

A regularized version of the Kuwabara-Kono force scheme for 2nd order convergence in DEM simulations of granular materials

Gabriel N. Bufolo^{1,*} and Yuri D. Sobral^{1,**}

¹Departamento de Matemática, Universidade de Brasília, Campus Universitário Darcy Ribeiro, 70.910-900 Brasília-DF, Brazil

Abstract. The Discrete Element Method is a technique widely used to simulate multi-particle systems, in particular granular materials. For conservative systems, the integration of the equations of motion is often performed via a Verlet-type method of order two, due to its second order accuracy and near energy conservation properties. However, when dissipative forces are included, such as in simulations of granular materials, the Verlet method no longer behaves as a second order method. For instance, when using the popular Kuwabara-Kono force scheme, the order of the Verlet method decreases to 1.5, due to the singular behavior of the damping force during particle collisions. In this work, we propose a regularization of the Kuwabara-Kono force model via mollification. We show numerically that the Verlet method combined with this regularized force model can integrate collisions with second order accuracy and that the coefficient of restitution of the system increases as a function of the regularization parameter.

1 Introduction

Consider two spherical particles, say P_1 and P_2 , in such a way that they will evolve to a purely normal collision. In this case, the motion of the particles is governed by Newton's second law of motion. The Discrete Element Method (DEM) algorithm provides a way to determine the contact force by establishing a relationship between the force and the overlap $\xi(t)$ between the two particles, defined as

$$\xi(t) := R_1 + R_2 - |\mathbf{x}_1(t) - \mathbf{x}_2(t)|, \quad (1)$$

where R_i and $\mathbf{x}_i(t)$ denote, respectively, the radius and position of the particle P_i . There are several force models that can be used to model the collision of the particles [1, 2] and, in this work, the one proposed by Kuwabara and Kono in [3] is used. It is given by

$$|\mathbf{F}_i(t)| = \tilde{k}_n \xi(t)^{3/2} + \gamma \xi'(t) \xi(t)^{1/2}, \quad (2)$$

where \tilde{k}_n is related to the stiffness of the material of the particles and γ is the damping constant. It is found that this model agrees reasonably well with experimental trends for both the coefficient of restitution and the collision duration [2].

In DEM simulations, some numerical integrator is used with Newton's second law. In this work, we concern ourselves mostly with Verlet-type methods [4]. When the force depends explicitly on the velocity, however, the standard Verlet method has to be adapted so that it retains second order accuracy [5]. It does so by first using a leapfrog method to find an approximation for the position

of the particle at t_{n+1} and then use this estimate to approximate the velocity of the particle at t_n via a centered finite difference of second order. For a one-dimensional motion along the axis defined by the centers of the particles, the adapted method is given by the iterative process

$$\begin{cases} \hat{v}_{n+\frac{1}{2}} &= v_{n-\frac{1}{2}} + hF(t_n, x_n, v_{n-\frac{1}{2}})/M; \\ \hat{x}_{n+1} &= x_n + h\hat{v}_{n+\frac{1}{2}}; \\ v_n &= \frac{\hat{x}_{n+1} - x_{n-1}}{2h}; \\ v_{n+\frac{1}{2}} &= v_{n-\frac{1}{2}} + hF(t_n, x_n, v_n)/M; \\ x_{n+1} &= x_n + hv_{n+\frac{1}{2}}, \end{cases} \quad (3)$$

where x and v denote, respectively, the position and the velocity of the particle, F denotes the total force acting on the particle, M is the mass of the particle and h the time step of the method. Further details regarding this method and its numerical properties can be found in [5, 6].

2 Order of the numerical integration with the Kuwabara-Kono model

2.1 Description of the problem

For this work, collision simulations were assembled in such a way that both particles have no angular motion and one of the particles is fixed, i.e. its position is not evolved in time. The center of the other particle is placed at a distance $R_1 + R_2$ of the center of the fixed particle, with an initial velocity of magnitude 1 m/s and in the direction of the fixed particle. Two such simulations were run, one using the Kuwabara-Kono force model given in eq. (2) and another one where the purely elastic (undamped) Hertz force

*e-mail: gbufolo7@gmail.com

**e-mail: ydsobral@unb.br

model was used instead. The order of the Verlet method in eq. (3) was determined for each of the simulations. The results are presented in fig. 1.

