1. Overview

A note about terminology: The term model is used in many fields that intersect with the proposal to follow, so a brief clarification of terms is necessary. Statistics uses the term model to describe the results of a regression analysis. Climate change researchers use the term model to describe a computational model and physical processes to determine how a system evolves over time. Thus, using the term model can be a source of confusion. To help in clarifying, I will employ the following conventions in this discussion: interpolation or regression model will be used to describe a statistical model that describes a single or multivariable model derived from observations; simulation or computational model will be used to describe the results of a climate or ice sheet model.

The purpose of this proposal is to map out the proposed tools to be developed as part of a dissertation in Computational and Data-Enabled Science and Engineering applied to SERAC ice sheet data. These four computational tools to be developed will form the basis for research on interpolation of time series of observation data of dynamic change in height of the ice sheet, generating spatial-temporal interpolations of large numbers of these time series, and comparing simulation data to those observations.

Methods developed with these proposed tools will help us better understand the changes that have occurred in the Greenland Ice Sheet over the past three decades for which airborne and satellite data is available. The development of tools to assist in the analysis will permit others to apply similar methods to observational data gathered for other parts of the cryosphere. In addition to comparing methods of working with irregular time series, the spatial and temporal distribution of change will be studied. Data visualization will be a key component of the analysis. Statistical models of the observations can then be compared model simulations to assist with validation of models and potentially for model initialization. Both of these applications contribute to better model simulations and thus more accurate predictions of future climate change. This work will focus specifically on dynamic change in the ice sheet.

2. Background

Human activities have been adding greenhouse gases to the atmosphere, primarily carbon dioxide, since at least 1750, at ever increasing rates. The impact of these gases has caused observed increases in global mean temperatures (IPCC, 2021). The graph in Figure 1, taken from IPCC AR6 (2022), shows the observed changes in global mean temperature and projection for the next century based on several model scenarios. The impact of these changes on the climate and the environment are only beginning to be understood; but, understanding the changes that have already occurred are essential to understanding the changes that will continue to occur until we are able to reduce emissions and restabilize the climate. Begin with discussing

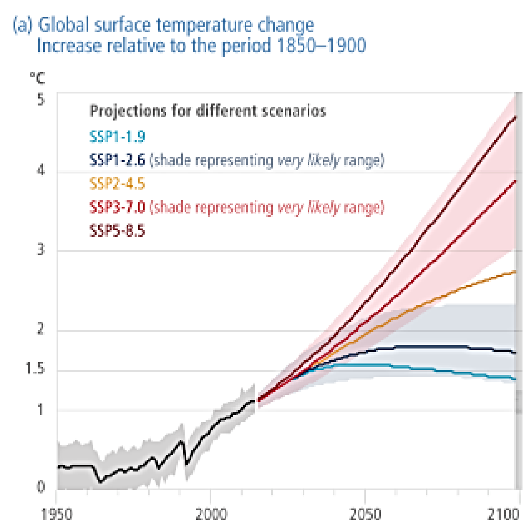

Figure 1. Adapted from IPCC AR6. (IPCC, 2022)Projected global mean temperature under various scenarios.

climate change broadly. The temperature changes to the climate are not equally distributed, and the poles are seeing more increases in temperature than areas closer to the equator. These changes have been driving a dramatic retreat of glacier ice since at least the 1990s (IPCC, 2021). Since that time, increased efforts to make detailed observations of glacial retreat, especially in the Arctic and Antarctic have been undertaken (Kimball et al., 2021; Su et al., 2015). Since Greenland and Antarctica have the largest stores of freshwater, their melting will have the largest impacts on seal-level rise in the long term (Chang et al., 2014; Studies, 2010). Understanding the impacts we have already had will be necessarily to accurately predict future changes that may be necessary to mitigate against (Bradley et al., 2018; Marzeion et al., 2012).

