A truly Newtonian softening length for disc simulations

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ABSTRACT

The softened point mass model is commonly used in simulations of gaseous discs including self-gravity while the value of associated length λ remains, to some degree, controversial. This ‘parameter’ is however fully constrained when, in a discretized disc, all fluid cells are demanded to obey Newton’s law. We examine the topology of solutions in this context, focusing on cylindrical cells more or less vertically elongated. We find that not only the nominal length depends critically on the cell’s shape (curvature, radial extension, height), but it is either a real or an imaginary number. Setting λ as a fraction of the local disc thickness – as usually done – is indeed not the optimal choice. We then propose a novel prescription valid irrespective of the disc properties and grid spacings. The benefit, which amounts to 2–3 more digits typically, is illustrated in a few concrete cases. A detailed mathematical analysis is in progress.

Key words: accretion, accretion discs – gravitation – methods: numerical.

1 INTRODUCTION

In simulations where a fluid is discretized on a computational grid, one must preliminary decide the way to treat matter contained inside each ‘numerical cell’, and how the physical quantities are assigned to the nodes. The problem is tricky when considering self-gravity because the Newtonian potential, namely at point P(r) (e.g. Kellogg 1929)

\[ \psi_{\text{cell}}(r) = -G \int_{\text{cell}} \frac{dm(r')}{|r - r'|}, \]

where dm is the elementary mass at P(r'), contains a diverging kernel that is difficult to manage. Except for the Cartesian geometry (MacMillan 1930; Waldvogel 1976), there is no closed-form for the above integral, and one must therefore employ specific techniques, which is rarely done (e.g. Ansorg, Kleinwächter & Meinel 2003; Huré & Pierens 2005; Li, Buoni & Li 2009). The singularity is usually avoided by raising the separation as follows (e.g. Binney & Tremaine 1987; Papaloizou & Lin 1989; Paardekooper 2012):

\[ |r - r'| \ll \sqrt{|r - r'|^2 + \lambda^2} \geq |\lambda| > 0, \]  

where λ is a ‘softening’ length. A small value is usually considered, typically the numerical resolution or the smallest scale available. This bare substitution does not economize the numerical quadrature, while replacing equation (1) by an analytical function offers much more flexibility. A common choice is the ‘softened’ point mass potential

\[ - \frac{G m}{\sqrt{|r - r'|^2 + \lambda^2}} \equiv \psi_{\text{Plum}}(r; r_0, \lambda), \]

also known as the Plummer potential for a sphere with centre r0, mass m, and core radius λ (e.g. Dejonghe 1987). In disc simulations, the role of the parameter is to account for the vertical extension of matter, and λ is thereby set to some fraction of the local thickness. In practical, authors often choose a constant value of the order of 0.6, to a factor 2 typically (Masset 2002; Baruteau, Meru & Paardekooper 2011; Meru & Bate 2012; Müller, Kley & Meru 2012), and sometimes a function of space (see e.g. table 1 in Huré & Pierens 2005).

It is clear that equation (3) does not corresponds precisely to the Newtonian potential of a numerical cell, unless λ satisfies

\[ \psi_{\text{Plum}}(r; \lambda) = \psi_{\text{cell}}(r) = 0, \]

everywhere, i.e.

\[ \lambda^2 = \left( \frac{G m}{\psi_{\text{cell}}} \right)^2 \geq |r - r_0|^2, \]

which is inevitably a complicated function of space and cell’s parameters (geometry/shape and density). This is especially true inside the cell and in close neighbourhood. At long range, the requested 1/|r - r_0| decline typical of Newtonian gravity is however achieved for any small value of the softening length as an expansion of equation (3) in \( \lambda^2/|r - r_0|^2 \ll 1 \) shows. At first sight, it could seem superfluous to try to ameliorate this parameter, but there is an essential point: in a discretized disc, almost all the grid cells are

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located far away from a given node $P(r)$, meaning that most cells are seen as distant cells. Finally, it is rather risky to be satisfied with a small but arbitrary value, in particular if a certain level accuracy is requested.

