Efficient modelling of particle collisions using a non-linear viscoelastic contact force

Shouryya Ray\textsuperscript{a,},\textsuperscript{*} Tobias Kempe\textsuperscript{a}, Jochen Fröhlich\textsuperscript{a}

\textsuperscript{a}Institut für Strömungsmechanik, Technische Universität Dresden, George-Bähr-Straße 3c, D-01062 Dresden, Germany

Abstract

In this paper the normal collision of spherical particles is investigated. The particle interaction is modelled in a macroscopic way using the Hertzian contact force with additional linear damping. The goal of the work is to develop an efficient approximate solution of sufficient accuracy for this problem which can be used in soft-sphere collision models for Discrete Element Methods and for particle transport in viscous fluids. First, by the choice of appropriate units, the number of governing parameters of the collision process is reduced to one, thus providing a dimensionless parameter that characterizes all such collisions up to dynamic similitude. It is a simple combination of known material parameters as well as initial conditions. A rigorous calculation of the collision time and restitution coefficient from the governing equations, in the form of a series expansion in this parameter is provided. Such a first principles calculation is particularly interesting from a theoretical perspective. Since the governing equations present some technical difficulties, the methods employed are also of interest from the point of view of the analytical technique. Using further approximations, compact expressions for the restitution coefficient and the collision time are then provided. These are used to implement an approximate algebraic rule for computing the desired stiffness and damping in the framework of the adaptive collision model (Kempe & Fröhlich, Journal of Fluid Mechanics, 709: 445-489, 2012). Numerical tests with binary as well as multiple particle collisions are included that illustrate the accuracy of the proposed method and its superiority in terms of numerical efficiency.

Keywords: Particle-laden flow, Discrete Element Method, collision modelling, Hertzian contact

1. Introduction and motivation

Particle laden flows and their numerical simulation are of major interest in a wide range of engineering applications as well as in fundamental research. A frequently used approach for the simulation of dynamic granular materials is the Discrete Element Method (DEM),

\textsuperscript{*}Corresponding author

Email address: Shouryya.Ray@tu-dresden.de (Shouryya Ray)

Preprint submitted to Elsevier February 27, 2015
The linear and angular momentum balance of the particles is solved to obtain their translational and rotational velocity. The hydrodynamic interaction between particles is often neglected or fluid forces are accounted for by simple empirical correlations and the particle interaction modelled using macroscopic collision models of various types. The accurate numerical modelling of the collision process, however, is crucial for the quality of the simulation in a vast regime of parameters.

Several numerical models for the collision process between particles and for the collision of particles with walls have been developed in the framework of the DEM, cf. [11–13]. These models can be divided into two groups: hard-sphere models and soft-sphere models. The hard sphere approach [2] is based on binary, quasi-instantaneous collisions. The post-collisional velocities are calculated from momentum conservation between the states before and after surface contact. Such models, however, are inappropriate for interface-resolving simulations since they introduce numerical errors. Soft-sphere models, on the other hand, usually require an excessively small time step if physically realistic material parameters are matched. In the soft-sphere approach the motion of the particles is calculated by numerically integrating the equations of motion of the particles during the collision process accounting for the contact forces acting on them. Typical for all soft-sphere models is that very small time steps must be used to ensure that for reasons of stability and accuracy the step size in time is substantially smaller than the duration of contact. The soft-sphere contact models are usually based on linear and non-linear spring damper models [11–13]. A commonly used model for time-resolved particle interactions in numerical simulations is a Hertzian contact force in combination with a linear damping [11, 14]. However, in contrast to linear spring models, no closed solution exists for this equation. One is hence forced to integrate numerically with a very small time step. This issue even leads some researchers to prefer linear spring models which are much easier to evaluate [13].

The discussion whether the linear or the non-linear approach is to be preferred seems unsettled in the community so far [13], and the present paper does not aim to compare these or to advocate one or the other. Instead, the mathematical properties of the equation of damped Hertzian contact are discussed and an efficient engineering approximation is proposed so as to reduce the cost of this model. This can enhance the efficiency of DEMs employing the physically more realistic non-linear approach.

Due to the time-step reduction required by many soft-sphere models, DEM practitioners often modify the material parameters of the collision model to alleviate this problem [9] and allow the use of larger time steps. The idea is to make the collision process softer, hence longer in time, at the price of increased numerical overlap of particles during collisions. Here as well, the approximation proposed in the present paper may be advantageous. Except for the linear models, the adjustment of parameters in the soft-sphere model is usually performed by trial and error. This is time consuming and prone to sub-optimal choice of values. A current trend in the modelling of particulate flows is that DEMs are enhanced by representations of the viscous effects of the continuous phase around the particles [9, 16]. In this framework, hard-sphere models are inapplicable as they cannot properly account for the coupling to the surrounding viscous fluid, thus introducing substantial numerical errors [8]. Here, soft-sphere models are required, with the drawbacks discussed above. As a remedy,
a systematic strategy was recently proposed to determine the parameters for a softened contact model [8]. It is based on imposing the duration of the contact between the particles during collisions according to some external constraint, such as a pre-selected time step. The coefficients in the model are then determined so as to maintain the exact restitution coefficient. This guarantees maximal physical realism under given constraints imposed by computational resources. The approach, termed Adaptive Collision Time Model (ACTM), was implemented and tested with particles in viscous fluids for single collisions [8] as well as for multiple simultaneous collisions [10].

Beyond that, the approach is very interesting for pure DEM without viscous fluid, as it provides an automated systematic approach to regularising the collision process. Another substantial advantage of this approach is that the original physical values of the coefficients can be introduced as bounds so that the original model is obtained again in a regular limit when the collision time is sufficiently reduced. This provides optimal commodity for the user.

In a simulation with many particles, each collision takes place with different velocities of the collision partners. Hence, when imposing the duration of contact and the restitution coefficient, one is forced to select the model coefficients for stiffness and damping for each collision individually. If no closed solution is available, this requires an iterative procedure as indeed used so far [8]. In the present paper, this is now improved by providing a direct solution to this problem, based on a systematically controlled approximation. The increased efficiency is demonstrated by suitable test cases and comparison to the original method.

The paper is structured as follows. First, an exact formal solution of the equation of motion is derived using nonlinear transformations and a parametric series expansion. Then, a rigorous calculation of the collision time and restitution coefficient is carried out. As a next step, compact analytical approximations are developed. These formulæ allow the direct computation of the physically relevant parameters, i.e. collision time and restitution coefficient, from the intrinsic material parameters. Afterwards, the inverse problem is addressed. The artificial lengthening of the collision time, while preserving the restitution coefficient, requires the computation of the appropriate stiffness and damping. Finally, numerical tests demonstrate the accuracy and efficiency of the proposed algorithm, including test runs in typical engineering settings.

