171 In Eq.(10), u_{in}/ϕ is the interstitial velocity, which is used for normalising the velocity magnitudes and
172 its components throughout this study. It should be noted that the simulation results include the velocity
173 magnitude and its components in the x, y, and z-directions for each lattice point at different time steps;
174 the analysis of which was carried out using ParaView ⁵⁶.

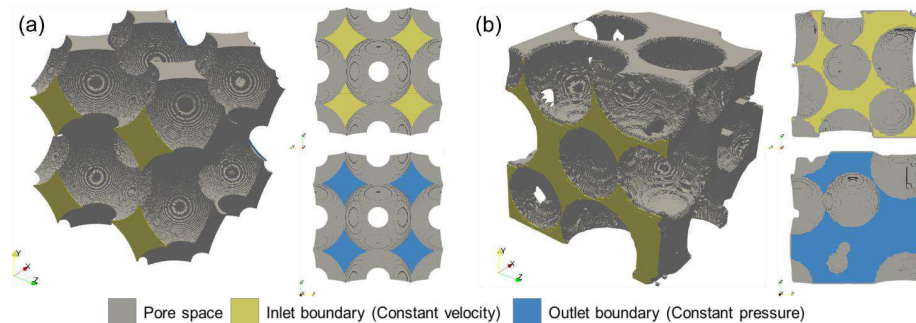
175 At the steady state conditions, the relative variations of the velocities are expected to be zero
176 throughout the computational domain, which would be ideal because of the numerical errors and the
177 possibility of the presence of the spatiotemporal evolving flow signatures, particularly at high Re .
178 Therefore, the convergence of the solution is monitored by finding the average normalised velocity
179 magnitudes at three different planar sheets perpendicular to the imposed flow direction (x-direction),
180 one at the middle and the other two at the first and third quarters of the domain and calculating its
181 relative variation over time. The solution is considered to be converged when the relative variations
182 of the average normalised velocity magnitudes become less than 5%. It should be noted that the
183 simulation continues after the convergence is achieved in order to capture any spatiotemporal
184 evolution of the flow signatures within the pore space.

185 2.2 Geometry of the porous structures

186 We study the fluid flow in two cubic porous media with the size of $200^3 \mu\text{m}^3$, consisting of spherical
 187 grain particles with the same diameter (D_p) of $100 \mu\text{m}$, as illustrated in Figure 1. The porous structures
 188 both have the porosity (ϕ) of $\sim 36\%$, calculated via obtaining the number of their fluid and solid voxels.
 189 The first structure shown in Figure 1-(a) is a regular porous domain, in which the grains are placed
 190 next to each other with the SC packing configuration. The other structure shown in Figure 1-(b) is a
 191 randomly-packed porous domain taken from a $600^3 \mu\text{m}^3$ beadpack image. The beadpack image is
 192 created and segmented by Prodanović and Bryant⁵⁷ to represent the experimental measurements of
 193 the coordinates of the centres of equally-sized spherical grain particles obtained by Finney⁵⁸. It has
 194 the voxel size, porosity, and absolute permeability of $2 \mu\text{m}$, 0.359 and $5.43 \times 10^{-12} \text{m}^2$ ⁵, respectively,
 195 been shown to be representative of packed-bed porous media, and used by scholars to investigate
 196 pore-scale transport in the other studies^{8,59,60}.

197 As the randomly-packed structure is sampled from the beadpack image, it is essential to
 198 investigate whether it is still representative of packed-bed porous media. There are different analysis
 199 techniques such as re-running the simulations where the primary flow direction is changed and
 200 obtaining the corresponding permeabilities⁶¹, or comparing the petrophysical properties such as
 201 porosity and permeability of the sampled medium with those of the original structure. The porosity
 202 and permeability of the randomly-packed sample are 0.36 and $5.01 \times 10^{-12} \text{m}^2$, quite close to those
 203 reported for the beadpack image in the literature, showing that the randomly-packed structure can be
 204 representative of packed-bed porous media.

205 We consider a lattice mesh size of $0.4 \mu\text{m}$ for the discretisation of the pore space, which is 5 times
 206 smaller than that of the voxels in the beadpack image. As a common approach for maintaining the
 207 stability of the solution in LBM at high-velocity conditions is to refine the lattice mesh⁶², the ultra-fine
 208 mesh size enables us to not only run the simulations at high Re but also capture the spatially-resolved
 209 complex flow signatures.



210 Figure 1. Geometries of the (a) regular SC-packed and (b) irregular randomly-packed porous
 211 structures. Fluid flows in the x-direction and constant velocity (Yellow) and pressure (Blue) boundary
 212 conditions are considered at the inlet and outlet boundaries, respectively.

213 3. Results

214 3.1 The evolution of the PDF of the velocity fields

215 3.1.1 SC-packed porous medium

216 The fluid flow simulations were conducted for the SC-packed porous medium, the pore velocity
 217 magnitudes and components both along and transverse to the imposed flow direction were extracted
 218 for each lattice point, normalised against the interstitial velocity, and their sample PDF were plotted
 219 at Re of 0.98 , 9.81 , and 98.14 in Figure 2, Figure 3, and Figure 4, respectively. In these figures, the
 220 simulation times (t) were normalised against the total simulation time (t_{Total}):

$$t^* = \frac{t}{t_{Total}} \quad (11)$$

221 The spatial distribution and streamlines of the velocity field at t_{Total} were also depicted for each Re to
 222 assist with the analysis of the PDFs. It should be emphasised that the effect of the inlet (constant
 223 velocity) boundary on the PDF of the velocities was minimised by excluding the first quarter of the
 224 flow domain when extracting the velocity data. Table 1 summarises the average normalised velocity
 225 magnitudes at the middle planar sheet perpendicular to the x-direction, used to check the
 226 convergence of the solution (as demonstrated earlier), assisting with the understanding of the
 227 evolution of the velocity fields at different Re and times. The PDFs can be also found in Supplementary
 228 Material.

229 Table 1. The average normalised velocity magnitudes at the middle planar sheet perpendicular to
 230 the x-direction in the SC-packed porous medium at different Re and normalised simulation times.

No.	Re	Average Normalised Velocity (-)				
		$t^* = 0.2$	$t^* = 0.4$	$t^* = 0.6$	$t^* = 0.8$	$t^* = 1.0$
1	0.98	0.95	1.31	1.53	1.57	1.60
2	9.81	1.52	2.03	1.77	1.58	1.60
3	98.14	1.07	1.53	1.71	1.71	1.67

231

232 According to Table 1 and Figure 2, the convergence of the solution at $Re = 0.98$ is achieved in
 233 $t^* = 0.6$, and the flow becomes fully developed throughout the domain. However, there are still small
 234 discrepancies in the tail of the PDFs (<0.5% of the velocity data), which could be attributed to the
 235 ultimate development of the velocity field at the centre of the pore throats with the highest velocities
 236 (Figure 2-(e)).

237 In Figure 2-(a), the PDF of the normalised x-direction velocity can be divided into three main parts:
 238 (i) the negative velocities, (ii) the positive velocities lower than 1.47, and (iii) the positive velocities
 239 higher than 1.47. The presence of the negative x-direction velocities in the non-tortuous SC-packed
 240 porous medium – in which there is no pathway opposite to the imposed flow direction hence no
 241 backflow – can only be due to the formation of the recirculating flow structures aligned with the
 242 imposed flow direction. Therefore, as no negative velocity is observed in Figure 2-(a) after the
 243 convergence of the solution, there must not be any flow recirculation in the imposed flow direction,
 244 suggesting the dominance of the Stokes (creeping) flow in the pore space, which is expected at low
 245 Re ⁶³. However, a number of small recirculating flows perpendicular to the imposed flow direction can
 246 be still spotted at the wake of the grain particles (see Figure 2-(e)). These regions are referred to as
 247 the stagnant zones, where the velocities are much lower than those at the main flow pathways hence
 248 the fluid flow is driven dominantly by the viscous forces⁶⁴. Therefore, as the fluid layers of lower
 249 energies flow inside these regions, they experience more details of the landscape at the fluid-solid
 250 interface, and viscous momentum is transmitted laterally across successive laminae of the fluid,
 251 generating small-scale and low-energy recirculating flow structures⁶⁵. The separation of the positive
 252 normalised velocities at 1.47 suggests the presence of two distinct flow signatures, which cannot be
 253 characterised with a single PDF. In Figure 2-(b) and (c), a perfectly symmetrical distribution is
 254 observed for the velocity components in the y- and z-directions, which is expected owing to the
 255 geometrical symmetry of the SC-packed domain in both directions. Interestingly, two different flow
 256 signatures are observed in these directions, separated at ~ 0.1 . Therefore, the distribution of the
 257 velocities lower than 0.1 should be described differently than the higher velocities. Such distinctive
 258 flow signatures are expected primarily because the flow characteristics in the main pathways away
 259 from the solid boundaries with high velocities (the high-velocity zones) are controlled by the inertial
 260 forces while the viscous forces are dominant in the stagnant regions as well as the vicinity of the solid
 261 boundaries at the main flow pathways (the low-velocity zones)⁶⁶. Here, we emphasise that the log-

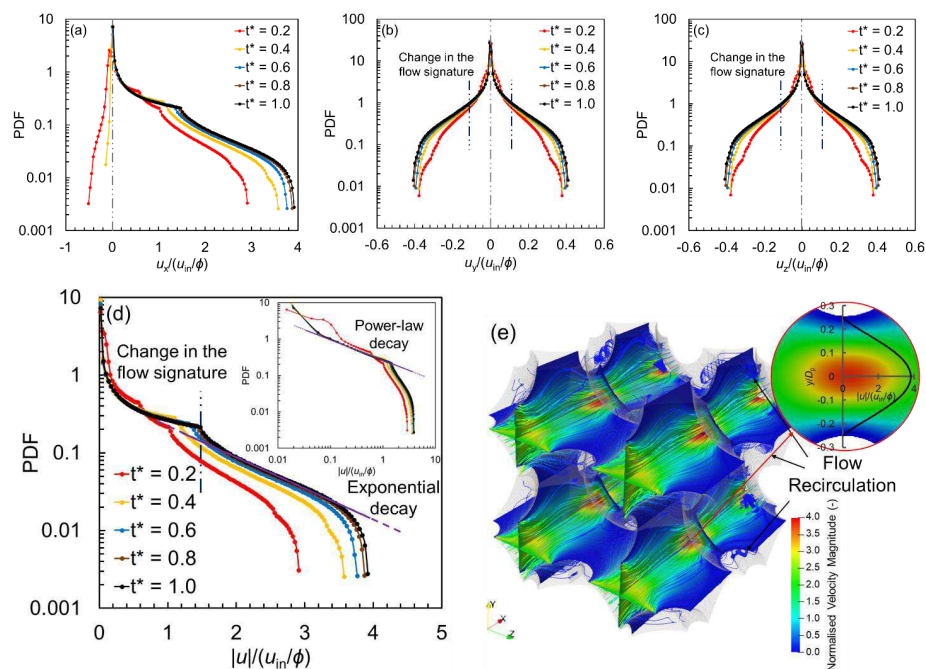
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262 log plot of the PDF of the velocity components has been also analysed to confirm the distinctive
 263 velocity values.