In this paper, we show that, if $\lambda$ is defined to faithfully reproduce the Newtonian potential of a cell, then not only it depends on the cell’s parameters and distance, but it can be an imaginary number, which is not common at all. A calculus aiming to extract the dipolar term in equation (1) – $\lambda$ in fact measures how $\psi_{\text{cell}}$ deviates from the monopole – is currently under way and will be the aim of an dedicated article. In the meanwhile, we present a simple method to estimate $\lambda$, combining some analytics and a simple numerical scheme. We work in cylindrical geometry, well suited to rotating systems like discs.

The article is organized as follows. In Section 2, we show in one dimension that the softening length can be either a real or imaginary number. This result is supported by a analytical development valid at long range. In Section 3, we illustrate the complicated topology of $\lambda$ associated with the potential of the cylindrical cell. By using Simpson’s rule, we determine the softening length with good accuracy. We then propose a new prescription valid for almost any distance and cell’s geometry (rigorously, with radial-to-azimuthal aspect ratio around unity). We show in Section 4 through a few concrete tests (regular and log, grid spacings, flared power-law discs, fully inhomogeneous density) that this new prescription gives much better results than the standard prescription. A concluding section summarizes the results. A few extensions of this work are discussed.

2 EVIDENCE FOR IMAGINARY SOFTENING LENGTHS

In order to estimate $\lambda$ from equation (5), we work in cylindrical coordinates well suited to rotating discs. The system is supposed to be discretized on a numerical grid where each cell is a cylindrical sector, as the one depicted in Fig. 1. The cell has centre $r_0(a, \theta_0, z_0)$, angular extension $\Delta \theta$, radial size $\Delta a$, and height $2h$. At this level, there is no particular constraint on the shape parameters (i.e. vertical-to-radial and radial-to-azimuthal extension ratios). We however make the assumption that the fluid density does not vary inside. The elementary mass is $dm = \rho a da d\theta' dz$, and $\rho$ is the constant density. If we set

$$I_{\text{cell}} = \int_{\theta_0-h}^{\theta_0+h} \int_{a_0-\Delta a/2}^{a_0+\Delta a/2} \int_{z_0-h}^{z_0+h} \rho a da d\theta' dz,$$

then $\psi_{\text{cell}}$ is just

$$\psi_{\text{cell}} = -\frac{Gm}{V} I_{\text{cell}},$$

where $m = \rho V$ is the mass of the cell and $V$ its volume. Then, according to equation (5), the softening length is

$$\lambda^2 = \left(\frac{V}{I_{\text{cell}}}\right)^2 - |r - r_0|^2.\quad (8)$$

To anticipate, we see that $\lambda^2$ can be negative, which implies an imaginary softening length. This situation means that the point mass potential is weaker than that of the cell, and must therefore be increased (by decreasing the separation $|r - r'|$).

2.1 Exact formula for the massive arc

We first integrate the kernel over the azimuth, i.e. calculate $I_{\text{arc}}$ in equation (6). This quantity is linked to the Newtonian potential of a homogeneous, massive arc with radius $a$, length $\ell = a \Delta \theta'$, and opening angle $\Delta \theta'$, namely

$$\psi_{\text{arc}}(r) = -\frac{Gm}{\ell_{\text{arc}}}.$$  (9)

It is traditionally expressed in terms of incomplete elliptic integral of the first kind

$$F(k, \phi) = \int_0^\phi \frac{d\theta'}{\sqrt{1 - k^2 \sin^2 \theta'}},$$

where $k \leq 1$ is the modulus. With the notations $P(r') = (\ell, \theta', Z)$, $P'(r' \equiv (a, \theta', z)$, we have

$$|r - r'|^2 = (a + R)^2 + \zeta^2 - 4 aR \sin^2 \phi,$$

where $\zeta = Z - z$ and $2 \phi = \pi + \theta - \theta'$, and so the modulus is given by

$$k^2 [(a + R)^2 + \zeta^2] = 4 aR. \quad (12)$$

We then have (Zhu 2005; Huré, Trova & Hersant 2014)