Ice sheet models have been developed to help model the flow of ice in the ice sheet, and how a changing climate can impact its behavior. Ice sheet models (ISMs) may be coupled with full or partial climate models to account for the feedbacks between ocean and ice sheet, and atmosphere and ice sheet (Fürst et al., 2015; Goelzer et al., 2017). Observations of the ice sheet collected over the last three decades aid in modeling the dynamics of the ice sheet through validating or initializing the models (Goelzer et al., 2018; Price et al., 2017).

Dramatic temperature changes near the poles are driving ice loss. Figure 2 shows the loss of ice mass in Greenland derived from ICESat data (Bolch et al., 2013). Loss of the entire Greenland Ice Sheet could account for as much as 20 feet (around 50 meters) of sea-level rise (Alley et al., 2005). Ice loss is currently accelerating (Kjeldsen et al., 2015; Rignot et al., 2011).

While some observational data collection has taken place at various glaciers for many

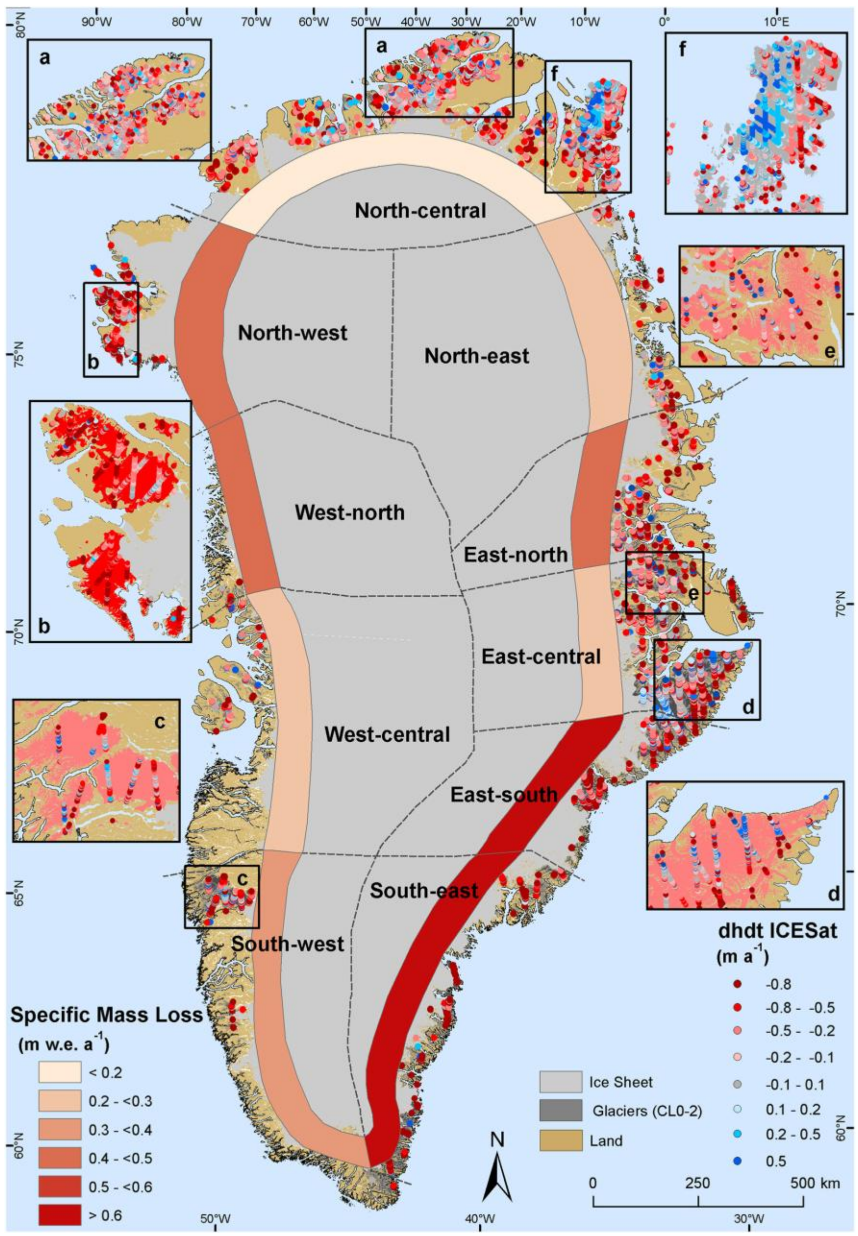

Figure 2. Mean mass changes for the 10 sectors and elevation changes for the GIC derived from ICESat points. Adapted from (Bolch et al., 2013).

