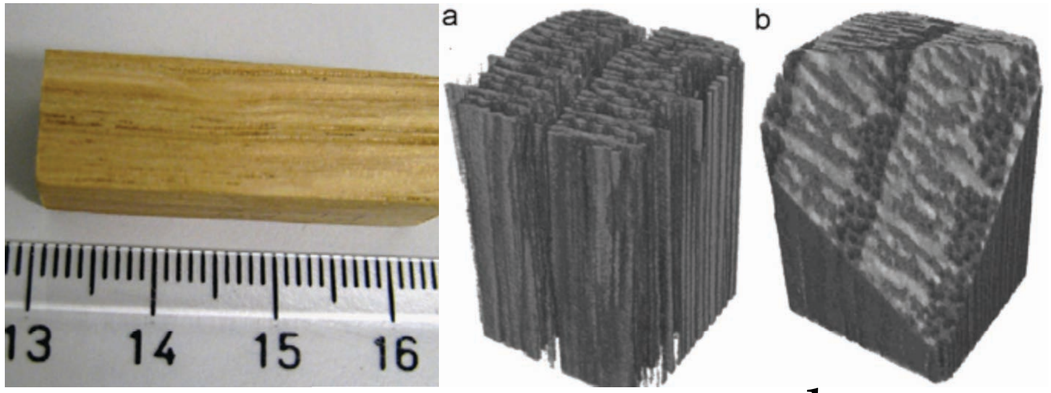
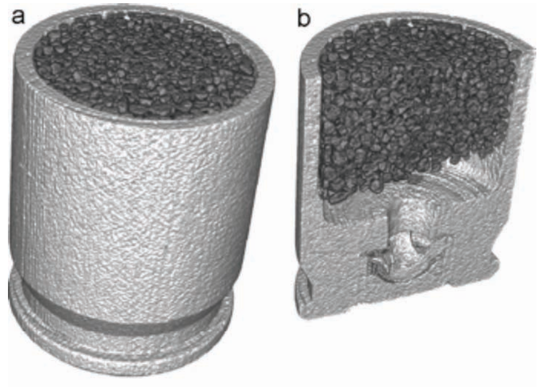
3D+ Visualization: Avizo, VisIt, and Mathematica via CHEM4581: Mathematical Methods in Chemistry

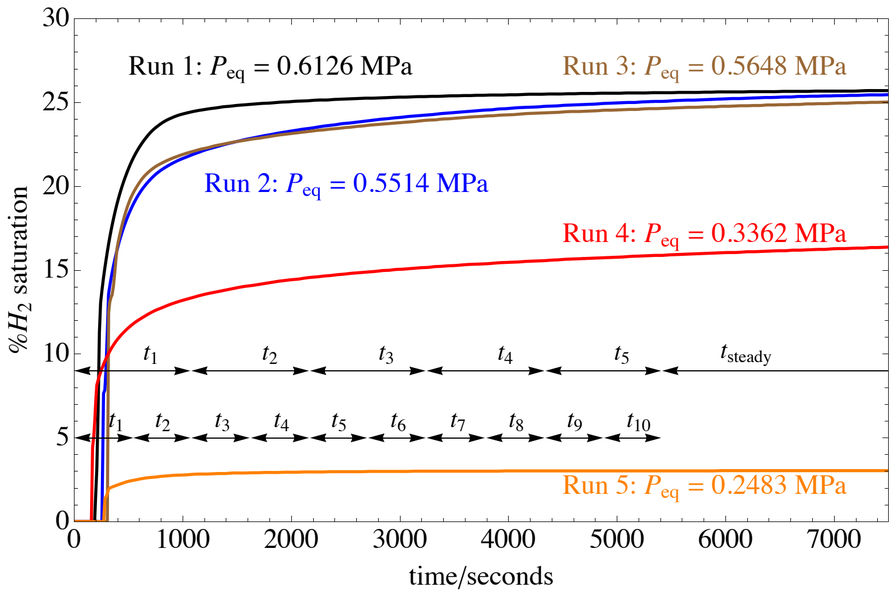
Les Butler - lbutler@lsu.edu, 329 Choppin Hall
Jinghua Ge - jinghuage@cct.lsu.edu, 5 Johnston Hall