2. Basic equation of the collision process

The situation of a normal particle-wall collision is illustrated in Figure 1. Particle deformation during contact is represented here by the overlap of the undeformed particle with the collision partner. The equation of motion governing the surface penetration $\zeta = \zeta(t)$ during the contact phase considered here is [8]

$$m_p\ddot{\zeta} = -d\dot{\zeta} - k\zeta^{3/2}$$

with $m_p$ the mass of the particle, $d$ the damping coefficient and $k$ a stiffness parameter, the last two being material properties. The overdot represents differentiation with respect to time $t$. The second term is the nonlinear restoring force originally derived by Hertz [5].
The first term on the right hand side of (1) corresponds to the damping, which is assumed to be linear. For \( d = 0 \) the behaviour is termed ideally elastic. The initial conditions at the beginning of the collision read \( \zeta(t = 0) = 0, \dot{\zeta}(t = 0) = u_{\text{in}}. \)

Equation (1) is more conveniently expressed in dimensionless form by defining new variables \( \tau, z \) with \( t = \tau t_* \) and \( \zeta = z u_{\text{in}} t_* \), which is tantamount to fixing the characteristic unit of velocity for the system as \( u_{\text{in}} \) and choosing \( t_* \) as the (at present arbitrary) unit of time. The first and second derivatives of \( \zeta \) can then be expressed as

\[
\dot{\zeta}(t) = u_{\text{in}} \dot{z}(\tau) \quad (2)
\]

and

\[
\ddot{\zeta}(t) = \frac{u_{\text{in}}}{t_*} \ddot{z}(\tau) \quad (3)
\]

Here and in all further cases of occurrence, the overdot denotes, when applied to a dimensionless quantity, differentiation with respect to the dimensionless time \( \tau \), unless stated otherwise. Dividing by the characteristic unit of force \( m_p u_{\text{in}} / t_* \), one obtains the dimensionless equation

\[
\ddot{z} + \frac{t_* d}{u_{\text{in}} m_p} z + \frac{k u_{\text{in}}^{1/2}}{m_p t_*^{5/2}} z^{3/2} = 0. \quad (4)
\]

Choosing the unit of time \( t_* \) as

\[
t_* = \sqrt[5]{\frac{m_p^2}{k^2 u_{\text{in}}}} \quad (5)
\]

yields the following equation for \( z(\tau) \):

\[
\ddot{z} + 2 \lambda \dot{z} + z^{3/2} = 0 \quad (6)
\]

with initial conditions \( z(\tau = 0) = 0, \dot{z}(\tau = 0) = 1 \) and the parameter \( \lambda \),

\[
\lambda = \frac{1}{2} \frac{t_* d}{m_p} = \frac{1}{2} \frac{d}{m_p} \sqrt[5]{\frac{m_p^2}{k^2 u_{\text{in}}}}. \quad (7)
\]

Following [8], the collision time \( T_c \), i.e. \( \tau_c \) in the non-dimensional setting, is obtained as the strictly positive root of \( \zeta \), i.e. the point of time when the surface penetration of the particle-wall system returns to zero. The restitution coefficient is then conveniently defined as

\[
e_{\text{dry}} = -\frac{u_{\text{out}}}{u_{\text{in}}} = -\frac{\dot{\zeta}(t = T_c)}{u_{\text{in}}} = -\dot{z}(\tau = \tau_c). \quad (8)
\]

The latter expression makes clear that the only way the restitution coefficient may depend on material and other input parameters is as a function of the parameter \( \lambda \) introduced above. Physically, one may interpret this as follows: All linearly damped normal Hertzian particle-wall collisions are, up to a characteristic parameter, similar. This characteristic parameter
is on one hand the restitution coefficient $e_{dry}$, which is easy to determine experimentally but cannot be calculated trivially from known material properties and initial conditions. The other option, introduced here, is $\lambda$, which cannot be measured directly but is readily calculated. At the heart of the present work is the convenient analytical conversion between the two. The case $\lambda = 0$ corresponds to the undamped case considered by Hertz [5], which is simply a conservative system, i.e. $e_{dry} = 1$, and is integrated readily. Furthermore, Hertz [5] gave the collision time as

$$T_{c,0} = \frac{2\sqrt{\pi} \Gamma(7/5)}{\Gamma(9/10)} \sqrt{\frac{25m_p^2}{16k^2u_{in}}},$$

with $\Gamma$ denoting the Gamma function. reads Evaluating the special functions to four significant figures, this yields $\tau_{c,0} = 3.218$ in dimensionless form.

3. Exact formal solution of the equation of motion

3.1. Introduction

The purpose of this section is to calculate rigorously from first principles, i.e. starting from the equation of motion (6) and using mathematically justifiable techniques, the physical parameters pertaining to the characterization of collisions in the chosen model. Such results are not only useful for the purpose of theoretical investigation, but are also instructive from the perspective of the analytical technique. Since these results are, to the best of our knowledge, not available in the existing literature, their derivation is presented in the following.

Due to the fractional power of $z$ in (6) and the initial condition $z(\tau = 0) = 0$, a naive power series solution for $z$ in $\tau$ is not possible. Furthermore, it is not desirable at all to have a series representation in $t$, since it is not a variable that is naturally small. On the other hand, especially in practical applications, very low values of $e_{dry}$ are unlikely to be of interest. By
consequence, $\lambda$ is a parameter that may be assumed small for practical purposes. Indeed, numerical examples show that if a lower bound of 0.4 is imposed on $e_{\text{dry}}$, $\lambda \leq 0.2$ may be safely assumed. In addition, as remarked earlier, the case $\lambda = 0$ has already been studied in detail and is, hence, well-understood [5]. Thus, in the following, the solution of the equation of motion is most conveniently expressed using series expansions in $\lambda$.

### 3.2. Solving the equation of motion

It will be found that the relevant mathematical operations are substantially facilitated when the problem is transformed to phase space $(z, \dot{z})$. Furthermore, the dimensionless velocity is now interpreted as a function of the penetration, i.e. $\dot{z} = \dot{z}(z)$. Using the relation $\ddot{z} = \frac{d\dot{z}}{d\tau} = \frac{dz}{d\tau} \frac{d\dot{z}}{dz} = \dot{z} \frac{d\dot{z}}{dz}$ the equation of motion expressed in these new variables now reads

$$\ddot{z} \frac{\partial \dot{z}}{\partial z} + 2\dot{z}^2 + z^{3/2} = 0. \quad (10)$$

In passing, observe that if the damping term were absent, this would reduce to an exact differential, with the solution given by the level curve of a potential function which is readily interpreted as the conserved total energy of the system. In fact, the energy method was the procedure followed by Hertz [5] when deriving the solution for the undamped case. The analysis here, on the other hand, needs to be more involved. It is now convenient to define

$$\dot{z} = \begin{cases} \sqrt{v_+} & \text{in} \\ -\sqrt{v_-} & \text{out} \end{cases} \quad (11)$$

where ‘in’ refers to the part of the collision during which the particle is compressed and the motion is directed into the wall, while ‘out’ describes the outward motion of the particle (Figure 2). By the chain rule, one has $\dot{z}d\dot{z} = \frac{1}{2}d\dot{v}_+$, where the choice of + and − is determined by (11). Finally, it is helpful to define $y := \sqrt{z}, dz = 2y dy$. Inserting these new variables into (10) yields the initial value problems of the two phases of motion:

$$\frac{\partial v_+}{\partial y} + 8\lambda y \sqrt{v_+} + 4y^4 = 0 \quad v_+(y = 0) = 1 \quad (12)$$

$$\frac{\partial v_-}{\partial y} - 8\lambda y \sqrt{v_-} + 4y^4 = 0 \quad v_-(y = 0) = e_{\text{dry}}^2. \quad (13)$$