264 The velocity PDFs in Figure 2-(d) exhibit two different signatures, similar to what observed for the
 265 positive velocities in the x-direction, and the separation point is 1.47. For the velocities higher than
 266 this distinctive value, an exponential decay can be fitted to the velocity distribution, which has been
 267 already observed in the other numerical and experimental studies^{7,67,41,68}. In fact, the exponential
 268 function can be used to characterise the flow in the main pathways where the inertial forces are
 269 dominant. The inset in Figure 2-(d) depicting the log-log PDF plot of the normalised velocities confirms
 270 that the velocity in the low-velocity zones should be characterised with a power-law PDF model
 271 instead.



272 Figure 2. Temporal evolution of the normalised velocity fields within the SC-packed porous structure
 273 at $Re = 0.98$: (a-d) log-linear PDF plot of the normalised velocity magnitude and its components in
 274 the x, y, and z-directions, and (e) the spatial distribution and streamlines of the velocity field at $t^* =$
 275 1.0. The inset in (d) is the log-log plot of the PDF of the normalised velocity magnitude.

276 According to Table 1 and Figure 3, the solution convergence at $Re = 9.81$ is obtained in $t^* = 0.8$,
 277 later than the convergence time of the previous case. The main reason for the delay in the
 278 convergence of the velocity is the formation of the recirculating flow structures oriented in the imposed
 279 flow direction at the stagnant regions. This can also be confirmed by investigating the PDF of the x-
 280 direction velocity component (Figure 3-(a)), where almost 5% of the velocity data become negative
 281 after $t^* = 0.6$. The recirculating flow structures could be of particular interest when investigating the
 282 transport of the scalar properties such as chemicals through porous media⁶⁹. It should be noted that
 283 the presence of the recirculating flow structures at the stagnant regions of regularly-packed porous

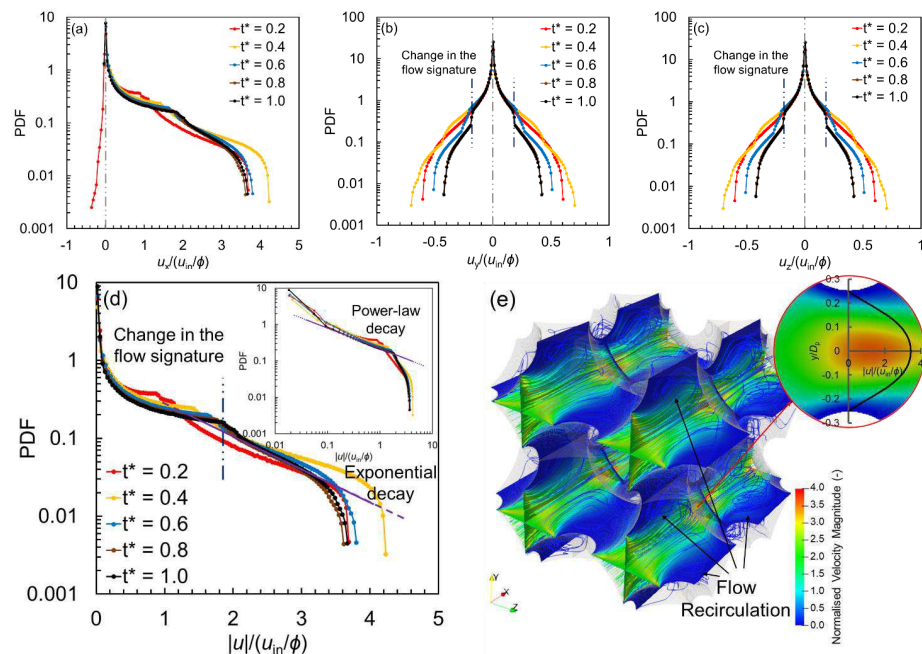
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284 media as well as their dependence on the pore structure have been experimentally investigated at
 285 high Re in the other studies^{70–72}. The ultra-fine mesh size considered in this study assisted us with
 286 capturing them even at smaller Re and confirming their size and orientation dependence on the
 287 velocity of the fluid flowing within the system.

288 The PDFs of the normalised velocities at $Re = 9.81$ and $t^* = 1.0$ in Figure 3-(a) to (d) are generally
 289 similar to the ones at $Re = 0.98$; however, they exhibit some distinguished features. Apart from the
 290 presence of the negative x-direction velocities and recirculating flows, which were discussed above,
 291 a clear separation of the velocity distributions in the y- and z-directions can be seen at the normalised
 292 value of ~ 0.2 . Besides, the distinctive point of the normalised velocity magnitudes is ~ 1.8 , which is
 293 higher than what captured in the previous case. This difference can be attributed to the size of the
 294 recirculating flow structures and the magnitude of the velocities in these regions. It can be seen in
 295 Figure 3-(e) that the recirculating flows are larger than those in Figure 2-(e), and they are extended
 296 from the stagnant regions to the main pathways hence influencing wider areas. Thus, the transmission
 297 of the viscous momentum across successive laminae of the fluid could even occur in the regions with
 298 higher velocities, which results in shifting the distinctive velocity to a higher value.



299 Figure 3. Temporal evolution of the normalised velocity fields within the SC-packed porous structure
 300 at $Re = 9.81$: (a-d) log-linear PDF plot of the normalised velocity magnitude and its components in
 301 the x, y, and z-directions, and (e) the spatial distribution and streamlines of the velocity field at $t^* =$
 302 1.0. The inset in (d) is the log-log plot of the PDF of the normalised velocity magnitude.

303 The PDF of the velocity magnitude and its components at $Re = 98.14$ is illustrated in Figure 4. The
 304 solution convergence is obtained in $t^* = 0.8$, according to Table 1; however, there are still some
 305 differences in the tail of the PDF of the normalised velocity magnitude and its x-direction component
 306 ($<2\%$ of the velocity data). The highest velocities are only found at the converging/diverging region of

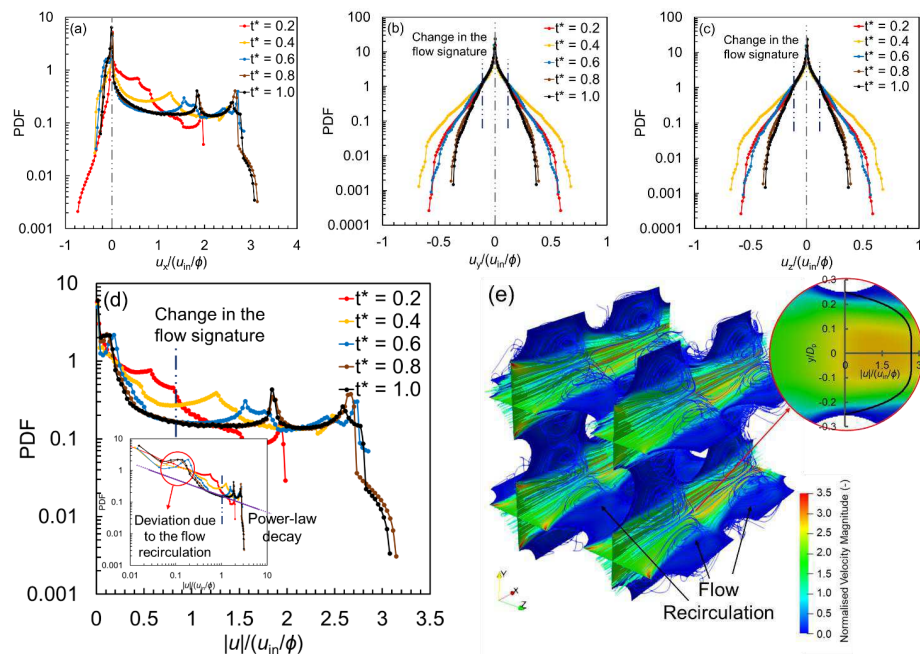
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307 the pore throats (see Figure 4-(e)); therefore, such differences could be due to the flow instabilities at
 308 these regions, a phenomenon captured experimentally at high Re in the other studies^{26,6}.

309 In Figure 4-(a), the PDF of the normalised x-direction velocity can be divided into three main parts:
 310 (i) the negative normalised velocities that are more than 23% of the x-direction velocity data, meaning
 311 the large-scale recirculating flow zones do exist in almost a quarter of the pore space (covering all the
 312 stagnant regions and extending into the main pathways), (ii) the positive normalised velocities lower
 313 than the distinctive value of 1.0 (the interstitial velocity), and (iii) the positive velocities higher than 1.0.
 314 The separation of the positive normalised velocities again confirms there are two distinctive flow
 315 signatures. However, the trend at the velocities higher than the distinctive velocity value is entirely
 316 different from what observed in Figure 2 and Figure 3, suggesting a new flow signature at the main
 317 pathways; this will be discussed in the next paragraph. In Figure 4-(b) and (c), a symmetrical
 318 distribution is observed for the velocity components in the y- and z-directions, and similar to the
 319 previous cases, the distribution of the velocity components lower than the distinctive value of 0.1
 320 should be characterised differently from the higher velocity components in these two directions.



321 Figure 4. Temporal evolution of the normalised velocity fields within the SC-packed porous structure
 322 at $Re = 98.14$: (a-d) log-linear PDF plot of the normalised velocity magnitude and its components in
 323 the x, y, and z-directions, and (e) the spatial distribution and streamlines of the velocity field at $t^* =$
 324 1.0. The inset in (d) is the log-log plot of the PDF of the normalised velocity magnitude.