$$I_{\text{arc}} = \sqrt{\frac{a}{R}} k \Delta F,$$

where $\Delta F(k, \phi_1, \phi_2) = F(k, \phi_1) - F(k, \phi_2), 2 \phi_1 = \pi + \theta - \theta'_0 + \Delta \theta'/2$, and $2 \phi_2 = \pi + \theta - \theta'_0 - \Delta \theta'/2$. So, the softening length associated with the arc is given by

$$\lambda^2 = \left(\frac{\ell}{I_{\text{arc}}}\right)^2 - |r - r'_0|^2.\quad (14)$$

By using equation (13), we find for $R > 0$

$$\frac{\lambda^2}{4aR} \equiv \frac{1}{k^2} \left[\frac{\Delta \theta'^2}{2 \Delta F} - 1\right] + \sin^2 \phi_0,$$

where $2 \phi_0 = \pi + \theta - \theta'_0$. The interpretation of this result is the following: the Plummer potential computed with $\lambda$ given by
equation (15) perfectly reproduces the Newtonian potential of a homogeneous arc everywhere in space. The occurrence of imaginary numbers for \( \lambda \), already perceptible in equation (8), can be understood from this latter formula: we have \( F(k, \phi) \geq \phi \) whatever \( k \) and \( \phi \leq 1 \), which means that weight is possibly given to the negative term \(-1/\kappa^2\).

Fig. 2 shows the normalized softening length \( \tilde{\lambda} \) versus \( R/a_0 \) and \( \theta - \theta_0' \equiv \alpha \) (in units of \( \pi \)) for an arc with opening angle \( \Delta \theta' = 0.01 \) (this value corresponds to a resolution number \( N_0 \equiv 2\pi/\Delta \theta' \approx 629 \) which is typical in high-resolution disc simulations). Depending on the field point, the softening length is either a real or a pure imaginary number. We see that it is also a complicated function of space, especially at short radii and in the vicinity of the arc (see the pinching in the figure at \( R/a_0 = 1 \) and \( \alpha \equiv \theta - \theta_0' = 0 \)). In contrast, for \( R/a_0 \gg 1 \) (i.e. at long range), \( \tilde{\lambda} \) is mainly a function of \( \alpha \). At long range, imaginary numbers are found for \( |\alpha| \geq \frac{\pi}{2} \) typically, which corresponds to field points located in the concave side of the arc (while real values are for the convex side of the arc). The length is zero for \( \alpha = \pm \frac{\pi}{2} \), which corresponds to the direction of the arc: matter located beyond and below the centre \( r_0 \) compensate somehow, and do not contribute at the actual expansion order.

2.2 Long-range behaviour for the massive arc

We can precisely catch the long-range behaviour of \( \lambda \) by writing \( F(k, \phi) \) as a double series in \( k \) and \( \phi \) around \( k \to 0 \), but an expansion up to order 3 is necessary here (Gradsteyn & Ryzhik 2007). One goes more straight to the point by expanding the kernel \( 1/|r - r'| \) over \( \alpha = \theta - \theta_0' \) before integration in azimuth. After some algebra detailed in Appendix A, we find

\[
I_{\text{arc}} = \frac{aR \Delta \theta'}{|r - r'|} \left[ 1 - \frac{aR \Delta \theta'}{|r - r'|} \cos \alpha \left( 1 - \text{sinc} \frac{\Delta \theta'}{2} \right) \right].
\]

For \( \Delta \theta'/2 \ll 1 \), which corresponds to arcs with a small opening angle, an expansion of the sine cardinal function leads to

\[
\tilde{\lambda}^2 = \frac{1}{2^6} \left( 1 - \text{sinc} \frac{\Delta \theta'}{2} \right) \cos \alpha \approx \frac{\Delta \theta'}{48} \cos \alpha.
\]

This is in agreement with what is observed in Fig. 2 for \( R/a_0 \gg 1 \): at long range, the length is independent on the radius and varies as \( \sqrt{\cos(\theta - \theta_0')} \) where the cosine can be positive or negative.

