homework II - first draft of final project

due 02/16/12, 09:30am, 300-020

Late homework can be dropped off in a box in front of Durand 217. Please mark clearly with date and time @drop off. We will take off 1/10 of points for each 24 hours late, every 12pm after due date. This homework will count 10% towards your final grade.

problem 1 - kinematics of growth

Despite tremendous improvements during the past 20 years, heart failure remains one of the most common, costly, disabling, and deadly medical conditions affecting more than 25 million people worldwide. Surgical strategies to reverse strain abnormalities in the ventricular wall are currently being recognized as a new paradigm for preventing the progression of heart failure. In an attempt to quantify cardiac changes in form and function, researchers in the lab of Prof. D. Craig Miller in the Department of Cardiothoracic Surgery at Stanford have developed a novel technique to measure infarct-induced changes of wall kinematics. Here you will analyze their data to characterize growth of the heart. Figure 1 shows four characteristic markers. The grey tetrahedron shows the marker positions $\boldsymbol{X}$ in the baseline state, i.e., before the infarct. The red tetrahedron shows the marker positions $\boldsymbol{x}$ in the grown state, i.e., seven weeks after the infarct.

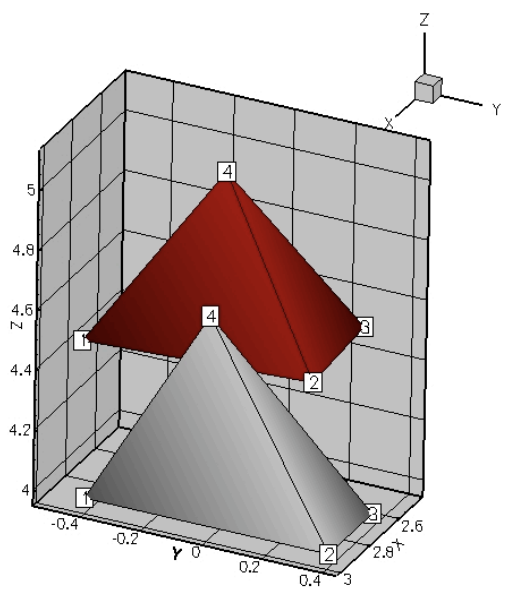


Fig. 1 Coordinates of ventricular beadset

$$\boldsymbol{X}_1 = [\ +2.80\ \ -0.27\ \ +3.75\ ]^t \qquad \boldsymbol{x}_1 = [\ +2.56\ \ -0.50\ \ +4.32\ ]^t$$
$$\boldsymbol{X}_2 = [\ +2.80\ \ +0.53\ \ +3.75\ ]^t \qquad \boldsymbol{x}_2 = [\ +2.57\ \ +0.39\ \ +4.31\ ]^t$$
$$\boldsymbol{X}_3 = [\ +2.50\ \ +0.52\ \ +3.75\ ]^t \qquad \boldsymbol{x}_3 = [\ +2.26\ \ +0.39\ \ +4.32\ ]^t$$
$$\boldsymbol{X}_4 = [\ +2.80\ \ +0.13\ \ +4.45\ ]^t \qquad \boldsymbol{x}_4 = [\ +2.60\ \ +0.07\ \ +4.85\ ]^t$$

The histologically measured fiber orientation angle for the displayed tetrahedron, measured against the horizontal axes, is $\alpha = 12.5^0$. The cardiac muscle fiber direction $\boldsymbol{N}^{\text{fib}}$ can then be expressed through the following unit vector.

$$\boldsymbol{N}^{\text{fib}} = [\,0.0\ \ -\cos(\alpha)\ \ +\sin(\alpha)\,]^t \qquad \text{with} \qquad \alpha = 12.5^0$$

The overall objective is this homework is to characterize the muscle fiber lengthening during growth. This is pretty straightforward if you solve the following substeps!

