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**Berichte des Fachgebiets für Strömungsmechanik  
Uwe Janoske (Hrsg.)**

Markus Bürger

**AN IMMERSED BOUNDARY  
METHOD FOR ARBITRARILY  
SHAPED LAGRANGIAN BODIES**



# **An Immersed Boundary Method for Arbitrarily Shaped Lagrangian Bodies**

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to obtain a doctoral degree (Dr.-Ing.)**

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TO MY FAMILY



# Preface

This dissertation was written during my time as a research associate at the Chair of Fluid Mechanics of the University of Wuppertal.

First of all, I would like to express my sincere gratitude to Prof. Dr.-Ing. habil. Uwe Janoske, whose expertise was invaluable in formulating the research questions and methodology. He continuously provided insightful discussions and feedback but also gave me the freedom to pursue my own questions and approaches. I also like to thank Prof. Dr.-Ing. Martin Böhle for kindly preparing the second report.

I would like to acknowledge all my colleagues from the Chair of Fluid Mechanics, with whom I shared moments of challenge, enthusiasm, and excitement. I will never forget our coffee breaks together. Special thanks to my colleague and friend Dr.-Ing. Uwe Fechter for proof-reading and helping me to prepare myself for my defense.

Further, I give thanks to Dr.-Ing. Carsten Dehning who sparked my interest in scientific work, unceasingly insisted on obtaining my doctorate, and finally never got tired of pushing me forward in my work.

A very special word of thanks goes to my family. You have been great over the years and never raised an eyebrow when I claimed my dissertation would be finished 'in the next two months' for nearly two years. To conclude, I want to thank you for all your unconditional support, loving encouragement, and inexhaustible patience in all these years.





# Kurzfassung

Ein großer Schwerpunkt der mechanischen Verfahrenstechnik befasst sich mit der Behandlung von Partikeln. Darunter fallen insbesondere der Transport, das Mischen und das Separieren bzw. Filtrieren von Partikeln. In der Regel werden in diesen Modellen die Partikel durch Punktmassen abgebildet und die Partikel-Fluid-Interaktion durch Widerstands- und Impulsaustauschmodelle unter der Annahme simpler, meist sphärischer Partikel herbeigeführt. Der Vorteil dieser Herangehensweise ist die in Bezug auf Speicherbedarf und Rechenaufwand kostengünstige Möglichkeit, eine sehr große Partikelzahl zu simulieren. Auf der anderen Seite werden Details wie Partikelgeometrie und das Strömungsfeld am Partikelrand nicht berücksichtigt. Aus dieser Situation heraus entstand die Motivation für diese Arbeit, welche eben solche Detailinformationen für partikelbehaftete Strömungen liefert. Die grundlegende Idee für diese Arbeit war die Anwendung der Immersed Boundary Methode. Dadurch ist es möglich, unabhängig vom zugrundeliegenden Rechengitter, Partikel mit beliebiger Geometrie in das Simulationssystem einzubetten.

Für detaillierte Partikelsimulationen mit beliebiger Partikelgeometrie wurde in dieser Arbeit **ABSFoam**, das Arbitrary-Body Simulation Toolkit für **OpenFOAM**<sup>®</sup>, entwickelt. Dabei war das Ziel, ein möglichst modulares, vielseitig anwendbares und erweiterbares Werkzeug zu schaffen, maßgebend.

Eine Reihe von Testfällen zeigt neben der vielseitigen Anwendbarkeit auch, dass **ABSFoam** valide Ergebnisse liefert. So wird zunächst an sphärischen Partikeln demonstriert, dass Widerstand und Auftrieb in der Scherströmung korrekt berechnet werden. Anschließend werden eine Reihe nichtsphärischer Partikel in der Scherströmung betrachtet. Die Rotationsgeschwindigkeit in Abhängigkeit des Schergradienten und die Variation der Rotationsgeschwindigkeit während einer Umdrehung stehen im Mittelpunkt der Beobachtung. Dem Fall von komplexgeometrischen, makroskopischen Körpern widmet sich der dritte Validierungsfall. Hier wird eine Kugelschüttung bestehend aus mehreren tausend Partikeln als ein komplexes geometrisches Objekt durchströmt. Die errechneten Druckverluste der Durchströmung werden mit

experimentellen Daten und einschlägig bekannten Annäherungsformeln verglichen. Der vierte Testfall dient nicht der Validierung. Vielmehr verdeutlicht er den Bedarf an detaillierten Partikelsimulationen. Es werden Partikeltrajektorien im Spalt eines Tellerseparators untersucht und dabei die Abscheideeigenschaft von Partikeln unterschiedlicher Geometrie untersucht.

