Title: Models to Predict Protein Biomaterial Performance (IMuBEAM WG)

Summary of the project:

This project aims at advancing in thee ability to predict biomaterial performance by the combined use of suitable experimental models to cover polymer features (chemistry, molecular weight), processing (e.g., fibers, films, sponges, hierarchical structure) and modeling at different length scales of materials structural hierarchy (from nano- to macroscopic), which has broad implications for many types of biomaterials for biomedical applications.
For more information about the workgroup see the link below:
https://www.imagwiki.nibib.nih.gov/content/integrated-multiscale-biomaterials-experiment-and-modeling-group-imubeam

Model Credibility Plan and Reusability updates

1. Sharing methods: papers

In an attempt to share and show the work we develop in the project, we have published several papers this year, with a focus on methodology and protocol papers to describe in detail the process of design, construction and computational analysis of silk proteins in the paper ("Silkworm silk-based materials and devices generated using bio-nanotechnology", published in Chemical Society Reviews, and the previously published "Predicting Silk Fiber Mechanical Properties through Multiscale Simulation and Protein Design", published in ACS biomaterials science & engineering), the methodology of biomaterial modeling ("Materials-by-design: computation, synthesis, and characterization from atoms to structures", published in Physica Scripta, and "Multiscale modeling of keratin, collagen, elastin and related human diseases: Perspectives from atomistic to coarse-grained molecular dynamics simulations", published in Extreme Mechanics Letters).

2. Reproducibility methods: sharing methods and codes

During this time we have been working on updating our IMAG consortium webpage https://www.imagwiki.nibib.nih.gov/content/integrated-multiscale-biomaterials-experiment-and-modeling-group-imubeam) to incorporate all the information relevant for the coding and methods for the project, as well as the minutes and slides from the monthly meetings where we discussed progress on each subproject. As an additional initiative, we aimed to create a website (http://lamm.mit.edu/silk-integrative-theory-experiment-project-sitep), to post new tutorials for modeling and sharing scripts, but we had to move to a new extension in order to make more user friendly.
Data management has been an issue as each group/person had their own storage depository. In order to overcome this problem and have a more accessible data, we plan as part of the daily work, to implement a new depository for the raw data generated for the project where all students, and postdocs will upload their data.
Finally, in an attempt to get a better idea on the people using the methodology described in our papers, we plan on make a search on the literature where our papers are cited.

3. Sharing methods: videos

Apart from the previous videos that we produce and share (a video showing the workflow with key points on the construction and computational analysis of silk biomaterials and a video showing the potential of using the hydrothermal liquid process to generate carbon materials to use as asphalts from different biomass sources) we just produced and submitted a video for the IMAG competition summarizing our

project, that will be posted and accessible both in Youtube and on our wikipage, and that can be found in the following link: https://vimeo.com/285941736 .

4. Reproducibility and reusability: sharing methods and codes

Sharing the model and reproducibility is an important consideration in our collaborative project and we are expanding our open collaborations with which we share all the methods generated in the project as well as scripts and codes. Some open collaborations where methodology and models were share are the groups of Dr. Jingjie Yeo (Institute Of High Performance Computing, Singapore), Prof. Tony Weiss (University of Sydney, Australia), Prof. Grace Gu (University of California-Berkeley, USA), Prof. Anna Tarakanova (University of Connecticut, USA), Prof. Wenwen Huang (Zhejiang University), Prof. Shengjie Ling (ShanghaiTech University, China), Prof. Flavia Libonati (University of Milano, Italy), Prof. Leila Deravi (Northeastern University, USA), Prof. Joyce Wong (Boston University, USA) or Prof. Guy Genin (Washington University in St Louis, USA).

5. Reproducibility and reusability: outreach

We started to expand our initial plans on symposium organization where computational science and model credibility and reusability outreach would be a key part of the agenda. We plan on applying to organize a symposium during the next American Chemistry Society National Meeting & Expo, which we consider as the most suitable platform for it. The symposium will be divided in 3 sessions, including a session on model credibility and model reusability. It will include an overview of methods, examples of outreach videos, summary of papers, as well as collaboration with colleagues, web sites and tutorials. This session will explore best practices, challenges and a vision forward for the community to broaden the reach of models and data for broad sharing across fields and labs.

Year	Aim	Task	Lab
1	Reproducibility	Update the IMAG consortium webpage to incorporate the minutes and slides of our monthly reports available, as well as to make accessible any relevant information about scripts and methods.	Buehler, Kaplan
	Reusability	Intensify interactions with IMAG-MSM Integrated multiscale biomaterials experiment and modeling WG. This includes dissemination of tools, data, software, training and related needs to organize per the broader community.	Buehler, Kaplan
	Outreach	Discussions to create and organize a symposium and seminars with a focus on the integration of multiscale modeling with experiment. A session of these events will focus on model credibility.	Buehler, Kaplan
	Outreach	Create a tutorial video that showcases the workflow of the project for a broad audience.	Buehler, Kaplan
	Data management	Use experimental outcomes to model protein variants for structure and mechanics	Buehler, Kaplan
2	Reproducibility	Create and update a new project webpage where we will post new tutorials for modeling, share scripts and provide regular updates on the work carried out in the frame of our collaborative project, both for scientists and layman audience.	Buehler, Kaplan
	Reusability	Expand interactions with non IMAG-MSM labs to intensify collaborations. Include dissemination of tools, data, software, training.	Buehler, Kaplan
	Reusability	Start exploring the impact of the work developed by the group by analyzing the citations in the literature of our papers.	Buehler, Kaplan
	Outreach	Organize a seminar for American Chemistry Society National Meeting & Expo where a session on model credibility will be held.	Buehler, Kaplan
	Data management	Create a common repository for the raw data generated for the project.	Buehler, Kaplan

3, 4	Reproducibility	Continue web site collection of tools, tutorials, trainings and software, as well as posting new information about the project in the blog.	Buehler, Kaplan
	Reusability	Continue integrating plans with IMAG-MSM Working Group	Buehler, Kaplan
	Reusability	Finish exploring the impact of the work developed by the group by analyzing the citations in the literature of our papers.	Buehler, Kaplan
	Outreach	Continue creating videos related to the work developed in our labs and dissemination through seminars focused on the integration of multiscale modeling with experiment.	Buehler, Kaplan
	Data management	Continue collecting data from the project and create guides on how to manage the data stored.	Buehler, Kaplan