1.1 Determine three vectors $\mathrm{d}\boldsymbol{X}_i$ that span the tetrahedron at baseline. Take an arbitrary point of the tetrahedron as origin, e.g., $\boldsymbol{X}_4$, and calculate the three vectors $\mathrm{d}\boldsymbol{X}_1$, $\mathrm{d}\boldsymbol{X}_2$, and $\mathrm{d}\boldsymbol{X}_3$ from the origin to any other point using the coordinates $\boldsymbol{X}$ at baseline such that $\mathrm{d}\boldsymbol{X}_i = \boldsymbol{X}_i - \boldsymbol{X}_4$ for $i = 1, 2, 3$.

1.2 Determine the same three vectors $\mathrm{d}\boldsymbol{x}_i$ that span the tetrahedron after growth. Take the same point as origin, e.g., $\boldsymbol{x}_4$, and calculate the vectors $\mathrm{d}\boldsymbol{x}_1$, $\mathrm{d}\boldsymbol{x}_2$, and $\mathrm{d}\boldsymbol{x}_3$ from the origin to any other point using the coordinates $\boldsymbol{x}$ after growth such that $\mathrm{d}\boldsymbol{x}_i = \boldsymbol{x}_i - \boldsymbol{x}_4$ for $i = 1, 2, 3$.

1.3 Determine the growth tensor $\boldsymbol{F}^{\mathrm{g}}$ that maps the baseline line elements $\mathrm{d}\boldsymbol{X}_i$ onto the grown line elements $\mathrm{d}\boldsymbol{x}_i$. The growth tensor maps line elements according to $\mathrm{d}\boldsymbol{x}_i = \boldsymbol{F}^{\mathrm{g}} \cdot \mathrm{d}\boldsymbol{X}_i$. The application of this mapping to all three line elements $\mathrm{d}\boldsymbol{X}_i$ defines three vector valued equations, i.e., nine equations to solve for the nine components of $\boldsymbol{F}^{\mathrm{g}}$. To obtain a more compact notation, rearrange all baseline line elements from [1] and all grown line elements from [2] in 3×3 matrices, i.e., $\boldsymbol{C} := [\ \mathrm{d}\boldsymbol{X}_1;\ \mathrm{d}\boldsymbol{X}_2;\ \mathrm{d}\boldsymbol{X}_3\ ]$ and $\boldsymbol{c} := [\ \mathrm{d}\boldsymbol{x}_1;\ \mathrm{d}\boldsymbol{x}_2;\ \mathrm{d}\boldsymbol{x}_3\ ]$. Now, determine the growth tensor $\boldsymbol{F}^{\mathrm{g}}$ by using the equation $\boldsymbol{F}^{\mathrm{g}} \cdot \boldsymbol{C} = \boldsymbol{c}$, thus $\boldsymbol{F}^{\mathrm{g}} = \boldsymbol{c} \cdot \boldsymbol{C}^{-1}$.

1.4 Control your results by calculating $\mathrm{d}\boldsymbol{x}_i = \boldsymbol{F}^{\mathrm{g}} \cdot \mathrm{d}\boldsymbol{X}_i$. Do the calculated grown line elements $\mathrm{d}\boldsymbol{x}_i$ match the ones you had calculated in [2]?

1.5 Determine the grown fiber direction $\boldsymbol{n}^{\mathrm{fib}} = \boldsymbol{F}^{\mathrm{g}} \cdot \boldsymbol{N}^{\mathrm{fib}}$. The growth tensor can be used to map the measured baseline fiber direction $\boldsymbol{N}^{\mathrm{fib}}$ onto the grown fiber direction $\boldsymbol{n}^{\mathrm{fib}}$. Determine $\boldsymbol{n}^{\mathrm{fib}}$ and comment on how $\boldsymbol{N}^{\mathrm{fib}}$ and $\boldsymbol{n}^{\mathrm{fib}}$ deviate.