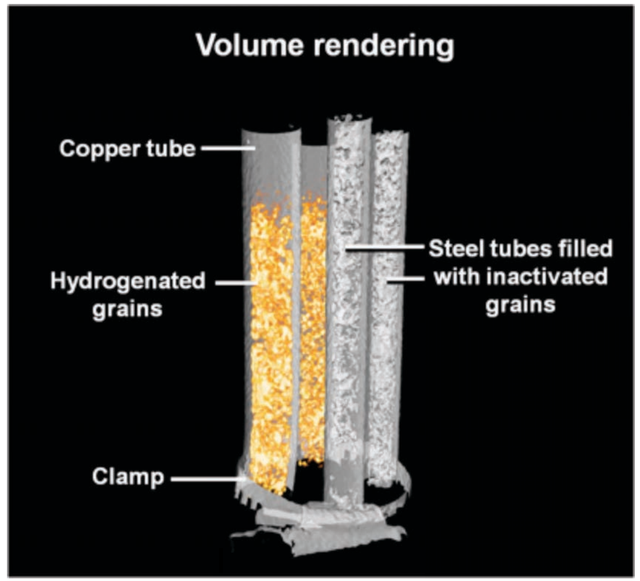


wood



cartridge





Approximate Schedule

Weeks 1-5: Installation on student laptops Mathematica, VisIt, ImageJ, and Filezilla. Lectures on data formats, data import, histograms, threshold and binarization. Labs on introduction to Avizo, VisIt. Mathematica homework on data formats, importing, histograms, image and contour plots, and opacity. 3D data acquisition.

Weeks 6-10: Lectures on erosion/dilation, distance/watershed transformation, and connected components analysis. Labs on segmentation, open/closing operations, label fields, and connected component output. Mathematica homework on erosion/dilation, distance/watershed transformation, connected components, and re-ordering of label fields.

Weeks 11-15: Lectures on inverse Radon transformation, affine transformation, texture, optimization, python scripting. Labs on scripting, affine transformation, brushes for manual editing. Mathematica homework on Radon transformation, affine transformation, optimization.

and VisTrails. Options for your own 3D data set.