For $\lambda$ assumed small, the the unknowns are now expressed in form of a series in powers of $\lambda$:

$$v_+ = \sum_{m=0}^{\infty} v_{+,m} \lambda^m \quad v_{+,m} = \frac{1}{m!} \left. \frac{\partial^m v_+}{\partial \lambda^m} \right|_{\lambda=0} \quad (14)$$

$$v_- = \sum_{m=0}^{\infty} v_{-,m} \lambda^m \quad v_{-,m} = \frac{1}{m!} \left. \frac{\partial^m v_-}{\partial \lambda^m} \right|_{\lambda=0} \quad (15)$$

Differentiating $m$ times with respect to $\lambda$ and evaluating at $\lambda = 0$ successively yields the equations determining $v_{\pm,m}$ for $m \geq 0$. For $m = 0$, this gives

$$v_{\pm,0} = 1 - \frac{4}{5}y^5 \quad (16)$$
Figure 2: Sketch of the compression (in) and the rebound phase (out) during the collision process (cf. Figure 1) with \( \hat{z} \) being the non-dimensional maximum surface penetration. a) Physical space, b) phase space

and for \( m \geq 1 \),

\[
m! \frac{\partial v_{\pm,m}}{\partial y} = \mp 8y \left. \frac{\partial^m \lambda \sqrt{v_{\pm}}}{\partial \lambda^m} \right|_{\lambda=0}\]

(17)

The right-hand side of (17) may be further simplified using the Leibniz formula,

\[
\left. \frac{\partial^m \lambda \sqrt{v_{\pm}}}{\partial \lambda^m} \right|_{\lambda=0} = \sum_{i=0}^{m} \binom{m}{i} \left. \frac{\partial^i \lambda}{\partial \lambda^i} \right|_{\lambda=0} \left. \frac{\partial^{m-i} \sqrt{v_{\pm}}}{\partial \lambda^{m-i}} \right|_{\lambda=0} .
\]

(18)

Only the term \( i = 1 \) survives, so that the higher order corrections are given by

\[
v_{+,m} = -\frac{8}{(m-1)!} \int_{0}^{y} \left. \frac{\partial^{m-1} \sqrt{v_{+}}}{\partial \lambda^{m-1}} \right|_{\lambda=0} y' \, dy' ;
\]

(19)

\[
v_{-,m} = \frac{1}{m!} \left. \frac{\partial^m e_{\text{dry}}^2}{\partial \lambda^m} \right|_{\lambda=0} + \frac{8}{(m-1)!} \int_{0}^{y} \left. \frac{\partial^{m-1} \sqrt{v_{-}}}{\partial \lambda^{m-1}} \right|_{\lambda=0} y' \, dy' .
\]

(20)

Since the \((m-1)\)-st derivative of \( v_{\pm} \) at \( \lambda = 0 \) can only involve \( v_{\pm,0}, \ldots, v_{\pm,m-1} \), equations (19), (20) yield well-defined recursions for \( v_{\pm,m} \). Furthermore, it is readily seen by mathematical induction, that \( v_{\pm,m} \) have a convergent Taylor series expansion around \( y = 0 \), and that the convergence radius is \((5/4)^{1/5}\). From conservation of energy, however, it can be deduced that \( z \leq (5/4)^{2/5}\), i.e. \( v_{\pm,m} \) can be represented by a power series on the whole domain of interest. A physical interpretation of these terms is discussed in Appendix A. Note also that derivatives of \( e_{\text{dry}} \) appear explicitly in the expressions for \( v_{-,m} \). This should not, however, be seen to imply that \( e_{\text{dry}} \) needs to be known \textit{a priori}. Indeed, it will be seen later that
$e_{\text{dry}}$ is uniquely determined by certain conditions that need to be fulfilled in order for the trajectory to be continuous in time and space.

To find a connection to the time domain, one may exploit the fact that $\dot{z} \, d\tau = d\,z$ to find (with $\hat{y}^2 = \hat{z}$ the maximum surface penetration)

$$\tau = \tau(y) = \begin{cases} \tau_+(y) := \int_0^y \frac{2dy'y'}{\sqrt{v_+}} & \text{in} \\ \tau_-(y) := \tau_+(\hat{y}) + \int_0^y \frac{2dy'y'}{\sqrt{v_-}} & \text{out} \end{cases}$$

(21)

In the classical sense, the problem is solved now. In order to obtain an explicit relation of the form $z = z(\tau)$, one would have to take the functional inverse and square the resultant expression. However, since it does not contribute to the calculation of the relevant physical properties $\hat{z}, e_{\text{dry}}$ and $\tau_c$, that part of the problem, though utterly non-trivial, will not be addressed here.

### 3.3. Calculation of the physical parameters

With the above solution (19)–(21) of the equation of motion at hand, it is now possible to calculate the significant physical quantities. Although the two primary parameters of interest are the restitution coefficient $e_{\text{dry}}$ and collision time $\tau_c$, the calculation of the maximum penetration $\hat{z}$ is required as an intermediate step and is therefore addressed first. From the definition of $\dot{z}$, it follows that $\dot{z} = 0$, which is equivalent to the more tractable condition

$$v_+(y = \hat{y}) = 0,$$

(22)

with $\hat{y}^2 = \hat{z}$ the maximum penetration. This equation uniquely determines $\hat{z}$ in terms of the smallest positive real root of $v_+$. Since the solution trajectory is required to be continuous, the velocity on both the inward and outward trajectory must both go to zero at the same value of $y$, yielding the condition

$$v_-(y = \hat{y}) = 0.$$

(23)

This uniquely determines $e_{\text{dry}}$. Finally, the collision time can be computed directly as

$$\tau_c = \tau_-(\hat{y}).$$

(24)

Obviously, each of these quantities depend on $\lambda$. For $\lambda = 0$, the classical case of the undamped Hertzian restoring force is obtained, for which the solutions are

$$\hat{y}_0 := \hat{y}(\lambda = 0) = (5/4)^{1/5},$$

(25)

$$e_{\text{dry}}(\lambda = 0) = 1,$$

(26)

$$\tau_{c,0} := \tau_c(\lambda = 0) = 3.218.$$

(27)

For $\lambda$ small, therefore, it is natural to develop the solutions in terms of a power series in $\lambda$ around $\lambda = 0$, whereby the respective governing equations are successively differentiated.
at \( \lambda = 0 \) using implicit differentiation, with the chain rule used to evaluate the Taylor coefficients. This gives
\[
\sqrt{z} = \hat{y}_0 - 0.748\lambda + 0.578\lambda^2 + O(\lambda^3)
\] (28)
and hence, finally, one obtains:
\[
\begin{align*}
\epsilon_{\text{dry}} & = 1 - 3.576\lambda - 5.131\lambda^2 + O(\lambda^3) \\
\tau_c & = \tau_{c,0} + 1.152\lambda + O(\lambda^2)
\end{align*}
\] (29) (30)
where the special functions and other constant numerical factors were evaluated to four significant digits. Details of the calculation procedure are provided in Appendix B.

4. Approximate method and results

While the solution (29), (30) derived in the previous section is formally correct, calculating the necessary quantities can be costly as higher-order terms must be included for sufficient accuracy. If, however, terms higher than quadratic are involved, then the expressions cannot be conveniently inverted. Indeed, by algebraic means, the inversion of (29), (30) cannot be carried out if quintic or higher-order terms are present. The inversion can be done using the theta function, which is a non-elementary special function and costly to evaluate. In the following, a more elegant procedure is developed, based on the fact that the expressions of \( \epsilon_{\text{dry}}(\lambda) \) or \( \tau_c(\lambda) \) can be resolved for \( \lambda \).

