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Comparative analysis of molecular dynamics and method of moments in two-dimensional concentric circular layers

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Abstract

In this manuscript, we undertake an examination of a classical plasma deployed on two finite co-planar surfaces: a circular region Ω_{in} into an annular region Ω_{out} with a gap in between. It is studied both from the point of view of statistical mechanics and the electrostatics of continua media. We employ a dual perspective: the first one is by using molecular dynamics (MD) simulations to find the system's positional correlation functions and velocity distributions. That by modeling the system as a classical two-dimensional Coulomb plasma of point-like charged particles q_1 and q_2 on the layers Ω_{in} and Ω_{out} respectively with no background density. The second one corresponds to a finite Surface Electrode (SE) composed of planar metallic layers displayed on the regions Ω_{in}, Ω_{out} at constant voltages V_{in}, V_{out} considering axial symmetry. The surface charge density is calculated by the Method of Moments (MoM) under the electrostatic approximation. Point-like and differential charges elements interact via a $1/r$—electric potential in both cases. The thermodynamic averages of the number density, and electric potential due to the plasma depend on the coupling and the charge ratio $\xi = q_1/q_2$ once the geometry of the layers is fixed. On the other hand, the fields due to the SE depend on the layer's geometry and their voltage. In the document, is defined a protocol to properly compare the systems. We show that there are values of the coupling parameter, where the thermodynamic averages computed via MD agree with the results of MoM for attractive $\xi = -1$ and repulsive layers $\xi = 1$.

Keywords: molecular dynamics, method of moments, Coulomb systems, long-range interaction

1. Introduction

In this study, we examine a metallic configuration comprising distinct layers denoted as Ω_{in} and Ω_{out}, collectively forming a gapped surface electrode (SE) devoid of background charge density. The inner layer is a disk $\Omega_{\text{in}} = \{(x,y) : \sqrt{x^2+y^2} \leqslant R_1\} \subset \mathbb{R}^2$ of radius $R_1 = R$ and the outer layer is an annular region $\Omega_{\text{out}} = \{(x,y) : R_2 \leqslant \sqrt{x^2+y^2} \leqslant R_3\} \subset \mathbb{R}^2$. The system can be also modeled as two-dimensional plasma where within Ω_{in}, reside N_1 particles with charge $q_1 \in \mathbb{R}$, while Ω_{out} holds N_2 particles with charge $q_2 \in \mathbb{R}$ (see figure 1). The foregoing study draws inspiration from [1], where the gapped SE was characterized by two-conductor flat regions with differing

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potentials and a distinct gap. Electric field and surface charge density analysis in that system involved resolving Laplace's equation with specified conditions.

In general, we can use electrostatics to compute steady and continuous distributions of charge $\sigma(\boldsymbol{r})$ on a metallic layers of the SE e.g. by solving Laplace equation $\nabla^2\Phi(\boldsymbol{r}) = 0$ for the electric potential $\Phi(\boldsymbol{r})$ with the proper boundary conditions. However, formally the charge on the layers at microscopical level is not continuous because it is quantized in packages having the value of electron charge. Additionally, the charge is never static since a charged metallic layer at a given temperature T implies motion of the charges in the microscopical level. Despite this, electrostatics is a good approximation in the macroscopic scale. In fact, the SE (continuous electrostatics) and the Coulomb plasma (discrete system) depicted in figure 1 are two models which can be used to describe the surface charge density in absence of density current $\boldsymbol{J}$. In the electrostatic system, the SE, density current by definition is zero since density charge is steady. In the case of the Coulomb plasma at the thermodynamic equilibrium charged particles move generating individually currents but null collectively $\boldsymbol{J} = 0$ since there is not direction of preference.

The $R_1 \longrightarrow R_2$ (gapless) and $R_3 \longrightarrow \infty$ (semi-infinite outer layer) limits of the gapped SE were studied in [2]. The SE was modeled as a two-dimensional classical Coulomb gas with $+q$ and $-q$ charges on the inner and outer electrodes. Equilibrium states and charge density were derived from Monte Carlo (MC) simulations. In that study, interactions followed an inverse power law potential $1/r$, where the coupling parameter Γ has been found inversely proportional to the system's temperature and proportional to q^2.

Furthermore, authors of [1] explored the electric vector potential and the Biot–Savart law analogy in electrostatics. These efforts set the zero stage for the present study, aiming to further analyze the system in question with the statistical mechanics approach. Subsequent sections detail our MC methodology, results, and implications within the previous electrostatics descriptions of the system.