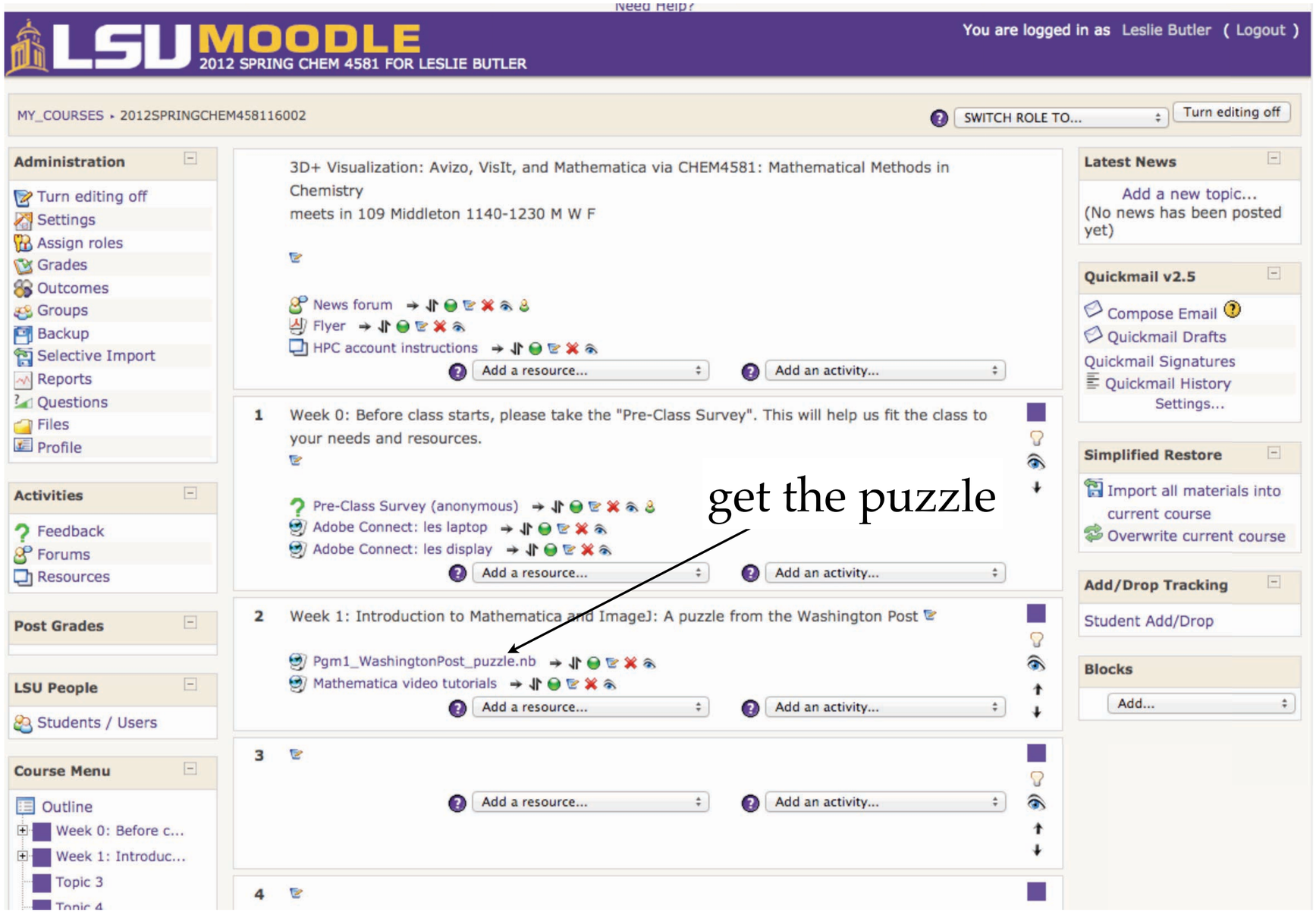
Grading

Grades will be based on homework, participation in labs, midterm, and final. There will be separating syllabi for undergraduates and graduate students.
We have consulted with the Honors College and for the undergraduates, this course can count for honors credit.

Assignments and exams will be graded on a point system. At midterm, the points will be totaled and scaled such that perfect score = 140%. Letter grades, A-F, assigned based on 90%, 80%, 70%, 60% or below. Procedure is repeated for assignments between midterm and final.

- Bonus points accumulated in first half of semester do not carry over to second half of semester.
- Missed assignments are allowed.
- There will be lots of assignments. Typically, started in class and finished as HW. Visualization is like chess; the more you practice, the better you get.

Moodle


Need Help?
LSU MOODLE
2012 SPRING CHEM 4581 FOR LESLIE BUTLER
You are logged in as Leslie Butler (Logout)
MY_COURSES ▸ 2012SPRINGCHEM458116002
SWITCH ROLE TO...
Turn editing off
Administration
Turn editing off
Settings
Assign roles
Grades
Outcomes
Groups
Backup
Selective Import
Reports
Questions
Files
Profile
Activities
Feedback
Forums
Resources
Post Grades
LSU People
Students / Users
Course Menu
Outline
Week 0: Before c...
Week 1: Introduc...
Topic 3
Topic 4
3D+ Visualization: Avizo, VisIt, and Mathematica via CHEM4581: Mathematical Methods in Chemistry
meets in 109 Middleton 1140-1230 M W F
News forum
Flyer
HPC account instructions
Add a resource...
Add an activity...
1 Week 0: Before class starts, please take the "Pre-Class Survey". This will help us fit the class to your needs and resources.
Pre-Class Survey (anonymous)
Adobe Connect: les laptop
Adobe Connect: les display
Add a resource...
Add an activity...
2 Week 1: Introduction to Mathematica and ImageJ: A puzzle from the Washington Post
Pgm1_WashingtonPost_puzzle.nb
Mathematica video tutorials
Add a resource...
Add an activity...
3
Add a resource...
Add an activity...
4
get the puzzle
Latest News
Add a new topic...
(No news has been posted yet)
Quickmail v2.5
Compose Email
Quickmail Drafts
Quickmail Signatures
Quickmail History
Settings...
Simplified Restore
Import all materials into current course
Overwrite current course
Add/Drop Tracking
Student Add/Drop
Blocks
Add...