3 THE CASE OF CYLINDRICAL CELLS

3.1 A numerical example

A closed-form for the potential of a homogeneous cylindrical cell, i.e. for \( I_{\text{cell}} \), is apparently missing yet so there is no equivalent to equation (15). We can employ numerical means.\(^1\) An illustration is given at Fig. 3 for a cylindrical cell with parameters \( a_0 \Delta \theta' = \Delta \alpha = 2\pi = 0.01 \). We see that zones where the length is real and imaginary are still present, while inverted with respect to the arc. The softening length is now imaginary at large radii for \( |\alpha| \lesssim \frac{\pi}{4} \). Again, the map is more complex in the vicinity of the cell, where real values are found inside the circle with radius \( R \leq a_0 \) typically. Fig. 4 is a zoom around \( r_0 \) and we see that imaginary numbers are indeed located at \( R/a_0 \gtrsim 1 \). We perceive dipole and quadrupole features which are very difficult to catch by analytical

\(^1\) In practical, the potential \( \psi_{\text{cell}} \) is determined from the contour integral reported by Huré et al. (2014). In the paper throughout, we use this accurate method to generate reference values.

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3.2 Central values
The softening length depends on several factors linked to the cell’s geometry, namely
(i) the polar shape factor ½λΔα/Δa,
(ii) the meridional shape factor 2h/Δa,
and on the relative altitude Z/h too. Exploring the solution of equation (4) by varying these quantities would be interesting but it is out of the scope of this paper. It is however worth noting that λ is particularly sensitive to 2h/Δa when this ratio is around unity. Actually, as the meridional shape factor is larger than unity and decreases, the solution has first a spherical geometry and λ is real. When 2h/Δa reaches unity (as in the canonical example above), a quadrupolar pattern quickly sets in (see Fig. 4), while imaginary solutions appear at R/0 > 1. Below unity, λ is mainly an imaginary number, except in the very close vicinity of the cell (and inside it) where λ remains real. The real-to-imaginary swing occurs for a variation of 10 per cent of 2h/Δa around unity typically.

3.3 Reliable estimate from Simpson’s rule
In the mid-plane of the cell, i.e. at Z = z0, we can rewrite equation (6) as follows:
Icell = 2 0 0+h 2 θ 0 0 0+1 Δa Λα (a, z) da,
(19)
where 0 must be regarded as function of a and z (it also depends on θ and Δθ and as well). Because Icell is essentially regular, 4 we can employ a classical quadrature scheme to estimate Icell, i.e. the double integral is replaced by a discrete summation with values of Λα, taken at different places (a, z). For the present purpose, Simpson’s rule has a sufficient accuracy. There are therefore nine nodes (a, z) involved in total, namely

2 There are two possible ways to get λ inside the cell and neighbourhood: from the formula for the potential of the polar cell (Huré 2012), or from the double expansion of F(κ, φ) around κ = 1 and φ = 2 (Van de Vel 1969). Despite efforts, we failed in producing a result. This question remains open.
3 The potential of a perfect cube is very close to that of a sphere, and there is no dipole contribution (Durand 1953).
4 In practical, 0 has large amplitude in the very close vicinity of the arc, and not always monotonic. Even, it is logarithmically diverging as soon as the modulus k = 1, which occurs for R = 0, for Z = z0. To avoid singular values, we can safely replace k by k in equation (12), where

k2[(a0 + R2 + ε2 + ε3)] = 4 a0R,
(20)
and ε = 1/100 min{ε1, ε2, ε3} for instance.

Figure 5. Central value of the softening length versus the meridional shape factor 2h/Δa of the grid, in units of the radial extension Δa (which is held fixed), for ½λΔα/Δa = 1 (black). The quadratic regression (with associated residuals) refers to equation (18). Also indicated (grey) is the central value when varying the polar shape factor ½λΔα/Δa in the range [0.1, 10]; see equation (B1) for the double fit.