A strategy to study two-dimensional plasmas is by using molecular dynamics (MD) simulations [3–11]. In the present study, we shall perform simulations in the NVT-ensemble by using Nosé–Hoover and Langevin thermostats. Our goal is to study the thermodynamic averages of number density and the potential as a function of $\beta = k_{\mathrm{B}}T$ for a fixed geometry of the SE. We aim to know if a coulomb plasma with a finite number of particles can be in agreement with the electrostatics of the SE.

The motivation behind this study stems from the electrostatic behavior of the gapped SE system comprising Ω_{in} and Ω_{out}. While prior research has shed light on this system's electromagnetic fields, our work extends the investigation into the realm of statistical mechanics. By delving into the interplay between MDs simulations and the Method of Moments technique, we aim to uncover the underlying principles governing the system's surface charge density and its correlation with the Coulomb's interaction between charges.

This document is structured as follows: We first delve into the Method of Moments, focusing on the derivation of surface charge density for a single circular layer and exploring the distinctive electrostatic behavior originating from the interactions governed by a Coulomb potential. Then, we describe the MDs techniques, together with the experimental protocol that is followed to make comparisons. Subsequently, we present and analyze results obtained through both the Method of Moments (MoM) and MD methods. The statistical results are contrasted against analytic descriptions of SE. These findings are discussed within the context of electrostatics and statistical mechanics, highlighting their broader implications. Finally, we conclude by summarizing our contributions.

2. Method of moments

In this section, we delve into the main concepts of the Method of Moments and its application to our system. From the point of view of the electrostatics of continuum, (see figure 1-right) charge is continuously distributed over the SE layers. The potential of the layers is known from the problem definition, but the surface charge distribution $\sigma(\boldsymbol{r})$ is unknown. To calculate the surface charge distribution on the layers we use the MoM. That method is often employed to study classical electromagnetic radiation [12–14], but it is also useful to derive surface charge densities in electrostatic systems [15, 16]. We start by examining the behavior of a single circular layer and exploring the derivation of surface charge density. Furthermore, we investigate the intricate interplay of interactions governed by the $1/r$ potential, shedding light on the unique electrostatic behavior of our system.

2.1. Single circular layer

First, we derive the surface charge density for a single circular layer configuration. This first step serves as the foundational study in a single component of the gapped SE system. The integral formula of the electrostatic potential is given by

$$\frac{1}{4\pi\epsilon_o}\int_{\Omega}\frac{\sigma(\boldsymbol{r}')}{|\boldsymbol{r}-\boldsymbol{r}'|}\mathrm{d}^2\boldsymbol{r} = \Phi(\boldsymbol{r}\in\Omega) = V_o,$$

with ϵ_o the permittivity of vacuum and V_o the voltage of the circular layer $\Omega = \{(x,y) : \sqrt{x^2+y^2} \leqslant R\} \subset \mathbb{R}^2$ of radius R. Since the system has azimuthal symmetry then potential electrostatic potential in the space is independent of the angular ϕ-coordinate $\Phi(\boldsymbol{r}) = \Phi(u,z)$. Therefore, the surface charge density is a function depending only of the radial $u = \sqrt{x^2+y^2}$ coordinate $\sigma(\boldsymbol{r}) = \sigma(u)$. Any location on the plate is given by $\boldsymbol{r}(u,\phi) = u\hat{u}(\phi)$, and the distance between two different points on the plate is

$$|\boldsymbol{r}-\boldsymbol{r}'| = \sqrt{u^2+(u')^2-2uu'\hat{u}(\phi)\cdot\hat{u}(\phi')},$$