http://www.washingtonpost.com/wp-srv/artsandliving/magazine/second-glance/20120115/index.html

Rare view - January 1, 2012

Find the **12** differences between the original photograph, top, and the altered photograph, bottom. (Degree of difficulty: Extreme)

Show Answers

#1

#2

A closer look - January 8, 2012

Find the **12** differences between the original photograph, top, and the altered photograph, bottom. (Degree of difficulty: Advanced)

Show Answers

#1

#2

A f looded downtown - January 15, 2012

Find the **12** differences between the original photograph, top, and the altered photograph, bottom. (Degree of difficulty: Advanced)

Show Answers

#1

#2

Standard image processing commands can solve the puzzle in about 0.3 seconds.

This output shows 12 components with sizes ranging from 278 pixels to 3,814 pixels.

{1 -> 327, 2 -> 308, 3 -> 278, 4 -> 598, 5 -> 1010, 6 -> 3814,
7 -> 485, 8 -> 1355, 9 -> 837, 10 -> 1632, 11 -> 2477, 12 -> 518}

And this is the code to find differences, plot differences, and list differences.

In[124]:=

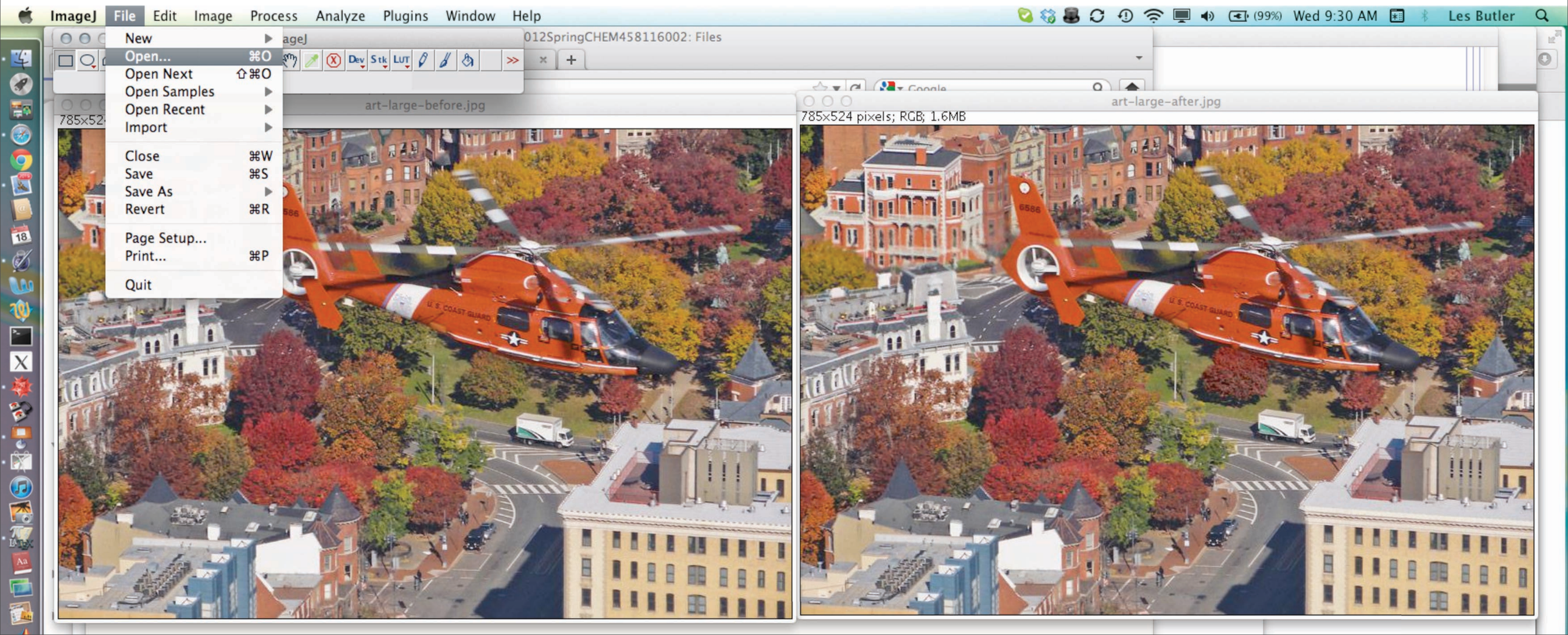
```
imageDifference = Dilation[Binarize[ImageDifference[imageAfter, imageBefore], 0.1], 4];
imagePerimeter = Dilation[EdgeDetect[imageDifference], 1];
imageComponents = MorphologicalComponents[imageDifference];
(* imageComponents// Colorize *)
ComponentMeasurements[imageComponents, "Count"]
GraphicsRow[{ImageAdd[imageBefore, imagePerimeter], ImageAdd[imageAfter, imagePerimeter]}, ImageSize → {800, 500}]
```