decades, more intense observational programs of more of the ice sheet has taken place since the 1990s. Both airborne and satellite observational regimes have occurred including the relatively recent ICESat and ICESat2 missions using laser altimetry, as well as GRACE gravimetry (Brenner et al., 2007; Csatho et al., 2014; Simonsen et al., 2021). This data provides frequent (seasonal) and accurate measurements that can contribute to the understanding of ice loss as it occurs. ICESat2 will provide the most detailed measurements of the ice sheet (Markus et al., 2017).

Once observations are obtained and processed, they must be further modeled using regression or spatial modeling methods to interpolate the results. Because multiple sensor missions are combined to produce data over longer periods of time than a single mission, the time series generated at any local position are irregular. Irregular time series have limitations on how they can be modeled, and a variety of different techniques have been developed (Collenteur, 2021; Salcedoa et al., 2012; Zhou et al., 2022). Regression techniques are among those employed, including spline-based and polynomial models (Shekhar et al., 2020). Gaussian process models are becoming more common (Gramacy, 2020). However, modeling a time series of observations at a single location does not fully generalize to the entire ice sheet. What is needed is a spatiotemporal model to combine the time series spread over the ice sheet into a simple model for a region (Li et al., 2014; MACEACHREN et al., 2010; Wang et al., 2018). Visualization of the resulting model is crucial.

To better share data with the geology and glaciology community, Ghub was formed as an online space to share results, research, data and code. Built on the University at Buffalo's computing resources, Ghub uses Jupyter notebooks running Python or R that can run on UB's computing cluster. Data from observations and ice sheet models are available from the site (Sperhac et al., 2020).

3. Data

The data for this analysis comes from NASA's laser altimetry data for the Greenland Ice Sheet (GrIS). The data is derived from multiple sensors and missions including NASA's Airborne Topographic Mapper (ATM) starting in 1993 through Operation Ice Bridge (OIB) and the Ice, Cloud and Elevation Satellite (ICESat). These missions produced more than 150,000 irregular time series distributed across Greenland. The processing of this data was described in Csatho, et al., 2014(Csatho et al., 2014). The data set has been extended from 2012 at the time of that paper to include data up to 2017. The altimetry data was processed using the Surface Elevation Reconstruction and Change Detection (SERAC) method to collect the measurements into patches of 1 km^2. Observations that fell the same region at the same time period were fit to analytic functions to produce a single observation in the time series. This process is described in detail in Csatho, et al., 2014, and provides for rigorous error estimation for each

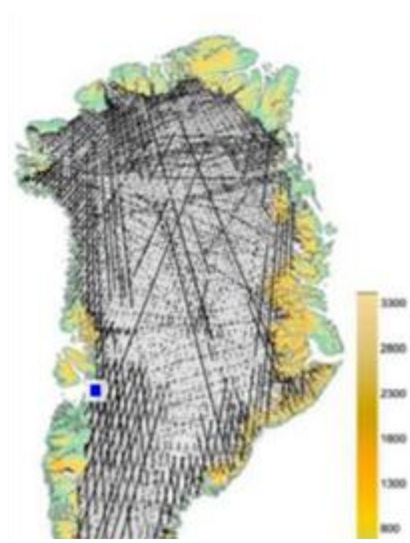

Figure 3. Locations of time series in the SERAC dataset (in black) as of 2014. (Csatho, et al., 2014.)

measurement in the series.(Csatho et al., 2014) The image in Figure 3 is adopted from Csatho, et al., 2014 to show the locations of the final time series.