# Abstract

A major focus of mechanical process engineering lies on handling particles. Particularly, this includes the process of transport, mixing, separation and filtration of particles. Usually, the particles are represented by point masses and the particle–fluid interaction is realised through resistance and momentum exchange models under the assumption of simple or even spherical particles. In terms of memory and computational effort, these methods are very cheap and efficient and allow simulations with a large number of particles. On the other hand, details such as particle geometry and the flow field in the particles’ vicinity is not taken into account. This situation was the motivation for this work which provides the desired detailed information for particle-laden flows. The basic idea of this work was the application of the immersed boundary method. Thus it is possible—independently of the underlying computational grid—to embed particles of any geometry into the simulation system.

**ABSFoam**, the Arbitrary–Body Simulation Toolkit for **OpenFOAM**<sup>®</sup>, was developed in this thesis for detailed particle simulations with arbitrary particle geometry. Further, the goal was to create a modular, versatile and expandable tool.

A number of test cases show the versatile applicability of **ABSFoam**, and the ability to provide valid results is also demonstrated. Based on spherical particles, it is first illustrated that lift and drag are accurately calculated in the shear flow field. Afterwards, a number of non-spherical particles are considered. Here, the rotational speed as a function of the shear gradient and the variation of the rotation speed during a single revolution are the center of attention. The third validation case is dedicated to geometrically complex, macroscopic bodies. In this case, a particle bed consisting of thousands of particles represents a geometrically complex object. The simulated pressure drops of the flow through these particle beds are then compared to experimental data and theoretical formulas. The last test case is not dedicated to validation. It rather raises the need for detailed particle simulations. The focal points of the observations are particle trajectories in the gap of disc stack separators and the variation of separation efficiency according to different particle geometries.



# Contents

<b>Preface</b>	<b>I</b>
<b>Kurzfassung</b>	<b>III</b>
<b>Abstract</b>	<b>V</b>
<b>List of Figures</b>	<b>IX</b>
<b>List of Tables</b>	<b>XI</b>
<b>List of Symbols</b>	<b>XIII</b>
<b>1 Introduction</b>	<b>1</b>
1.1 Notations and naming conventions . . . . .	2
1.2 Basic principles of Lagrangian multiphase systems . . . . .	3
1.3 The Immersed boundary method (IBM) . . . . .	5
1.3.1 The continuous forcing approach . . . . .	6
1.3.2 The discrete forcing approach . . . . .	10
1.3.3 The cut–cell finite–volume method . . . . .	19
1.4 The discrete element method (DEM) . . . . .	21
1.4.1 Hydrodynamic force . . . . .	22
1.4.2 Hydrostatic force . . . . .	25
1.4.3 Contact force . . . . .	26
1.4.4 Conservative force . . . . .	26
1.4.5 Other forces . . . . .	27
1.5 Stokesian dynamics (SD) . . . . .	28
1.6 The level–set method . . . . .	29
1.7 The chimera grid or overset mesh method . . . . .	31
1.8 Continuous grid adaption . . . . .	32
1.9 Tabular overview of literature . . . . .	32
1.10 About this work . . . . .	35

<b>2</b>	<b>Simulation model</b>	<b>39</b>
2.1	Implementation of the immersed boundary method . . . . .	39
2.1.1	Software architecture . . . . .	39
2.1.2	Numerical approach . . . . .	46
2.1.3	Parallelisation and efficiency issues . . . . .	52
2.2	Implementation of potential forces . . . . .	59
2.2.1	General consideration . . . . .	59
2.2.2	Numerical calculation by surface integration . . . . .	62
<b>3</b>	<b>Numerical studies and validation</b>	<b>67</b>
3.1	Lift and drag of spherical particles . . . . .	68
3.1.1	Computational setup . . . . .	69
3.1.2	Results . . . . .	70
3.2	Rotation of non-spherical particles . . . . .	71
3.2.1	Computational setup . . . . .	73
3.2.2	Results . . . . .	74
3.3	Flow resistance of packed beds . . . . .	77
3.3.1	Description of flow and pressure drop in packed beds . . . . .	77
3.3.2	Construction of packed beds . . . . .	80
3.3.3	Conducted experiments and their results . . . . .	81
3.3.4	Computational setup . . . . .	83
3.3.5	Results . . . . .	86
3.4	Properties of heteromorphic particles in disc stack separators . . . . .	88
3.4.1	A short introduction to fluid flows in disc stack separators . . . . .	89
3.4.2	Computational setup . . . . .	92
3.4.3	Results . . . . .	96
<b>4</b>	<b>Conclusion und Outlook</b>	<b>101</b>
	<b>Bibliography</b>	<b>105</b>
	<b>Index</b>	<b>119</b>