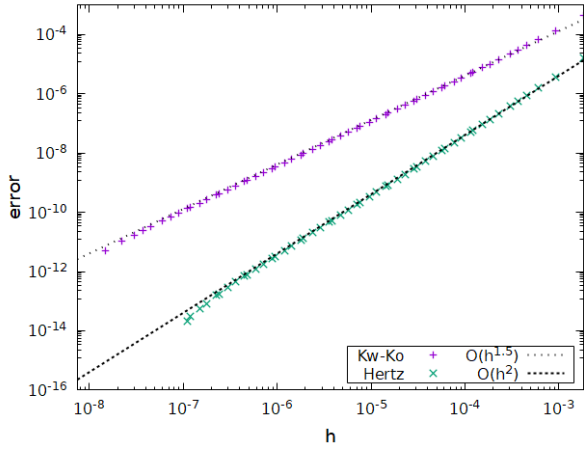


Figure 1: Order analyses of the position of the moving particle involved in the binary normal collision. The usual Hertz model has no damping term, which means that $\gamma = 0$ in eq. (2) in this case. The parameters used for the simulations were $\rho = 19300 \text{ kg/m}^3$, $R = 1 \text{ m}$, $\tilde{k}_n \approx 4.4 \times 10^{10} \text{ N/m}^{1.5}$, $\gamma \approx 1.1 \times 10^9 \text{ kg/(m}^{0.5}\text{s)}$ and $T \approx 0.012 \text{ s}$.

The results of the order analysis depicted in fig. 1 reveal an unexpected behavior. When the purely elastic force model is used, the accumulated error in the position decreases as $O(h^2)$, as it is expected when eq. (3) is used to integrate the motion of the particle. However, when the full Kuwabara-Kono force model is used, the curve approximating the accumulated error in the position decreases as $O(h^{1.5})$, which does not agree with the expected order of eq. (3).

The inclusion of the dissipation term in the model penalized the order of the Verlet algorithm given by eq. (3). The cause of this order reduction, therefore, has to lie in the $\xi^{1/2}$ term in eq. (2): in fact, when there is a transition from $\xi = 0$ to $\xi > 0$, the derivative of the term $\xi^{1/2}$ becomes unbounded. It seems that this issue has not yet been observed nor discussed in the literature.

2.2 Numerical analysis of the penalization of the order of the numerical scheme

In order to formally analyze the order reduction of eq. (3) caused by the dissipation term in eq. (2), we devised a simplified problem which retains the essential feature we believe is behind the issue identified in section 2.1 [7]. In this simplified problem, the nonlinearity retains the general form ξ^q , for $0 < q < 1$. Note that, for the Kuwabara-Kono force model, $q = 1/2$. We were able to formally prove [7] that the error of the leapfrog method applied to the simplified problem decreases as h^{1+q} , thus confirming the suppositions in the last paragraph of the previous section. We want to be able to retain the appropriate physics brought by the Kuwabara-Kono force model and the $O(h^2)$

of the Verlet-type integration given by eq. (3). Thus, we have chosen to remove the singularity brought by the nonlinearity $\xi^{1/2}$.

3 A regularized force model

3.1 Mollifiers

Let $\phi : \mathbb{R} \rightarrow \mathbb{R}$ be defined as

$$\phi(x) := \begin{cases} \frac{1}{C} \exp\left(\frac{1}{x^2 - 1}\right) & \text{if } -1 < x < 1; \\ 0 & \text{otherwise,} \end{cases} \quad (4)$$

where C is chosen such that the integral of $\phi(x)$ equals 1. The function defined by eq. (4) is called the ‘‘standard mollifier’’ [8], and can be seen in fig. 2(a).