Seasonal changes have been extracted and we will be analyzing the dynamic interannual changes, Δh. Positive change represents an increase over the reference height for the patch, while a negative change represents a decrease from the reference height. While regression methods do allow us to account for other variables in our models, we will be modeling the dynamic change only based on the time input.

Some of the time series, particularly from the interior of Greenland, are quite short and contain fewer than ten datapoints in the processed dataset. However, time series from locations near the coast may have observations from multiple missions stretching over twenty years and contain as many fifty datapoints.

4. Tools to be developed and Timeline

4.1. Interpolation Tool

The first tool will consist of a set of Jupyter Notebooks to be posted on Ghub using primarily R code. Python will be used within R as necessary. The fundamental purpose of this tool is to permit exploration and comparison of regression models for time series data. The tool is developed using the SERAC time series; however, it is intended that the tool can also serve a more general purpose.

The tool will be presented as a set of related Notebooks linked together in the following structure.

I. Data Exploration
II. Model Construction
  A. Polynomial Model
    i. Outlier & Influential Point Detection
    ii. Hyperparameter Setting
  B. Loess Model
    i. Outlier & Influential Point Detection
    ii. Hyperparameter Setting
  C. ALPS
  D. Gaussian Process Model
    i. Outlier & Influential Point Detection
    ii. Hyperparameter Setting
III. Model Comparison
  A. Two Model Comparison
  B. Three Model Comparison
  C. Four Model Comparison

Data Exploration: Any good data analysis process should begin with data exploration and visualization. The first Jupyter Notebook will include a set of functions to aid in visualizing the time series, decomposing any seasonal component of the time series, examining rates of change of the time series, and perhaps other methods. This notebook is intended to be the most general tool and considers the needs of users who may not only be analyzing previous cleaned data.

Model Construction: Three of the four regression models (polynomial(James et al., 2021), Loess(Cleveland & Devlin, 1988), and Gaussian process(Santner et al., 2003)) will be handled with their own set of Notebooks. (ALPS has all of these functions in its own approximation tool already on Ghub (Shekhar et al., 2020), so I won't be reproducing that here.) The main page for each of the regression models with provide for importing the data set from a file and creating the model. Parameters are set, to the extent possible, as variables outside the main code chunks to make changing values as easy as possible. The notebook will include a selection of graphing options, code to save the regression model output and confidence intervals as files and saving the visualizations with file names that connect back to the model type and the time series ID code. Each interpolation model type will have their own model construction page. An example of one of the plots for one of the model types is shown in Figure 4.