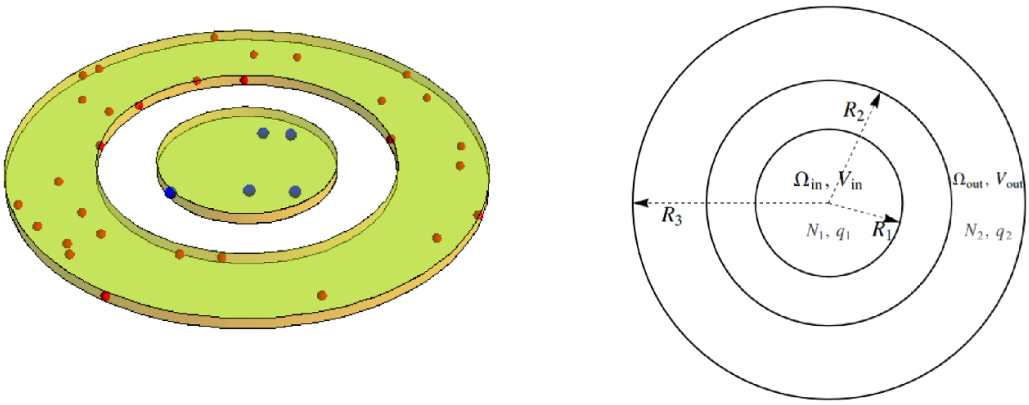

Figure 1. The system. Two metallic sheets Ω_{in} and Ω_{out} with no background density charge having N_1 particles of charge q_1 and N_2 particles of charge q_2.

with $\hat{u}(\phi) = (\cos\phi, \sin\phi, 0)$ written in Cartesian coordinates. Hence, the potential on the metallic layer can be calculated from

$$\frac{1}{4\pi\epsilon_o}\int_0^R\int_0^{2\pi}\frac{\sigma(u)}{\sqrt{u^2+(u')^2-2uu'\cos(\phi-\phi')}}u'\mathrm{d}u'\mathrm{d}\phi' = \Phi(\boldsymbol{r}\in\Omega) = V_o.$$

We aim to obtain the surface charge density σ from the previous integral equation. The strategy is to expand σ into a truncated series of functions as follows,

$$\sigma(u) = \sum_{n=0}^{N}\sigma_n f_n(u),$$

with $\{f_n(u)\}_{n=1,\ldots,N}$ the set of basis functions where σ_n is the nth coefficient for the surface charge density in that basis. Then,

$$\frac{1}{4\pi\epsilon_o}\sum_{n=0}^{N}\sigma_n\int_0^R\int_{-\phi}^{2\pi-\phi}\frac{f_n(u')}{\sqrt{u^2+(u')^2-2uu'\cos(\beta)}}u'\mathrm{d}u'\mathrm{d}\beta' = \Phi((u,\phi,0)\in\Omega) = V_o,$$

where we have used the change of variable $\beta = \phi' - \phi$. Note that the choice of $\phi\in[0,2\pi]$ only ranges the surface of the plate, then

$$\frac{1}{4\pi\epsilon_o}\sum_{n=0}^{N}\sigma_n\int_0^R\left[\int_0^{2\pi}\frac{\mathrm{d}\beta}{\sqrt{u^2+(u')^2-2uu'\cos(\beta)}}\right]f_n(u')\,u'\mathrm{d}u' = \Phi((u,0,0)\in\Omega) = V_o.$$

The angular integral can be evaluated straightforwardly since it is related to the complete elliptic function of the first kind[4],

$$\int_0^{2\pi}\frac{\mathrm{d}\beta}{\sqrt{u^2+(u')^2-2uu'\cos(\beta)}} = \frac{4}{|u-u'|}K\left(-\frac{4uu'}{|u-u'|^2}\right), \tag{1}$$

where the elliptic function is given by

$$K(\chi) = \int_0^{\pi/2}\frac{\mathrm{d}\theta}{\sqrt{1-\chi\sin^2\theta}}.$$

The potential evaluated on the sheet is computed from

$$\frac{1}{\pi\epsilon_o}\sum_{n=0}^{N}\sigma_n\int_0^R\frac{f_n(u')}{|u-u'|}K\left(-\frac{4uu'}{|u-u'|^2}\right)u'\mathrm{d}u' = \Phi((u,0,0)\in\Omega) = V_o.$$

In this case, we can choose the value of u in the interval $[0,R]$. We shall define $\mathcal{N}+1$ equally spaced discrete values at the radial coordinate $u_0,\ldots,u_{\mathcal{N}}$ with $u_n = nR/\mathcal{N}$, to define $\mathcal{N}$

[4] This integral can be simplified by introducing

$$\zeta(u',u) := \sqrt{(u')^2+u^2-2u'u} = |u-u'|, \text{ and } \xi := \frac{4u'u}{\zeta(u',u)^2} = \frac{4u'u}{|u-u'|^2}.$$

Changing the β variable with $\beta = 2t$ leads to

$$\begin{aligned}(u')^2+u^2-2u'u\cos\beta &= (u')^2+u^2-2u'u+2u'u(1-\cos\beta)\\ &= \left((u')^2+u^2-2u'u\right)+4u'u\sin^2 t\\ &= \zeta(u',u)^2+\xi\zeta(u',u)^2\sin^2 t\\ &= \zeta(u',u)^2\left(1+\xi\sin^2 t\right) = |u-u'|^2\left(1+\xi\sin^2 t\right).\end{aligned}$$