For any $\epsilon \in (0, \infty)$, one can then define the real function

$$\phi_\epsilon(x) := \frac{1}{\epsilon} \phi\left(\frac{x}{\epsilon}\right). \quad (5)$$

The function ϕ_ϵ is called the ϵ -mollifier, it is supported on the interval $[-\epsilon, \epsilon]$, and its integral remains equal to 1.

Given $f : \mathbb{R} \rightarrow \mathbb{R}$ a locally integrable function, one can define its ϵ -mollification as the convolution of ϕ_ϵ and f , denoted by $\phi_\epsilon * f$. This new function has the desired property of being infinitely differentiable in \mathbb{R} , while being almost the same function as the original function f . The quality of the approximation of f by $\phi_\epsilon * f$ improves as $\epsilon \rightarrow 0$.

3.2 Extended square root and ϵ -shift

In order to properly calculate $\phi_\epsilon * f$, the function f must be defined on $[-\epsilon, \infty)$. In the case of the square root function, this is not true. For this reason, we extend the square root to negative numbers via $\sqrt{x} = 0$ if $x < 0$ (while maintaining the same notation).

The ϵ -mollification of this square root does not vanish at $x = 0$, as illustrated in fig. 2(b). This could pose a problem for the force model. A way to prevent this is to define the right-shift function,

$$\tau_\epsilon : \mathbb{R} \rightarrow \mathbb{R}; \quad \tau_\epsilon(x) = x - \epsilon. \quad (6)$$

Then, the ϵ -shifted ϵ -mollification of $\sqrt{\cdot} \circ \tau_\epsilon$, which is depicted in fig. 2(c), is always zero when $x = 0$. For convenience of notation, from now on we define

$${}_\epsilon\sqrt{\cdot} := \phi_\epsilon * \left(\sqrt{\cdot} \circ \tau_\epsilon\right). \quad (7)$$

3.3 Regularized normal force model

Based on the discussion in the subsections above, we propose a regularized model for the normal contact force in which the $\sqrt{\cdot}$ term in eq. (2) is substituted by ${}_\epsilon\sqrt{\cdot}$, as defined in eq. (7). Therefore, we obtain

$$|\mathbf{F}_i(t)| = k\xi(t)^{3/2} + \gamma\xi'(t) {}_\epsilon\sqrt{\xi(t)}. \quad (8)$$

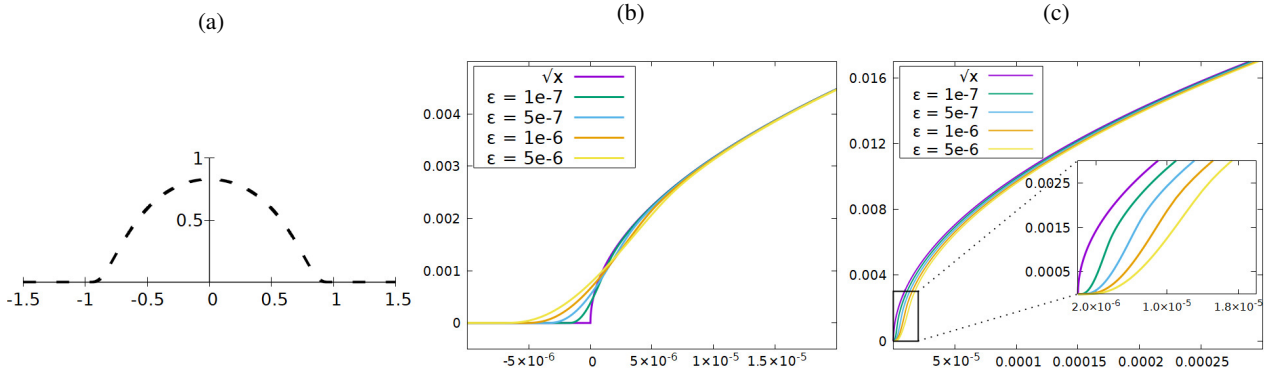


Figure 2: In (a), the plot of the standard mollifier. In (b), comparison between $\sqrt{\cdot}$ and the ϵ -mollification of \sqrt{x} for different values of ϵ . In (c), comparison between $\sqrt{\cdot}$ and the ϵ -mollification of $(\sqrt{\cdot} \circ \tau_\epsilon)$, $\epsilon\sqrt{\cdot}$, for different values of ϵ . In both plots, the purple curve is \sqrt{x} , for comparison. Notice how all curves in (c) go through (0,0). In both figures, mollifications were computed using a composite midpoint rule with 1000 sub-intervals.