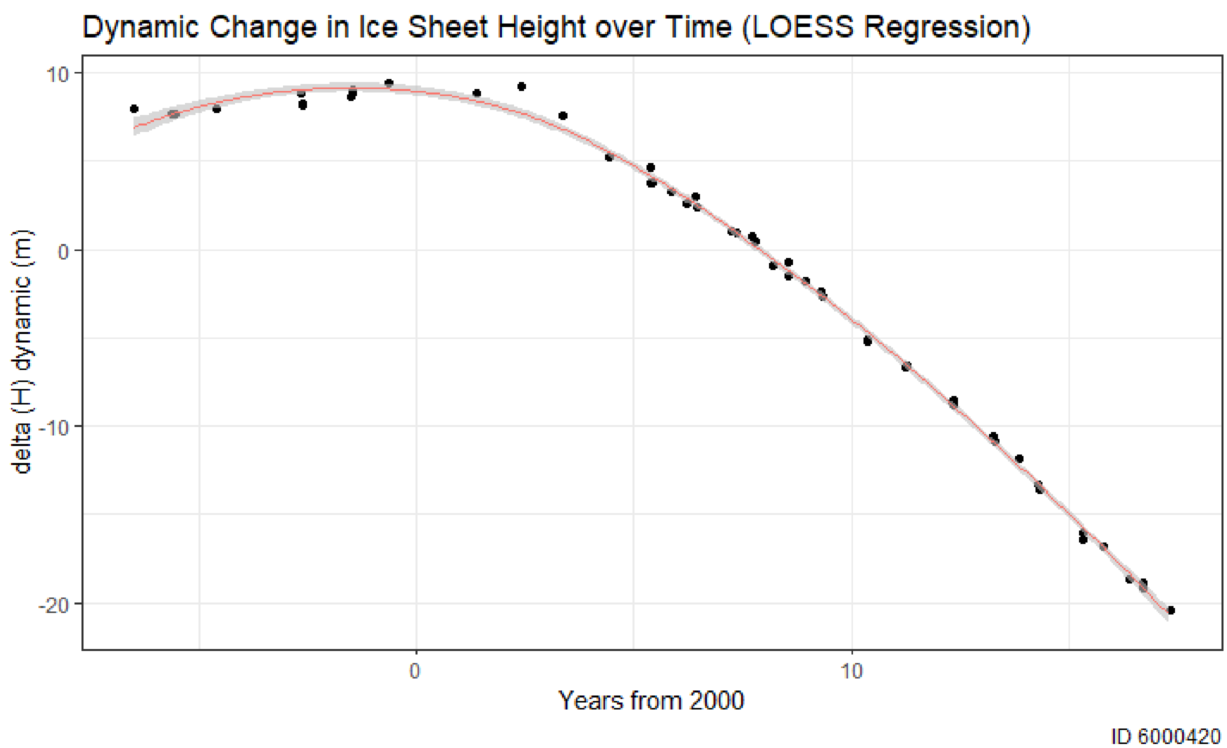

Figure 4. An example of the Loess Regression plot notebook.

Separate from but related to each of the three regression models, will be associated with it a notebook page for selecting one or more hyperparameters. For the polynomial model, the parameter selection is for the degree of the polynomial; for the Loess model, the parameter selection is for the span; for the Gaussian process model the parameter selection will be (at least) for the correlation length. Functions to aid in this selection will include cross validation and elbow plots of various measurements to assess the best setting for the given time series. Functions selected for inclusion will depend on the specific model, at least in part. Table 1 shows an example output for a cross validation analysis of model fit for polynomial degree selection.

Degree	1	2	3	4	5
MSE	13.2059100	0.6130251	0.3504036	0.2410928	0.4872951

Table 1. The results of cross validation on fitting the best polynomial degree for a time series. The minimum mean square error (MSE) suggests a fourth-degree polynomial may be the best fit for this specific time series without overfitting.

In addition to the hyperparameter selection functions, outlier and influential point functions will be included in a separate page. Each of the polynomial, Loess, and Gaussian process models will have a similar set of analyses available, but which points are potentially considered outliers or influential points will depend on the model (as error estimation differs between models). Visualization of the impact of point removal will be included. It is possible that classification of the time series could be incorporated as part of the hyperparameter selection tool for each type of regression model (for instance, controlling degree selection for polynomials, span selection for Loess and correlation length for Gaussian process regression).

The ALPS model will not include these the hyperparameter selection or outlier detection methods because they already exist in the ALPS approximation tool (Shekhar et al., 2020). The model construction notebook intended here will call to the ALPS code in Python from within R primarily for the sake of consistent visualization of all the model types. There is no need to recreate functionality that already exists in the ALPS tool.

Model Comparison: The final three notebooks of this tool will allow for comparing two, three or four models with each other for the same time series, plotted on the same graph. The four-model case has the simplest code. All four models will be run on the same data set and plotted on the same graph options. As with the individual model notebooks, the interpolation results can be combined into a single dataframe and saved to a common file. The two-model and three-model comparison tools will function similarly, but users can select which of two or three of the interpolation models will be graphed and saved. An example of the output graphs is shown in Figure 5.

