Analysis and Improvement of the

Time-Driven Discrete Element Method

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Vorwort

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Abstract of the Dissertation

Several processes in nature as well as many industrial applications involve static or dynamic granular materials. Granulates can adopt solid, liquid or gas like states and thereby reveal intriguing physical phenomena not observable in its versatility for any other form of matter. The frequent occurrence of phase transitions and the related characteristics thereby strongly affect their processing quality and economics. This situation demands for prediction methods for the behavior of granulates. In this context simulations provide a feasible alternative to experimental investigations. Advantageous are their better reproducibility, their less expenditure of time and their lower costs. Several different simulation approaches are applicable to granular materials. The time-driven Discrete Element Method turns out to be the most complex but also as the most general method. It is based on tracking each particle's movement and its interactions with the surrounding over time. The method provides detailed information on particle positions, orientations and translational and angular velocities. These properties are obtained by integrating numerically a set of fully deterministic differential equations which are explicitly depending on the contact forces.

The time-driven Discrete Element Method is a simulation approach which has been used in a wide variety of scientific fields for more than thirty years. With the tremendous increase in available computer power, especially in the last years, the method is more and more developing to the state of the art simulation technique for granular materials. Despite of the long time of usage, model advances and theoretical and experimental studies are not harmonized in the different branches of application, providing a large potential for improvements.

Therefore, the scope of this work is a review of methods and models based on theoretical considerations and experimental data from literature. Through model advances it is intended to contribute to a general enhancement of techniques, which are then directly available for simulations.

In detail, force displacement models which are usually separated in normal and tangential direction are reviewed for a broad range of experimental data. Model improvements and new methods for the derivation of simulation parameters are proposed. For a special combination of force models an analytical solution is derived, which is later used as a benchmark case for the evaluation of different integration schemes. With the Discrete Element Method even today being mostly limited to simple spherical bodies a method for the implementation of complex shapes based on multi-sphere particles is reviewed. The applicability of this approach is verified based on a study on collision properties under different impact situations. As a final application outlining the advantages of particle orientated modeling the Discrete Element Method incorporating the derived improvements is used for a comparative study of mixing on grates.

Contents

Glossary

Latin Glossary:

Variable	Unit	Denotation
a	$[m/s^2]$	acceleration
A	$[1/m]$	normal force model parameter
A	$[-]$	tangential force model parameter
b	$[m/s^3]$	first time derivative of the acceleration
B	$[-]$	tangential force model parameter
c	$[-]$	dimensionless exponent
c	$[m/s^4]$	second time derivative of the acceleration
C	$[-]$	tangential force model parameter
d	$[m]$	diameter
D	$[-]$	tangential force model parameter
D	$[m]$	normalized particle depth
$\overline{D}$	$[m]$	mean normalized particle depth
$\widetilde{D}$	$[m]$	fluctuating normalized particle depth
e	$[-]$	coefficient of restitution
E	$[kg/(m\,s^2)]$	Young's modulus
$\vec{\tilde{E}}$	$[-]$	unit vectors in the inertial frame
$\vec{E}$	$[-]$	unit vectors in the body fixed frame
$\vec{F}$	$[kg\ m/s^2]$	force vector
g	$[m/s^2]$	acceleration of gravity
$\vec{g}$	$[m/s^2]$	acceleration of gravity vector
G	$[kg/(m\,s^2)]$	shear modulus
h	$[m]$	height
h_r	$[m/s]$	position related integration scheme parameter
h_v	$[m/s^2]$	velocity related integration scheme parameter
i	$[-]$	integral indices
I	$[-]$	integral indices
I	$[kg\ m^2]$	inertia tensor
$\hat{I}$	$[kg\ m^2]$	inertia tensor along principal axis
j	$[-]$	integral indices
J	$[-]$	integral indices
k	$[-]$	integral indices
k	$[kg/s^2]$	linear stiffness
$\widetilde{k}$	$[kg/(m^{1/2}s^2)]$	non-linear stiffness
K	$[-]$	integral indices
l	$[-]$	integral indices
l	$[m]$	length

L	$[-]$	integral indices
L	$[m]$	length
Δl	$[m]$	amplitude
m	$[kg]$	mass
m	$[-]$	integral indices
M	$[-]$	integral indices
$\vec{M}$	$[kg\ m^2/s^2]$	moment vector
n	$[-]$	set of coefficients
n	$[-]$	integral indices
$\vec{n}$	$[-]$	normal vector
N	$[-]$	integral indices
o	$[-]$	integral indices
O	$[-]$	error order
O	$[-]$	integral indices
p	$[-]$	normal force model parameter
p_y , $\widetilde{p}_y$	$[N/m^2]$	materials yield point
$\vec{p}$	$[m/s]$	standard deviation of fluctuating velocities
p	$[m/s]$	scalar standard deviation of fluctuating velocities
$\vec{P}^t$	$[m/s]$	velocity based mixing property
P^t	$[m/s]$	scalar velocity based mixing property
$\Delta\vec{P}$	$[kg\ m/s]$	change of momentum
q	$[-]$	normal force model parameter
Q^t	$[m/s]$	position based time averaged mixing property
r	$[m]$	radius
r	$[-]$	non-dimensional radius
r	$[m]$	position
r_V	$[m]$	evaluation radius
R	$[m]$	radius
s	$[1/m]$	normal force model parameter
s	$[m]$	coordinate of the contact point
t	$[s]$	time
t'	$[s]$	time
Δt	$[s]$	time step
$\vec{t}$	$[-]$	tangential vector
t^n	$[s]$	duration of a collision
v	$[m/s]$	velocity
v_{00}	$[(m/s)^{\chi_2}]$	normal force model parameter
$\vec{v}$	$[m/s]$	velocity vector
$\bar{\vec{v}}$	$[m/s]$	mean velocity vector
$\tilde{\vec{v}}$	$[m/s]$	fluctuating velocity vector
w	$[-]$	weighting factor