325 Given the imposed flow is in the x-direction, the PDF of the normalised velocity magnitude is quite
 326 similar to its x-direction component. According to the log-linear PDF plot in Figure 4-(d), the velocities
 327 higher than the interstitial velocity exhibit a Laplace PDF (with two distinguished location parameters
 328 of 1.84 and 2.58), which is entirely different from the exponential behaviour observed for the high
 329 velocities at lower Re . This interesting behaviour can be simply attributed to the fact that a fluid jet
 330 enters the pore space at such a high Re and flows through the main pathways. Since the pore

331 structure is regular and non-tortuous, there is no obstacle to change the flow direction. As a result,
 332 the flow keeps being fully turbulent within these regions and the velocity profile would not become
 333 parabolic, similar to the turbulent velocity profile in pipes⁷³. Therefore, the PDF of the velocity at the
 334 main pathways with the turbulent flow regime changes to the Laplace with the location parameter of
 335 2.58.

336 It should be noted that the Laplace model for the high velocities may not be necessarily observed
 337 in the other porous media as the pore structure can highly influence the trajectory of the main flow
 338 pathways, this will be discussed in Section 3.1.2. The reason for having another location parameter
 339 at 1.84 is that the turbulent flow in the pores located closer to the inlet boundary is still influenced by
 340 the inlet boundary conditions, resulting in a similar distribution but with a lower location parameter,
 341 which could be of particular interest for the studies investigating the effect of the boundary flow in
 342 transport phenomena in porous media. According to the log-log PDF plot in Figure 4-(d), the velocities
 343 lower than 1.0 can be still characterised with a power-law PDF model similar to the results at low Re ,
 344 confirming the presence of a viscous (laminar) flow regime in the vicinity of the solid boundaries with
 345 no-slip boundary conditions, surrounding the turbulent flow regions. The deviations from the power-
 346 law decay around the normalised velocity of 0.1 are also caused by the recirculating flows.

347 As discussed above, the PDF of the velocity magnitude as well as its components in the SC-
 348 packed porous medium must be quantified with two models regardless of Re . Table 2 summarises
 349 the type and parameter(s) of the PDF models fitted to the distribution of the normalised velocity
 350 magnitudes at both low- and high-velocity zones. As can be seen, while the exponent of the power-
 351 law functions in the low-velocity regions (k) does not exhibit any clear sensitivity to Re , the rate
 352 parameter of the exponential functions in the high-velocity regions (λ) becomes higher when Re
 353 increases; a direct proportionality observed at low Re in the other studies^{7,59}.

354 Table 2. Summary of the type and parameter(s) of the models fitted to the PDF of the velocity
 355 magnitudes in the SC-packed porous structure. u^* here the normalised velocity magnitude,
 356 $|u|/(u_{in}/\phi)$.

No.	Re	PDF model		Distinctive normalised velocity magnitude (-)
		Low-velocity zones	High-velocity zones	
1	0.98	$PDF \propto u^{*-k}, k = 0.571$	$PDF \propto e^{-\lambda u^*}, \lambda = 0.936$	1.47
2	9.81	$PDF \propto u^{*-k}, k = 0.559$	$PDF \propto e^{-\lambda u^*}, \lambda = 1.140$	1.80
3	98.14	$PDF \propto u^{*-k}, k = 0.623$	$PDF \propto e^{\frac{ u^*-\mu }{b}}, \mu = 1.84, 2.58$ $b = 3.44, 1.21$	1.00

357
 358

3.1.2 Randomly-packed porous medium

359 We conducted the fluid flow simulations for the randomly-packed porous medium at Re of 1.16,
 360 11.59, and 115.85, extracted the velocity magnitudes and its components, normalised them against
 361 the interstitial velocity, and plotted their sample PDF evolutions at various times in Figure 5, Figure 6,
 362 and Figure 7, respectively, together with the spatial distribution and streamlines of the velocity field at
 363 t_{total} . The average normalised velocity magnitudes at the middle planar sheet perpendicular to the
 364 x-direction, which were used to check the convergence of the solution, are provided in Table 3. These
 365 velocities help with the analysis of the evolution of the velocity fields at different Re and times. The
 366 PDFs are also available in Supplementary Material.

367 Table 3. The average normalised velocity magnitudes at the middle planar sheet perpendicular to
 368 the x-direction in the randomly-packed porous medium at different Re and normalised simulation
 369 times.

No.	Re	Average Normalised Velocity (-)
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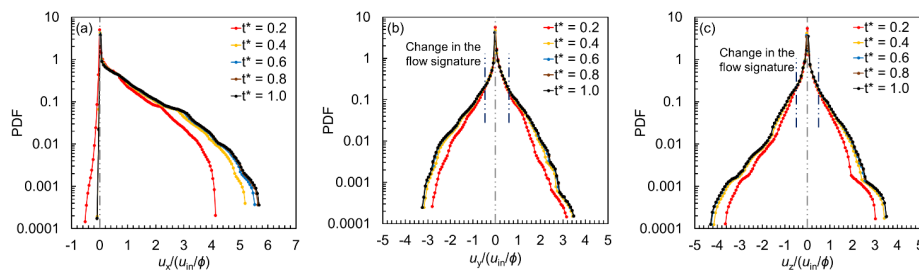
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	$t^* = 0.2$	$t^* = 0.4$	$t^* = 0.6$	$t^* = 0.8$	$t^* = 1.0$
1	1.16	0.81	1.08	1.16	1.17
2	11.59	1.20	1.39	1.25	1.21
3	115.85	1.19	1.65	1.62	1.52

370

371 According to Table 3 and Figure 5, the solution convergence at $Re = 1.16$ is obtained in $t^* = 0.6$.
 372 The PDF of the normalised x-direction velocity in Figure 5-(a) can be divided into (i) the negative
 373 velocities, (ii) the positive velocities lower than 1.0, and (iii) the positive velocities higher than 1.0,
 374 similar to the results in Figure 2-(a) for the SC-packed porous medium. The separation of the positive
 375 normalised x-direction velocities at 1.0 confirms the presence of two different flow signatures. This
 376 separation, however, is not as clear as that of the SC-packed porous medium. It should be noted that
 377 the presence of the negative x-direction velocities here would not be necessarily due to the
 378 recirculating flows, simply because it is likely to have the flow pathways opposite to the imposed flow
 379 direction hence the backflow may occur^{42,43}. Apart from that, the trajectory of the main flow pathways
 380 essentially depends on the arrangement of the solid particles; therefore, the recirculating flows in
 381 directions other than the imposed flow direction may exist in a tortuous porous medium, enhancing
 382 the transport between the main flow pathways and the stagnant zones. The tortuosity of the randomly-
 383 packed porous structure is 1.2 (see⁶⁰), close to that of the SC-packed structure (i.e. 1.0), implying
 384 the main flow pathways must be still aligned with the x-direction. Since almost 0.1% of the x-direction
 385 velocity data are negative, it can be elucidated that there is almost no streamwise flow recirculation
 386 and the Stokes flow is dominant throughout the domain at such a low Re . The evolution of the PDFs
 387 of the normalised velocities in the y- and z- directions are provided in Figure 5-(b) and (c), respectively.
 388 As expected, the distributions are no longer symmetric essentially due to the geometrical asymmetry
 389 of the domain, and two different functions are required to characterise the velocity in both directions.

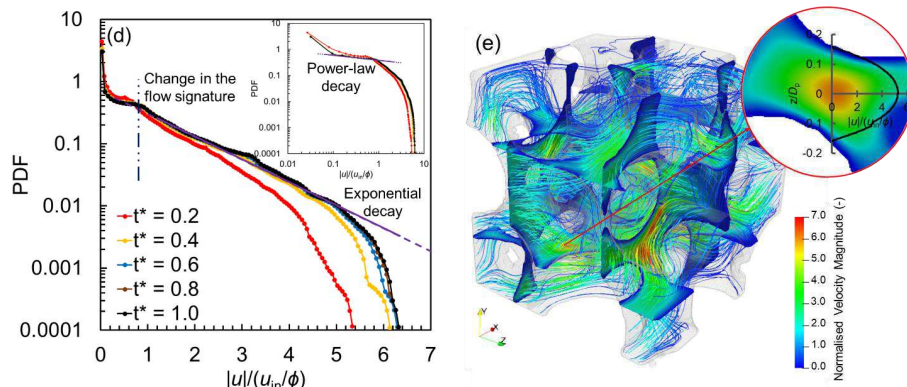
390 The velocity PDFs in Figure 5-(d) exhibit two different signatures, and the distinction point is 1.05.
 391 The velocities higher than this distinction point are required to be characterised with an exponential
 392 PDF model (see log-linear PDF plot) whereas a power-law model describes the PDF of the lower
 393 velocities (see log-log PDF plot).



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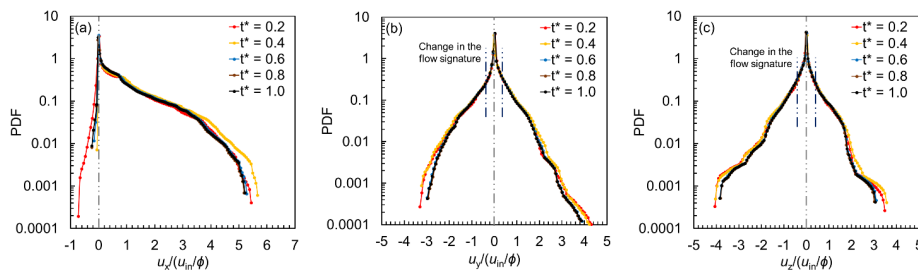
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394 Figure 5. Temporal evolution of the normalised velocity fields within the randomly-packed porous
 395 structure at $Re = 1.16$: (a-d) log-linear PDF plot of the normalised velocity magnitude and its
 396 components in the x, y, and z-directions, and (e) the spatial distribution and streamlines of the
 397 velocity field at $t^* = 1.0$. The inset in (d) is the log-log plot of the PDF of the normalised velocity
 398 magnitude.