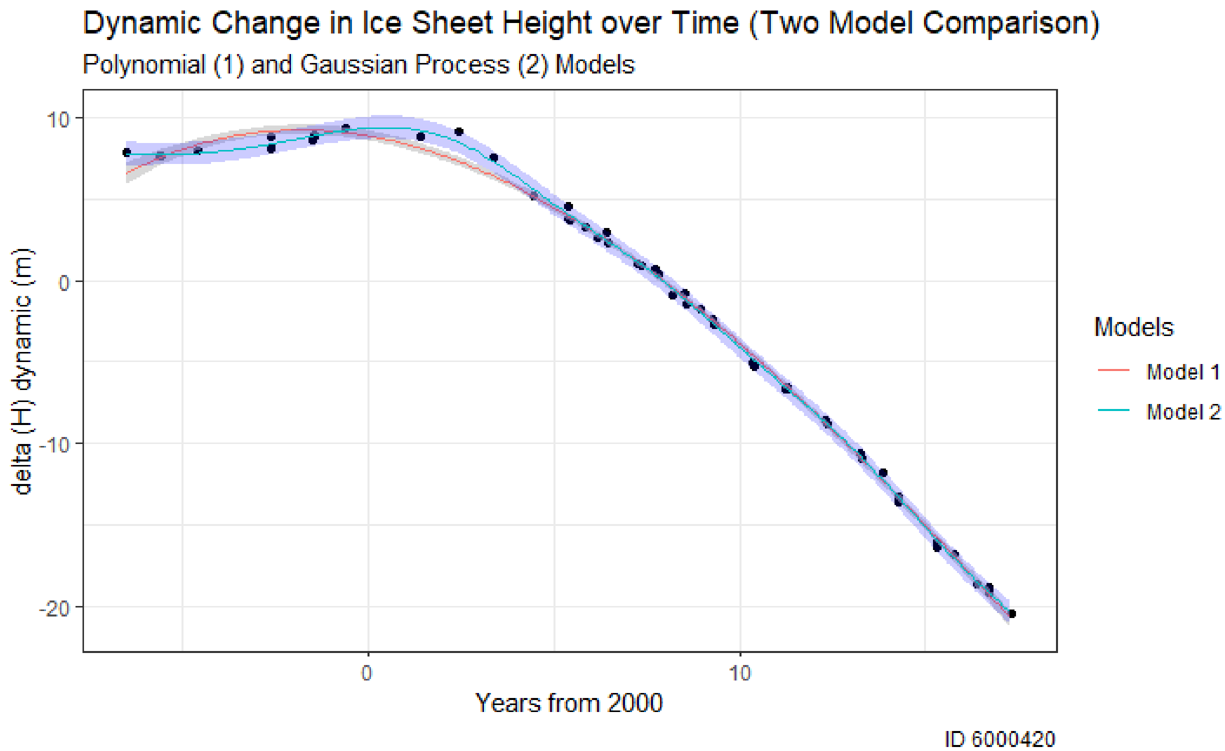

Figure 5. A comparison of the polynomial model fit (degree 3) against the Gaussian Process Regression fit.

At present, this tool has seen significant development already. The individual model and model comparison pages are very far along. The main issue to be resolved here in calling the Python code for ALPS from within R. The outlier detection functions need to be cleaned up for each of the regression models. The hyperparameter selection functions and data exploration codes are in progress.

The language R was chosen here as the coding language, rather than primarily using Python, in order to use the package RobustGaSP (Gu et al., 2019). The interpolations developed here will be the basis for the spatial modeling to follow. The ggplot2 package will be used for data visualization (Wickham et al.).

Significant work was done on these tools during the fall semester 2021 and will form much of the analytical basis for a journal paper that is also in progress. My current estimate for completion of the entire tool and the related paper is approximately the end of spring semester 2022.

4.2 Batch Processing Tool

The second tool is a batch processing tool. The primary purpose of the batch processing tool was originally to prepare data for the spatial-temporal model (described in Section 4.3). This tool is an extension of Tool 1 (Section 4.1), but also preparatory to the spatial-temporal tool; however, because it seemed like it could be useful for other applications, I felt was best left as a standalone tool for the purpose of posting it to Ghub. The batch processing tool when complete will ingest an entire tile of SERAC time series data and process all the time series in that tile for a given model. At present, the data is preprocessed and saved to a file using a combination of Excel and Python. The R code then reads that file and processes all the time series with Gaussian process regression to produce a regular time series. All that data is added to a dataframe. At the end of the process, the dataframe will contain all the processed time series. The processed and unprocessed data can then be called and graphed together one time series at a time, in a faceted graph, or in an animation.

