Introducing Our Team

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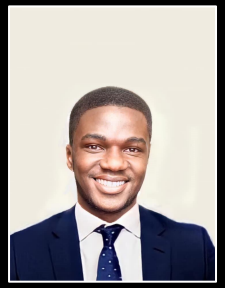
(Lead Mentor)

Christopher Lanclos
(Co-Mentor)

Jinwei Liu
(Co-Mentor)

Jean-Pierre
Bianchi
(Student)



Ayomide
Olatunde
(Student)

Christopher
Metellus
(Student)

Team Landmarks

Thursday:
- Met together and created introduction video

Friday:
- Created GitHub repository
- Ideation, finding carbon nanotube database
- Basic render of carbon nanotube (CNT) made in Blender
- More research into CNTs, may influence project scope

Saturday:
- Benchmark render using VM compute configs
- More angles of CNT renders captured
- Attempts at rendering Blender files using CloudyCluster is made

Sunday:
- Web pages connected for GitHub site
- Lack of communication → slow progress

Monday:
- GitHub site completed
- Resorting to using Google Cloud

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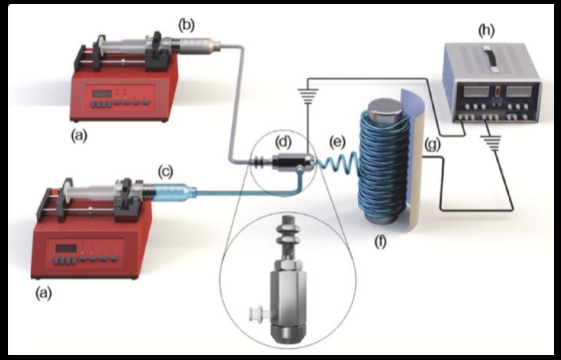
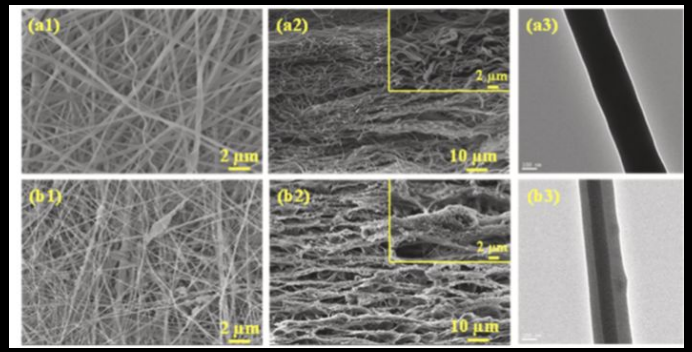
Team Demonstration Video

GitHub Link: https://qrgo.page.link/tGLCW

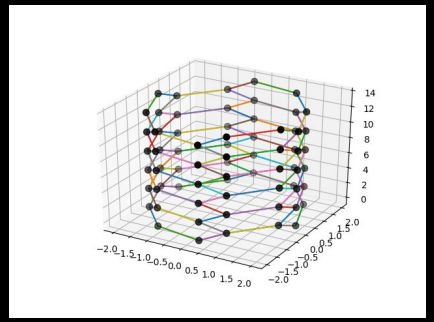
Seawater filter with nanotubes





Nanotube Creation with Python

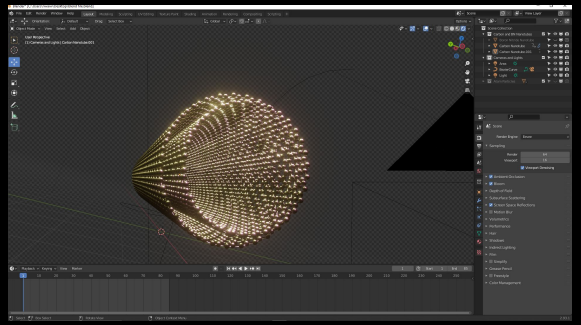
```python
from ase.build import nanotube
cnt1 = nanotube(6, 0, length=400)  # see ase doc for significance of parameters
bond_length = 1.4  # we give the covalent bond length so we can easily plot them (bonds are not real)
cnt2 = nanotube(3, 3, length=6, bond=bond_length, symbol='Si')  # generates 72 atoms

# https://wiki.fysik.dtu.dk/ase/ase/neighborlist.html?highlight=covalent%20bond#building-neighbor-lists
from ase.neighborlist import neighbor_list
d = neighbor_list('d', cnt2, bond_length)

# ase gives atoms locations, but not the covalent bonds between them
# so we have to do it ourselves (or use complex software used by chemists)

# # let's get the distances between every atom
# from ase.geometry import get_distances
positions = cnt2.positions
# xyz, dist = get_distances(positions, p2=None, cell=None, pbc=None)
# covalent bonds exist only between closest ones, ie at bond_length
dist = sc.cdist(positions,positions)
# argwhere does fantastic job at finding all bonded atoms (indices) with condition
bondsidx = np.argwhere((dist < bond_length*1.1) * (dist > bond_length*0.9))

# let's get the xyz coordinates of every atom in the nanotube
x,y,z = positions.T

fig = plt.figure()
# https://jakevdp.github.io/PythonDataScienceHandbook/04.12-three-dimensional-plotting.html
ax = plt.axes(projection='3d')  # we want a 3D scatter plot to see all atoms
ax.scatter(x,y,z,c='black',s=50)
```



