

Performance Variation of the Albany Land-Ice Code at Sandia National Labs

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Abstract

Albany Land-Ice is a numerical ice sheet model being maintained and developed in part by scientists at Sandia National Labs. With many contributors actively working on the model, improvements in one area may inadvertently affect performance in other ways. In this project, we explore the use of automated changepoint detection methods and visualization tools to detect changes in the runtime of nightly test runs. Generalized likelihood ratio methods are used to evaluate the significance of candidate changepoints. Jupyter notebook and the Plotly package for Python are used to display findings and show interactive plots of multiple test cases. Building off of the changepoint model, we perform paired analysis of different test cases to evaluate one against the other. The resulting notebooks and models are currently being integrated into automated processes and email reports at Sandia.

1 Introduction

To understand the effects of climate change, accurate and high-performance models must be developed to predict the state of our Earth, looking decades into the future. One of these prediction tasks is the increase in sea level, which is largely affected by the dynamics of land ice sheets. The Albany Land-Ice model is being developed at Sandia National Labs and Los Alamos National Labs, and is intended for use with various high-performance computing architectures [8]. In addition to generating realistic, accurate predictions of land ice geometry, these models must efficiently handle model large, high-resolution data.

The core components of the model are the Albany PDE framework and Trilinos nonlinear solvers. With many scientists actively contributing to both code bases, model improvements in one area can occasionally affect performance in other areas. In particular, this project is concerned with unexpected changes in simulation time, in terms of wall-clock time. Until recently, changes in performance could go unnoticed for weeks or months. The current solution uses automatically generated plots, which must be reviewed manually; and simple statistical tests, which can detect the presence of changes but not always the point at which they occur.

To improve the performance monitoring process, we explore using changepoint detection models and creating automatically-generated visualizations to:

- Measure the likelihood of a change in performance
- Detect the most likely location of a change, and relate it to Git commit metadata
- Show performance trends over time

With a changepoint model in place, we can also identify the data that is relevant to present-day decisions. For example, we can compare times from test cases run on different computing architectures, while excluding data that is no longer relevant.

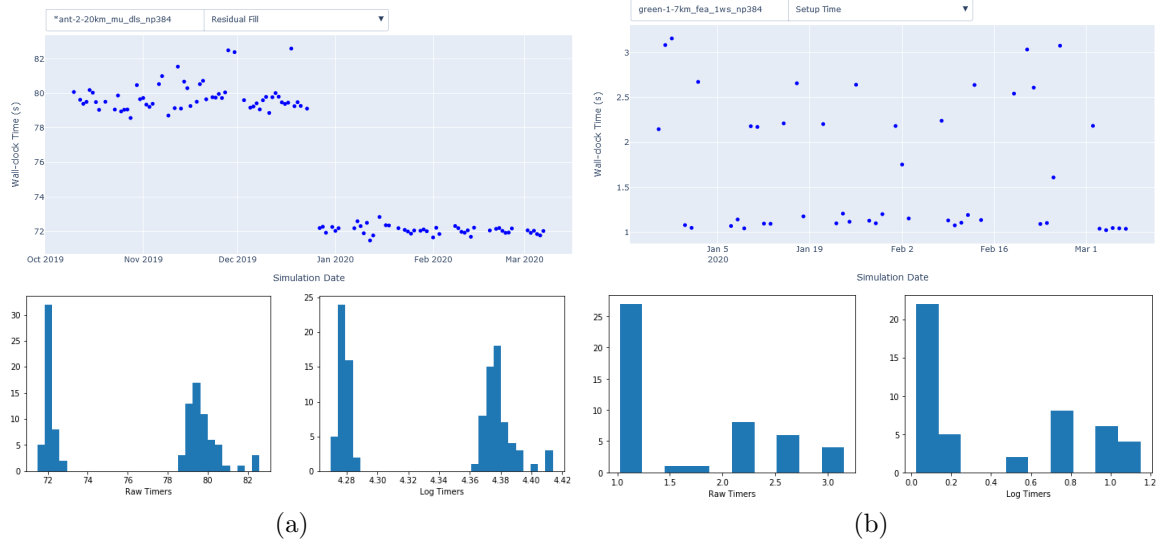


Figure 1: Time series plot and histogram of various timers, as either the raw data (subplot bottom left) or log-transformed data (bottom right). In (a), each portion of the data roughly fits either a normal or lognormal distribution, but with some outliers. In (b), the data does not seem to fit any standard parameterized distribution.

In section 2, we cover the dataset of test cases and timers. In section 3, we discuss methods for changepoint detection and visualization libraries. In section 4, we show the results of our methods on the actual timer data as well as some basic simulated examples. Lastly, in section 5 we recap the project experience, and discuss potential improvements for the future.