Hence, the integrand can be written as

$$\int_0^{2\pi}\frac{\mathrm{d}\beta}{\sqrt{u^2+u'2-2uu'\cos(\beta)}} = \frac{4}{|u-u'|}\int_0^{\pi/2}\frac{\mathrm{d}t}{\sqrt{(1+\xi\sin^2 t)}} = \frac{4}{|u-u'|}K(-\xi).$$

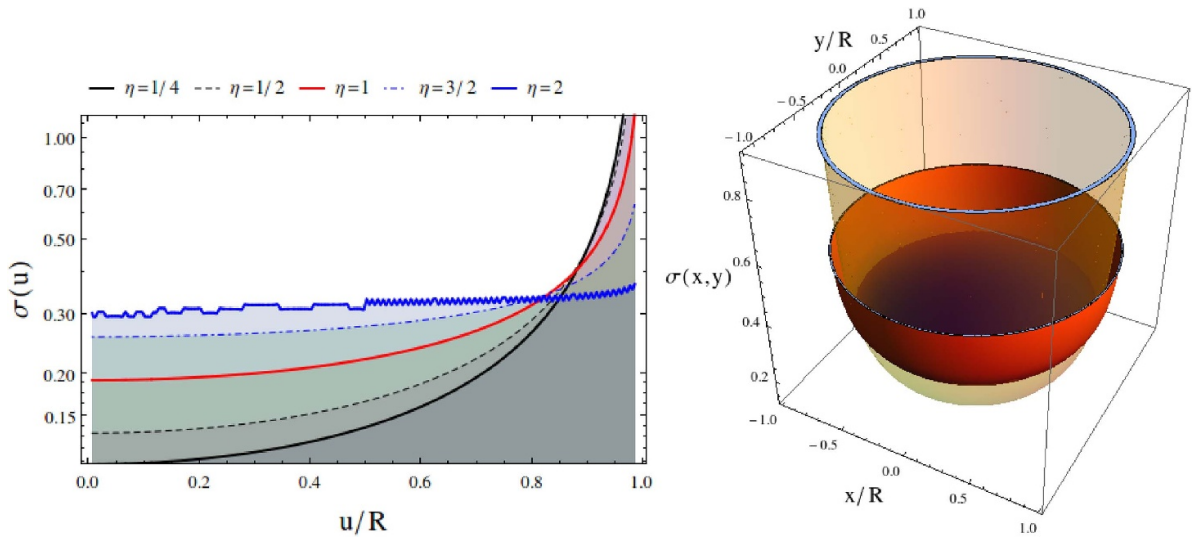

Figure 2. Surface charge density of the singular circular plate at a constant voltage according to MoM. (left) Profile of the charge density. (right) Surface density charge for $\eta = 1/2$ (transparent surface) and $\eta = 3/2$ (solid surface).

intervals $U_n := [u_n, u_{n+1}]$ with centers located at $u_n^{(c)} = (u_n + u_{n+1})/2$, then

$$\frac{1}{\pi\epsilon_o}\sum_{n=0}^{N}\sigma_n\int_0^R \frac{f_n(u')}{|u_m^{(c)}-u'|}K\left(-\frac{4u_m^{(c)}u'}{|u_m^{(c)}-u'|^2}\right)u'\mathrm{d}u' = \Phi\left(\left(u_m^{(c)},0,0\right)\in\Omega\right) = V_o,$$

which can be written as a linear set of algebraic equations that can be inverted to find the σ_n coefficients, as follows

$$\sum_{n=0}^{\mathcal{N}} M_{mn}\sigma_n = \Phi_m \;\therefore\; \sigma_m = \sum_{n=0}^{\mathcal{N}} M_{mn}^{-1}\Phi_n = \sum_{n=0}^{\mathcal{N}} M_{mn}^{-1}\{V_o\}_n,$$

with

$$M_{mn} = \frac{1}{\pi\epsilon_o}\int_0^R \frac{f_n(u')}{|u_m^{(c)}-u'|}K\left(-\frac{4u_m^{(c)}u'}{|u_m^{(c)}-u'|^2}\right)u'\mathrm{d}u'$$

being a square matrix and $\Phi_m = \Phi\left((u_m^{(c)},0,0)\in\Omega\right)$ a vector of constant entries V_o.