Figure 4. Same legend and same colour code as for Fig. 3, but zoomed around the numerical cell (boundary in dashed white line). Interior values are out of range of the colour code (λ ~ 0.0021 at the centre).
4 WHAT DOES THIS CHANGE FOR DISC SIMULATIONS?

4.1 A new prescription

On the basis of the results above and various tests performed, we can propose a new prescription for $\lambda$ which makes the softened point mass potential very close to the Newtonian potential of a cylindrical cell by combining: (i) the numerical value computed at the cell’s centre (the fit has sufficient accuracy), and (ii) the 9-point stencil. For a given cell with shape parameters ($\ell_1, \ell_2, \ell_3$) and centre $r_0$, the recipe is as follows:

(i) $\lambda$ is given by equation (18) or equation (B1), if $r = r_0$,

(ii) otherwise, $\lambda$ is given by equations (8) and (21).

This composite formula is a priori easy to include into numerical codes.

4.2 Two numerical tests

By adding the contribution of individual cells, one can determine the total potential of any kind of inhomogeneous system, where each cell has its own shape parameters, density, and associated softening length. We have therefore performed several concrete tests, in order to check the efficiency of this new prescription for $\lambda$. It is in particular interesting to compare with the standard prescription where $\lambda \propto h$.

Among possibilities, we have selected two configurations: (i) a fully homogeneous and flat disc, and (ii) a power-law density disc with constant aspect ratio. In both cases, the disc is axially symmetrical, and has inner edge at $a_{in} = 0.5$. The numerical grid consists of $N_k$ nodes in radius, and $N_\theta$ node in azimuth. In the vertical direction, there is a unique node located in the disc mid-plane. There are therefore $(N_k - 1)(N_\theta - 1)$ cells in total and the same amount of nodes. In practical, we use $N_k = 2 \times N_\theta = 64$ (which leads to $\Delta \theta' \approx 0.1$; see below for higher resolutions). In addition, we have considered two types of grid: one grid with regular spacing, and one with log spacing. In this latter case, we have the relationship

$$\frac{2h}{\Delta a} = \frac{\eta}{\pi N_\theta},$$

(22)

where $\eta = h/a$ is the disc aspect ratio.

At each radius $R$ in the mid-plane, the reference potential is reconstructed by adding individual contributions. In parallel, we perform the same summation but using the Plummer potential (i) with the new prescription, and (ii) with the standard prescription where $\lambda \propto h$ (in practical, we take $\lambda = 0.6h$). Fig. 8 shows the deviations observed for the homogeneous flat disc. We see that this an improvement by 2–4 digits depending on the radius in the disc. Results are much better close to the outer edge. We have also considered an inhomogeneous version by simply multiplying the density field of each cell by a random factor in the range [1, 2]. The results are plotted in the same figure and the conclusions are unchanged.

Fig. 9 shows the same results but for the flared, power-law density disc where $\rho(a) = \frac{1}{4} \Delta \theta'$ and $\rho(a) \propto a^{-2.5}$, which is typical. The new prescription is again better, while the benefit is a little bit reduced for the grid with regular spacing. For the grid with log spacing, potential values are improved by almost two more digits.
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Figure 8. Relative error for potential values (decimal log scale) with respect to the reference (see text) for the standard prescription with $\lambda/h = 0.6$ (green) and for the present prescription (see Section 3.1). The disc is fully homogeneous and flat with inner edge at $a_{in} = 0.5$ (plain lines); the azimuthal number is $N_\theta = 64$ and radial number $N_R = N_\theta/2$. Two grids are used: regular spacing (left-hand panel) and log spacing (right-hand panel). The label on the curves give the average deviation. For the fully inhomogeneous density field (dashed lines; see text), errors are azimuthally averaged.

Figure 9. Same legend and same conditions as for Fig. 8 but for the flared, power-law density disc (see text).

