spack Documentation

Release 0.1

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Contents

Code available on Github, and documentation at Read the Docs.

CHAPTER 1

A 2D or 3D sphere packing analysis package

This package exists to enable fast, simple, and easy analysis of packings of spheres (3D) and disks (2D). It was developed for use in a Granular Materials lab, so some of the methods reflect that.

CHAPTER 2

Installation

This library requires numpy at a minimum, which you will probably want to have installed before installing this. Optionally, you may want vapory and povray are required for making pretty pictures, and Voronoi tessellations are provided by tess. The optional dependencies can be installed at any time, at which point the associated methods (*scene()* and *tess()*) will work.

To install, use `pip` (or `easy_install`):

```
pip install --user spack
```

Or to install from Github:

```
pip install --user git+git://github.com/wackywendell/spack@master
```

CHAPTER 3

Example Usage

Make a *Packing*:

```
>>> from spack import Packing
>>> from numpy import array, pi
>>> L = 2.0066668050219723
>>> diameters = array([ 0.96,  0.97,  0.98,  0.99,  1.  ,  1.01,  1.02,  1.03,  1.04])
>>> locs = array([[ 1.40776762,  1.26647724,  0.73389219],
...               [ 0.58704249,  2.11399   ,  1.52956579],
...               [ 1.75917911,  0.54290089,  1.27577478],
...               [ 2.13750384,  0.87508242,  0.21938647],
...               [ 1.07283961,  0.87692084,  1.9060841 ],
...               [ 0.09550267,  1.94404465,  0.56463369],
...               [ 1.07636871,  2.1942971 ,  0.63752152],
...               [ 0.49922725,  1.20002224,  1.13360082],
...               [-0.27724757,  1.62152603,  1.67262247]])
>>> pack = Packing(locs, diameters, L=L)
```

How many contacts are in my packing?

```
>>> pack.contacts()
Contacts(Nc=25, stable=25, floaters=0)
>>> # 25 contacts found
>>> # 25 contacts required for stability (for a packing of 9 particles)
>>> # 0 floaters
```

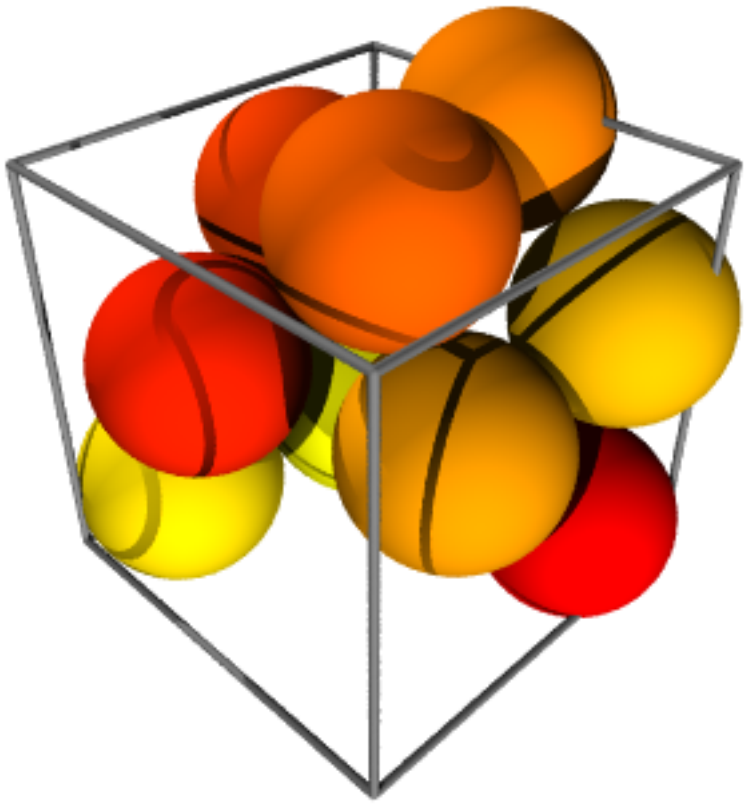
What are its highest resonant frequencies?

```
>>> freqs = pack.DM_freqs()
>>> for f in reversed(sorted(freqs)[-4:]):
...     print('{:.4f}'.format(f))
0.7018
0.6717
0.6416
0.6375
```

What does it look like? (requires *vapory* package and *povray* program)

```
>>> size = 400
>>> sc = pack.scene(rot=pi/4, camera_dist=2, cmap='autumn')
>>> sc.render('example-packing.png', width=size, height=size, antialiasing=0.0001)
```

Colors indicate diameter, with floaters drawn in gray.



docs/example-packing.png

Let's look at all sides, using *moviepy*:

```
>>> from moviepy.editor import VideoClip
>>> import moviepy.editor as mpy
>>>
>>> duration = 10
>>> def make_frame(t):
...     return (
...                 pack.scene(rot=(t/duration + .125)*2.*pi,
...                            camera_dist=2, cmap='autumn', bgcolor=[1,1,1])
...                 .render(width=size, height=size, antialiasing=0.001)
...             )
>>> vc = VideoClip(make_frame, duration=duration)
>>>
```

```
>>> vc.write_gif("example-packing.gif",fps=24)
```

And this is the output:

There are a few other methods for things like finding the backbone of the packing (*backbone()*), the adjacency matrix (*neighbors()*), or getting the Voronoi tessellation (*tess()*, requires tess). See the Reference for more details.