There are several choice of basis functions $\{f_u(n)\}_{n=0,\ldots,\mathcal{N}}$. One of the simplest choices is the C_0 basis defined as

$$f_n(u) = \begin{cases} 1 & u\in U_n = [u_n, u_{n+1}], \\ 0 & \text{otherwise}, \end{cases}$$

for which the M_{mn} matrix becomes

$$M_{mn} = \frac{1}{\pi\epsilon_o}\int_{U_n}\frac{u'\mathrm{d}u'}{|u_m^{(c)}-u'|}K\left(-\frac{4u_m^{(c)}u'}{|u_m^{(c)}-u'|^2}\right).$$

If the number of the interval divisions is large $\mathcal{N} >> 1$ one can use a mid-point approximation, leading to the simpler discrete term

$$M_{mn} = \frac{1}{\pi\epsilon_o}\frac{u_n^{(c)}\Delta u_n}{|u_m^{(c)}-u_n^{(c)}|}K\left(-\frac{4u_m^{(c)}u_n^{(c)}}{|u_m^{(c)}-u_n^{(c)}|^2}\right) \quad \text{for} \quad m\neq n,$$

with $\Delta u_n = u_{n+1} - u_n$. However, it is often advisable to perform numerical integration through sophisticated techniques to obtain accurate values of M_{mn}. In this manuscript, these integrals are evaluated by using the *Global Adaptive* method set by default in function *NIntegrate* of Wolfram Mathematica 9.0 [17]. The MoM is a versatile method and it can be easily generalized for other long-range potentials of the form $1/r^\eta$ with $\eta\in\mathbb{R}^+$ (as demonstrated in appendix A). The value of η is related with the type of interaction between particles long-range/short-range interactions. Commonly, $n\leqslant 1$ is related to long-range interactions e.g. $\eta = 1$ for the Coulomb potential. On the other hand, large values of that exponent are related to short-range interactions, the limit case $\eta\to\infty$ corresponds to the hard-sphere potential. Other particular values of that power are $\eta = 2, 3$ related to dipolar interactions and the Lenard–Jones potential which combines attractive and repulsive inverse power law potentials including $\eta = 6$ and $\eta = 12$. For the case of a single circular plate, the voltage V_o plays a scaling role for the charge density, thus one can set that voltage as one. In figure 2-left we show the surface charge density profile for standard $1/r$-interaction potential (red-solid line) for the circular plate. It occurs that surface charge density in the electrostatic approximation diverges at the sheet border, that is $\lim_{u\to R}\sigma(u) = \infty$. Numerically, we do not reach that limit since we compute the vector $\sigma(u_m^{(c)}) = \sigma_m$ and the largest value σ_N is located at $R - \Delta u_{\mathcal{N}}/2$ which approaches to the border as $\mathcal{N}\longrightarrow\infty$, where $\sigma_{\mathcal{N}\to\infty}\longrightarrow\infty$. Note that the surface charge density tends to be infinite on the layer border not only for the Coulomb potential $\eta = 1$ but also for $\eta = 1/2$ and $1/4$ (see figure 2) according to the MoM. This is a feature of these long-range interaction potentials and the fact that the system does not have a neutralizing background potential. In contrast, the surface charge density has a finite value on the layer border for $\eta = 3/2$ and 2 and larger values of η corresponding to short-range interaction potential. One has to take into account that in all cases the MoM calculates the surface charge distribution under the condition that the metallic layer

is an equipotential surface embedded into a tridimensional space.

2.2. Two layers

The MoM for concentric circular layers (see figure 1) can be straightforwardly generalized by following an analogous procedure to the one described for one circular plate. A generalization of this procedure to the gapped SE is presented in appendix B. Summarizing, two basis functions $\{f_n(u)\}_{n=1,\ldots,2\mathcal{N}}$ are employed to expand the surface charge density: the first $n=1,\ldots,\mathcal{N}$ bases are employed for the inner layer and the complementary $n=\mathcal{N}+1,\ldots,2\mathcal{N}$ are used for the second layer. The surface charge density between these elements is

$$\sigma_m = V_{\text{in}}\sum_{n=1}^{\mathcal{N}} M^{-1}_{m,n} + V_{\text{out}}\sum_{n=\mathcal{N}+1}^{2\mathcal{N}} M^{-1}_{m,n} \qquad m=1,\ldots,2\mathcal{N}, \tag{2}$$

with $M_{m,n}$ a $2\mathcal{N}\times 2\mathcal{N}$ matrix given by

$$M_{mn} = \int_{u_{n-1}}^{u_n} I\left(u_m^{(c)},u'\right)u'\mathrm{d}u' \ \textbf{if}\ n=1,\ldots,\mathcal{N},$$
$$\textbf{otherwise}\int_{u_n}^{u_{n+1}} I\left(u_m^{(c)},u'\right)u'\mathrm{d}u',$$

and

$$I(u,u') = \frac{1}{\pi\epsilon_o}\frac{1}{|u-u'|}K\left(-\frac{4uu'}{|u-u'|^2}\right).$$