The goal here is to further develop the code to allow for a single notebook to call the SERAC data on Ghub in the notebook. Ideally, a processed version of the SERAC data would be available for use. The present version of the code uses only the Gaussian process model; however, adapting it for the other three models will not be that difficult once the first tool (particularly calling ALPS from within R) is completed.

I also have a batch processing outlier and influential point detection code developed for the Gaussian process model. The present version of the code saves a series of analyses to a dataframe for further analysis so that each time series does not have to be inspected by hand one time series at a time. This function would be used to determine rejection criteria (if any) for a time series, and then another version of this tool would permit points that meet selected criteria to be flagged so that it can be easily filtered when processed. The goal here would be to extend this code to permit other regression models to be used.

The outlier detection functions can be seen as an extension of the analysis of uncertainty quantification. My work with outlier detection with the various models shows that Gaussian processes lead to fewer points being flagged as outliers, suggesting that its uncertainty measures are of higher quality. Output of the analysis to a dataframe can aid in determination of appropriate rejection criteria consistent with the scale of the data being analyzed.

The notebooks for this tool will be organized as follows:

I. Batch Processing
   A. Polynomial
   B. Loess
   C. ALPS
   D. Gaussian Process
II. Outlier and Influential Point Flags
   A. Polynomial
   B. Loess
   C. ALPS
   D. Gaussian Process

This tool continues the work of the first tool (Section 4.1). It will mostly operate in the R programming language, though it will call to Python code to employ the ALPS model in the batch processing. In R, the RobustGaSP package will be used for the Gaussian process models (Gu et al., 2019), ggplot2 for visualization (Wickham et al.), and EnvStats will be used for outlier detection (Millard & Kowarik, 2013). Processed models will be output to a file for later use, and each time series will be processed separately, so this is an ideal environment for incorporating parallel processing methods to speed up the computation.

The current timeline for completion of this tool is approximately mid-summer 2022.

4.3 Spatial-Temporal Interpolation and Visualization Tool

This research started with the goal of this third tool in mind: to produce a spatial-temporal model of the dynamic change in the ice sheet. This research is only in its very preliminary stages, but it would use partial parallel emulation (Gaussian process) to model observations both in space and time (Cressie & Wilke, 2011). The primary batch processing tool above is meant to feed into this modeling process.

At present I have been able to process a small set of time series to produce a coarse model of a small patch of the ice sheet. The first goal would be to increase the amount of data being processed from 37 time series to several hundred at a time.

Some challenges remain such as whether to use only (t, x, y) data (one temporal, two spatial variables) or to try to use (t, x, y, z) data (one temporal, three spatial) to produce the model. The challenge has been in obtaining reference height data at (x, y) locations where there are no observations. I believe this can be overcome through using Gaussian processes to predict the z-variable. Other alternatives are possible, but at present have been set aside to produce a working model. At present it remains unclear whether the three-variable or four-variable model inputs works better.

The other challenge is to produce a meaningful visualization of the result. I have experimented with heatmaps, animated to show the time variable, although the initial low resolution and small color variation produced less than exciting results. Similar issues with a point-plot. I have also experimented with static contour graphs at a single point in time. This may be a viable alternative. I would also like to produce 3D visualizations. This would require a different graphics package, but there are several options available to experiment with. Selecting an appropriate section of the ice sheet where something interesting is happening remains a challenge.

The output of these tools will be savable to a dataframe and file. Likewise, any visualizations will be saved to a file.