Let's use another program and the same "standard" image processing commands.
First, run this cell in Mathematica:

- **Export the before and after jpgs.**

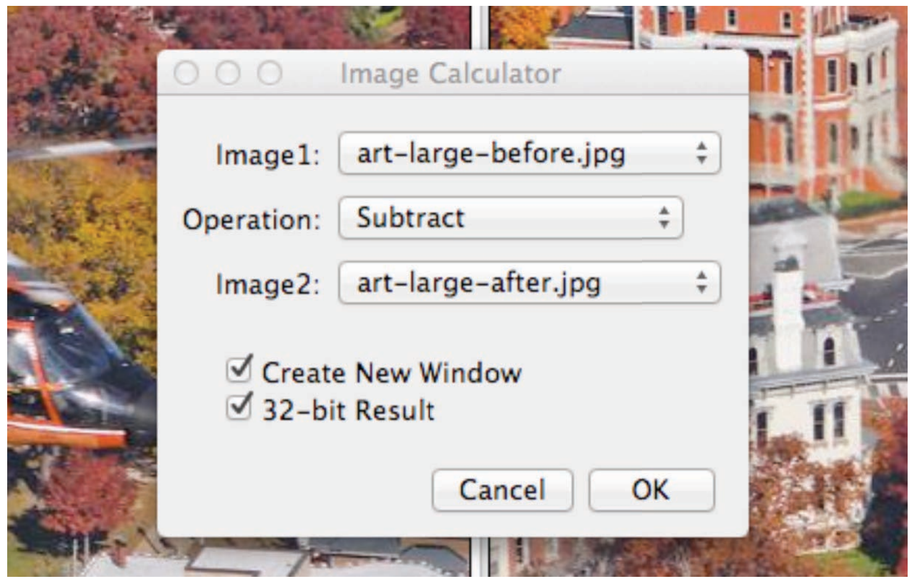
```
In[129]:= Export[NotebookDirectory[] <> "art-large-before.jpg", imageBefore, "JPG"]
          Export[NotebookDirectory[] <> "art-large-after.jpg", imageAfter, "JPG"]

Out[129]= /Users/les/Documents/Class/4581_Spr12/art-large-before.jpg

Out[130]= /Users/les/Documents/Class/4581_Spr12/art-large-after.jpg
```

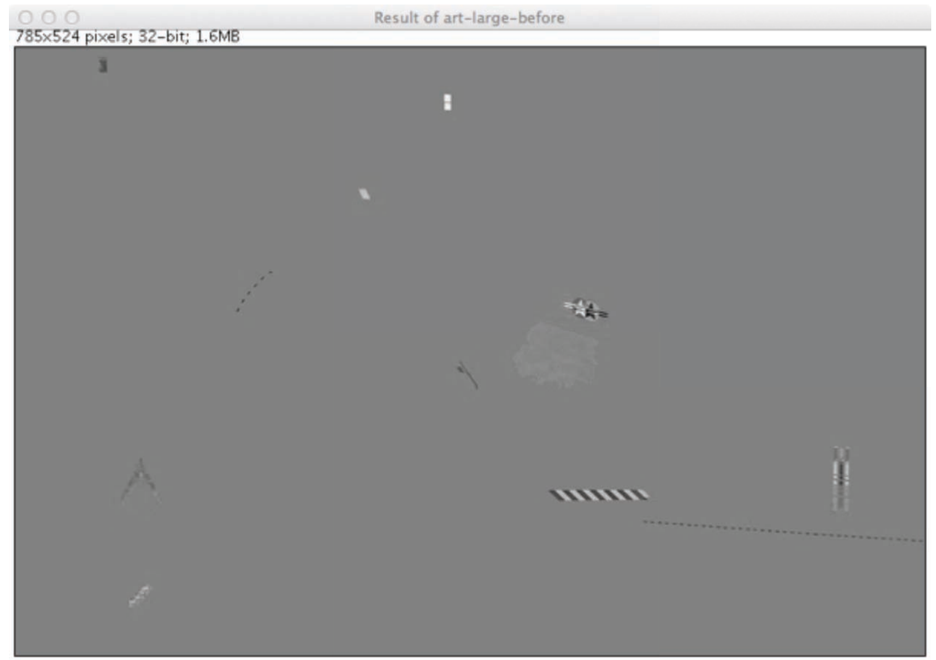
Second, open ImageJ and then open
the two files, "art-large-before.jpg" and "...-after.jpg"