To this end, consider the following ansatz with \( A, B, C \) denoting free parameters whose values are to be determined appropriately:
\[
\begin{align*}
\epsilon_{\text{dry}} & = \exp\left(-\frac{\alpha\lambda\tau_{c,0}}{\sqrt{1-C\lambda}}\right) \\
\tau_c & = \tau_{c,0} \sqrt{1-A\lambda-B\lambda^2}
\end{align*}
\] (31) (32)
The reason one may expect (31), (32) to be a more convenient choice than the simple power series (29), (30) for describing the required quantities is because they mimic to a great extent the relationships that are valid in the case of the damped harmonic oscillation. The equation of motion governing a dimensionless simple harmonic oscillation with linear damping is obtained if the power \( \frac{3}{2} \) is replaced by unity in (6), which is readily solved explicitly in closed form and yields the behaviour \( \log \epsilon_{\text{dry}} \propto -\delta \tau_c \) and \( \tau_c \propto (1-\delta^2)^{-1/2} \), where \( \delta \) corresponds to the damping ratio.

The value of most of the free parameters in (31), (32) can be determined directly from the solution (29), (30) found in Section 3. Differentiating (31) at \( \lambda = 0 \) yields the two equations
\[
\begin{align*}
\frac{\partial \epsilon_{\text{dry}}}{\partial \lambda}\big|_{\lambda=0} & = \alpha \tau_{c,0} \\
\frac{\partial^2 \epsilon_{\text{dry}}}{\partial \lambda^2}\big|_{\lambda=0} & = \alpha \tau_{c,0} (\alpha \tau_{c,0} - C)
\end{align*}
\] (33) (34)
The derivatives are given by (29), so that one obtains
\[
\alpha = 1.111 \quad \text{and} \quad C = 0.744
\] (35)
Likewise, differentiating (32) yields
\[ \frac{\partial \tau_c}{\partial \lambda} \bigg|_{\lambda=0} = \frac{1}{2} \tau_{c,0} A , \] (36)
so that
\[ A = 0.716 . \] (37)

The method is difficult to employ for determining the remaining free parameter \( B \), because it requires knowledge of the second-order correction to \( \tau_c \), which in turn necessitates the summation of divergent terms (in the form of derivatives of terms like \( (1 - \frac{1}{5} y^5)^{-1/2} \) with respect to \( y \) at \( y = \tilde{y}_0 \)) and improper divergent integrals. This appears, in fact, to be a characteristic shared by corrections to the collision time of all non-zero orders. For the first-order correction, the regularization of the result could be carried out by hand, because the indefinite integral underlying the divergent improper integral could be carried out in closed form and the cancellation of the divergent terms could be done away with in a straightforward manner. For higher order corrections, the integrals become increasingly involved; so much so, that even for the second-order term, the integration could not be carried out by hand. Thus the calculation of \( B \) by self-consistent methods is a highly non-trivial task which may be addressed in a future investigation.

For the present study, it shall suffice to obtain an approximation by a method similar to data-fitting. To this end, the dimensionless collision time is determined from numerically calculated solutions of the governing equation (6) for several values of \( \lambda \). The numerical integration was carried out using a Runge-Kutta method with an adaptive step size, employing the routine \texttt{ode45} of \textsc{Matlab}\textsuperscript{TM}. Equation (32) predicts that \( (\tau_{c,0}/\tau_c)^2 + A\lambda \) is a linear function of \( \lambda^2 \). Linear regression of the same yields
\[ B = 0.830 . \] (38)

The result of this section now is the approximation (31), (32) with the parameter values given in (35), (37) and (38). This shall serve as a convenient alternative to the series expansions (29), (30) for the purposes of the subsequent sections. In spite of the simple nature of the approximate formul\ae\ proposed in this section, their accuracy is very high in the practically interesting parameter range (\( \lambda \leq 0.2 \)). For a given value of \( \lambda \), the values of \( \epsilon_{\text{dry}} \) and \( \tau_c \) calculated from the closed-form expressions (31) and (32) were compared with the corresponding values obtained from a numerical Runge-Kutta solution of equation (6). It was found that the expression (32) for \( \tau_c \) has a maximum relative error of \( 2.2 \times 10^{-4} \). Likewise, the relative error of the approximation (31) does not exceed \( 4.9 \times 10^{-3} \) for the values of \( \lambda \) considered here. This may be seen as a numerical validation of the solutions derived in Section 3.3.

5. Application to the inverse problem

5.1. Inverse problem

In practice, one is often interested in a sort of inverse problem to the one discussed above. The ACTM of [5] imposes \( \epsilon_{\text{dry}} \) and \( T_c \) and determines the values of the parameters \( k \) and \( d \)
such that this is obtained individually for each collision. The problem, then, is to choose the appropriate parameters $k, d$ depending on the incident velocity $u_{\text{in}}$, given the mass of the particle $m_p$, collision time $T_c$ and restitution coefficient $e_{\text{dry}}$. To the best of our knowledge, a non-numerical means of achieving this is not known in the literature, although Kempe and Fröhlich [8] provide a practicable numerical iterative scheme.

5.2. Subroutine for direct parameter adaption

Equation (31) allows to solve for $\lambda$, yielding

$$
\lambda = \frac{1}{\alpha^2 \tau_{c,0}^2} \left( -\frac{1}{2} C \eta + \sqrt{\frac{1}{4} C^2 \eta^2 + \alpha^2 \tau_{c,0}^2 \eta} \right),
$$

where $\eta = (\log e_{\text{dry}})^2$ for convenience. Only the positive root of the quadratic equation is physically relevant. The values to be used in (39) are $\tau_{c,0} = 3.218 \ [5]$ and $\alpha = 1.111, C = 0.744$ from Section 4. When the collision time $T_c$ is imposed in physical units, relation (31) can be inserted into (32) in order to calculate the unit of time

$$
t_*= \frac{T_c}{\tau_{c,0}} \sqrt{1 - A \lambda - B \lambda^2},
$$

where the values $A = 0.716$ and $B = 0.830$ from Section 4 are to be used. With the definitions of $t_*$ and $\lambda$, namely (7) and (5) respectively, one finally obtains the physical material parameters

$$
d = \frac{2 \lambda m_p}{t_*},
$$

$$
k = \frac{m_p}{\sqrt{u_{\text{in}} t_*^5}}.
$$

For given material parameters of the particles, $m_p$ and $e_{\text{dry}}$, this provides a routine to compute from given impact velocity $u_{\text{in}}$ and desired collision time $T_c$ the parameters $k$ and $d$ in the governing equation (1).

6. Numerical results

6.1. Validation and assessment for binary particle-particle collisions

In this section numerical tests of the proposed subroutine for parameter adaption are presented. In particular, the accuracy and efficiency of the results obtained using the developed method is investigated. Table 1 provides data of test runs for various values of $e_{\text{dry}}$ and compares the performance with that of the quasi-Newton iterations developed by Kempe & Fröhlich [8] to compute the desired damping and stiffness. Since the standard Newton iteration scheme requires the calculation of the Jacobi matrix for each iteration step, it was replaced by a Broyden approximation. The convergence criterion in the iterative scheme was based on the residual of the rebound velocity and collision time and was set to $10^{-6}$. A
striking feature of the new algorithm is that the computation time is practically negligible for all cases. This is because all the underlying calculations involve at most the evaluation of elementary mathematical functions. On the other hand, the CPU time used by the iterative procedure shows a general trend of increasing CPU time for decreasing values of $e_{\text{dry}}$, and always yields larger times than that required by the present method.

