# Organized Disorder: Packing in Microscopic and Macroscopic Systems

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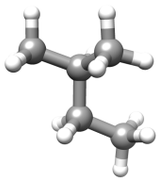
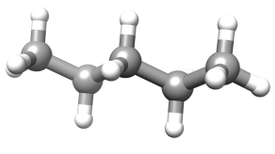
## Abstract

How does shape affect a molecule or object's ability to pack? We compared the packing abilities of pentane molecules to Runts candies to investigate how shape affects packing as well as to make a conceptual connection between the macroscopic and the microscopic worlds. Using UCSF Chimera [1], we constructed cyclopentane, isopentane, neopentane, and n-pentane (a natural model and a manipulated model.) We then ran molecular simulations using Gromacs 4.5.5 [2] to sample the densities of the molecules' liquid state at 0 degrees centigrade (273.15 K) and then again at nearly absolute zero (0 K). We compared the densities and packing abilities of the candies and molecules, and the Runts' ability to pack was analogous to the similarly shaped molecules' ability to pack.

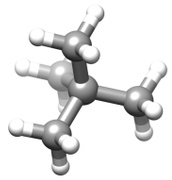
**Isopentane**



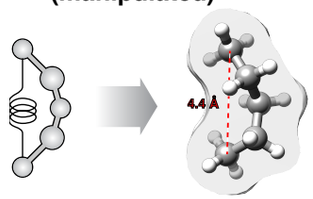
**N-pentane**



**Neopentane**



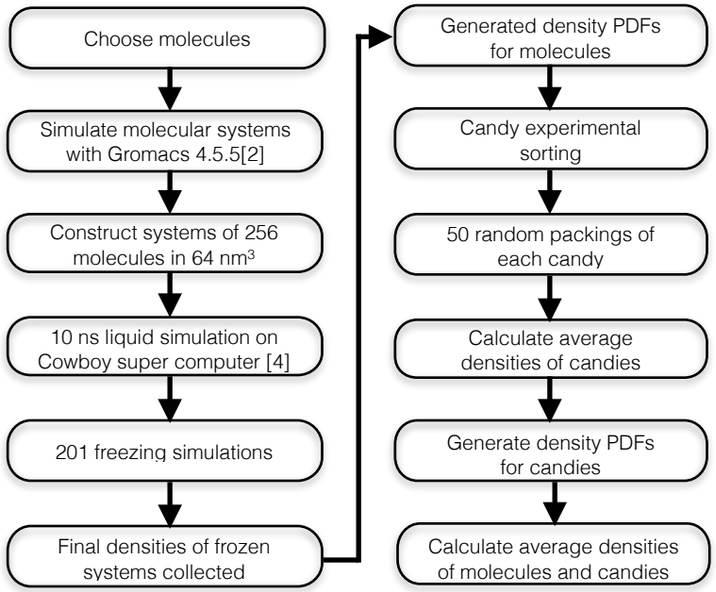
**N-pentane (manipulated)**



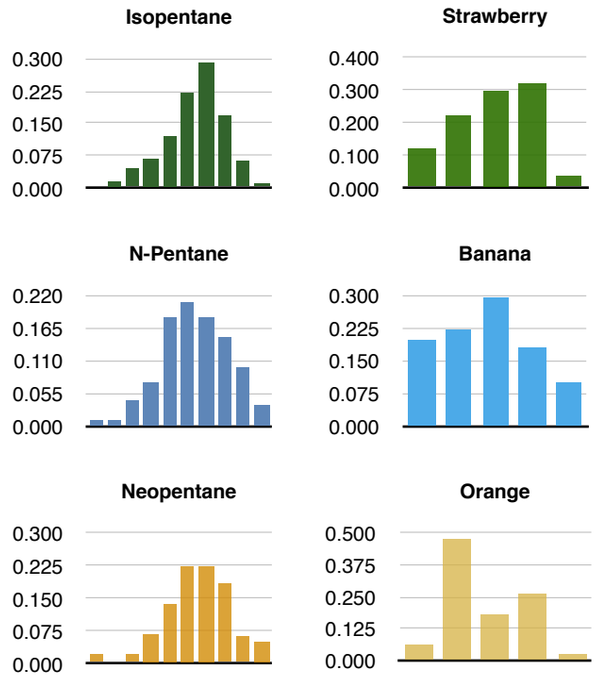

## Problem

- How systems pack dictates macroscopic properties in a glass state.
- Glass states are difficult to access experimentally.
- What is the optimum shape of a particle to increase density of a system? [1]

## Method




## Results




## Conclusion

- Shape affects how densely a system packs.
- Packing in the microscopic and macroscopic worlds is analogous.

| Average Densities of Candies (g/cm³) | |
|---|---|
| **Strawberry** | **1.039** |
| Banana | 0.965 |
| Orange | 0.927 |

| Average Densities of Molecules (g/cm³) | |
|---|---|
| **Isopentane** | **0.826** |
| N-Pentane | 0.823 |
| Neopentane | 0.818 |

## Application

- Increasing density and therefore quantity of a substance such as grain by changing shape of particles from spheres to ellipsoids. [1]
- Understanding which fuels are more dense according to molecular shape so that a fuel can "pack more punch" by having more fuel in a given volume.
- Grandparent University: making a connection between the macroscopic and microscopic worlds for children and their grandparents to learn about chemistry.

GRANDPARENT UNIVERSITY

## References

[1] Donev, et al. (2004) Science. 5660: 990-993

[2] Hess, et al. (2008) J. Chem. Theory Comput. 4:435-447.

[3] Peterson, et al. (2004) J Comput. Chem. 25:1605-1612.

[4] The computing for this project was performed at the OSU High Perfomance Computing Center at Oklahoma State University supported in part through the National Science Foundation grant OCI - 1126330.