1.6 Determine the fiber stretch upon growth $\lambda^{\mathrm{g}} = \sqrt{\boldsymbol{n}^{\mathrm{fib}} \cdot \boldsymbol{n}^{\mathrm{fib}}}$. Since the fiber orientation $\boldsymbol{N}^{\mathrm{fib}}$ was given as a unit vector, the length of the grown vector $\boldsymbol{n}^{\mathrm{fib}} = \boldsymbol{F}^{\mathrm{g}} \cdot \boldsymbol{N}^{\mathrm{fib}}$ corresponds to the relative change in fiber length, i.e., the amount of growth along the fiber direction, $\lambda^{\mathrm{g}} = \sqrt{\boldsymbol{n}^{\mathrm{fib}} \cdot \boldsymbol{n}^{\mathrm{fib}}} = \sqrt{\boldsymbol{N}^{\mathrm{fib}} \cdot \boldsymbol{F}^{\mathrm{g}\,\mathrm{t}} \cdot \boldsymbol{F}^{\mathrm{g}} \cdot \boldsymbol{N}^{\mathrm{fib}}}$.

1.7 Determine the Green Lagrange growth strain $\boldsymbol{E}^{\mathrm{g}} = \frac{1}{2}\left[\, \boldsymbol{F}^{\mathrm{g}\,\mathrm{t}} \cdot \boldsymbol{F}^{\mathrm{g}} - \boldsymbol{I} \,\right]$. $\boldsymbol{E}^{\mathrm{g}}$ is called the Green Lagrange strain tensor and it is used to characterize growth strains with respect to the reference configuration in a finite strain setting.

1.8 Determine the displacement gradient tensor $\boldsymbol{H}^{\mathrm{g}} = \boldsymbol{F}^{\mathrm{g}} - \boldsymbol{I}$. $\boldsymbol{H}^{\mathrm{g}} = \nabla \boldsymbol{u}$ is the non-symmetric displacement gradient tensor which can also be expressed as $\boldsymbol{H}^{\mathrm{g}} = \partial \boldsymbol{u} \,/\, \partial \boldsymbol{X} = \partial[\boldsymbol{x} - \boldsymbol{X}] \,/\, \partial \boldsymbol{X} = \boldsymbol{F}^{\mathrm{g}} - \boldsymbol{I}$.

1.9 Determine the small strain tensor $\boldsymbol{\epsilon}^{\mathrm{g}} = \frac{1}{2}\left(\boldsymbol{H}^{\mathrm{g}} + \boldsymbol{H}^{\mathrm{g}\,\mathrm{t}}\right)$. Compare the small strain approximation $\boldsymbol{\epsilon}$ with the large strain Green Lagrange tensor $\boldsymbol{E}^{\mathrm{g}}$ and comment on your results.

1.10 Determine the normal strain $\epsilon_n^g = \boldsymbol{N}^{\text{fib}} \cdot \boldsymbol{\epsilon}^g \cdot \boldsymbol{N}^{\text{fib}}$. Compare the small strain approximation of the normal strain ϵ_n with the large strain fiber stretch λ^g.

1.11 Determine the volume change $J^g = \det(F^g)$ and compare it with the small strain volume dilation $e^g = \text{tr}(\boldsymbol{\epsilon}^g)$. What does this imply in terms of tissue growth?

You can use MATLAB to solve the matrix and vector operations. If you choose to do so, you must deliver a printout of your MATLAB code with the homework. You can find additional details in the lecture notes from the fourth class.

problem 2 - shaping your research project

To structure your thoughts for your final project, read the attached paper by George M. Whitesides *"Writing a Paper"* as a guideline.

2.1 Sketch a *bulleted outline* for your project. This does not need to be your final layout, it is just meant to organize your ideas. Identify the sections and subsections of your paper.

2.2.a If you plan to write a scientific paper, identify a key *hypothesis*. The purpose of the hypothesis is to provide focus throughout the manuscript. A good hypothesis is objectively testable, non-trivial, and specific. For example, you could hypothesize that cardiac growth in athletes is reversible and vanishes gradually upon detraining. If you plan a finite element analysis, a reasonable hypothesis might involve regional variations in density or volume growth in relation to strain, stress, shape or something similar.

2.2.b If you plan to write a review paper, it might be more difficult to *keep focus*. In one sentence, specify precisely which aspects of growth you want to review. Remember the characteristics of your last homework, i.e., type of tissue, type of growth, scale you look at, mechanical driving force, disease specific or training, etc.

2.3 Identify *three key references* for your work and at least *three additional references* that you consider relevant. If you work in a group identify *five key references* for your work and at least *five additional references*. Create a bibliography and submit it with this homework.