Moreover, the present subroutine does not trade off accuracy for efficiency, at least not to any significant extent. To quantify this aspect, the equations of motion were solved with the adapted parameter values $k_{\text{appr}}, \theta_{\text{appr}}$ given by new method using a third-order Runge-Kutta solver. This is similar to how the algorithm would be employed in practice, as shown in the next section. On this basis the restitution coefficient $e_{\text{appr}}^{\text{dry}}$ and the collision time $T_{\text{c}}^{\text{appr}}$ were determined. The quality of the result can then be quantified by the relative errors

$$
e_{\text{dry}}^{\text{appr}} := \left| 1 - \frac{e_{\text{appr}}}{e_{\text{dry}}} \right| \quad \text{and} \quad T_{\text{c}}^{\text{appr}} := \left| 1 - \frac{T_{\text{c}}^{\text{appr}}}{T_{\text{c}}} \right|$$

with respect to the preset target values $e_{\text{dry}}$ and $T_{\text{c}}$. From Table 1, it is apparent that accuracy is indeed not compromised by the new direct method. In all cases of potential practical relevance ($e_{\text{dry}} > 0.7$), the relative error in the restitution coefficient is $e_{\text{dry}}^{\text{appr}} \sim 10^{-4}$ and does not exceed 1.3%, which is excellent. For obvious reasons, the accuracy decreases when lowering $e_{\text{dry}}$. Even for $e_{\text{dry}}$ as low as 0.4, the relative error is $e_{\text{dry}}^{\text{appr}} \sim 3\%$, which is acceptable. In the time domain, the collision time that results from the parameter adjustment by the present method agrees up to a relative error $e_{\text{c}}^{\text{appr}} \sim 10^{-4}$ with the pre-set target value.

The computation times for the Newton iteration scheme given in Table 1 is for a much more stringent convergence criterion. Hence, one may ask what the computational effort is, if the required accuracy of the Newton scheme is reduced to that of the direct approximate scheme, simply by stopping the iterations earlier. The resulting timings are reported in Table 2. It turns out that in the extreme case of $e_{\text{dry}} = 0.4$, the CPU time required when relaxing accuracy is reduced by a factor of nearly 6.3. For $e_{\text{dry}} = 0.95$ used later in Section 6.2, the saving obtained when lowering the accuracy of the iterative scheme is negligible. In all cases, even with the relaxed convergence criterion, the required time is orders of magnitude higher than the direct scheme, because even the initialisation and execution of 4-5 iteration steps is much costlier than the evaluation of elementary functions.

In summary, one can conclude that the subroutine proposed in this paper enables a computationally cheap and at the same time sufficiently accurate implementation of the concept of parameter-adapted time-stretched collision modelling developed in [8].
| $\epsilon_{\text{dry}}$ | ACTM | present |
|----------------|-------|---------|
|                | $n_{\text{it}}$ | $t_{\text{CPU}}$ [s] | $k$ | $d$ | $u_{\text{out}}$ | $T_c$ | $t_{\text{CPU}}$ [s] | $k$ | $d$ | $u_{\text{out}}$ | $T_c$ | $\epsilon_{\text{dry}}$ | $\epsilon_{T_c}$ |
| 1.00           | 1     | 60699.0 | 0   | $-1$ | $10^{-2}$ | 2.76 $\times 10^{-7}$ | 60694.4 | 0.00000 | $-1.00000$ | $1.00000 \times 10^{-2}$ | 3.50 $\times 10^{-12}$ | 0 |
| 0.95           | 5     | 0.0234  | 61491.7 | 0.30165 | $-0.95$ | $10^{-2}$ | 2.88 $\times 10^{-7}$ | 61491.7 | 0.30165 | $-0.95000$ | $1.00001 \times 10^{-2}$ | 7.71 $\times 10^{-7}$ | 7.6 $\times 10^{-5}$ |
| 0.90           | 5     | 0.0234  | 62369.2 | 0.61964 | $-0.90$ | $10^{-2}$ | 2.86 $\times 10^{-7}$ | 62371.9 | 0.61966 | $-0.90000$ | $0.99998 \times 10^{-2}$ | 1.33 $\times 10^{-5}$ | 1.7 $\times 10^{-5}$ |
| 0.80           | 13    | 0.0507  | 64418.6 | 1.31209 | $-0.80$ | $10^{-2}$ | 2.86 $\times 10^{-7}$ | 64437.6 | 1.31340 | $-0.79979$ | 0.99991 $\times 10^{-2}$ | 2.63 $\times 10^{-4}$ | 9.5 $\times 10^{-5}$ |
| 0.70           | 8     | 0.0351  | 66985.7 | 2.09541 | $-0.70$ | $10^{-2}$ | 2.87 $\times 10^{-7}$ | 67042.7 | 2.10348 | $-0.69906$ | 0.99982 $\times 10^{-2}$ | 1.34 $\times 10^{-3}$ | 1.8 $\times 10^{-4}$ |
| 0.60           | 19    | 0.0646  | 70299.5 | 2.99798 | $-0.60$ | $10^{-2}$ | 2.82 $\times 10^{-7}$ | 70434.0 | 3.02380 | $-0.59734$ | 0.99979 $\times 10^{-2}$ | 6.05 $\times 10^{-3}$ | 2.1 $\times 10^{-4}$ |
| 0.50           | 60    | 0.1679  | 74735.8 | 4.06030 | $-0.4999$ | $10^{-2}$ | 2.75 $\times 10^{-7}$ | 75047.0 | 4.12956 | $-0.49396$ | 1.00000 $\times 10^{-2}$ | 1.21 $\times 10^{-2}$ | 2.5 $\times 10^{-6}$ |
| 0.40           | 76    | 0.1992  | 80999.5 | 5.35192 | $-0.3998$ | $10^{-2}$ | 2.88 $\times 10^{-7}$ | 81738.6 | 5.51951 | $-0.38797$ | 1.00085 $\times 10^{-2}$ | 1.34 $\times 10^{-2}$ | 8.5 $\times 10^{-4}$ |

Table 1: Summary of test runs for cases. The results achieved by the method presented in Section 5.2 (heading: present) are compared with those of the Newton iterations in [8]. The situation simulated is depicted in Figure 1 with initial condition $u_{\text{in}} = 1$, material parameters particle density $\varrho = 7800$ and radius $R_p = 10^{-2}$. The pre-set collision time was $T_c = 10^{-2}$ and the target restitution coefficient $\epsilon_{\text{dry}}$ was varied as documented in the first column. The cases with $\epsilon_{\text{dry}} < 0.7$ are fictitious, in the sense that they are unlikely to be of practical interest as of now, and are included to show the integrity of the presented method even in such extremes.
6.2. Application to multiple particles sedimenting on a rough surface

The final test case deals with the sedimentation of 100 randomly distributed particles and their impact on a layer of 195 fixed particles arranged in hexagonal packing (Fig. 3a) very similar to the simulations presented in [10]. The main difference is that the fluid is neglected in the present case corresponding to an infinite Stokes number of the particles. The goal of the simulations is to compare the results obtained with the original scheme [8] to the results of the approximate inverse procedure developed in Section 5 when the procedure is employed in a practical application with multiple simultaneous collisions.

