COS 126 – Atomic Theory of Matter



Raise your hand and ask





- No universal acceptance of the atomic nature of matter
- Botanist Robert Brown notices erratic motion of pollen grains in water. This motion is later called: *Brownian motion*



- Einstein publishes a revolutionary paper:
- Brownian motion is caused by smaller moving particles colliding with the larger pollen grains.
- Density of particles affects displacement in Brownian motion



 Jean Baptist Perrin experimentally validated Einstein's theory and equations.

Your Task: Redo Perrin's experiments!
Not so difficult with computers and your COS126 skills

Goal of the Assignment

Calculate Avogadro's number

- Using Einstein's equations
- Using fluorescent imaging
- Input data
 - Sequence of images
 - Each image is a rectangle of pixels
 - Each pixel is either light or dark
- Output
 - Estimate of Avogadro's number

Atomic Theory Overview

- Brownian Motion
 - Random collision of molecules
 - Displacement over time fits a Gaussian distribution



Atomic Theory Overview

- Avogadro's Number
 - Number of atoms needed to equal substance's atomic mass in grams
 - N_A atoms of Carbon-12 = 12 grams
 - Can calculate from Brownian Motion
 - Variance of Gaussian distribution is a function of resistance in water, number of molecules



Record a video of particles undergoing Brownian motion



Convert the video into a sequence of frames

video



Frames

Identify **Beads** in every frame

3









Displacements

Given as input



video



7.1833 4.7932 2.1693

5.5287

5.4292

2.1893

5.7294

Displacements



Beads

 $oldsymbol{0}$

frame i

0

frame i+1

BeadFinder.java Detects all the "Beads" in a given frame.

BeadTracker.java

Outputs displacements of beads over successive frames.

Number

Avogadro's

Avogadro.java Computes Avogadro's number from a given set of displacements.

Blob.java Represents + a set of adjacent pixels.

+ readme.txt Shows performance analysis.

Assignment: Four Programs

- Blob.java
 - Represents a set of adjacent pixels.
- BeadFinder.java
 - Detects all the *Beads* in a given image.
- BeadTracker.java
 - Outputs displacements of beads over consecutive frames.
- Avogadro.java
 - Computes Avogadro's number from a given set of displacements.
- readme.txt
 - Shows performance analysis.

Blob.java

API for representing particles (blobs) in water

- public Blob()
- public void add(int i, int j)
- public int mass() // number of pixels
- public double distanceTo(Blob b) // from center (average)
- public String toString()
- Only need three values to efficiently store
 - Do not store the positions of every pixel in the blob



Blob Challenges

Format numbers in a nice way

- String.format("%2d (%8.4f, %8.4f)", mass, cx, cy);
- (Use same format in System.out.printf())
- E.g., "%6.3f" -> _2.354
- E.g., "%10.4e" -> 1.2535e-23
- Thoroughly test
 - Create a simple main()

Blobs and Beads

- Blob: Any group of adjacent light pixels.
 Not X
- How many blobs are there?
- Bead: A blob with a number of pixels that is at least min.
- How many beads are there? (assume min=5)



BeadFinder.java

- Locate all blobs in a given image
 - And identify large blobs (called beads)

API

- public BeadFinder(Picture picture, double threshold)
 - Calculate luminance (see Luminance.java, 3.1)
 - Include pixels with a luminance >= threshold
 - Find blobs with DFS (see Percolation.java, 2.4)
 - The hard part, next slide...
- public Blob[] getBeads(int minSize)
 - Returns all beads with at least minSize pixels
 - Array must be of size equal to number of beads

BeadFinder.java

An Image



Input:

A Luminance Threshold **tau**

BeadFinder.java

BeadFinder: Original Image



BeadFinder: Applying Luminance Threshold tau



- Use boolean[][] array to mark visited
- Traverse image pixel by pixel
 - Dark pixel
 - Mark as visited, continue
 - Light pixel
 - Create new blob, call DFS

DFS algorithm

- Base case: simply return if
 - Pixel out-of-bounds
 - Pixel has been visited
 - Pixel is dark (and mark as visited)
- Add pixel to current blob, mark as visited
- Recursively visit up, down, left, and right neighbors



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BeadFinder Challenges

- Data structure for the collection of blobs
 - Store them any way you like
 - But be aware of memory use and timing

BeadFinder Challenges

- Data structure for the collection of blobs
 - Store them any way you like
 - But be aware of memory use and timing
- Array of blobs?
 - But how big should the array be?
- Linked list of blobs?
 - Memory efficient, but harder to implement
 - Avoid traversing whole list to add a blob!
- Anything else?
 - Submit your (extra) object classes

BeadTracker.java

- Track beads between successive images
- Single main function
 - Take in a series of images
 - Output distance traversed by all beads for each time-step
 - For each bead found at time t+1, find closest bead at time t and calculate distance
 - Not the other way around!
 - Don't include if distance > 25 pixels (new bead)



BeadTracker Challenges

Reading multiple input files

- java-introcs BeadTracker 25 180.0 25.0 run_1/*.jpg
- Expands files in alphabetical order
- End up as args[0], args[1], ...
- Avoiding running out of memory
 - How?
- Recompiling
 - Recompile if Blob or BeadFinder change

BeadTracker Challenges

Reading multiple input files

- java-introcs BeadTracker 25 180.0 25.0 run_1/*.jpg
- Expands files in alphabetical order
- End up as args[0], args[1], …
- Avoiding running out of memory
 - Do not open all picture files at same time
 - Only two need to be open at a time
- Recompiling
 - Recompile if Blob or BeadFinder change

Avogadro.java

- Analyze Brownian motion of all calculated displacements
 - Lots of crazy formulas, all given, pretty straightforward
 - Be careful about units in the math, convert pixels to meters, etc.
- Can test without the other parts working
 - We provide sample input files
 - Can work on it while waiting for help

Conclusion: Final Tips

Avoiding subtle bugs in BeadFinder

- Double check what happens at corner cases (e.g. at boundary pixels, or when luminance == tau, or mass == cutoff)
- Common errors in BeadFinder
 - NullPointerException
 - StackOverflowError (e.g., if no base case)
 - No output (need to add print statements)
- Look at Possible Progress Steps
 - Click ► to expand!

Conclusion: Final Tips

- Avoid *magic numbers*
 - Define constants
- No Checkstyle or other errors/warnings
- Testing with a main()
- There is a limit of twenty (20) times that you may click the Check Submitted Files to receive feedback from the TigerFile auto-grader
 - So, test locally! I.e., on your laptop before using TigerFile to run test cases

Conclusion: Final Tips

Timing analysis - *doubling method!*

- Wild cards
 - The frames use the following naming convention:
 - frame00000.jpg, frame00001.jpg ... frame00198.jpg, frame00199.jpg
 - On command line:
 - 10 frames? run_1/frame0000*.jpg
 - 20 frames? run_1/frame000[01]*.jpg
 - 40 frames? run_1/frame000[0123]*.jpg
 - 100 frames? run_1/frame000*.jpg
 - 200 frames? run_1/frame*.jpg
 - 400 frames? run_1/frame*.jpg run_1/frame*.jpg



References

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