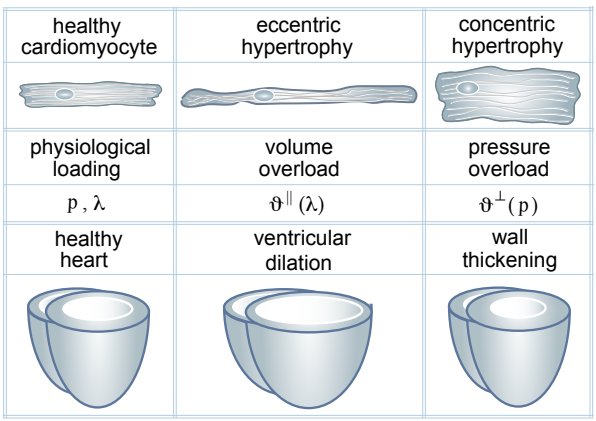
2.4 Identify a catchy *opening sentence*. This sentence is meant to catch the attention of the reader. If you plan on writing something disease related, this sentence should reflect the medical importance of your work. For example, this sentence can state the number of people affected, the health care cost involved, or the predicted growth of this disease. Provide a citation to back up your statement.

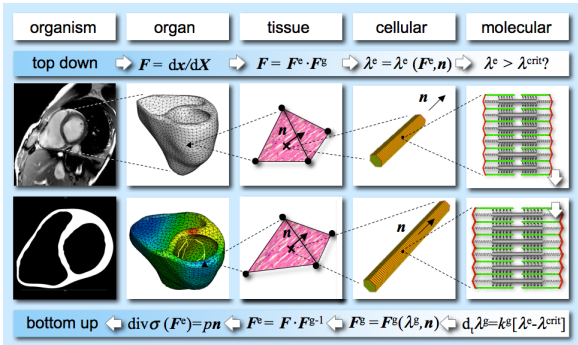
2.5 Summarize the *current knowledge* citing the literature you have listed in your bibliography file. This section will later be part of your Introduction section.

2.5.a If you plan to write a scientific paper, consider breaking the current knowledge section into two paragraphs, one on the biological nature and one mechanical modeling.

2.5.b If you plan to write a review paper, consider breaking the current knowledge section into two or three paragraphs for the individual aspects you plan to review and compare.

2.6 Create a schematic drawing that summarizes your project. The figures below show two samples of schematic drawings. If you like, you can draft this drawing by hand first. Ultimately, this figure will go into the introduction of your paper, to give the reader a quick overview about your work.





Schematic of data transfer between organism, organ, tissue, cellular, and molecular levels. We test the hypothesis that the overstretch-induced serial addition of sarcomeres on the molecular level translates into cardiac dilation on the organ level.

Although these sub-problems seem to require just a few words, put some effort into structuring your work - this will definitely pay off in the end.

Whitesides' Group: Writing a Paper**

By *George M. Whitesides**

1. What is a Scientific Paper?

A paper is an organized description of hypotheses, data and conclusions, intended to instruct the reader. Papers are a central part of research. If your research does not generate papers, it might just as well not have been done. "Interesting and unpublished" is equivalent to "non-existent".

Realize that your objective in research is to formulate and test hypotheses, to draw conclusions from these tests, and to teach these conclusions to others. Your objective is not to "collect data".

A paper is not just an archival device for storing a completed research program; it is also a structure for *planning* your research in progress. If you clearly understand the purpose and form of a paper, it can be immensely useful to you in *organizing* and conducting your research. A good outline for the paper is also a good plan for the research program. You should write and rewrite these plans/outlines throughout the course of the research. At the beginning, you will have mostly plan; at the end, mostly outline. The continuous effort to understand, analyze, summarize, and reformulate hypotheses on paper will be immensely more efficient for you than a process in which you collect data and only start to organize them when their collection is "complete".

2. Outlines

2.1. The Reason for Outlines

I emphasize the central place of an outline in writing papers, preparing seminars, and planning research. I especially believe that for you, and for me, it is most *efficient* to write papers from outlines. An *outline* is a written plan of the organization of a paper, *including* the data on which it rests. You should, in fact, think of an outline as a carefully organized and presented set of data, with attendant objectives, hypotheses, and conclusions, rather than an outline of text.