The computational domain is \( \Omega = [0, L] \times [0, L] \times [0, L] \) with \( L = 1.5 \). Periodic boundary conditions were applied in the \( x \)- and \( z \)-directions. The gravitational acceleration is \( g = 9.81 \) and the density of the particles is \( \varrho_p = 1200 \), with the particle diameter \( D = 0.1154 \). The mobile particles are placed randomly in the subdomain \( \Omega_1 = [0.1, 1.4] \times [0.3, 1.2] \times [0.1, 1.4] \), and their velocity is initialised with zero. Once these particles are released from their initial position (Figure 3a), they are accelerated by gravity towards the fixed layer and then collide with the bed or with other mobile particles. At the same time they are subjected to a dissipation of kinetic energy when undergoing collisions. Two different cases are considered.

In Case 1, the coefficient of restitution is set to \( e_{\text{dry}} = 0.95 \) and in Case 2 the value is \( e_{\text{dry}} = 0.7 \). The simulations were run with \( \Delta t = 5 \times 10^{-4} \) for 5000 steps, corresponding to a non-dimensional simulation time of \( t = 2.5 \). This situation is depicted in Figure 3b for Case 1. The particles are coloured by the absolute value of their velocity from red \( (u_p = 2) \) to blue \( (u_p = 0) \) showing that not all the particles come to rest at the end of the simulation if the damping is weak.

The collision process is elucidated by computing the various components of the total energy of the particles. The potential energy, the kinetic energy and the energy stored by deformation of the springs in the collision model are defined as

\[
E_{\text{pot}} = \sum_{i=1}^{n_p} m_{p,i} g y_{p,i}
\]  

Table 2: Number of iterations \( n_{\text{it}} \) and computation time \( t_{\text{CPU}} \) for the quasi-Newton iteration scheme of [8] with the convergence criterion at par with the accuracy achieved by the present method (cf. Table 1).

| \( e_{\text{dry}} \) | \( n_{\text{it}} \) | \( t_{\text{CPU}} \) [s] |
|---------------------|----------------|---------------------|
| 1                   | 0              | —                   |
| 0.95                | 4              | 0.0234              |
| 0.90                | 4              | 0.0234              |
| 0.80                | 4              | 0.0234              |
| 0.70                | 4              | 0.0234              |
| 0.60                | 4              | 0.0234              |
| 0.50                | 5              | 0.0313              |
| 0.40                | 5              | 0.0313              |
Figure 3: Sedimentation of 100 particles at infinite Stokes number and impact on a layer of 195 fixed particles in hexagonal packing. a) Initial configuration at $t = 0$, b) situation at the end of the simulation $t = 2.5$. The particles are coloured by the absolute value of their velocity from red ($u_p = 2$) to blue ($u_p = 0$).

The total energy in the computational domain then is

$$E_{\text{tot}} = E_{\text{pot}} + E_{\text{kin}} + E_{\text{spring}}$$

(47)

The fractions of energy are displayed in Figure 4a and Figure 4b for Case 1 and 2, respectively. As already mentioned above, in Case 1 the particles do not come to rest at the end of the simulation, reflected by their kinetic energy not being zero at the end of the simulation. In contrast to this, the kinetic energy of the particles at $t = 2.5$ is zero for Case 2. Obviously, no significant differences of the various fractions of the energy are observed if the iterative or if the approximate method is used. The slight differences in Case 1 rather result from the fact that extremely small differences in the collision process can yield different particle trajectories, in turn leading to subsequent differences, as in a billiard system, without changing the overall behaviour of the ensemble.

To further elucidate the efficiency of the two numerical procedures, the CPU times of the old and the new scheme are compiled in Table 3. Here, $t_{\text{tot}}$ is the overall CPU time required for the whole simulation including overhead, $t_{\text{par}}$ the time spent in the particle routines, $t_{\text{coeff}}$ is the part of $t_{\text{par}}$ required for the determination of stiffness and damping, $n_{\text{col}}$ the overall
number of collisions and, finally, $t_{\text{col}}$ is the average time required per collision. Obviously, the numerical effort is substantially reduced for all values of $e_{\text{dry}}$ if the new approximate method is used. The results presented in this section confirm the accuracy, robustness and efficiency of the proposed method.

7. Concluding remarks

In this paper, normal particle-wall collisions were studied by modelling the elastic interaction with a repulsive Hertzian contact force, with an additional damping force linear in the velocity accounting for dissipative effects.

First, the equation of motion (1) was converted to its dimensionless form (6). This reduces the number of parameters in the equation to a single constant $\lambda$ depending on the material parameters $k, d$ and the impact velocity $u_0$. In particular, the physically relevant and practically interesting properties, the collision time $T_c$ (dimensionless: $\tau_c$) and restitution coefficient $e_{\text{dry}}$, hence, can only depend on this particular combination of physical input parameters. This is conceptually and technically analogous to the damping ratio, or its inverse, the quality factor, which are familiar from the simple harmonic oscillator, the latter more so from $LC$ circuits in electrical engineering. In contrast, earlier works [8, 11] typically use a three-parameter family of input variables $k, d, u_0$. While the use of $e_{\text{dry}}$ to label cases is helpful in practice, the proposed nondimensionalization and the subsequent analytical investigation establishes in a straightforward manner the one-to-one correspondence between the important experimental parameter $e_{\text{dry}}$ and the parameter $\lambda$, which is easy to obtain from material parameters. Furthermore, it demonstrates that different parameters with the same $e_{\text{dry}}$ have solutions that are identical up to a linear scaling of space and time.
| Method | $e_{\text{dry}}$ $t_{\text{tot}}$ [s] | $t_{\text{par}}$ [s] | $t_{\text{coeff}}$ [s] | $n_{\text{col}}$ | $t_{\text{col}}$ [s] |
|--------|---------------------------|-----------------|--------------------------|----------------|-----------------|
| Newton | 0.95  836.46  812.78 | 221.49 | 21950 | 0.01009 | |
|        | 0.90  839.22  815.23 | 229.71 | 22362 | 0.01027 | |
|        | 0.80  783.91  760.36 | 186.57 | 16605 | 0.01134 | |
|        | 0.70  734.28  711.93 | 142.86 | 11687 | 0.01222 | |
| present| 0.95  597.76  578.45 | 1.953 $\times 10^{-2}$ | 21111 | 9.72 $\times 10^{-7}$ | |
|        | 0.90  601.75  582.09 | 3.516 $\times 10^{-2}$ | 22974 | 9.05 $\times 10^{-7}$ | |
|        | 0.80  591.66  572.28 | 2.344 $\times 10^{-2}$ | 18845 | 8.32 $\times 10^{-7}$ | |
|        | 0.70  591.19  571.71 | 7.813 $\times 10^{-3}$ | 11829 | 8.38 $\times 10^{-7}$ | |

Table 3: CPU time required for the sedimentation test case with various values of the restitution coefficient using the ACTM with Newton iterations [8] and the present direct method (39)–(42) for the computation of stiffness and damping.