399 The evolutions of the PDFs of the normalised velocity magnitude and its components at $Re =$
 400 11.59 are illustrated in Figure 6. According to Table 3, the solution convergence is obtained in $t^* =$
 401 0.6 , and the trends of the PDFs are generally similar to those at $Re = 1.16$. However, a higher number
 402 of the negative x-direction velocity data ($\sim 0.9\%$ of the velocity data) is observed in Figure 6-(a)
 403 compared to those in Figure 5-(a), implying the formation of the recirculating flows at the stagnant
 404 zones. However, these flow structures are not numerous and large enough to influence the flow field;
 405 therefore, no delay in the solution convergence is observed. This fact can also be confirmed by
 406 investigating the separation point of the flow signatures in Figure 6-(d). As observed, the separation
 407 point is 0.82 , lower than that of the previous case, suggesting limited low-velocity zones, in which the
 408 flow is likely to become recirculated, and wider high-velocity regions, where the flow can be
 409 characterised with an exponential PDF model.

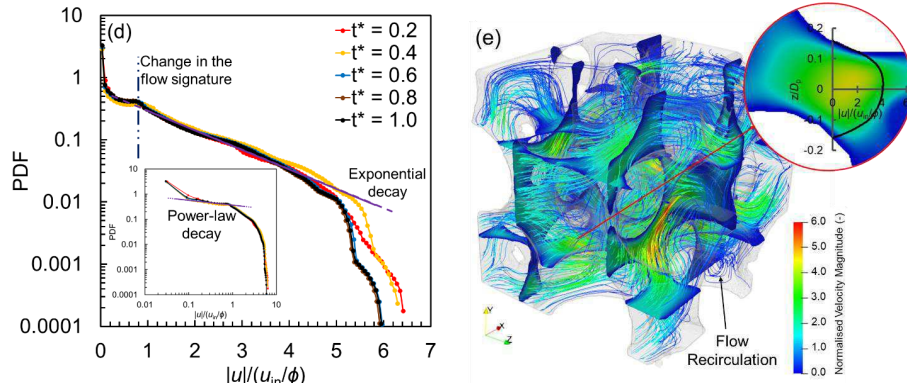
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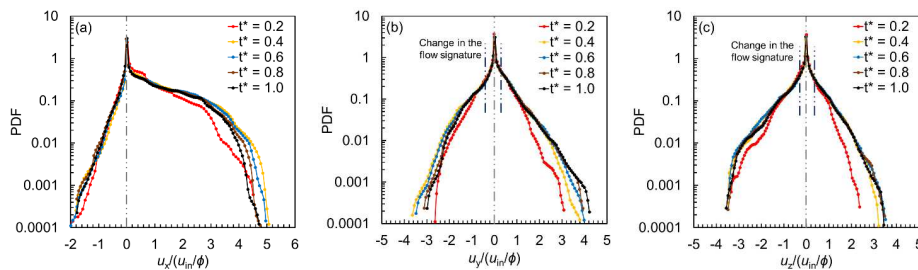
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411 Figure 6. Temporal evolution of the normalised velocity fields within the randomly-packed porous
 412 structure at $Re = 11.59$: (a-d) log-linear PDF plot of the normalised velocity magnitude and its
 413 components in the x, y, and z-directions, and (e) the spatial distribution and streamlines of the
 414 velocity field at $t^* = 1.0$. The inset in (d) is the log-log plot of the PDF of the normalised velocity
 415 magnitude.

416 The PDF of the velocity magnitude and its components at $Re = 115.85$ is illustrated in Figure 7.
 417 As evidenced by the average velocities presented in Table 3, the solution convergence is obtained in
 418 $t^* = 0.8$, and the flow becomes fully developed in many regions. However, there are still discrepancies
 419 in the PDF of the normalised velocity magnitude and its x-direction component at the values higher
 420 than 3.6, covering almost 3.0% of the velocity data. These discrepancies can be related to the
 421 instability of the flow at the converging/diverging pore throats and the large-scale high-velocity vortical
 422 structures in the main flow pathways (see Figure 7-(e)).

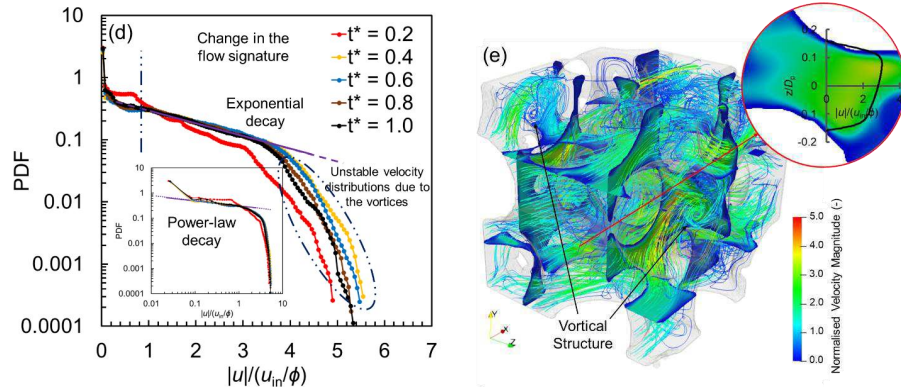
423 The PDF of the normalised x-direction velocities is shown in Figure 7-(a). The separation of the
 424 positive normalised velocities at 0.8 confirms the presence of two distinctive flow signatures (which
 425 will be discussed later). The negative velocities are almost 13% of the velocity data, significantly
 426 higher than those in the lower Re . Moreover, in contrast to the PDF of the velocities shown in Figure
 427 5 and Figure 6 at lower Re , the discrepancies are observed in the tail of the PDF at both negative and
 428 positive x-direction velocities after the convergence of the solution, a behaviour that can be also seen
 429 in the PDF of the normalised velocities in the y- and z-directions (Figure 7-(b) and (c)). Such
 430 discrepancies essentially cannot be caused by the flow recirculation (which would be expected to
 431 form in the stagnant zones), and they are due to the presence of the high-velocity vortical structures
 432 in the main flow pathways, confirming the dominance of the turbulent flow regime.



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433 Figure 7. Temporal evolution of the normalised velocity fields within the randomly-packed porous
 434 structure at $Re = 115.85$: (a-d) log-linear PDF plot of the normalised velocity magnitude and its
 435 components in the x, y, and z-directions, and (e) the spatial distribution and streamlines of the
 436 velocity field at $t^* = 1.0$. The inset in (d) is the log-log plot of the PDF of the normalised velocity
 437 magnitude.

438 The log-linear PDF plot of the normalised velocity magnitude in Figure 7-(d) is fairly similar to that
 439 of the x-direction velocity, as expected, and an exponential function can be used to characterise the
 440 velocity distribution, in contrast to what observed for the SC-packed structure in Figure 4-(d). The
 441 underlying reason for such a different flow signature is that the main flow pathways in the SC-packed
 442 medium are all aligned with the imposed flow direction. Thus, the velocity profile of the fluid jet entering
 443 this non-tortuous structure would not be disturbed significantly by the solid boundaries. Consequently,
 444 the flow keeps its turbulent (non-parabolic) characteristics when flowing in the main pathways, a
 445 Laplace function can be used to characterise the flow in these regions, and obvious boundaries would
 446 be created between the low- and high-velocity zones, all perpendicular to the imposed flow direction.
 447 On the other hand, when the fluid flows in the randomly-packed medium with a higher tortuosity (i.e.
 448 more disturbances from the solid boundaries), the flow cannot keep its non-parabolic characteristics
 449 and its velocity profile becomes influenced by the no-slip boundary conditions hence an exponential
 450 decay is observed in the PDF of the velocities, similar to the results for lower Re .

451 As discussed above, the distribution of the velocity magnitude and its components in the
 452 randomly-packed porous medium must be quantified with two functions at various Re . The type and
 453 parameter(s) of the PDF models fitted to the distribution of the normalised velocity magnitudes at both
 454 low- and high-velocity zones are summarised in Table 4. In the low-velocity regions, it is observed
 455 that k still does not show a clear and strong sensitivity to Re whereas comparing its values to those
 456 reported in Table 2 reveals its dependence on the pore structure, suggesting the evolution of the
 457 distribution of the velocity magnitude from power-law toward flat and uniform behaviour when the
 458 heterogeneity increases. It should be noted that the flat distribution of the velocity in the low-velocity
 459 zones has been observed in the other studies^{43,74}. In the high-velocity regions, λ shows an inverse
 460 proportionality to Re , in contrast to the observations in Table 2. Such a contradiction suggests that λ
 461 must be sensitive to both Re and the tortuosity of the porous structure.

462 Table 4. Summary of the type and parameter(s) of the models fitted to the PDF of the velocity
 463 magnitudes in the randomly-packed porous structure. u^* here the normalised velocity magnitude,
 464 $|u|/(u_{in}/\phi)$.

No.	Re	PDF model
-----	------	-----------

	Low-velocity zones	High-velocity zones	Distinctive normalised velocity magnitude (-)
1	1.16 $PDF \propto u^{*-k}, k = 0.218$	$PDF \propto e^{-\lambda u^*}, \lambda = 0.835$	1.00
2	11.59 $PDF \propto u^{*-k}, k = 0.291$	$PDF \propto e^{-\lambda u^*}, \lambda = 0.773$	0.82
3	115.85 $PDF \propto u^{*-k}, k = 0.316$	$PDF \propto e^{-\lambda u^*}, \lambda = 0.507$	0.80

465

466 As discussed above, the negative x-direction velocities can be directly correlated to the flow
 467 recirculation. Thus, the effect of the pore space heterogeneity on the formation of the recirculating
 468 flow structures can be understood by comparing the distribution of the negative x-direction velocities
 469 of the randomly-packed structure with that of the SC-packed medium. Referring to the PDF of the
 470 velocities, the fractions of the negative x-direction velocities in the SC-packed porous structure are
 471 markedly higher than those in the randomly-packed structure. This evidently demonstrates that it is
 472 more likely to observe the flow recirculation in the wake of grain particles in the orderly-packed
 473 structures, where the trajectory of the main flow pathways is less distorted, and there are clear
 474 boundary surfaces between the low-velocity stagnant zones and the high-velocity main pathways;
 475 this will be discussed further in Section 3.2.