# List of Figures

1.1	The hybrid principle of chimera grids / overset meshes. . . . .	31
2.1	Software architecture of the simulation model. . . . .	40
2.2	The integration of <b>ABSFoam</b> into the CFD solver. . . . .	41
2.3	The flow chart of the <b>particle manager</b> . . . . .	42
2.4	The integration of <b>constraints</b> , <b>contact models</b> , and <b>potential models</b> into <b>ABSFoam</b> . . . . .	45
2.5	The numerical structure of <b>ABSFoam</b> . . . . .	47
2.6	The fluid–solid-coupling and the solid–fluid-coupling in <b>ABSFoam</b> . . . . .	51
2.7	The distribution of particles to the processing units. . . . .	54
2.8	An infinitesimal cone of solid angle $d\theta$ and apex $\mathbf{x}_j$ , penetrating the surface $\mathcal{S}_{b_i}$ at point $\mathbf{x}_i$ with cross section $d\mathbf{A}_i$ . . . . .	63
3.1	Case setup according to Nirschl [90]. . . . .	68
3.2	Drag coefficients depending on the dimensionless wall distance $\frac{h}{d_p}$ for various particle Reynolds numbers $Re_p$ . . . . .	70
3.3	Lift coefficients depending on the dimensionless wall distance $\frac{h}{d_p}$ for various particle Reynolds numbers $Re_p$ . . . . .	71
3.4	Case setup according to Choi et al. [20]. . . . .	72
3.5	The particles with different shapes. . . . .	73
3.6	The rotational speeds depending on the shear rate for different particle shapes. . . . .	74
3.7	Angular velocities over the dimensionless time $t^*$ for different particle shapes at shear gradient $\dot{\gamma} = 1 \text{ s}^{-1}$ . . . . .	75
3.8	Biconcave at an inclination of $90^\circ$ . . . . .	76
3.9	Biconcave at an inclination of $180^\circ$ . . . . .	76
3.10	The contribution of shear forces and pressure per face area to the total torque. . . . .	77
3.11	The construction of packed beds: The process of filling a cylinder with spheres is simulated using the <b>Bullet</b> physics engine of <b>Blender</b> . . . . .	81



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3.12	Constructed packed beds with variable distributions of particle diameter $d_p$ . . . . .	82
3.13	Constructed packed beds with variable porosity $\epsilon = 50\%..90\%$ . . . . .	83
3.14	The computational domain of fluid simulation in packed beds as a rectangular subsection. . . . .	84
3.15	The immersion of the packed bed into the computational domain. . . . .	85
3.16	Visualisation of the flow velocity profile at the end of the packed bed. . . . .	86
3.17	The pressure drop in the numerical experiments using ABSFoam and the experiments of Gupte [50]. . . . .	87
3.18	The pressure drop in the numerical experiments using ABSFoam and the estimations of Ergun's equation (Eqn. 3.17). . . . .	88
3.19	Design principle of a disc stack separator. . . . .	89
3.20	The coordinate system and the velocity components of a disc stack separator. . . . .	91
3.21	The simulated subdomain of the single gap. . . . .	92
3.22	The analytical Gol'din profile according to the given parameter set (Table 3.7). . . . .	94
3.23	The computational subdomain. . . . .	95
3.24	Trajectories of particles for different starting positions, shapes, and initial inclinations. . . . .	98
3.25	The influence of different initial inclinations. . . . .	99
3.26	Angle $\theta_{\text{Gol'din}}$ between the particles' main axis and the flow velocity vector due to Gol'din [47]. . . . .	100
3.27	Comparison of the settling lengths for different geometries and initial inclinations. . . . .	100