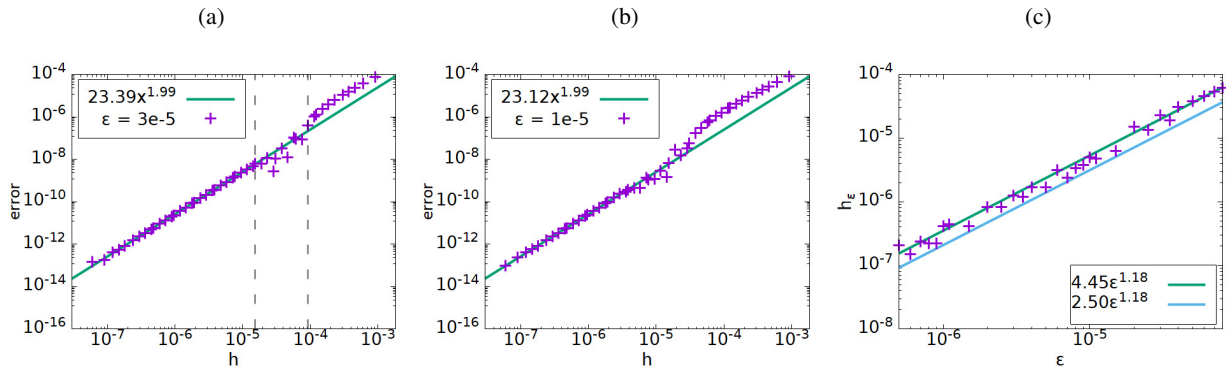


Figure 3: In (a) and (b), order analyses of the integration method shown in eq. (3) associated with the proposed model described in eq. (8), for different values of ϵ . The physical system being simulated is a binary normal collision and the position of one of these particles is the variable whose order is being analyzed. In (c), computed value of h_ϵ as a function of ϵ . The green line is the best fit of the data to a power law, while the blue line is “safe” choice for h based on all values of ϵ tested. In all plots, the values of the parameters used are presented in the caption of fig. 1.

We performed simulations for different values of ϵ . The results are displayed in section 3.3 and indicate that the error decreases as $O(h^2)$, as desired.

Because of the regions of error oscillations (whose boundaries are highlighted in fig. 3(a) and depend on the choice of ϵ), it is necessary that the value of h belongs to the leftmost region of the plot in fig. 3(a), for the chosen value of ϵ . In these regions, where the size of h is comparable to the size of ϵ , the mollified force model given in eq. (8) is not sampled enough times near zero to provide an adequate calculation of the mollified square-root function. Thus, an adequate combination of ϵ and h must be selected. To quantitatively understand how this selection must be made, we performed the order analyses for different values of ϵ and h . For each of these analyses, we selected the biggest value of h , called h_ϵ , such that the error decreases as $O(h^2)$ for all $h < h_\epsilon$. The results are presented in fig. 3(c). Any pair (ϵ, h_ϵ) below the blue line

is a valid choice for which the regularized model in eq. (8) integrated with eq. (3) will produce an (expected) $O(h^2)$ decay of the error for the values of \tilde{k}_n and γ given in the caption of fig. 1.

Further details on how to efficiently implement the regularized force model are available in [6].

3.4 Physical behavior of the regularized model

In order to evaluate the effect of the regularized model proposed in eq. (8) on the physics of the problem — in particular the effects of the choice of the ϵ parameter — we performed some simulations. The setup is identical to the one described in section 2.1. The results are shown in fig. 4(a).