476

3.2 Analysis of the flow in the low-velocity regions

477

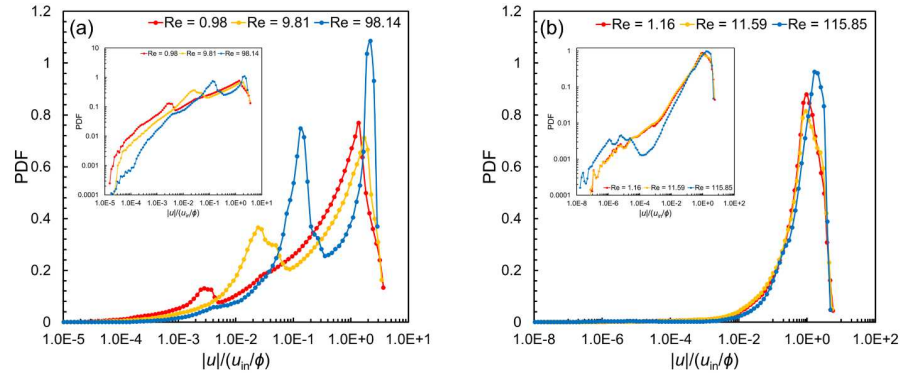
478 In Section 3, the analysis of the PDF of the velocity magnitude and its components in both porous
 479 structures at different Re confirmed that two different PDF models should be employed to characterise
 480 the flow field in porous media, regardless of the packing and heterogeneity of the porous structure.
 481 Referring to the velocity PDF data at different Re indicates that at least more than 65% and 45% of
 482 the velocity magnitudes in the SC- and randomly-packed structures are lower than the distinction
 483 point of the flow signatures, respectively. We provide further insights into the features of the velocity
 484 distribution at the low-velocity regions because it essentially controls the longitudinal dispersion of the
 485 scalar parameters being transported in porous media⁷⁵⁻⁷⁷. The PDF of the converged normalised
 486 velocity magnitudes, sampled uniformly in bins of their logarithm, for both SC- and randomly-packed
 487 porous structures are provided in Figure 8, on semi- and doubly-logarithmic axes. As observed, the
 488 flow signatures at lower velocities are quite similar to each other, exhibiting a tube-like behaviour, see
 489⁵⁹, which is expected since both porous structures are not heterogeneous. Besides, the characteristics
 489 of the flow in the two lower Re , where the flow regime is laminar, are closer to each other at the high
 490 normalised velocities, compared to the trend observed for the highest Re , where the flow becomes
 491 turbulent. In particular, it can be seen that the change of the flow behaviour from laminar to turbulent
 492 regime results in the spread of the high-velocity peak becoming narrower, taller, and occurring at a
 493 higher normalised velocity.

494

495 The insights into the effect of the pore structure on the flow behaviour can be obtained via
 496 investigating the trend and the range of the velocity PDFs. As observed in Figure 8-(a), the PDF of
 497 the normalised velocity in the SC-packed medium exhibits a bimodal behaviour, and the variations of
 498 the velocities are almost six orders of magnitude ($10^{-5} - 10^1$), regardless of Re . The bimodal trend of
 499 the velocity PDF is expected because there are clear and connected boundary surfaces between the
 500 low-velocity stagnant zones and the high-velocity main pathways; these boundaries have been
 501 observed in the other experimental and modelling works studying transport in the homogeneous
 ordered porous structures^{72,78,79}.

502

503 It is also observed that the first peak, representing the recirculating flow structures, becomes taller
 504 and shifts toward higher normalised velocity values when Re increases. This behaviour supports our
 505 discussion regarding the effect of Re on the size of the recirculating flows and their velocities
 presented in Section 3.1.1.



506 Figure 8. Probability density function (PDF) of the converged velocity magnitudes for the (a) SC-
 507 packed and (b) randomly-packed porous structures on semi-logarithmic axes. The inset in each plot
 508 is the same PDF on doubly logarithmic axes.

509 In Figure 8-(b), a unimodal trend is observed for the PDF of the velocity in the randomly-packed
 510 medium at different Re and the variations of the velocities are almost nine orders of magnitude (10^{-8}
 511 $- 10^1$). The unimodal trend of the velocity PDF indicates the random arrangement of the solid particles
 512 has caused the formation of a limited number of recirculating flow structures. Comparing the trend
 513 and wider variations of the velocity PDF in the randomly-packed medium to that of the SC-packed
 514 medium confirms that the tortuosity, even being small, plays a key role in controlling the spatial
 515 distribution and size of the low- and high-velocity regions as well as the possibility of formation of
 516 different flow structures in the pore space. Such distinctive characteristics are essential to be
 517 considered when studying the transport of the scalar phenomena in porous media as they are
 518 inherently influenced by the flow signature.

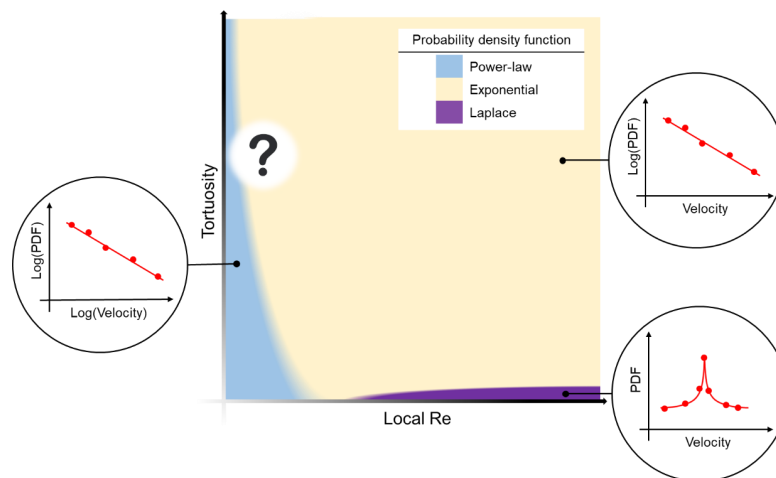
519 **3.3 Tortuosity and local Re : The key parameters to understanding different flow**
 520 **signatures in porous media**

521 The analysis of the PDFs in the previous sections indicates that the flow characteristics in a given
 522 porous medium depend upon the competition of the viscous and inertial driving forces as well as the
 523 geometry of the pore structure. Therefore, the type and extent of the flow signatures can be correlated
 524 to the tortuosity and flow rate. In this section, according to the insights obtained in the previous
 525 sections into the effect of the flow regime and pore structure on the flow behaviour, we propose a
 526 general framework for determination of the most possible flow signatures and their velocity PDFs in
 527 a packed-bed porous structure with respect to its tortuosity and local Re .

528 Figure 9 illustrates the colour map of the PDFs versus the tortuosity and local Re . As evidenced
 529 by our discussion in the previous sections, the flow in porous media can be described with three
 530 possible velocity PDFs:

- 531 i. Power-law PDF: Regardless of the tortuosity, the power-law PDF is most likely to be found
 532 in the vicinity of the solid boundaries and the stagnant regions (such as dead-end pores
 533 or the wake of the solid particles), where the local Re is small and the flow is highly
 534 influenced by the solid-fluid interface. In addition, analysis of the distinction points at which
 535 the PDF of the velocity changes from the power-law (to either exponential or Laplace)
 536 shows that increasing the tortuosity results in shrinkage of the range of the power-law PDF
 537 dominance. It should be noted that investigations on the flow characteristics in highly-

- 538 tortuous and heterogeneous structures are required to provide reliable insights into high-
 539 tortuosity conditions.
- 540 ii. Exponential PDF: The exponential PDF can be found in the main pathways where the fluid
 541 flows with a higher velocity and the effect of the inertia is not negligible. The prevalence of
 542 this flow signature in an individual pore highly depends on the extent the viscous forces
 543 can be transmitted from the solid-fluid interface toward the pore centre and shape the
 544 velocity profile. Therefore, the exponential PDF would be expected to be seen in the main
 545 pathways of tortuous porous media at moderate and high local Re while at non-tortuous
 546 media, it is likely to be found only at moderate local Re .
- 547 iii. Laplace PDF: This PDF can only be seen in the main pathways of non-tortuous porous
 548 media at the high local Re where there is almost no solid obstacle in front of the flow and
 549 the velocity profile is non-parabolic.



550
 551 Figure 9. Proposed colour map of the PDFs of the velocity fields as a function of the tortuosity and
 552 local Re .

553 It should be noted that the above framework is qualitative and created based on the analysis of
 554 the velocity PDFs in backed-bed structures; therefore, its application in its current form might only be
 555 limited to the fields concerned with packed-bed porous media. We believe more modelling and
 556 experimental studies with a focus on the other potential key factor such as porosity, surface
 557 roughness, and particle size distribution assist with obtaining a better understanding of the flow
 558 dependency on the properties of the host medium. The fruits of these future studies are essential
 559 to be used for quantifying the proposed framework. Geostatistical analysis of the velocity data can also
 560 help with establishing a robust correlation between the microscale flow details and the macroscale
 561 effective properties such as permeability in different regimes.

562 **4. Conclusions**

563 In this work, we conducted single-phase fluid flow simulation using LBM to shed light on the pore-
 564 scale flow characteristics in 3D SC- and randomly-packed porous structures. The ultra-fine mesh size
 565 considered in the simulations made it possible to carry out the simulations at three orders of
 566 magnitude of Re , covering laminar to turbulent flow regimes, and capture different flow signatures.
 567 The following conclusions can be drawn from this study:

- 568 i. Regardless of the pore structure, the pore velocity fields in porous media at different Re cannot
 569 be characterised with a single PDF because the flow signature at the main pathways, where the
 570 velocity magnitudes are higher hence most of the fluid transport is carried, is different from that
 571 of the low-velocity regions such as the wake of the solid particles and the vicinity of the solid
 572 boundaries, where the velocity is lower. These flow signatures exhibit their own specific behaviour
 573 in the PDF plot of the velocity magnitude, and there is always a distinction point, at which the
 574 velocity PDFs meet.
 575 ii. The velocities lower than the distinction point can be characterised by a power-law PDF model
 576 for both SC- and randomly-packed porous media. The velocities higher than the distinctive value,
 577 however, should be described with a different PDF model. The analysis of the PDFs of the
 578 velocities suggests the exponential model when Re is low and the flow is laminar. When Re is
 579 high and the flow is turbulent, the velocity exhibits a Laplace PDF for the SC-packed medium with
 580 the tortuosity of 1.0, owing to the fact that the main flow pathways are all aligned with the imposed
 581 flow direction. For the randomly-packed medium with the tortuosity of 1.2, however, the flow
 582 signature is quite similar to that of lower Re hence could be characterised by an exponential PDF
 583 model.
 584 iii. As expected, the PDF of the positive x-direction velocities have the same characteristics as those
 585 of the velocity magnitudes. The presence of the negative x-direction velocities can be due to
 586 recirculating flows oriented in the flow direction, vortical structures, or simply backflow. It was
 587 observed that the negative velocities are created due to the flow recirculation at the stagnant
 588 regions for the non-tortuous SC-packed medium while they are caused by the backflow at low Re
 589 and vortical structures at highest Re .
 590 iv. Analysis of the velocity data in y- and z- directions shows that the velocity components
 591 perpendicular to the imposed flow direction should be also characterised by two different PDFs,
 592 and there is a distinctive point in these directions too.
 593 v. Analysis of the flow in the low-velocity zones shows that the distribution of the velocities in these
 594 regions as well as the boundary between the low- and high-velocities highly depends on the
 595 arrangement of the solid particles and tortuosity of the porous structure. For the SC-packed
 596 medium, the regular arrangement of the solid particles causes a clear and connected boundary
 597 to form between these two flow signatures. Such a clear boundary, however, does not exist for
 598 the randomly-packed tortuous medium.
 599

600 5. Supplementary Material

601 The PDFs of the velocities (magnitude as well as components) for both SC- and randomly-packed
 602 porous media can be found in Supplementary Material. All the figures reported in Section 3 have been
 603 extracted by referring to and analysing these PDF data.