3. MDs

In this section, the SE system is modeled as N_1, N_2 distribution of classical electric charges (with nominal values q_1 and q_2) confined to planar geometries Ω_1 and Ω_2, respectively (see figure 1). The coarse-grained method is used to model charged particles, which collide elastically with the layer boundaries $\partial\Omega_1$, $\partial\Omega_2$ and interacting with each other via a Coulomb-like potential of the form

$$\Phi(\boldsymbol{r}_{ij}) = \frac{1}{4\pi\epsilon_o}\frac{q_i q_j}{|\boldsymbol{r}_i-\boldsymbol{r}_j|} \ \text{ if } \ |\boldsymbol{r}_i-\boldsymbol{r}_j|>2b, \text{ otherwise } \infty.$$

We employ two different MD techniques. In the first one, we consider hard-disk interactions with a radius of particles denoted by b, in addition to Coulomb interactions. For that technique, we employ the Langevin thermostat. In the second simulation, we eliminate hard-disk interactions and employ the Nose–Hoover thermostat. In both cases, we implement a Verlet algorithm to numerically integrate the equations of motion. Point-like charges remain on the layers, ensuring that particles in Ω_1 did not mix with particles in Ω_2. Using two thermostats serves two primary purposes. Firstly, it ensures consistency in benchmarking by comparing MD results with both thermostats against analytical and numerical results as we shall do in sections 5.2 and 5.3. This reinforces our initial thesis when consistency is achieved and identifies errors when discrepancies arise. Secondly, the choice between the Langevin and Nose–Hoover thermostats has specific advantages and disadvantages. The Langevin thermostat converges easily with spherical particles and thermalizes rapidly, but it assumes a Gaussian noise and adjusts the velocity distribution to that of an ideal gas. Conversely, the Nose–Hoover thermostat does not inherently conform to the ideal gas distribution, especially under strong coupling conditions. As it will be shown later the simulations indicate that increasing β values through MD with the Nose–Hoover thermostat provides insight into the recovery of electrostatics as the system moves away from the thermodynamic limit.

For convenience, we introduce the parameter $\xi = q_2/q_1$, i.e. the ratio between the two types of charges. We restrict that parameter in the range $-1\leqslant\xi\leqslant 1$ fixing the charge of the inner layer $q_1=q$ and varying the charge of the outer layer in the range $-q\leqslant q_2\leqslant q$.

We do not compensate the particles' repulsion on the layers e.g. by introducing a neutralizing background on each layer, since we look for charge configurations that make layers equipotential surfaces, as it occurs in electrostatics. In every simulation, we set the number of particles to $N_1=N_2=N/2$ on the layers with $N\in 2\mathbb{N}$ the total number of particles, thus being a globally neutral system when $\xi=-1$.

In MD simulations, we compute the number density $n(\boldsymbol{r})$ (i.e. number of particles per unit of area) that enables the computation of the surface charge density, as follows,

$$\sigma(u) = \begin{cases} n(u)\,q & 0\leqslant u\leqslant R_1,\\ n(u)\,\xi q & R_2\leqslant u\leqslant R_3,\\ 0 & \text{otherwise.}\end{cases} \tag{3}$$

The number density is computed by counting the particles in

$$\boldsymbol{ann}(u,\Delta u) := \left\{(u',\phi)\in\mathbb{R}^2 : u<|(u',\phi)|<u+\Delta u\right\}$$

e.g. concentric annular regions of thickness Δu and dividing by the area of those regions.

4. Numerical experiment protocol

In order to perform proper comparisons between the results of the approaches in the study, we follow an experimental design. This is necessary because the starting parameters of MoM and MD are different, even for the common geometry defined by R_1, R_2 and R_3. Regarding the MoM, one has to set the layers' potential V_{in} and V_{out}. On the other hand, MD requires establishing the number of particles of each layer N_1, N_2, the charge ratio ξ, and the temperature T, since the system is in the canonical ensemble. Of course, the starting parameters of MoM and MD are related by the electrostatic energy