CHAPTER 4

Full Contents

4.1 Example Usage of spack

This is an ipython notebook in `spack/docs/example-usage.ipynb`, demonstrating how to use `spack`.

First, we import our modules:

```
import spack
from math import pi
```

Now we put in some data.

The data below is from a simple packing I made using `pyparm.packmin`. Normally you'd load your own data from a file.

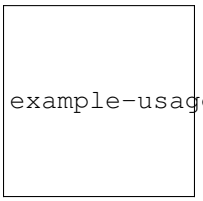
```
L = 2.0066668050219723
diameters = [ 0.96,  0.97,  0.98,  0.99,  1.  ,  1.01,  1.02,  1.03,  1.04]
locs = [[ 1.40776762,  1.26647724,  0.73389219],
        [ 0.58704249,  2.11399   ,  1.52956579],
        [ 1.75917911,  0.54290089,  1.27577478],
        [ 2.13750384,  0.87508242,  0.21938647],
        [ 1.07283961,  0.87692084,  1.9060841 ],
        [ 0.09550267,  1.94404465,  0.56463369],
        [ 1.07636871,  2.1942971 ,  0.63752152],
        [ 0.49922725,  1.20002224,  1.13360082],
        [-0.27724757,  1.62152603,  1.67262247]]
```

Now we make the packing:

```
pack = spack.Packing(locs, diameters, L=L)
```

What does it look like?

```
size = 400
sc = pack.scene(rot=pi/4, camera_dist=2, cmap='autumn', bgcolor=[1,1,1])
sc.render('ipython', width=size, height=size, antialiasing=0.001)
```



Let's make a movie!

```
from moviepy.editor import VideoClip
import moviepy.editor as mpy

duration = 10
def make_frame(t):
    return (
                pack.scene(rot=(t/duration + .125)*2.*pi,
                           camera_dist=2, cmap='autumn', bgcolor=[1,1,1])
                .render(width=size, height=size, antialiasing=0.001)
            )
vc = VideoClip(make_frame, duration=duration)
```

Write the movie to file. This takes about 10 minutes on my machine to render all 240 frames, but it does give you some pretty spiffy output.

```
vc.write_gif("example-packing.gif",fps=24)
```

```
[MoviePy] >>>> Building file example-packing.gif
[MoviePy] Generating GIF frames...
[MoviePy] Optimizing the GIF with ImageMagick...
[MoviePy] >>>> File example-packing.gif is ready !
```

And display the movie, in an ipython notebook.

```
from IPython.display import Image
Image(url="example-packing.gif")
```

4.2 Reference

spack: a package for spherical packing analysis

class spack.**Packing**(*rs*, *diameters*, *shear=0.0*, *L=1.0*)

A class representing a packing of spheres in a periodic box.

class Backbone(*indices*, *adjacency*)

__getnewargs__()

Return self as a plain tuple. Used by copy and pickle.

__getstate__()

Exclude the OrderedDict from pickling

__repr__()

Return a nicely formatted representation string

adjacency

Alias for field number 1

indices

Alias for field number 0

class Packing.**Contacts**(*Nc*, *stable*, *floaters*)

Nc

Alias for field number 0

__getnewargs__()
Return self as a plain tuple. Used by copy and pickle.

__getstate__()
Exclude the OrderedDict from pickling

__repr__()
Return a nicely formatted representation string

floaters
Alias for field number 2

stable
Alias for field number 1

Packing.**DM**(*masses=None*)
Dynamical matrix for array rs, size ds. Assumes epsilon is the same for all.

Parameters **masses** (*an array of length N of the masses of the particles.*) –

Packing.**DM_freqs**(*masses=None*)
Find the frequencies corresponding to the eigenvalues of the dynamical matrix.

This is just a short wrapper around DM().

class Packing.**Neighbors**(*adjacency*, *diffs*)

__getnewargs__()
Return self as a plain tuple. Used by copy and pickle.

__getstate__()
Exclude the OrderedDict from pickling

__repr__()
Return a nicely formatted representation string

adjacency
Alias for field number 0

diffs
Alias for field number 1

Packing.**backbone**(*tol=1e-08*)
Returns (backbone indices, neighbor matrix)

Packing.**cages**(*M=10000*, *R=None*, *Rfactor=1.2*, *padding=0.1*, *Mfactor=0.1*)
Find all cages in the current "packing".