604 6. Acknowledgement

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 606 (EP/R511808/1).

607 7. Appendix A: Validation of the code

608 Fluid flow through a cylindrical tube driven by a pressure gradient known as Poiseuille flow is
 609 extensively used as a benchmark to verify the accuracy and convergence of various CFD methods
 610 ^{51,52}. The exact analytical solution for Poiseuille flow in a cylindrical coordinate can be expressed as
 611 ⁸⁰:

$$u_x(r) = \frac{1}{4\nu} \left(-\frac{\partial p}{\partial x} \right) (R^2 - r^2) \quad (\text{A1})$$

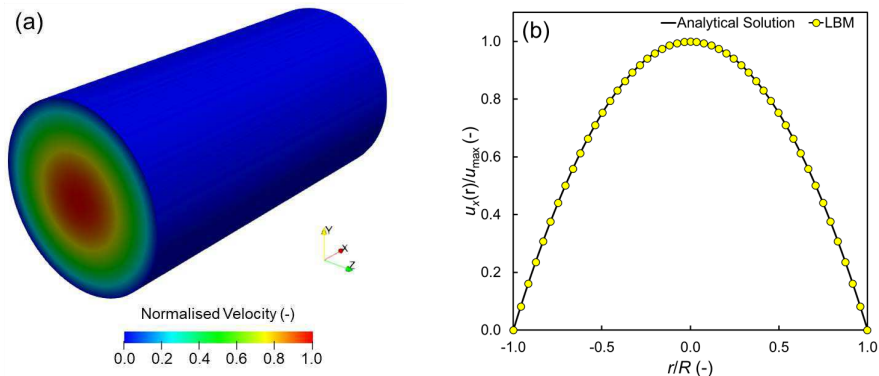
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612 where $u_x(r)$ is the axial velocity, $\frac{\partial p}{\partial x}$ is the pressure gradient, R is the radius of the cylindrical tube,
 613 and r is the distance from the centreline of the tube.

614 We validated the developed code by simulating Poiseuille flow in a cylindrical tube (having the
 615 diameter of $100\ \mu\text{m}$ and resolution of $1\ \mu\text{m}$ per lattice length) and comparing the velocity profile along
 616 the diameter of the tube against that of the analytical solution. The results are presented in Figure A1,
 617 showing that the normalised velocities in the x-direction obtained from the numerical solution agree
 618 perfectly with the exact analytical solution.



619 Figure A1. Poiseuille flow through a cylindrical tube: (a) normalised velocity field obtained via the
 620 numerical simulation, and (b) comparison between the velocity profiles along the diameter of the
 621 tube obtained via the numerical simulation and the exact analytical solution.