An outline itself contains little text. If you and I can agree on the details of the outline (that is, on the data and organization), the supporting text can be assembled fairly easily. If we do *not* agree on the outline, any text is useless. Much of the *time* in writing a paper goes into the text; most of the *thought* goes into the organization of the data and into the analysis. It can be relatively efficient in time to go through several (even many) cycles of an outline before beginning to write text; writing many versions of the full text of a paper is slow.

All writing that I do—papers, reports, proposals (and, of course, slides for seminars)—I do from outlines. I urge you to learn how to use them as well.

2.2. How Should You Construct an Outline?

The classical approach is to start with a blank piece of paper, and write down, in any order, all important ideas that occur to you concerning the paper. Ask yourself the obvious questions: "Why did I do this work?"; "What does it mean?"; "What hypotheses did I mean to test?"; "What ones did I actually test?"; "What were the results? Did the work yield a new method of compound? What?"; "What measurements did I make?"; "What compounds? How were they characterized?". Sketch possible equations, figures, and schemes. It is essential to try to get the major ideas. If you start the research to test one hypothesis, and decide, when you see what you have, that the data really seem to test some other hypothesis better, don't worry. Write them both down, and pick the best combinations of hypotheses, objectives, and data. Often the objectives of a paper when it is finished are different from those used to justify starting the work. Much of good science is opportunistic and revisionist.

When you have written down what you can, start with another piece of paper and try to organize the jumble of the first one. Sort all of your ideas into three major heaps (1–3).

1. Introduction

Why did I do the work? What were the central motivations and hypotheses?

2. Results and Discussion

What were the results? How were compounds made and characterized? What was measured?

3. Conclusions

What does it all mean? What hypotheses were proved or disproved? What did I learn? Why does it make a difference?

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[**] The text is based on a handout created on October 4, 1989.

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Next, take each of these sections, and organize it on yet finer scale. Concentrate on organizing the *data*. Construct figures, tables, and schemes to present the data as clearly and compactly as possible. This process can be slow—I may sketch a figure five to ten times in different ways trying to decide how it is most clear (and looks best aesthetically).

Finally, put everything—outline of sections, tables, sketches of figures, equations—in good order.

When you are satisfied that you have included *all* the data (or that you know what additional data you intend to collect), and have a plausible organization, give the outline to me. Simply indicate where missing data will go, how you think (hypothesize) they will look, and how you will interpret them if your hypothesis is correct. I will take this outline, add my opinions, suggest changes, and return it to you. It usually takes four to five iterations (often with additional experiments) to agree on an outline. When we *have* agreed, the data are usually in (or close to) final form (that is, the tables, figures, etc., in the outline will be the tables, figures,... in the paper).

You can then start writing, with some assurance that much of your prose will be used.

The key to efficient use of your and my time is that we start exchanging outlines and proposals as early in a project as possible. *Do not, under any circumstances, wait until the collection of data is "complete" before starting to write an outline.* No project is ever complete, and it saves enormous effort and much time to propose a plausible paper and outline as soon as you see the basic structure of a project. Even if we decide to do significant additional work before seriously organizing a paper, the effort of writing an outline will have helped to guide the research.

2.3. The Outline

What an outline should contain:

1. Title

2. Authors

3. Abstract

Do *not* write an abstract. That can be done when the paper is complete.

4. Introduction

The first paragraph or two should be written out completely. Pay particular attention to the opening sentence. Ideally, it should state concisely the objective of the work, and indicate why this objective is important.

In general, the Introduction should have these elements:

- The *objectives* of the work.
- The *justification* for these objectives: Why is the work important?
- *Background*: Who else has done what? How? What have *we* done previously?
- *Guidance to the reader*: What should the reader watch for in the paper? What are the interesting high points? What strategy did we use?
- *Summary/conclusion*: What should the reader expect as conclusion? In advanced versions of the outline, you should also include all the sections that will go in the Experimental section (at the level of paragraph subheadings) and indicate what information will go in the Microfilm section.