5 CONCLUDING REMARKS

In this article, we have proposed a new prescription for the softening length which enables to reproduce the Newtonian potential and the associated acceleration field from the Plummer formula with a very good level of accuracy. A major result is the occurrence of purely imaginary lengths, which was not envisaged before. Not only the location in space but also the grid shape plays a decisive role. Besides, the nominal value is generally not a fraction of the local thickness (unless a very special tuning of the grid parameters), in contrast with the current standard.

This study is preliminary and can be continued in several ways. As announced, a full dipolar expansion of the potential of the cylindrical cell is currently in progress. An analytical formula for $\lambda$ would actually be of great help not only to understand how the length depends on the cell’s shape, but also to avoid the evaluation of the elliptic integrals $F(k, \phi)$. Actually, the extra computational cost when using equations (21) and (8) instead of a constant $\lambda/h$ is due to the evaluation of $F(k, \phi)$ (18 evaluations in total for each cell). If the grid is fixed, this can be done once for all, but it is obvious that any approximation for this special function would reduce the computing time. It would also be interesting to understand how this prescription is modified if vertical stratification of matter is accounted for (for instance with a Gaussian profile). Another challenge concerns the derivation of the softening length in the case of spherical and Cartesian geometries. In the meanwhile, we plan to investigate how this prescription impacts on hydrodynamical simulations since acceleration fields are much accurate with this method (Trova, Pierens, & Huré, in preparation).

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Figure 10. Same legend as for Figs 8 and 9 but for various azimuthal resolution numbers $N_\theta$. The deviations are computed at the radius located at half-sampling, using the two kinds of grid: regular spacing (plain circles) and log. spacing (crosses).

4.3 Resolution effects

Fig. 10 gives the deviation observed at half-sampling in radius for $N_\theta \in \{32, 64, 128, 256, 512, 1024\}$ while maintaining $N_R = N_\theta/2$ and $a_{in} = 0.5$, for the two configurations considered above. This confirms that accuracy can be significantly improved by 2–3 orders of magnitude with respect to the standard case where $\lambda \propto h$ whatever the resolution.
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APPENDIX A: SOFTENING LENGTH ASSOCIATED WITH THE MASSIVE ARC. LONG-RANGE BEHAVIOUR

The relative distance is given by

$$r - r' = \sqrt{(R \cos \theta - a \cos \theta')^2 + (Z - z)^2},$$

$$= (a + R)^2 + \xi^2 - 4aR \sin^2 \phi,$$

where \(\xi = Z - z\) and \(2\phi = \pi + \theta - \theta'\). If we introduce the angle \(\alpha' = \theta' - \theta_0\), then

$$2\phi_0 = \pi + \theta - \theta_0' = \pi + \theta - \theta + (\theta' - \theta_0) = 2\phi + \alpha',$$

and so \(\sin^2 \phi = \sin^2(\phi_0 - \alpha' / 2)\). From simple trigonometric rules, we find

$$|r - r'|^2 = D_1^2 - 4aR \sin \alpha' \sin \left(\frac{\alpha'}{2} - 2\phi_0\right),$$

where \(D_1 = (a + R)^2 + \xi^2 - 4aR \sin^2 \phi_0\). We can directly deduce \(\lambda\) from equation (2). Provided \(\frac{\alpha'}{2} \ll 1\), we have

$$\frac{1}{|r - r'|} \approx \frac{1}{D_1} \left[1 + \frac{2aR}{D_1^2} \sin \alpha' \sin \left(\frac{\alpha'}{2} - 2\phi_0\right)\right].$$

(A4)

Since

$$\int \sin \frac{x}{2} \sin \left(\frac{x}{2} - x_0\right) \, dx = \frac{1}{2} [x \cos x_0 - \sin(x - x_0)],$$

(A5)

and \(\int \sin \theta \, d\theta = 2 \sqrt{1 - \sin^2 \theta}\), the integral over the shifted azimuth \(\alpha'\) has bounds \(\pm \frac{\alpha'}{2}\), and we have

$$\int \frac{\sin \frac{x}{2} \sin \left(\frac{x}{2} - x_0\right)}{2} \, dx = \frac{1}{2} [x \cos x_0 - \sin(x - x_0)].$$

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