The algorithm uses Monte Carlo: it finds M random points within a sphere of radius R from each particle, and sees if that particle could sit there without conflicting with other particles. Then (number of accepted points) / (number of test points) * (volume of sphere) is the volume of the cage.

The algorithm is adaptive: if not enough test points are accepted (n < M * Mfactor), it tries more test points. If any test points are within *padding* of the edge, *R* is (temporarily) expanded.

Parameters

- **M**(*Number of points in the sphere to test*) –
- **R**(*Size of sphere to test (will be expanded if necessary)*) –
- **Rfactor**(*How much to increase R by when the cage doesn't fit*) –

- **padding** (*How much larger the sphere should be than the cage (if it isn't, the sphere is*) – expanded)
- **Mfactor** (*Mfactor * M is the minimum number of points to find per cage. If they aren't*) – found, more points are tested.

Returns

- **points** (*a list of (A x 3) lists, A indeterminate (but larger than M * Mfactor), with each*) – list corresponding to the points within one cage.
- **Vs** (*The approximate volumes of each cage.*)

Packing.**contacts**(*tol=1e-08*)
Returns (number of backbone contacts, stable number, number of floaters)

Packing.**dist**(*other*, *tol=1e-08*, *maxt=1000000*)
Returns the distance between two packings, with the particles paired up in the most efficient way, and also with center-of-mass accounted for.

Packing.**dist_tree**(*other*, *tol=1e-08*)
Find the distance between two packings.

Requires pyparm.

Packing.**forces**()
Find Fij on each particle, assuming a harmonic potential, U = 1/2 (1 - r/σ)^2

Returns a dxNxN matrix.

Packing.**neighbors**(*tol=1e-08*)
For a set of particles at xs,ys with diameters diameters, finds the distance vector matrix (d x N x N) and the adjacency matrix.

Assumes box size 1, returns (adjacency matrix, diffs)

Packing.**paired_dists**(*other*, *match_com=True*)

Returns the distance between two packings, assuming particle 1 of packing 1 goes with particle 2 of packing 2.

Distance is calculated as :math:‘d = sqrt{sum_i left(

ec r_i ominus_ ec{L} ec s_i

ight)^2‘, where :math:‘

ec r_i‘ are the particles from one packing, :math:‘

ec s_i‘ are the particles from the other packing, and :math:‘ominus_

ec{L}‘ means “shortest distance given periodic boundary conditions in a box of shape :math:‘

ec{L}‘”.

other : Another *Packing*. match_com : Subtract off center-of-mass motion as well.

For *match_com* = *True*, this yields

:math:‘d = sqrt{sum_i left(

ec{r}_{i} ominus_ ec{L} ec{s}_{i} -

ec{delta} ight)^2}‘

Minimized over ‘

ec delta‘. It does this by actually evaluating

:math:‘d = sqrt{

rac{1}{N}sum_{leftlangle i,j ight angle

}left(

ec{r}_{ij} ominus_ ec{L} ec{s}_{ij} ight)^2}‘,

which turns out to be equivalent.

Packing.**phi**
Volume of the spheres in the box.

Packing.**plot_contacts**(*ax=None*, *tol=0*, *reshape=True*, ***kw*)
Designed for use with plot_disks, this will plot a line between neighboring particles.

Packing.**plot_disks**(*ax=None*, *color=None*, *alpha=0.4*, *reshape=True*)
Plot the packing as a set of disks.

Color can be None (uses the standard sets), ‘diameter’ (colors by diameter), or a list of colors.

‘reshape’ means set axis scaled, etc.

Packing.**scene**(*pack*, *cmap=None*, *rot=0*, *camera_height=0.7*, *camera_dist=1.5*, *angle=None*, *light-strength=1.1*, *orthographic=False*, *pad=None*, *floater_color=(0.6, 0.6, 0.6)*, *bg-color=(1, 1, 1)*, *box_color=(0.5, 0.5, 0.5)*, *group_indexes=None*, *clip=False*)
Render a 3D scene.

Requires *vapory* package, which requires the *povray* binary.

Parameters

- **cmap** (*a colormap*) –
- **box_color** (*Color to draw the box. 'None' => don't draw box.*) –
- **floater_color** (*Color for floaters. 'None' => same color as non-floaters (use cmap).*) –
- **group_indexes** (*a list of indexes for each "group" that should remain*) – together on the same side of the box.
- **clip** (*clip the spheres at the edge of the box.*) –

Returns scene

Return type vapory.Scene, which can be rendered using its *.render()* method.

Packing.**size_indices**(*tol=1e-08*)
Returns [idx of sigma1, idx of sigma2, ...]

Packing.**tess**()
Get a *tess.Container* instance of this.

Requires *tess*.

CHAPTER 5

Indices and tables

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