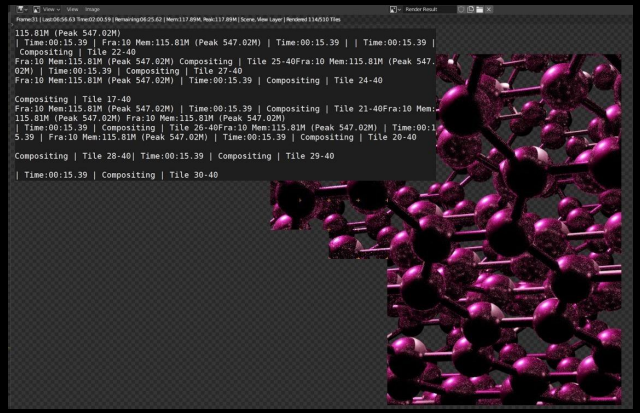
Problem: This is possible, but very time consuming.

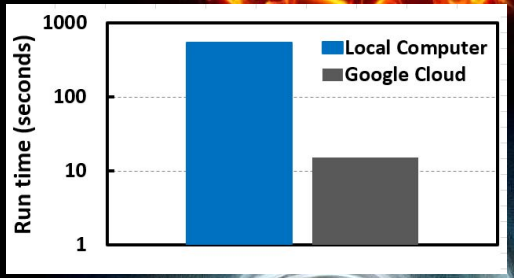
Cloudycluster for Rendering

Nanotube in Blender

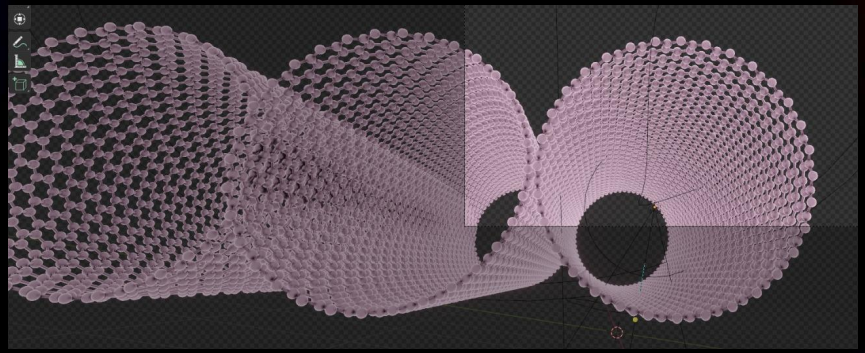


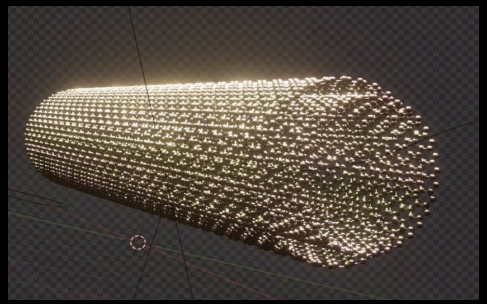
Approximate Render Time:
120’ on Desktop, 15’ on Cloudy Cluster

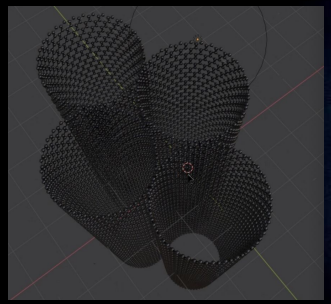




Using Blender to Create Carbon Nanotubes

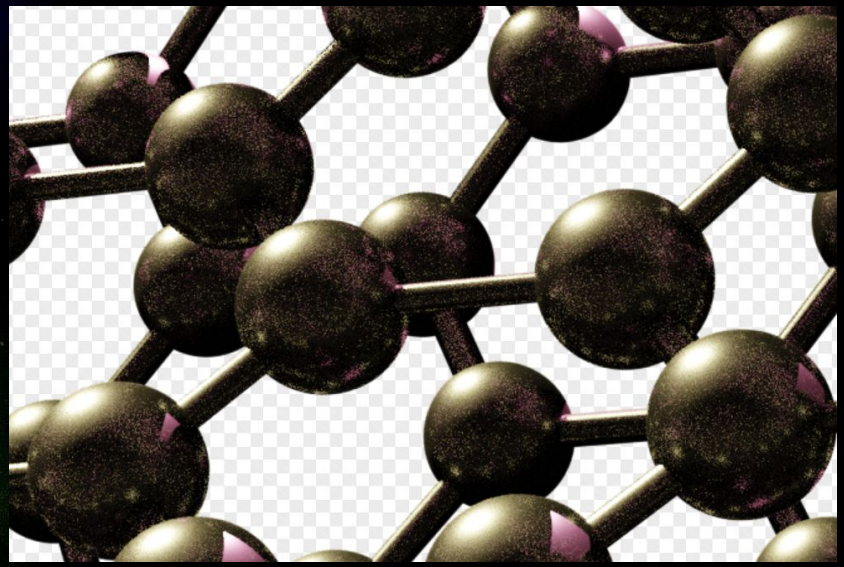






Website Link:
https://rollercoaster111.github.io/renderblender.io/main.html

Using Blender to Create Carbon Nanotubes



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The Render Benders have arrived!

Questions?