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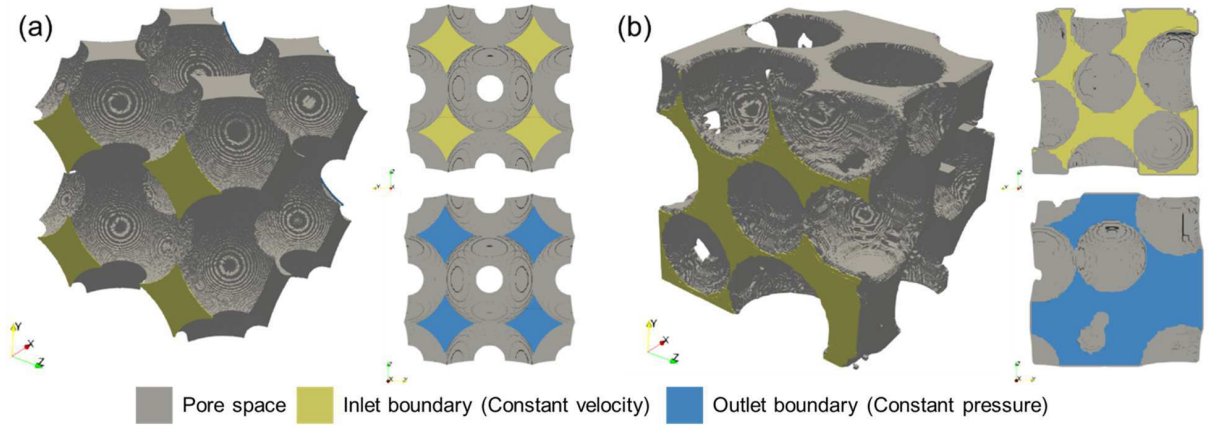
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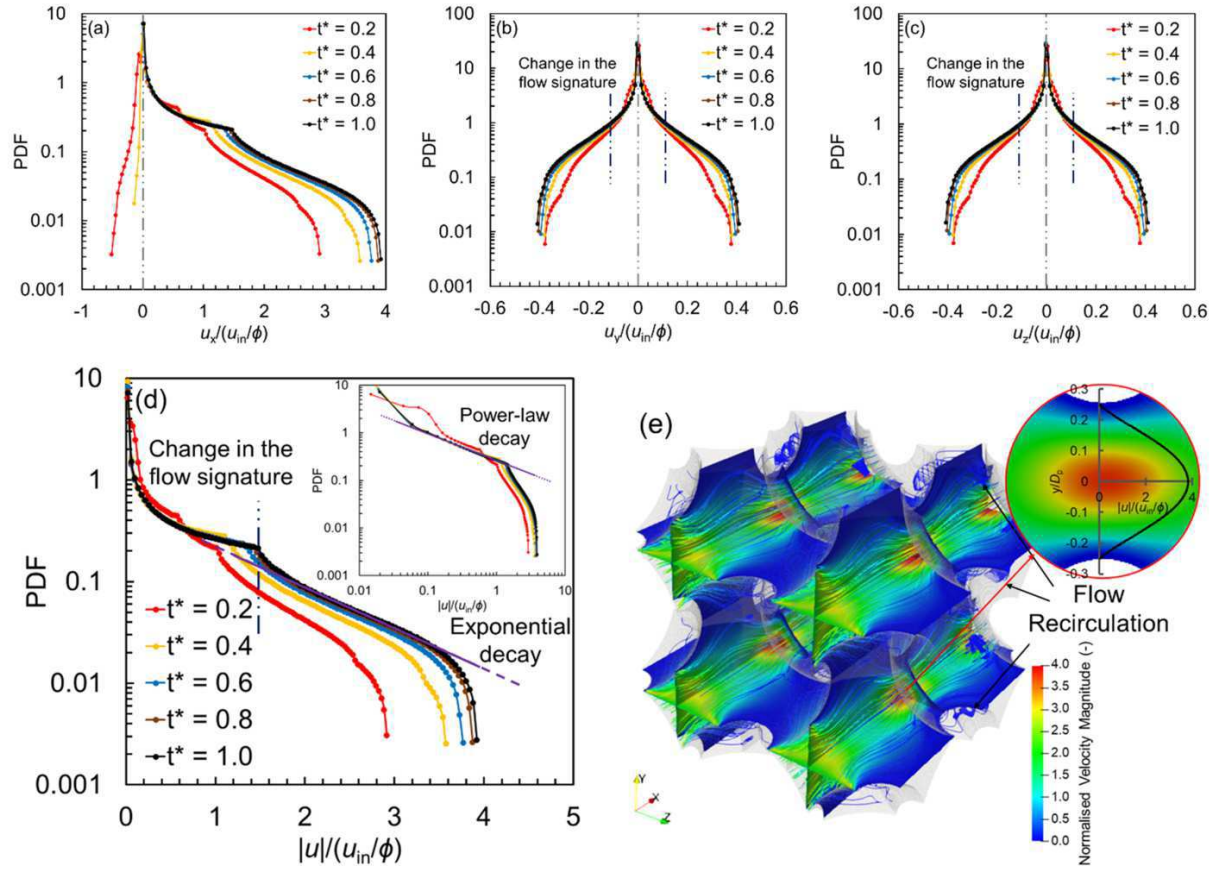
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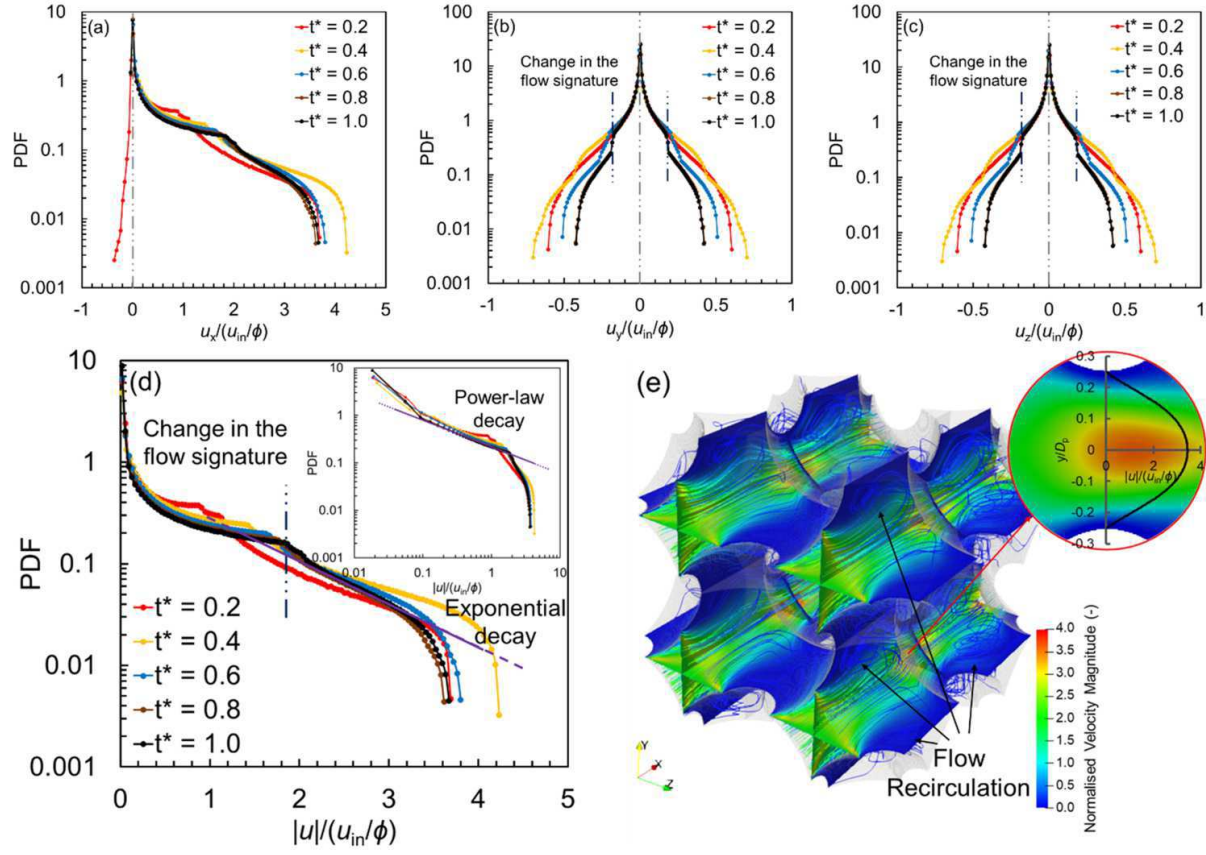
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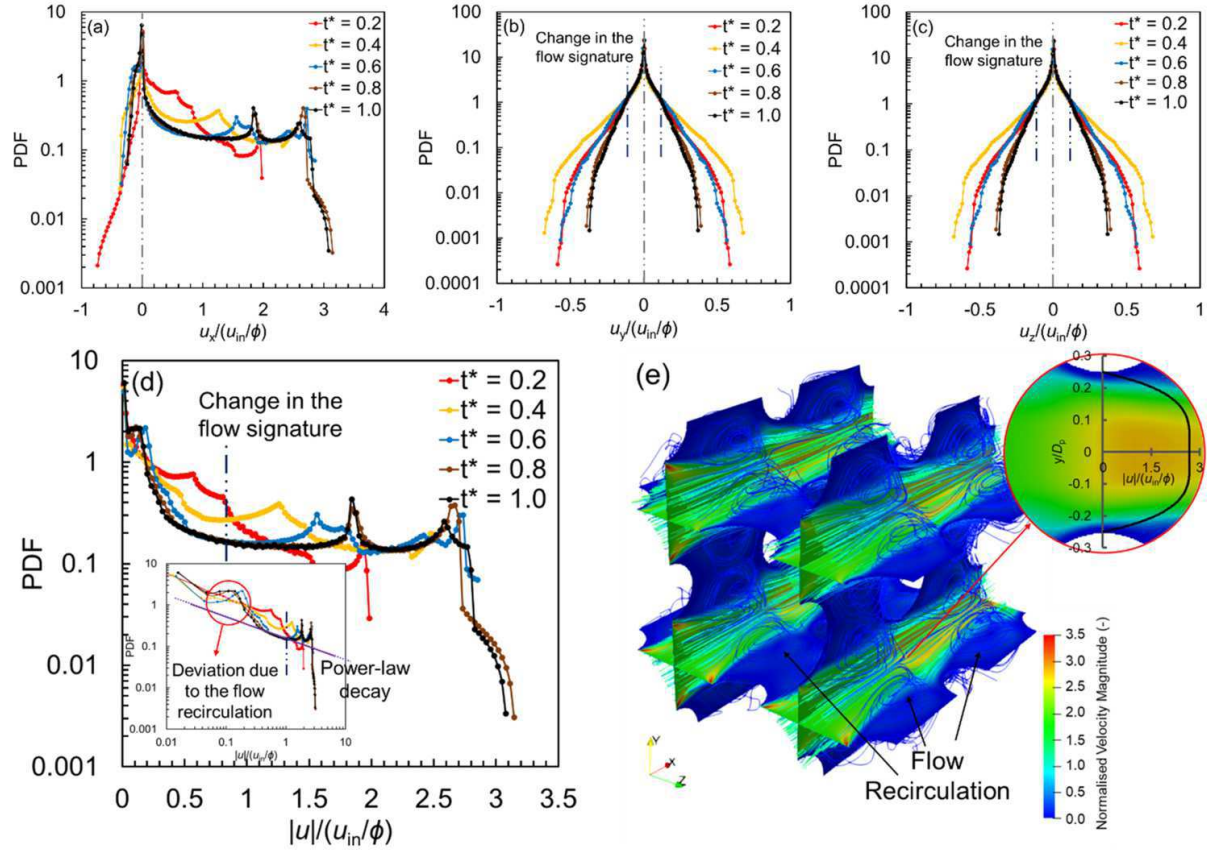
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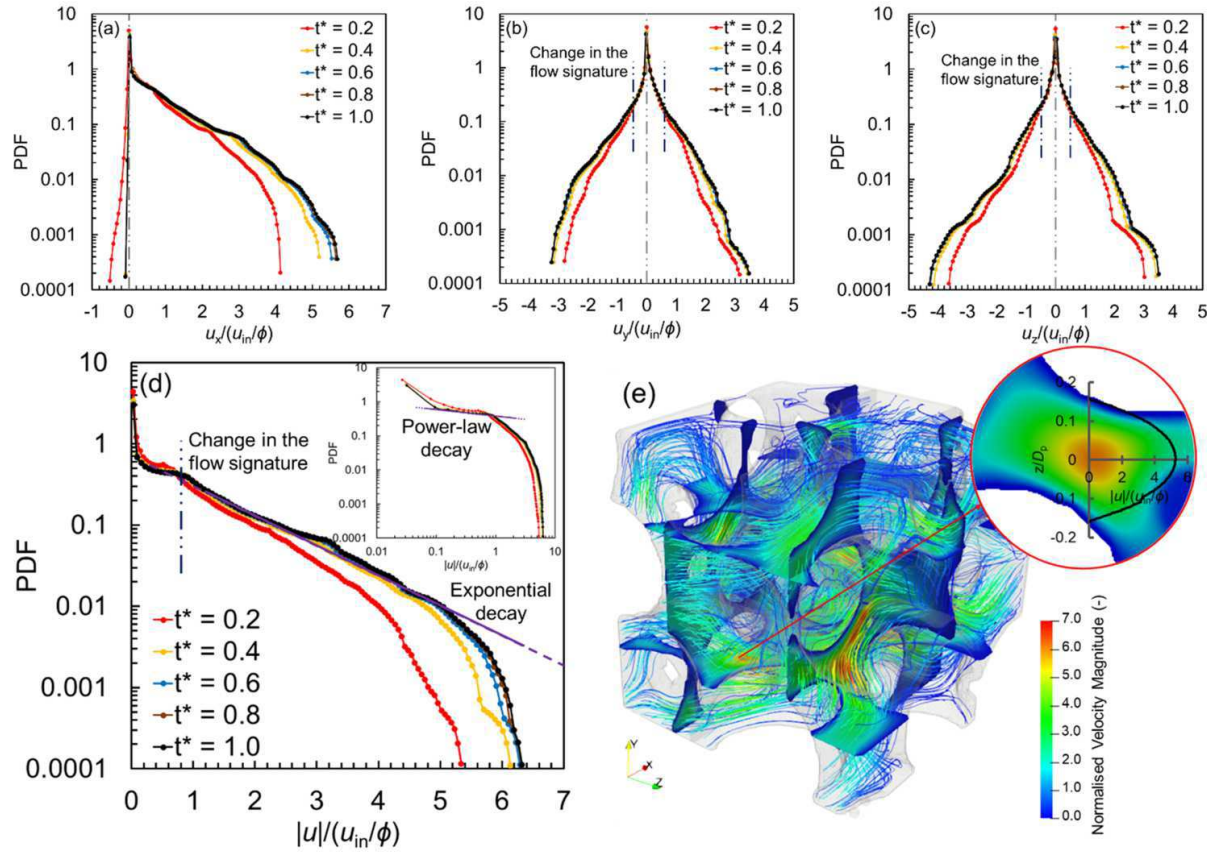