W	$[m]$	grate width
$\vec{W}$	$[1/s]$	angular velocity vector
$\vec{x}$	$[m]$	position vector
x	$[m]$	Cartesian coordinates
x	[varying]	independent variable
X	$[m]$	distance between particle centers
y	[varying]	dependent variable
y	$[m]$	Cartesian coordinates
z	$[m]$	Cartesian coordinates

Greek Glossary:

Variable	Unit	Denotation
α	$[rad]$	collision angle
α	$[rad]$	grate declination
α_l	$[kg\, m^{1-p} / s^2]$	empirical material stiffness during loading
α_{ul}	$[kg\, m^{1-p-q} / s^2]$	empirical material stiffness during unloading
β^n	$[-]$	damping ratio
β_1	$[-]$	sliding coefficient of tangential restitution
β_0	$[-]$	sticking coefficient of tangential restitution
β	$[-]$	effective coefficient of tangential restitution
β	$[rad]$	rebound angle
β	$[rad]$	grate inclination
γ	$[kg/s]$	velocity proportional damping coefficient
$\widehat{\gamma}$	$[kg/(s\, m^{1/4})]$	non-linear damping coefficient
$\bar{\gamma}, \hat{\gamma}$	$[1/s]$	dissipation coefficient
$\widetilde{\gamma}$	$[kg/(s\, m^{1/2})]$	non-linear damping coefficient
$\breve{\gamma}$	$[kg/(s\, m^{\widetilde{\Theta}})]$	non-linear damping coefficient
δ	$[1/s]$	frequency
δ	$[m]$	overlap or normal displacement
$\delta^V, \delta^{\Delta x}, \delta^x, \delta^d$	$[-]$	binary condition functions
ε^n	$[kg\, m^2/s^2]$	characteristic energy
ε	$[-]$	integration method parameter
ε	$[rad]$	tilting angle
η	$[-]$	material property
$\widetilde{\Theta}$	$[-]$	dimensionless exponent
θ	$[s^\eta/m^\eta]$	material property
θ	$[rad]$	angle of revolution
$\dot{\theta}$	$[1/s]$	angular velocity
ι	$[rad]$	tilting angle
κ	$[-]$	tangential to normal stiffness ratio
Λ	$[-]$	rotation matrix

$\Delta\Lambda$	$[-]$	incremental rotation matrix
μ	$[-]$	friction coefficient
ν	$[-]$	Poisson's ratio
ξ	$[m]$	overlap or normal displacement
ξ^t	$[m]$	elongation of the spring in tangential direction
$\vec{\xi}^t$	$[m]$	elongation vector of the tangential spring
$\dot{\xi}$	$[m/s]$	normal displacement rate
$\ddot{\xi}$	$[m/s^2]$	normal acceleration
ξ_f	$[m]$	final resulting displacement
ξ_r	$[-]$	displacement ratio
ξ_y	$[m]$	displacement at yield point
$\dot{\xi}_y$	$[m/s]$	displacement rate at yield point
ξ_0^t	$[m]$	micro structural surface roughness
O	$[-]$	Heaviside function
$\vec{\pi}$	$[kg\ m^2/s]$	angular momentum
ρ	$[kg/m^3]$	density
ς	$[-]$	functional relation
ϕ	$[kg\,m^2/s^2]$	continuous potential
ϕ	$[\text{varying}]$	measurable quantity
$\vec{\varphi}$	$[rad]$	angle of revolution
χ_1	$[(m/s)^{\chi_2}]$	normal force model parameter
χ_2, χ_4	$[-]$	normal force model parameter
χ_3	$[m^{\chi_4} \cdot s^{1-\chi_4}]$	normal force model parameter
χ^2	$[\text{varying}]$	weighted sum of squares
$\vec{\psi}$	$[-]$	vectorial rotation angle
ψ	$[-]$	normal force model parameter
ψ_1	$[-]$	dimensionless initial tangential velocity
ψ_2	$[-]$	dimensionless final tangential velocity
ω	$[1/s]$	frequency
ω	$[1/s]$	angular velocity
$\vec{\omega}$	$[1/s]$	angular velocity vector

Subscripts:

Variable	Denotation
0	initial
$analy$	analytical
bot	bottom
c	critical
CG	center of gravity
eff	effective
el	elastic

exp	experimental
$diss$	dissipative
f	final
$F0$	at zero force
i	integer indices
j	integer indices
k	integer indices
l	loading
m	mean
max	maximal
min	minimal
mod	model
num	numerical
$nonel$	non-elastic
p	predicted
PP	particle/particle
pt	potential derived
PW	particle/wall
rl	reloading
s	relative to the contact point
$t \pm n \cdot \Delta t$	at time $t \pm n \cdot \Delta t$
top	top
ul	unloading
x	relative to the x-axis
y	relative to the y-axis
z	relative to the z-axis

Superscripts:

Variable	Denotation
-1	inverse
$'$	final collision quantity
*	state of reversion
n	normal direction
t	tangential direction
T	transposed