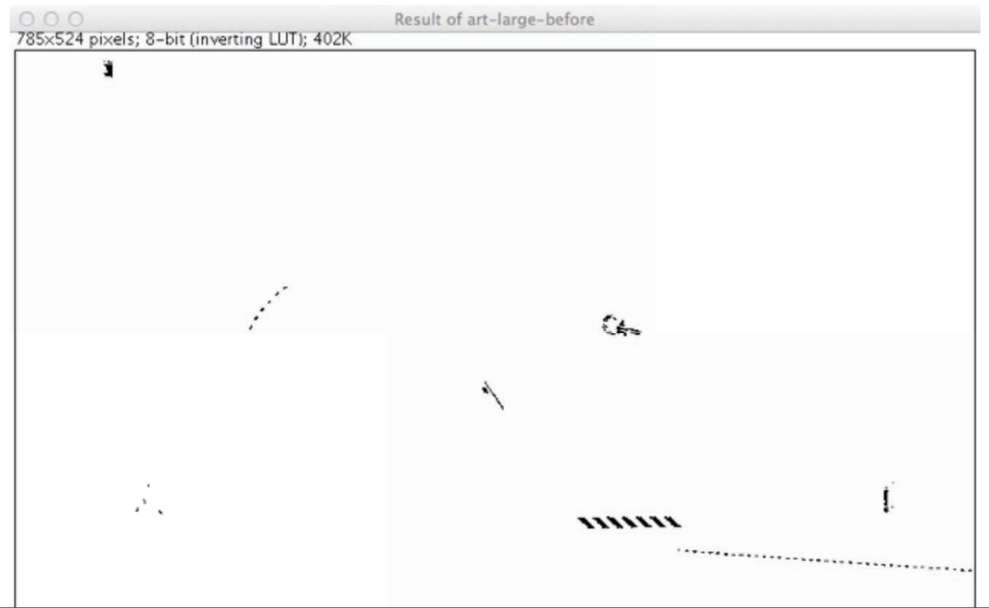
In ImageJ

1) Process/Image Calculator to get this grayscale image





2) Make the image binary with Process/Binary/Make Binary

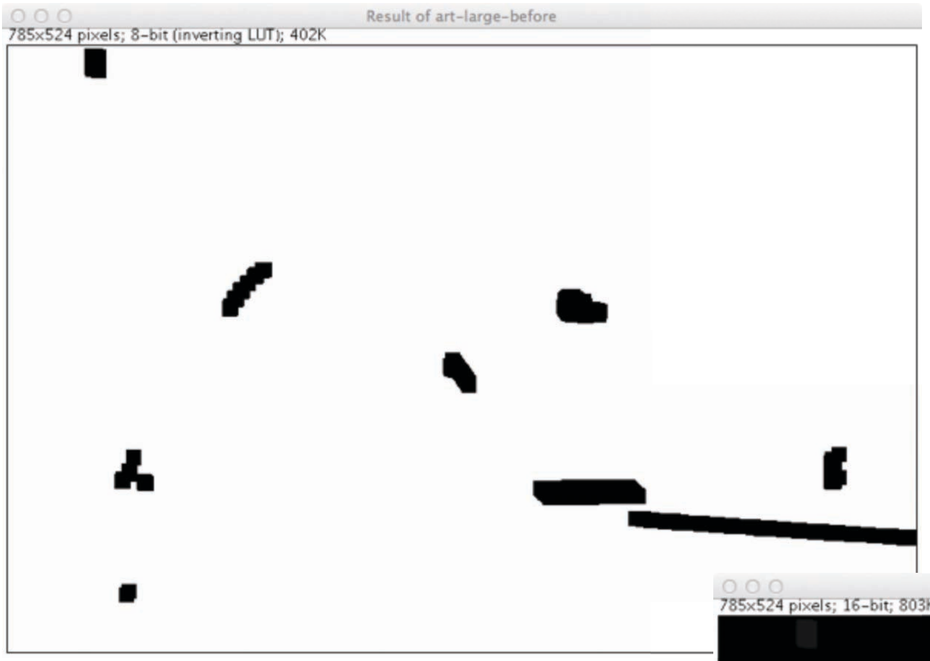


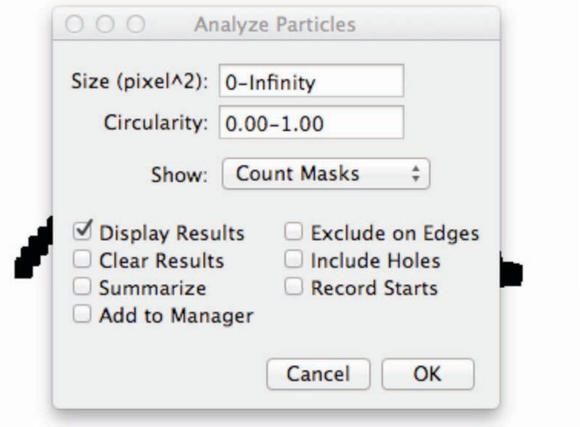
In ImageJ

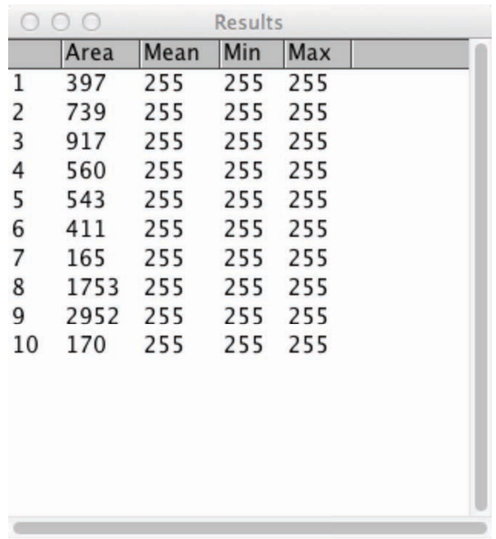
3) Make the objects bigger with dilation. Do Process/Binary/Dialate about 5 times.

In ImageJ

4) Next, a component analysis. Do Analyze/Analyze Particles...







Results

	Area	Mean	Min	Max
1	397	255	255	255
2	739	255	255	255
3	917	255	255	255
4	560	255	255	255
5	543	255	255	255
6	411	255	255	255
7	165	255	255	255
8	1753	255	255	255
9	2952	255	255	255
10	170	255	255	255

Count Masks of Result of art-large-before.tif

785x524 pixels; 16-bit; 803K

Results

	Area	Mean	Min	Max
1	397	255	255	255
2	739	255	255	255
3	917	255	255	255
4	560	255	255	255
5	543	255	255	255
6	411	255	255	255
7	165	255	255	255
8	1753	255	255	255
9	2952	255	255	255
10	170	255	255	255

Rare view - January 1, 2012

Find the **12** differences between the original photograph, top, and the altered photograph, bottom. (Degree of difficulty: Extreme)