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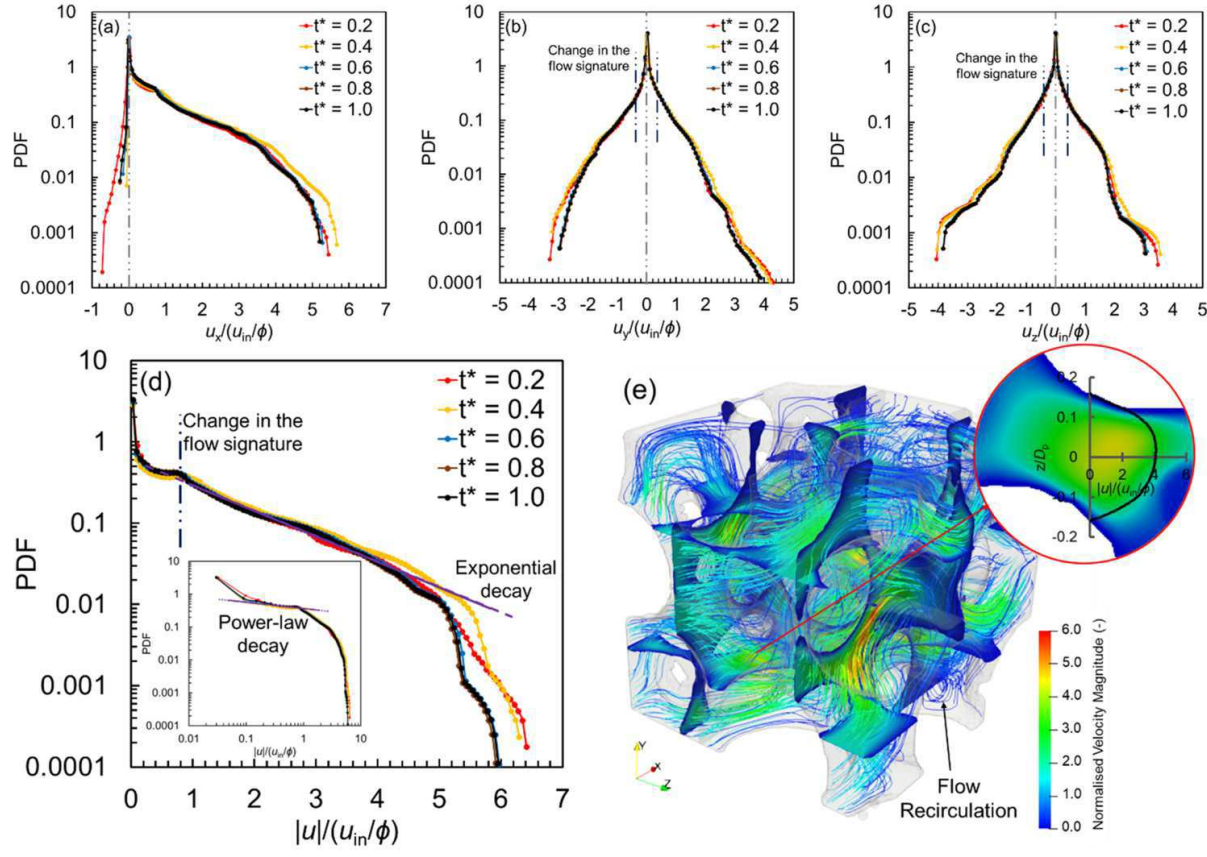
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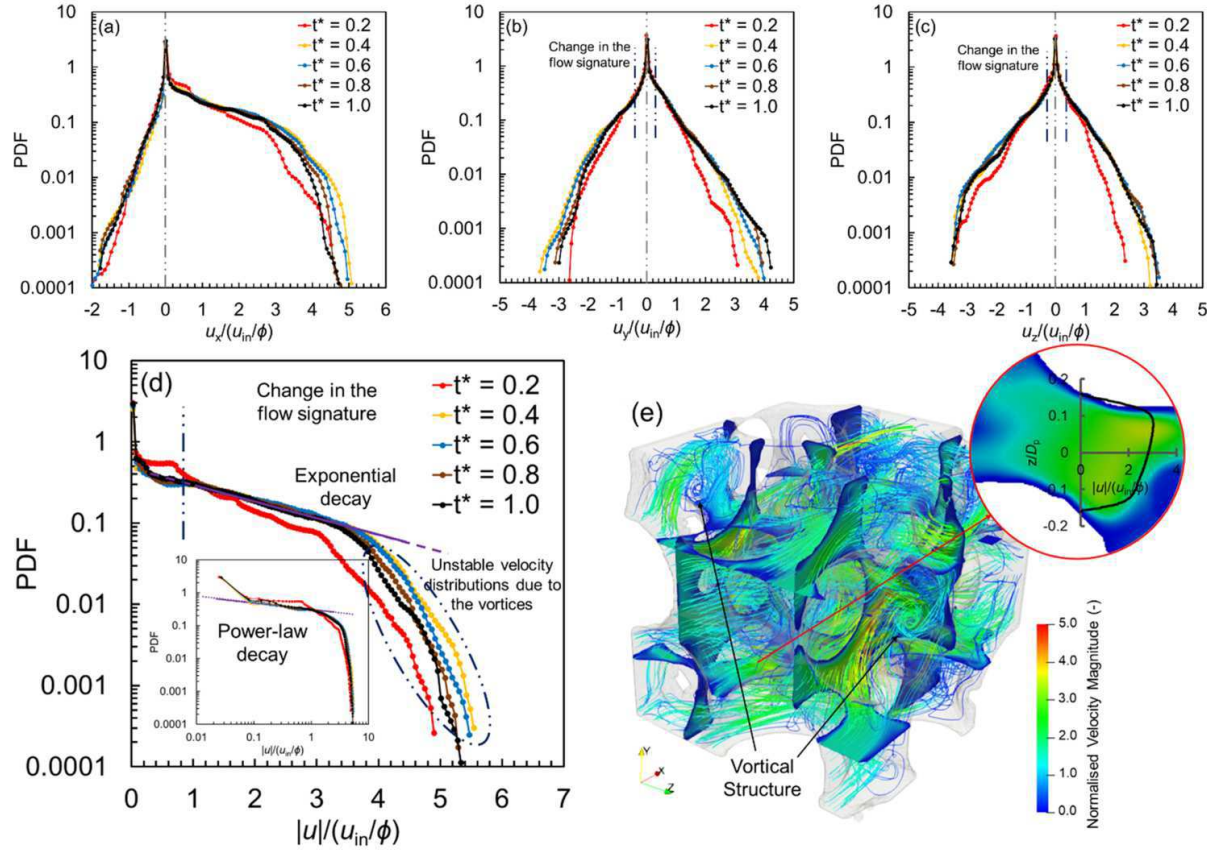
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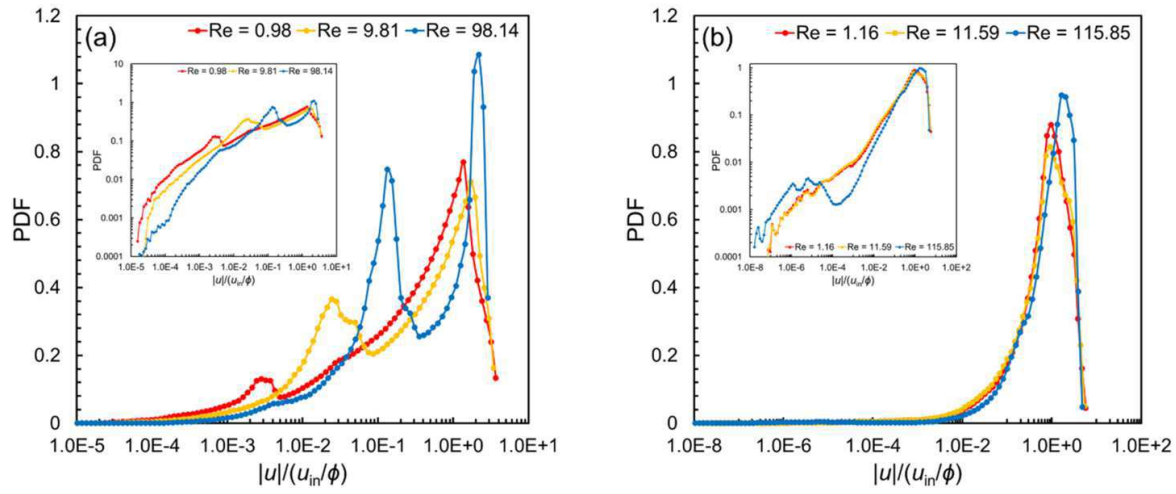
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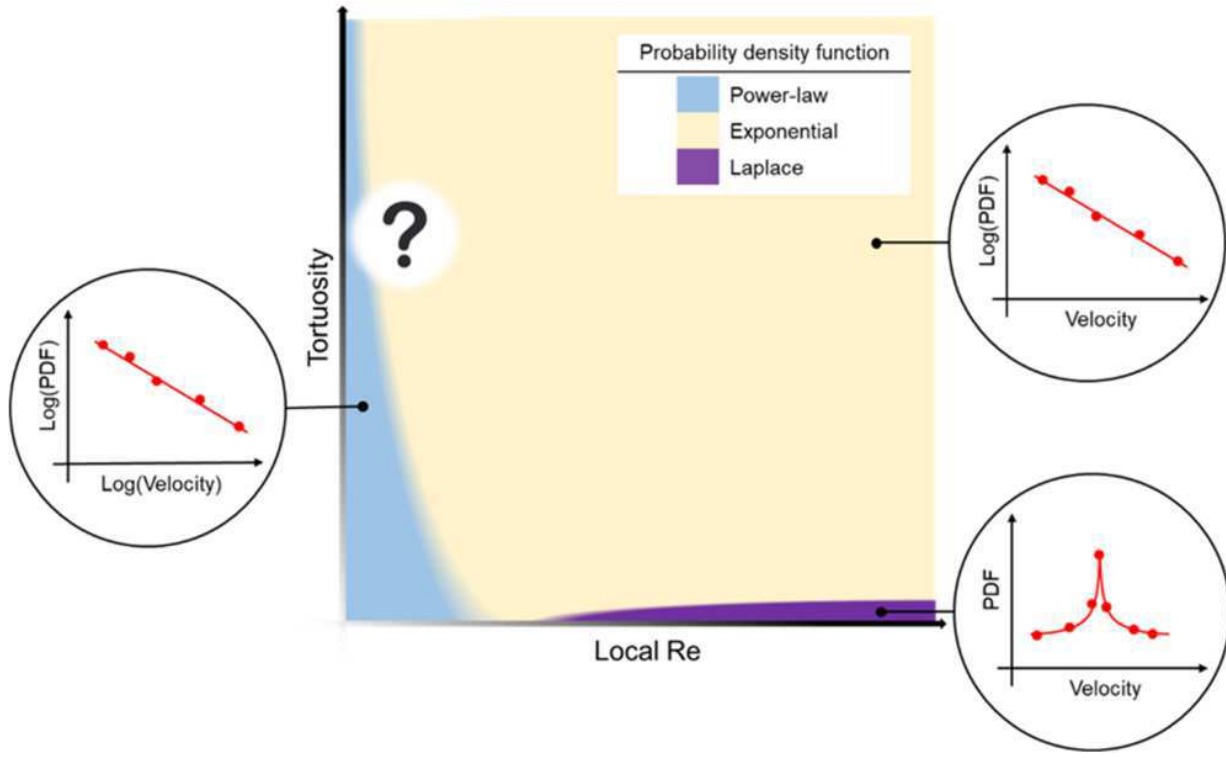
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