RadialDF

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This package provides the radial distribution function to analyze the radial density of particles around other particles. The package provides a single function *inner_rdf()* that calculates the RDF but excludes the border regions (as they would require n-dimensional intersection of shapes, which isn't computationally feasible).

A future version, if my short attention span permits it, will provide an `rdf` function that handles the 2D and 3D cases with the inclusion of the border regions.

CHAPTER

ONE

EXAMPLE

```
from radialdf import inner_rdf
import numpy as np
import plotly.graph_objs as go

# Generate 10000 random particles with 3 coordinates between 0 and 100
particles = np.random.rand(10000, 3) * 100
# Define a volume from 0 to 100 on 3 axes
box = [[0, 100]] * 3
# Check the radial distribution, which should be pretty boring and flat
g = inner_rdf(box, particles, 20, 0.2)
go.Figure(go.Scatter(x=[i * 0.2 for i in range(21)], y=g)).show()
```

1.1 radialdf package

1.1.1 Module contents

Radial Distribution Function module

radialdf.**inner_rdf**(*boundary*, *particles*, *r*, *dr*)

Computes the radial distribution function, showing the average density of other particles around each particle sampled in concentric shells of thickness `dr` within a maximum radius of `r`. This function stays a distance of `r` away from all borders as it currently does not deal with border effects. It will calculate the RDF only for those particles located at least `r` away from each border.

The `particles` argument should have an (n, k) shape where n is the amount of particles and k the number of dimensions.

The `boundary` argument should have shape (k, 2) where each row is the mimimum and maximum of a dimension of the volume within which particles should have been placed. An example for 3d-data would be `[[0, 100], [0, 200], [0, 100]]` for a 100x200x100 box.

Parameters

- **boundary** (*np.ndarray-like with shape (k, 2)*) – The limits for each dimension of the particles. Used to normalize to volume and exclude boundary particles.
- **particles** (*np.ndarray-like with shape (n, k)*) – The particles to investigate.
- **r** (*float*) – The maximum search radius, and the boundary exclusion size
- **dr** (*float*) – Resolution of the RDF. Thickness of the radial shells whose particle density is the basis of the RDF.

radialdf.**rdf**(*boundary*, *particles*, *r*, *dr*)

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