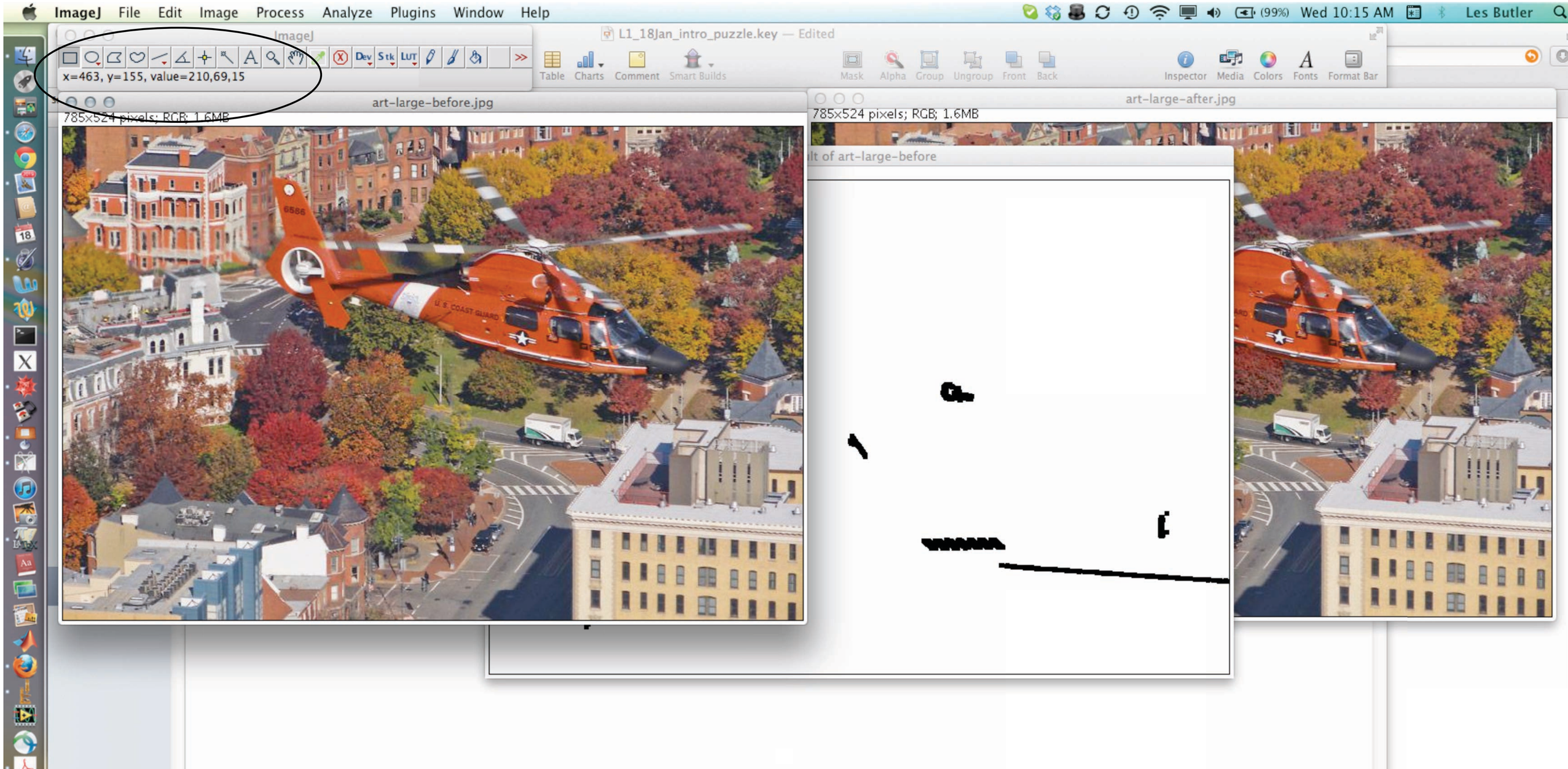
Hide Answers

#1

#2

In ImageJ

5) Let's look at the numbers in the picture. Put the cursor on the "red" helicopter and note the x, y, and value displays. The values are (red,green,blue) as 8-bit numbers.



Number formats common in imaging:
binary: 0, 1
byte (8 bits): 0... 255
unsigned integer 16 (16 bits): 0 to 65,535
signed integer 16: -32,768 to 32,767
real: ambiguous
real32: could be little-endian or big-endian
real64: could be little-endian or big-endian

In Mathematica, use the Help/Documentation Center and search for BinaryData to get more information.

■ Step by step

In[210]:=
```
imageDifference = ColorConvert[ImageDifference[imageAfter, imageBefore], "Grayscale"];
ImageQ[imageDifference]
imageDifference
```

Out[211]= True