This work will continuing using the RobustGaSP package in R for the spatial-temporal interpolations (Gu et al., 2019). While initial visualizations are currently employing ggplot2 (Wickham et al.), three-dimensional visualizations will be desirable; however, which package or packages will be useful for that purpose is yet to be determined. Some parts of the ice sheet are more dynamic than others. This work will focus on the most dynamic areas, not only because they are the most interesting, but also because they tend to involve the most densely packed observations and will thus provide the most accurate models. Visualizations of both the model interpolation and the errors are desired. Results may be compared to other DEMs at particular points in time to confirm reasonableness.

This work is only in the most preliminary stages. I expect that this work would lead to a second journal article. I estimate completion in the fall semester 2022.

4.4 Comparing Observations to Ice Sheet Simulations Tool

The fourth tool to be developed will be to link computational ice sheet model (ISM) outputs to the observational data. This tool would match up a location in an ice sheet model to the observational data that is closest to it and compare the results using a set of metrics (Fyke et al., 2018). The differences in resolution of the observational data versus the computational outputs are likely to be of different sizes. This may lead to more than one time series falling into the computational model patch, or several computational model patches falling into a single observational data patch. What to do in each of these circumstances will have to be determined.

A potential challenge associated with this would be in finding the point that is closest to a given location. With a dataframe containing the boundaries of each tile, searching within a single tile for the closest point would not be difficult, however, if the position is near a tile boundary, it is conceivable that the closest time series in the data set is in a different tile than the location itself. While I don't think this would happen a majority of the time, it is the case that along the coast, glaciers near each other may behave quite differently, so there is the possibility this search method could lead to misleading results. A dataset of all the locations for all the time series in a single file would facilitate this search and avoid the potential problem noted above. A version of the location data in this form would also facilitate constructing spatial models in Tool 3 (Section 4.3) where the patch to be modeled straddles one or more tiles.

The most difficult to model sections of the ice sheet for simulations to predict are the most dynamic portions. Sections of the ice sheet can be connected to other parts of the ice sheet through drainage basins. By using identified catchment basins, we can extract sections of the ice sheet with interconnected dynamics and model them together (Pitcher et al., 2016). Identifying simulation cells that overlap the catchment basin could then be fed into a loop to select appropriate time series in the SERAC data. These selected time series could then be modeled either individually (using Tool 1 or Tool 2, Sections 4.1 and 4.2), or could be modeled spatiotemporally (using Tool 3, Section 4.3).

As with previous tools, this one will be developed primarily in R. There are a variety of packages capable of working with spatial data (Lovelace et al., 2017). Data from the simulation models will be needed. Most of the code to select the appropriate time series or model outputs will have to be written. Visualization tools may be adapted from spatial modeling tool (Section 4.3), or new methods may be implemented. Measures of discrepancy between the two models may be compared to other methods of model validation, as well as measures of uncertainty within the models.

The research for this tool has not begun. My current timeline for completion is spring semester 2023.

5. Significance

Understanding the impacts of climate change on the Greenland Ice Sheet is important for understanding recent changes locally, but also for predicting future changes and modeling sea-level rise. Analysis of the existing observational data can provide insights for both local behavior of the ice sheet as well as understanding total recent mass loss.

Visualization of features can aid in understanding how regional effects are connected and can help to incorporate temporal factors into the overall picture.

Connecting the observational data to computational ice sheet models (ISM) can aid in model initialization and model validation.(Goelzer et al., 2017)

As the time series data is extended to include ICESat2 data, analyzes can be quickly reprocessed to update our understanding after the inclusion of the new data.(Csatho, 2020)

In addition, the tools developed here can also aid other researchers with analysis of their time series, both as applies to other observational ice sheet data sets, but also for other types of time series data sets.

6. Research Timeline

The research timeline for completion of each tool and associated paper (where this applies) is expected to approximately follow the table below:

Tool 1 (Section 4.1) Model Comparison Tool	Spring Semester 2022
Tool 2 (Section 4.2) Batch Processing Tool	Mid-summer 2022
Tool 3 (Section 4.3) Spatial-Temporal Tool	Fall Semester 2022
Tool 4 (Section 4.4) Matching to ISM Tool	Spring Semester 2023
Thesis Completion	Summer 2023

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