# List of Tables

1.1	The tabular summary of the literature. . . . .	33
3.1	General boundary conditions. . . . .	67
3.2	Boundary conditions of the CFD calculation. . . . .	69
3.3	Boundary conditions of the CFD calculation. . . . .	74
3.4	Statistical parameters of packed beds with variable width. . . . .	82
3.5	Statistical parameters of constructed packed beds. . . . .	84
3.6	Boundary conditions of the CFD calculation. . . . .	84
3.7	Properties used for the simulation. . . . .	93
3.8	Boundary conditions of the CFD calculation. . . . .	94
3.9	Definition of initial inclinations. . . . .	95



# List of Symbols

## Dimensionless Numbers

$Co$	The Courant number
$Eu$	The Euler number
$Kn$	The Knudsen number
$Q$	The dimensionless volume flow
$Re_p$	The particle Reynolds number
$Re_s$	The separator Reynolds number
$St_s$	The separator Stokes number

## Operators

$\langle x y \rangle$	The correlation function of $x$ and $y$
$\mathbf{x} \times \mathbf{y}$	The cross product of $\mathbf{x}$ and $\mathbf{y}$
DDT	Discrete time stepping operator
$\frac{D}{Dt}$	The covariant derivative of $(\cdot)$ w. r. t. time
$\frac{\partial}{\partial x}$	The partial derivative w. r. t. $x$
$\Delta$	The laplacian ( $\nabla^2$ ) of a mapping
$\delta_{ij}$	The Kronecker delta
Id	The identity tensor
$n \cdot$	The $n^{\text{th}}$ time step of $(\cdot)$
$\nabla$	The gradient of a mapping
$\nabla \times$	The curl of a mapping
$\nabla \cdot$	The divergence of a mapping
$\ \cdot\ _{L^p}$	$L^p$ -norm of Lebesgue spaces
$\ \cdot\ _p$	$p$ -norm in Euclidean space
$(a_i)_i$	The column vector $\mathbf{a} = (a_0, \dots, a_{n-1})^T \in \mathbb{R}^n$

$(a_{ij})_{ij}$	The row vector of column vectors $(\mathbf{a}_j)_j^T = (\mathbf{a}_0, \dots, \mathbf{a}_{m-1}) \in \mathbb{R}^{n \times m}$
$\cdot \parallel$	The tangential part of $(\cdot)$ w. r. t. a surface
$\cdot \perp$	The perpendicular part of $(\cdot)$ w. r. t. a surface
$\cdot *$	The intermediate solution of $(\cdot)$
$\Theta$	The Landau symbol to denote asymptotic equality
$\cdot^T$	The transpose of the vector or matrix $(\cdot)$

### Technical Terms

$B_{\Omega_f, \Delta}$	The bounding box of $\Omega_{f, \Delta}$
$c_{BG}$	The <b>background grid</b> cell of a <b>background grid</b>
$\mathcal{C}_{G_\Delta}$	The centre of the grid cell $G_\Delta$ of the discretised fluid domain $\Omega_{f, \Delta}$
$(i \xleftarrow{d} j)$	The MPI receive command of data $d$ from processing unit $j$ to $i$
$(i \xrightarrow{d} j)$	The MPI send command of data $d$ from processing unit $i$ to $j$
$\mathcal{C}_{s_\Delta}$	The centre of the surface element $s_\Delta$ of a surface triangulation
$d_{BG}$	The integer distance of two <b>background grid</b> cells in a <b>background grid</b>
$g_{BG}$	The <b>background grid</b> granularity <span style="float: right;">[m]</span>
$G_\Delta$	The grid cell in the discretised fluid domain $\Omega_{f, \Delta}$
$\mathfrak{M}_k$	The master processing unit of body $k$
$N_{BG}$	The neighbourhood of <b>background grid</b> cells in a <b>background grid</b>
$\Omega_{f, \Delta}$	The discretisation of the fluid domain $\Omega_f$
$\Omega_{f, \Delta}^l$	The part $\Omega_f$ , that belongs to processing unit $l$
$r_b$	The radius of a spatially resolved body <span style="float: right;">[m]</span>
$r_{BG}$	The <b>background grid</b> radius
$\mathcal{S}_{b, \Delta}$	The triangulation of $\mathcal{S}_b$
$\mathcal{S}_{b, \Delta}^l$	The part of $\mathcal{S}_{b, \Delta}$ , that resides in $\Omega_{f, \Delta}^l$
$\overline{\mathcal{S}_{b, \Delta}}$	The volume (as a set) enclosed by $\mathcal{S}_{b, \Delta}$
$s_\Delta$	The surface element of a surface triangulation
$\mathfrak{S}_k$	The slave processing units of body $k$