Next, an exact formal solution of the governing equation using nonlinear transformations and a series in the parameter $\lambda$ was proposed, providing a rigorous calculation of $e_{\text{dry}}$ and $\tau_c$ from the equation of motion. Owing to the technical difficulties presented by the governing equation, the analysis is necessarily involved, the methods and technique employed may be instructive, and the results may be of use in theoretical considerations. The approach is also quite flexible, and a similar analysis would be applicable to more general settings, such as the extension to fully nonlinear models, i.e. a nonlinear spring force in combination with a nonlinear dissipative force as considered in [2, 3, 7]. This may be the subject of future investigation.

Subsequently, an approximation based on the exact solution was proposed, yielding compact and convenient formulæ for $e_{\text{dry}}$ and $\tau_c$. Inverse formulæ were derived on that basis, enabling a very efficient and accurate calculation of the required stiffness and damping from the given input parameters, i.e. the desired collision time $T_c$ and restitution coefficient $e_{\text{dry}}$. These were then applied to an engineering context. The quasi-Newton iteration scheme in the original ACTM was replaced by the direct approximate solution developed here. Numerical tests on binary and multiple particle collisions confirm the accuracy and efficiency of the proposed method.

**Acknowledgements**

The computations in Section 6 were performed at ZIH, TU Dresden. The first author also wishes to express his gratitude to the Martin-Andersen-Nexo-Gymnasium Dresden for providing the appropriate framework within their school curriculum for carrying out parts of the research.
Appendix A. Physical interpretation of the coefficients \( v_{\pm,m} \)

It may be instructive to discuss the physical meaning of the coefficients \( v_{\pm,m} \) in the series expansion in powers of \( \lambda \) of \( v_{\pm} \), equations (19)-(20). First, it is readily seen that the zeroth-order term is

\[
v_{+,0} = v_{-,0} = 1 - \frac{4}{5} y^5,
\]

as obtained in (16). The fact that the two expressions are equal indicates reversibility. Indeed, for \( \lambda = 0 \), one has the classical oscillation problem with Hertzian restoring force, which is a conservative system. Moreover, upon inspection of the functional dependence, it is evident that the zeroth-order term expresses conservation of mechanical energy itself. The kinetic energy per unit mass and in dimensionless form is given by

\[
E_{\text{kin}} = \frac{1}{2} \dot{z}^2 = \frac{1}{2} v_{\pm}
\]
depending on which part of the trajectory is considered. Thus, the auxiliary variables \( v_{\pm} \) are proportional to the kinetic energy. The potential energy associated with the Hertz contact force (dimensionless and per unit mass) is

\[
E_{\text{pot}} = \frac{2}{5} z^{5/2} = \frac{2}{5} y^5.
\]

For both the inward and outward motion of the particle, the conservation of energy

\[
\frac{1}{2} v_{\pm} + 2 y^5 = E_{\text{kin}} + E_{\text{pot}} = \text{const.} \tag{A.1}
\]
is valid to zeroth-order in \( \lambda \). Now consider the more involved first-order corrections. Equations (19)-(20) yield

\[
v_{+,1} = -8 \int_0^y \sqrt{1 - \frac{4}{5} y^5} y' \, dy' \tag{A.2}
\]

\[
v_{-,1} = \frac{\partial e_{\text{dry}}^2}{\partial \lambda} \bigg|_{\lambda=0} + 8 \int_0^y \sqrt{1 - \frac{4}{5} y^5} \, dy' y' \tag{A.3}
\]

Both integrals can be evaluated analytically to give

\[
v_{+,1} = -\frac{16}{7} y^2 \sqrt{1 - \frac{4}{5} y^5} - \frac{20}{7} y^2 2 F_1 \left( \frac{2}{5}; \frac{7}{5}; \frac{4}{5} y^5 \right)
\]

with \( 2 F_1 \) denoting the hypergeometric function [cf. [1] Chapter 15, pp. 555]. A similar expression results for \( v_{-,1} \). The integral representations are actually more conducive for physical interpretation. Indeed, both expressions can be interpreted as work done by the dissipative force. In case of \( v_{-,1} \), there is an added constant term, because the initial condition \( v_-(y = 0) = e_{\text{dry}}^2 \) depends on \( \lambda \), unlike the much more straightforward case \( v_+(y = 0) = 1 \). For this reason, the +, or inward, branch of the trajectory shall be discussed in the following. Since \( 2ydy = dz \),

\[
\frac{1}{2} v_{+,1} = -2 \int_0^z \sqrt{1 - \frac{4}{5} z^{5/2}} \, dz'. \tag{A.4}
\]
On the other hand, from $v_+ = v_{+,0} + \mathcal{O}(\lambda)$, it follows that to first order in $\lambda$, the work done by the damping force is

$$W_+^{\text{diss}} = -2\lambda \int_0^z \dot{z} \, dz' = -2\lambda \int_0^z \sqrt{v_{+,0}} \, dz' + \mathcal{O}(\lambda^2) = \frac{1}{2} v_{+,1} \lambda + \mathcal{O}(\lambda^2) . \quad (A.5)$$

Thus, $v_{\pm,1}$ are essentially first-order corrections in the energy balance due to the work done by the dissipative term in the equations of motion.

**Appendix B. Calculations of first order corrections**

In the following, the necessary calculations to determine the first order corrections for three physically useful quantities are performed. These are the surface penetration $\dot{z} = \dot{y}^2$, the restitution coefficient $e_{\text{dry}}$ and the collision time $\tau_c$.

**Maximum surface penetration** A necessary condition fulfilled by the point of maximum penetration is $\dot{z} = 0$, hence the solution must obey $v_+ (\dot{y}) = 0$. To zeroth order, this yields

$$1 - \frac{4}{5} \dot{y}_0^5 = 0 , \quad (B.1)$$

and hence $\dot{y} = \sqrt[5]{5/4} + \mathcal{O}(\lambda)$. This is the same solution as one would estimate using conservation of energy, since to zeroth order in $\lambda$, the dissipation of energy, i.e. work done by the damping force is negligible. Differentiating $v_+ (\dot{y})$ once with respect to $\lambda$ and using the chain rule to account for the fact that $\dot{y} = \dot{y}(\lambda)$, one obtains at $\lambda = 0$ the condition

$$\frac{\partial v_+}{\partial y} \bigg|_{y=\dot{y}_0} \frac{\partial \dot{y}}{\partial \lambda} \bigg|_{\lambda=0} + v_{+,1} (y = \dot{y}_0) = 0 ,$$

or

$$-4 \dot{y}_0^4 \frac{\partial \dot{y}}{\partial \lambda} \bigg|_{\lambda=0} - 8 \int_0^{\dot{y}_0} \sqrt{1 - \frac{4}{5} y^5} \, dy = 0 \quad (B.2)$$

Carrying out the integration gives

$$\dot{y} = \sqrt[5]{\frac{5}{4}} - \frac{1}{2} \sqrt[5]{\frac{16}{25} \pi \Gamma \left( \frac{7}{5} \right) \lambda} + \mathcal{O}(\lambda^2) . \quad (B.3)$$

