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Uwe Janoske (Hrsg.)

Markus Bürger

AN IMMERSED BOUNDARY METHOD FOR ARBITRARILY SHAPED LAGRANGIAN BODIES

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An Immersed Boundary Method for Arbitrarily Shaped Lagrangian Bodies

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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.

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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 detailierte Partikelsimulationen mit beliebiger Partikelgeometrie wurde in dieser Arbeit ABSFoam, das Arbitrary–Body Simulation Toolkit für OpenFOAM®, 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®, 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.

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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
$\boldsymbol{x} \times \boldsymbol{y}$	The cross product of $\boldsymbol{x}$ and $\boldsymbol{y}$
DDT	Discrete time stepping operator
$\frac{\mathrm{D}\,\cdot}{\mathrm{D}t}$	The covariant derivative of $(\,\cdot\,)$ w. r. t. time
$\frac{\partial\,\cdot}{\partial x}$	The partial derivative w. r. t. x
Δ	The laplacian (∇^2) of a mapping
δ_{ij}	The Kronecker delta
Id	The identity tensor
${}^{n}\,\cdot$	The n^{th} time step of $(\,\cdot\,)$
∇	The gradient of a mapping
$\nabla\times$	The curl of a mapping
$\nabla\cdot$	The divergence of a mapping
$\lVert \cdot \rVert_{L^p}$	L^p-norm of Lebesgue spaces
$\lVert \cdot \rVert_p$	p-norm in Euclidean space
$(a_i)_i$	The column vector $\boldsymbol{a} = (a_0, \ldots, a_{n-1})^T \in \mathbb{R}^n$

$(a_{ij})_{ij}$	The row vector of column vectors $(\boldsymbol{a}_j)_j^T = (\boldsymbol{a}_0, \dots, \boldsymbol{a}_{m-1}) \in \mathbb{R}^{n\times m}$
$\cdot^{\parallel}$	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 $(\cdot)$
Θ	The Landau symbol to denote asymptoptic equality
$\cdot^{T}$	The transpose of the vector or matrix $(\cdot)$

Technical Terms

$B_{\Omega_{\mathrm{f},\Delta}}$	The bounding box of $\Omega_{\mathrm{f},\Delta}$	
c_{BG}	The background grid cell of a background grid	
$\boldsymbol{C}_{G_\Delta}$	The centre of the grid cell G_Δ of the discretised fluid domain $\Omega_{\mathrm{f},\Delta}$	
$\left(i \xleftarrow{d} j\right)$	The MPI receive command of data d from processing unit j to i	
$\left(i \xrightarrow{d} j\right)$	The MPI send command of data d from processing unit i to j	
$\boldsymbol{C}_{\boldsymbol{s}_\Delta}$	The centre of the surface element $\boldsymbol{s}_\Delta$ of a surface triangulation	
d_{BG}	The integer distance of two background grid cells in a background grid	
g_{BG}	The background grid granularity	[m]
G_Δ	The grid cell in the discretised fluid domain $\Omega_{\mathrm{f},\Delta}$	
$\mathfrak{M}_k$	The master processing unit of body k	
N_{BG}	The neighbourhood of background grid cells in a background grid	
$\Omega_{\mathrm{f},\Delta}$	The discretisation of the fluid domain Ω_{f}	
$\Omega^{\mathrm{l}}_{\mathrm{f},\Delta}$	The part Ω_{f}, that belongs to processing unit l	
r_{b}	The radius of a spatially resolved body	[m]
r_{BG}	The background grid radius	
$\mathcal{S}_{\mathrm{b}\Delta}$	The triangulation of $\mathcal{S}_{\mathrm{b}}$	
$\mathcal{S}^{\mathrm{l}}_{\mathrm{b}\Delta}$	The part of $\mathcal{S}_{\mathrm{b}\Delta}$, that resides in $\Omega^{\mathrm{l}}_{\mathrm{f},\Delta}$	
$\overline{\mathcal{S}_{\mathrm{b}\Delta,}}$	The volume (as a set) enclosed by $\mathcal{S}_{\mathrm{b}\Delta}$	
$\boldsymbol{s}_\Delta$	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	$[\mathrm{kg\,m^2\,s^{-2}}]$
$\boldsymbol{a}$	The acceleration vector	$[\mathrm{m\,s^{-2}}]$