### Variables, Functions, Coefficients, Constants

$A$	Hamaker's constant <span style="float: right;">[kg m<sup>2</sup> s<sup>-2</sup>]</span>
$\mathbf{a}$	The acceleration vector <span style="float: right;">[m s<sup>-2</sup>]</span>

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$\alpha_{\text{ds}}$	The disc angle	[°]
$\mathbf{a}_p$	The acceleration of the particle	[m s <sup>-2</sup> ]
$\boldsymbol{\alpha}_p$	The rotation angle vector of the particle	[rad]
$A_s$	The surface area of the solid fraction in a packed bed	[m <sup>2</sup> ]
$C_c$	The Cunningham correction factor	
$C_d$	The drag coefficient	
$C_r$	The variation of the $x^r$ -distribution	
$C_{\text{vdW}}$	The London–van der Waals constant	[kg m <sup>8</sup> /s <sup>2</sup> ]
$d$	The Euklidean distance	[m]
$d_{32}$	The Sauter mean diameter of a packed bed	[m]
$dA$	The measure of an infinitesimal surface area	[m <sup>2</sup> ]
$d\mathbf{A}$	The infinitesimal surface vector	[m <sup>2</sup> ]
$\delta$	The distribution function	
$\delta_h$	The discrete distribution function	
$d_h$	The hydraulic diameter of a packed bed	[m]
$\mathbf{d}_p$	The particle displacement vector	[m]
$d_p$	The particle diameter	[m]
$ds$	The measure of an infinitesimal curve segment	[m]
$\mathbf{ds}$	The vector of an infinitesimal curve segment	[m]
$d_{\text{sphere}100}$	The critical particle diameter	[m]
$D_T$	The thermophoretic coefficient	[kg m <sup>2</sup> s <sup>-2</sup> K <sup>-1</sup> ]
$dV$	The measure of an infinitesimal volume	[m <sup>3</sup> ]
$\epsilon$	The porosity of a porous medium	
$\boldsymbol{\eta}(t)$	Stochastic noise term	
$\mathbf{f}$	The volume force source term	[kg m <sup>-2</sup> s <sup>-2</sup> ]
$\mathbf{F}$	A general force vector	[kg m s <sup>-2</sup> ]
$\mathbf{F}_B$	The Brownian force	[kg m s <sup>-2</sup> ]
$\mathbf{F}_d$	The drag force	[kg m s <sup>-2</sup> ]
$\mathbf{F}_l$	The lift force	[kg m s <sup>-2</sup> ]
$\mathbf{F}_p$	The pressure force	[kg m s <sup>-2</sup> ]
$\tilde{\mathbf{f}}$	The kinematic body force source term	[m s <sup>-2</sup> ]
$\Gamma_{\text{ib}}$	The boundary (as a topol. set) of the immersed boundary	