5. Results and Discussion

The results and discussion are usually combined. This section should be organized according to major topics. The separate parts should have subheadings in boldface to make this organization clear, and to help the reader scan through the final text to find the parts of interest. The following list includes examples of phrases that might plausibly serve as section headings:

- Synthesis of Alkane Thiols
- Characterization of Monolayers
- Absolute Configuration of the Vicinal Diol Unit
- Hysteresis Correlates with Roughness of the Surface
- Dependence of the Rate Constant on Temperature
- The Rate of Self-Exchange Decreases with the Polarity of the Solvent

Try to make these section headings as specific and information-rich as possible. For example, the phrase "The Rate of Self-Exchange Decreases with The Polarity of The Solvent" is obviously longer than "Measurement of Rates", but much more useful to the reader. In general, try to cover the major common points:

- Synthesis of starting materials
- Characterization of products
- Methods of characterization
- Methods of measurement
- Results (rate constants, contact angles, whatever)

In the outline, do not write any significant amount of text, but get all the data in their proper place: Any text should simply indicate what will go in that section.

- Section Headings
- Figures (*with* captions)
- Schemes (with captions and footnotes)
- Equations
- Tables (correctly formatted)

Remember to think of a paper as a collection of experimental results, summarized as clearly and economically as possible in figures, tables, equations, and schemes. The text in the paper serves just to explain the data, and is secondary. The more information can be compressed into tables, equations, etc., the shorter and more readable the paper will be.

6. Conclusions

In the outline, summarize the conclusions of the paper as a list of short phrases or sentences. Do not repeat what is in the Results section, unless special emphasis is needed. The Conclusions section should be just that, and not a summary. It should add a new, higher level of analysis, and should indicate explicitly the significance of the work.

7. Experimental

Include, in the correct order to correspond to the order in the Results section, all of the paragraph subheadings of the Experimental section.

2.4. In Summary

- Start writing possible outlines for papers *early* in a project. Do not wait until the "end". The end may never come.
- Organize the outline and the paper around easily assimilated data—tables, equations, figures, schemes—rather than around text.
- Organize in order of importance, not in chronological order. An important detail in writing papers concerns the weight to be given to topics. Neophytes often organize a paper in terms of chronology: that is, they give a recitation of their experimental program, starting with their cherished initial failures and leading up to a climactic successful finale. *This approach is completely wrong*. *Start with the most important results*, and put the secondary results later, if at all. The reader usually does not care how you arrived at your big results, only what they are. Shorter papers are easier to read than longer ones.

3. Some Points of Style

- Do not use nouns as adjectives:

Not:
ATP formation; reaction product
But:
formation of ATP; product of the reaction

- The word "this" must always be followed by a noun, so that its reference is explicit.

Not:
This is a fast reaction; This leads us to conclude
But:
This reaction is fast; This observation leads us to conclude

- Describe experimental results uniformly in the past tense.

Not:
Addition of water *gives* product.
But:
Addition of water *gave* product.

- Use the active voice whenever possible.

Not:
It was observed that the solution turned red.
But:
The solution turned red. *or*
We observed that the solution turned red.

- Complete all comparisons.

Not:
The yield was higher using bromine.
But:
The yield was higher using bromine than chlorine.

- Type all papers double-spaced (not single- or one-and-a-half-spaced), and leave two spaces after colons, and after periods at the end of sentences. Leave generous margins.

Assume that we will write all papers using the style of the American Chemical Society. You can get a good idea of this style from three sources:

- *The journals*. Simply look at articles in the journals and copy the organization you see there.
- *Previous papers from the group*. By looking at previous papers, you can see exactly how a paper should "look". If what you wrote looks different, it probably is not what we want.
- *The ACS Handbook for Authors*. Useful, detailed, especially the section on references, pp. 173–229.

I also suggest you read Strunk and White, *The Elements of Style* (Macmillan: New York, 1979, 3rd ed.) to get a sense for usage. A number of other books on scientific writing are in the group library; these books all contain useful advice, but are not lively reading. There are also several excellent books on the design of graphs and figures.