α_{ds}	The disc angle	[°]
$\boldsymbol{a}_{\mathrm{p}}$	The acceleration of the particle	$[\mathrm{m\,s^{-2}}]$
$\boldsymbol{\alpha}_{\mathrm{p}}$	The rotation angle vector of the particle	[rad]
A_{s}	The surface area of the solid fraction in a packed bed	$[\mathrm{m^2}]$
C_{c}	The Cunningham correction factor	
C_{d}	The drag coefficient	
C_r	The variation of the x^r-distribution	
C_{vdW}	The London–van der Waals constant	$[\mathrm{kg\,m^8/s^2}]$
d	The Euklidean distance	[m]
d_{32}	The Sauter mean diameter of a packed bed	[m]
$\mathrm{d}A$	The measure of an infinitesimal surface area	$[\mathrm{m^2}]$
$\mathrm{d}\boldsymbol{A}$	The infinitesimal surface vector	$[\mathrm{m^2}]$
δ	The distribution function	
δ_{h}	The discrete distribution function	
d_{h}	The hydraulic diameter of a packed bed	[m]
$\boldsymbol{d}_{\mathrm{p}}$	The particle displacement vector	[m]
d_{p}	The particle diameter	[m]
$\mathrm{d}s$	The measure of an infinitesimal curve segment	[m]
$\mathrm{d}\boldsymbol{s}$	The vector of an infinitesimal curve segment	[m]
$d_{\mathrm{sphere}_{100}}$	The critical particle diameter	[m]
D_{T}	The thermophoretic coefficient	$[\mathrm{kg\,m^2\,s^{-2}\,K^{-1}}]$
$\mathrm{d}V$	The measure of an infinitesimal volume	$[\mathrm{m^3}]$
ϵ	The porosity of a porous medium	
$\boldsymbol{\eta}(t)$	Stochastic noise term	
$\boldsymbol{f}$	The volume force source term	$[\mathrm{kg\,m^{-2}\,s^{-2}}]$
$\boldsymbol{F}$	A general force vector	$[\mathrm{kg\,m\,s^{-2}}]$
$\boldsymbol{F}_{\mathrm{B}}$	The Brownian force	$[\mathrm{kg\,m\,s^{-2}}]$
$\boldsymbol{F}_{\mathrm{d}}$	The drag force	$[\mathrm{kg\,m\,s^{-2}}]$
$\boldsymbol{F}_{\mathrm{l}}$	The lift force	$[\mathrm{kg\,m\,s^{-2}}]$
$\boldsymbol{F}_{p}$	The pressure force	$[\mathrm{kg\,m\,s^{-2}}]$
$\tilde{\boldsymbol{f}}$	The kinematic body force source term	$[\mathrm{m\,s^{-2}}]$
Γ_{ib}	The boundary (as a topol. set) of the immersed boundary	

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

$r_{\mathrm{o_s}}$	The outer disc stack radius of the subsection	[m]
$\boldsymbol{\sigma}$	The Cauchy stress tensor	[kg m^{-1} s^{-2}]
S_{b}	The surface (as a measure) of the body	[m^2]
$\mathcal{S}_{\mathrm{b}}$	The surface (as a set) of the body	
Σ	The equivalent clarification area	[m^2]
s	The mass source term	[kg m^{-3} s^{-1}]
$\tilde{s}$	The kinematic mass source term	[s^{-1}]
s_{p}	The particle scaling factor for the STL geometry	
S_{V}	The specific surface of a packed bed	[m^{-1}]
$\boldsymbol{\tau}$	The deviatoric stress tensor	[kg m^{-1} s^{-2}]
$\boldsymbol{T}$	A general torque vector	[kg m^2 s^{-2}]
τ	The tortuosity of a packed bed	
$\theta_{\mathrm{Gol'din}}$	The angle against the flow velocity vector due to Gol'din	[°]
$\boldsymbol{u}$	The fluid velocity	[m s^{-1}]
$\boldsymbol{u}_{\mathrm{b}}$	The velocity of the spatially resolved body	[m s^{-1}]
$\boldsymbol{u}_{\mathrm{ib}}$	The boundary velocity	[m s^{-1}]
$\boldsymbol{u}_{\infty}$	The superficial velocity of a packed bed	[m s^{-1}]
$\bar{\boldsymbol{u}}$	The fluid intrinsic velocity in a packed bed	[m s^{-1}]
$\boldsymbol{u}_{\mathrm{p}}$	The velocity of the (point) particle	[m s^{-1}]
u_{p_∞}	The terminal particle velocity	[m s^{-1}]
V_{b}	The volume (as a measure) of the body	[m^3]
$\mathcal{V}_{\mathrm{b}}$	The volume (as a set) of the body	
$\dot{V}_{\mathrm{c}}$	The critical volume flow	[m^3 s^{-1}]
$\dot{V}$	The total volume flow	[m^3 s^{-1}]
$\dot{V}\|_{N\,\mathrm{gaps}}$	The total volume flow through N disc gaps	[m^3 s^{-1}]
V_{f}	The volume of the fluid fraction in a packed bed	[m^3]
V_{s}	The volume of the solid fraction in a packed bed	[m^3]
V_{total}	The total volume of a packed bed	[m^3]
W	The work in a force field	[kg m^2 s^{-2}]
$\boldsymbol{X}$	The curve describing the immersed boundary	
$\boldsymbol{x}$	A point in the domain	
$\boldsymbol{X}^e$	The curve describing the body surface	