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$g$	The gravitational acceleration	$[\text{m s}^{-2}]$
$\mathbf{g}$	The gravitational acceleration vector	$[\text{m s}^{-2}]$
$\boldsymbol{\gamma}$	The deformation rate tensor	$[\text{s}^{-1}]$
$b$	The disc gap height	$[\text{m}]$
$K$	The intrinsic permeability of the medium	$[\text{m}^2]$
$\kappa$	A spring constant	$[\text{kg s}^{-2}]$
$k_B$	Boltzmann's constant	$[\text{kg m}^2 \text{s}^{-2} \text{K}^{-1}]$
$L$	The characteristic physical length	$[\text{m}]$
$\lambda$	The mean free path	$[\text{m}]$
$\mu$	The dynamic viscosity	$[\text{kg m}^{-1} \text{s}^{-1}]$
$m_p$	The particle mass	$[\text{kg}]$
$M_{k,r}$	The $k^{\text{th}}$ moment moment of the $x^r$ -distribution	
$\mathcal{M}$	Mohr's portion factor; usually 0.8	
$\nu$	The kinematic viscosity	$[\text{m}^2 \text{s}^{-1}]$
$\mathbf{n}$	The outward pointing normal	
$\Omega_c$	A control volume in the physical domain	
$\Omega_f$	The fluid domain	
$\omega$	The angular velocity	$[\text{rad s}^{-1}]$
$\boldsymbol{\omega}$	The axis of rotation; also the curl of the fluid $\frac{1}{2} \nabla \times \mathbf{u}$	$[\text{rad s}^{-1}]$
$\boldsymbol{\omega}_p$	The angular velocity vector of the particle	$[\text{rad s}^{-1}]$
$\dot{\boldsymbol{\omega}}_p$	The angular acceleration vector of the particle	$[\text{rad s}^{-2}]$
$\mathbf{O}_\omega$	The origin of the rotational axis	
$p$	The pressure	$[\text{kg m}^{-1} \text{s}^{-2}]$
$\varphi$	The level-set function	
$\Phi$	The scalar potential energy	$[\text{kg m}^2 \text{s}^{-2}]$
$\tilde{p}$	The kinematic pressure	$[\text{m}^2 \text{s}^{-2}]$
$\rho_\infty$	The constant fluid reference density	$[\text{kg m}^{-3}]$
$\rho_f$	The fluid density	$[\text{kg m}^{-3}]$
RHS	The right-hand side of an equation	
$r_i$	The inner disc stack radius	$[\text{m}]$
$r_{is}$	The inner disc stack radius of the subsection	$[\text{m}]$
$r_o$	The outer disc stack radius	$[\text{m}]$

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$r_{o_s}$	The outer disc stack radius of the subsection	[m]
$\boldsymbol{\sigma}$	The Cauchy stress tensor	[kg m <sup>-1</sup> s <sup>-2</sup> ]
$S_b$	The surface (as a measure) of the body	[m <sup>2</sup> ]
$\mathcal{S}_b$	The surface (as a set) of the body	
$\Sigma$	The equivalent clarification area	[m <sup>2</sup> ]
$s$	The mass source term	[kg m <sup>-3</sup> s <sup>-1</sup> ]
$\bar{s}$	The kinematic mass source term	[s <sup>-1</sup> ]
$s_p$	The particle scaling factor for the STL geometry	
$S_V$	The specific surface of a packed bed	[m <sup>-1</sup> ]
$\boldsymbol{\tau}$	The deviatoric stress tensor	[kg m <sup>-1</sup> s <sup>-2</sup> ]
$\boldsymbol{T}$	A general torque vector	[kg m <sup>2</sup> s <sup>-2</sup> ]
$\tau$	The tortuosity of a packed bed	
$\theta_{\text{Gol'din}}$	The angle against the flow velocity vector due to Gol'din	[°]
$\boldsymbol{u}$	The fluid velocity	[m s <sup>-1</sup> ]
$\boldsymbol{u}_b$	The velocity of the spatially resolved body	[m s <sup>-1</sup> ]
$\boldsymbol{u}_{ib}$	The boundary velocity	[m s <sup>-1</sup> ]
$\boldsymbol{u}_\infty$	The superficial velocity of a packed bed	[m s <sup>-1</sup> ]
$\bar{\boldsymbol{u}}$	The fluid intrinsic velocity in a packed bed	[m s <sup>-1</sup> ]
$\boldsymbol{u}_p$	The velocity of the (point) particle	[m s <sup>-1</sup> ]
$u_{p_\infty}$	The terminal particle velocity	[m s <sup>-1</sup> ]
$V_b$	The volume (as a measure) of the body	[m <sup>3</sup> ]
$\mathcal{V}_b$	The volume (as a set) of the body	
$\dot{V}_c$	The critical volume flow	[m <sup>3</sup> s <sup>-1</sup> ]
$\dot{V}$	The total volume flow	[m <sup>3</sup> s <sup>-1</sup> ]
$\dot{V} _{N_{\text{gaps}}}$	The total volume flow through $N$ disc gaps	[m <sup>3</sup> s <sup>-1</sup> ]
$V_f$	The volume of the fluid fraction in a packed bed	[m <sup>3</sup> ]
$V_s$	The volume of the solid fraction in a packed bed	[m <sup>3</sup> ]
$V_{\text{total}}$	The total volume of a packed bed	[m <sup>3</sup> ]
$W$	The work in a force field	[kg m <sup>2</sup> s <sup>-2</sup> ]
$\boldsymbol{X}$	The curve describing the immersed boundary	
$\boldsymbol{x}$	A point in the domain	
$\boldsymbol{X}^e$	The curve describing the body surface	