**Restitution coefficient** Continuity of the solution requires, that $v_- (\dot{y}) = v_+ (\dot{y}) = 0$. Again, to zeroth order, one readily finds $e_{\text{dry}} |_{\lambda=0} = 1$, which is an obvious consequence of conservation of energy (the dissipation through damping being first order and higher in $\lambda$). Differentiating the expression for $v_- (\dot{y})$ yields

$$\frac{\partial v_-}{\partial y} \bigg|_{y=\dot{y}_0} \frac{\partial \dot{y}}{\partial \lambda} \bigg|_{\lambda=0} + v_{-,1} (y = \dot{y}_0) = 0$$

and hence

$$\frac{\partial e_{\text{dry}}}{\partial \lambda} \bigg|_{\lambda=0} = 2 \dot{y}_0^4 \frac{\partial \dot{y}}{\partial \lambda} \bigg|_{\lambda=0} - 4 \int_0^{\dot{y}_0} \sqrt{1 - \frac{4}{5} y^5} \, dy = -8 \int_0^{\dot{y}_0} \sqrt{1 - \frac{4}{5} y^5} \, dy , \quad (B.4)$$

so that finally

$$e_{\text{dry}} = 1 - 2 \sqrt[5]{\frac{25}{16} \pi \Gamma \left( \frac{7}{5} \right) \lambda} + \mathcal{O}(\lambda^2) \quad (B.5)$$
Collision time  This is, in principle, a straightforward computation of the integral
\[
\tau_c = \int_0^\hat{y} \left( \frac{1}{\sqrt{v_+}} + \frac{1}{\sqrt{v_-}} \right) 2y \, dy
\]  \hspace{1cm} (B.6)

Since \( v_+ = v_{+0} + v_{+1} \lambda + \cdots \), this gives
\[
\tau_c = \int_0^\hat{y} \left[ \frac{1}{\sqrt{v_{+0}}} \left( 1 + \frac{v_{+1}}{v_{+0}} \lambda + O(\lambda^2) \right)^{-1/2} + \frac{1}{\sqrt{v_{-0}}} \left( 1 + \frac{v_{-1}}{v_{-0}} \lambda + O(\lambda^2) \right)^{-1/2} \right] 2y \, dy
\]  \hspace{1cm} (B.7)

using (16), (A.3) and (B.5), as well as the Taylor series representation of \((1 + x)^{-1/2}\). For \( \lambda = 0 \), the integral is straightforward, yielding the same result as Hertz [5]:
\[
\tau_c = \frac{2\sqrt{\pi} \Gamma\left(\frac{7}{5}\right)}{\Gamma\left(\frac{9}{10}\right)} \sqrt{\frac{25}{16} + O(\lambda^2)} \]  \hspace{1cm} (B.8)

For the first-order correction, differentiating with respect to \( \lambda \) and setting \( \lambda = 0 \) gives
\[
\left. \frac{\partial \tau_c}{\partial \lambda} \right|_{\lambda=0} = -\frac{1}{2} \sqrt{\frac{16}{25}} \sqrt{\frac{\pi}{\Gamma\left(\frac{7}{5}\right)}} \frac{1}{\sqrt{1 - \frac{4}{5}y^5}} \bigg|_{y=\hat{y}_0} + \frac{5}{16} \sqrt{\frac{\pi}{\Gamma\left(\frac{7}{5}\right)}} \int_0^{\hat{y}_0} \frac{4y \, dy}{\sqrt{1 - \frac{4}{5}y^5}}. \]  \hspace{1cm} (B.9)

Both terms are divergent: The first term on the right hand side has a simple pole at \( y = \hat{y}_0 \) and the integrand in the second term diverges too fast for \( y \to \hat{y}_0 \). The result can, however, be regularized by calculating the integral first for general \( y < \hat{y}_0 \) and then taking the limit of the whole expression for \( y \to \hat{y}_0 \). The antiderivative of the function \( y \left( 1 - \frac{4}{5}y^5 \right)^{-3/2} \) contains a term \( \sim (1 - \frac{4}{5}y^5)^{-1/2} \), which cancels with the first singularity in (B.9), yielding
\[
\left. \frac{\partial \tau_c}{\partial \lambda} \right|_{\lambda=0} = \frac{2}{5} y_0 \sqrt{\frac{\pi}{\Gamma\left(\frac{7}{5}\right)}} \frac{\Gamma\left(\frac{7}{5}\right)}{\Gamma\left(\frac{9}{10}\right)} 2F_1\left(\frac{3}{5}, \frac{1}{2}; \frac{7}{5}; 1\right). \]  \hspace{1cm} (B.10)

This can be simplified to yield
\[
\tau_c = \frac{2\sqrt{\pi} \Gamma\left(\frac{7}{5}\right)}{\Gamma\left(\frac{9}{10}\right)} \sqrt{\frac{25}{16} + \frac{5}{9} \frac{4 \cdot 5^4}{\Gamma\left(\frac{7}{5}\right)} \Gamma\left(\frac{9}{10}\right)} \lambda + O(\lambda^2). \]  \hspace{1cm} (B.11)
References

[1] Abramowitz, A., Irene, A., 1965. Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables. Dover, New York.
[2] Crowe, C., 2006. Multiphase Flow Handbook. CRC Press.
[3] Crowe, C., Sommerfeld, M., Tsuji, Y., 1998. Multiphase Flows with Droplets and Particles. CRC Press, New York.
[4] Cundall, P. A., Strack, O. D. L., 1979. A discrete numerical model for granular assemblies. Geotechnique 29, 47–65.
[5] Hertz, H., 1882. Über die berührung fester elastischer körper. J. Reine Angew. Math. 92, 156–171.
[6] Hoomans, B. P. B., Kuipers, J. A. M., Briels, W. J., van Swaaij, W. P. M., 1996. Discrete particle simulation of bubble and slug formation in a two-dimensional gas-fluidised bed: a hard-sphere approach. Chem. Eng. Sci. 51, 99–108.
[7] Kawabara, G., Kono, K., 1987. Restitution coefficient in a collision between two spheres. Jpn. J. Appl. Phys. 1 26, 1230–1233.
[8] Kempe, T., Fröhlich, J., 2012. Collision modeling for the interface-resolved simulation of spherical particles in viscous fluids. J. Fluid Mech. 709, 445–489.
[9] Kempe, T., Fröhlich, J., 2012. An improved immersed boundary method with direct forcing for the simulation of particle laden flows. J. Comput. Phys. 231, 3663–3684.
[10] Kempe, T., Vowinckel, B., Fröhlich, J., 2014. On the relevance of collision modeling for interface-resolving simulations of sediment transport in open channel flow. Int. J. Multiphase Flow 58, 214–235.
[11] Kruggel-Emden, H., Simsek, E., Rickelt, S., Wirtz, S., Scherer, V., 2007. Review and extension of normal force models for the discrete element method. Powder Technol. 171, 157–173.
[12] Kruggel-Emden, H., Wirtz, S., Scherer, V., 2008. Selection of optimal models for the discrete element method: The single particle perspective. In: ASME 2008 Pressure Vessels and Piping Conference. American Society of Mechanical Engineers, pp. 123–135.
[13] Kruggel-Emden, H., Wirtz, S., Scherer, V., 2009. Applicable contact force models for the discrete element method: the single particle perspective. Journal of Pressure Vessel Technology 131 (2), 024001.
[14] Lee, J., Herrmann, H. J., 1993. Angle of repose and angle of marginal stability: molecular dynamics of granular particles. J. Phys. A: Mathematical and General 26 (2), 373.
[15] Pöschel, T., Schwager, T., 2005. Computational Granular Dynamics: Models and Algorithms. Springer.
[16] Uhlmann, M., 2005. An immersed boundary method with direct forcing for the simulation of particulate flows. J. Comput. Phys. 209, 448–476.