We also performed qualitative comparisons of the coefficient of restitution for binary collisions with different impact velocities using eq. (8) with the numerical results obtained with eq. (2) presented in [1]. This comparison

can be seen in fig. 4(b), which shows that collisions become more elastic (e_n closer to 1) as the value of ϵ increases, especially for very low normal impact velocities. Nevertheless, the results above indicate that the regularized model in eq. (8) can be used as a viable alternative to model normal forces in DEM simulations. The regularized model's restitution coefficient being closer to 1 seems to be inconsequential for most real life applications as, in most cases, energy dissipation primarily stems from friction in long-lasting contacts rather than normal damping in dense granular flows [9]. Further studies in real life scenarios still need to be carried out to thoroughly assess the effect of the regularized model proposed in eq. (8).

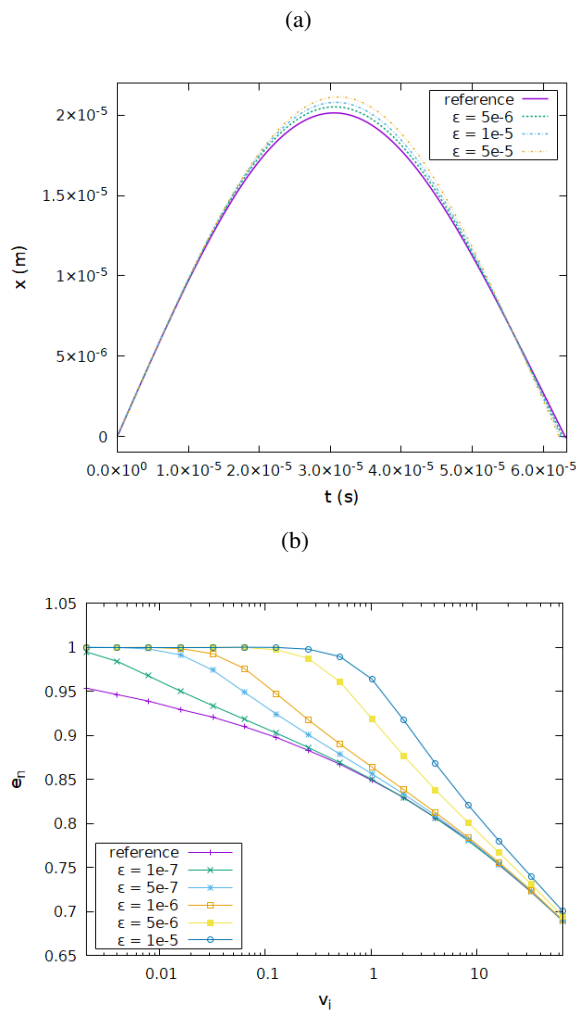


Figure 4: In (a), time evolution of the position of the mobile particle in a normal binary collision using the regularized model in eq. (8), for different values of ϵ . The reference curve uses the Kuwabara-Kono force model, given in eq. (2), instead. The impact velocity used is 1 m/s and the values of the remaining parameters are $\rho = 1300 \text{ kg/m}^3$, $r = 3 \text{ mm}$, $\tilde{k}_n \approx 9 \times 10^7 \text{ N/m}^{1.5}$, $\gamma = 190 \text{ kg/m}^{0.5}\text{s}$, $h = 2^{-23} \text{ s}$. In (b), visualization of the dependence of the coefficient of normal restitution on the impact velocity, for different values of ϵ . Reference curve obtained from [1] and the parameters of the simulations are the same in (a).

4 Conclusions

We have proposed a regularized force model, based on an extension of the Kuwabara-Kono model, in which the square-root function appearing in the dissipation term is replaced by an ϵ -shifted ϵ -mollified square-root function. This function, which is infinitely differentiable, allows for an actual order 2 integration of the equations of motion in DEM with the method described in eq. (3). The regularized force model, however, mimics slightly softer materials and slightly less dissipative collisions with respect to a similar simulation carried out for the same parameters using the standard Kuwabara-Kono model. Fully characterizing the regularized model and its implications on the motion of large granular assemblies is one of our current research interests.

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