2 Data and Processing

The data are provided by Sandia. When nightly performance tests are run, timers and metadata are collected with `ctest` and saved in `.json` files, starting in October 2019. Test runs are done on the Blake and Waterman (since Jan 2020) test beds [14]. Figures A.1 and A.2 show the various test cases, and Figure A.3 shows the timers that are collected during the modeling process. Notably, we rarely have known instances of performance changes. Thus, our evaluation of detection methods relies mostly on human judgment and simulated data.

The lack of known changes also makes it difficult to test the distribution of the data, since each time series could contain data from multiple distributions. There are many combinations of test cases and timers, making it prohibitive to visually inspect each one. Based on a small sample, we conclude that the normal or lognormal distribution describes most of our data reasonably, except for occasional outliers in the positive direction. In Figure 1, we show two cases where the changepoints (or lack thereof) are visually obvious. In the first case, the data and log-transformed data both pass a normality test [4] (using the implementation of `scipy.stats.normaltest`), with the log-transformed data fitting slightly better. In the second case, the data seems to belong to two distributions, but they are not separated by a single changepoint.

Another observation is that changes may happen with as few as three observations in between. Hence, our methods cannot rely on having even a medium amount of data.

Algorithm 1 The single changepoint detection algorithm. Parameters are the significance level, α , and the number of large changes to consider, k . Input is assumed to be roughly normal. Returns a set C of viable changepoint candidates, along with a map S from the candidates to their t-statistics.

```

function SINGLECHANGEPOINT( $x_{1:n}, \alpha, k$ )
   $C = []$ 
   $S = \{\}$ 
   $t^* = t_{n-2}^{1-\alpha/(2(n-1))}$ 
   $\mathcal{K} = \text{ARGSORTDESC}(|x_{2:n} - x_{1:n-1}|)$ 
  for  $\nu \in \mathcal{K}_{1:\max(n,k)}$  do
     $t = \text{TTEST}(x_{1:\nu-1}, x_{\nu:n})$ 
    if  $|t| > t^*$  and  $|t| > t_{\max}$  then
       $C \leftarrow [C, \nu]$ 
       $S \leftarrow S \cup \{\nu \rightarrow t\}$ 
    end if
  end for
  return  $C, S$ 
end function

```

3 Methods

The task of identifying changes in performance falls in the category of problems known as changepoint detection; see [1], [13], [3] for a complete description of this type of problem.

3.1 Single Changepoint Detection

The basic building block of changepoint detection algorithms is single changepoint detection: given a univariate time series x_1, x_2, \dots, x_n such that $\{x_i\}_{i=1}^{\nu-1}$ are i.i.d. with distribution f_0 , and $\{x_i\}_{i=\nu}^n$ are i.i.d. with distribution f_1 ; what is the best estimate of ν ? The conventional approach assumes a known baseline distribution f_0 (and sometimes f_1 as well).

Since we have many separate time series, each potentially changing multiple times, we need a method which requires limited knowledge of f_0 and f_1 . In the most general case, nonparametric models can theoretically detect any change in distribution, but they can be less powerful than parametric models. Since our sample size is limited, we assume a lognormal distribution, based on our findings in Section 2.

Given a potential changepoint ν , we can perform a two-sample t -test of $\{x_i\}_{i=1}^{\nu-1}$ and $\{x_i\}_{i=\nu}^n$. We found that Student's t -test, assuming equal variances, worked reasonably well, although a future improvement could be to use Welch's t -test which is robust to unequal variance.

To find the most likely changepoint, we can apply the t -test to each candidate changepoint. However, we must adjust our desired significance level for multiple hypothesis testing. The simplest solution is the Bonferroni correction [2], i.e. testing each candidate at a significance level of $\alpha/(n-1)$, where α is our original desired significance level. Figure 2 shows an example of this test. This correction is known to be overly conservative for large numbers of tests. To alleviate this, we test only the $\min(k, n-1)$ largest changes (by absolute value) in the time series; a typical value of k could be between 3 and 10. Lower values of k allow for more powerful tests, but are more susceptible to outliers clogging the list of the largest changes. Algorithm 1 shows pseudocode for this building block algorithm.

The multiple t -test method above can also be viewed as a generalized likelihood ratio test. Define two families of hypotheses: the null hypothesis states that $\{x_i\}_{i=1}^n$ belongs to a single distribution, while the alternative states that there exists some $\nu \in \{2, 3, \dots, n\}$ such that $\{x_i\}_{i=1}^{\nu-1}$ and $\{x_i\}_{i=\nu}^n$ are separate distributions. The test statistic is found by maximizing the likelihood of each hypothesis and taking the likelihood ratio. Assuming equal variance, Student's t -test is equivalent to the likelihood

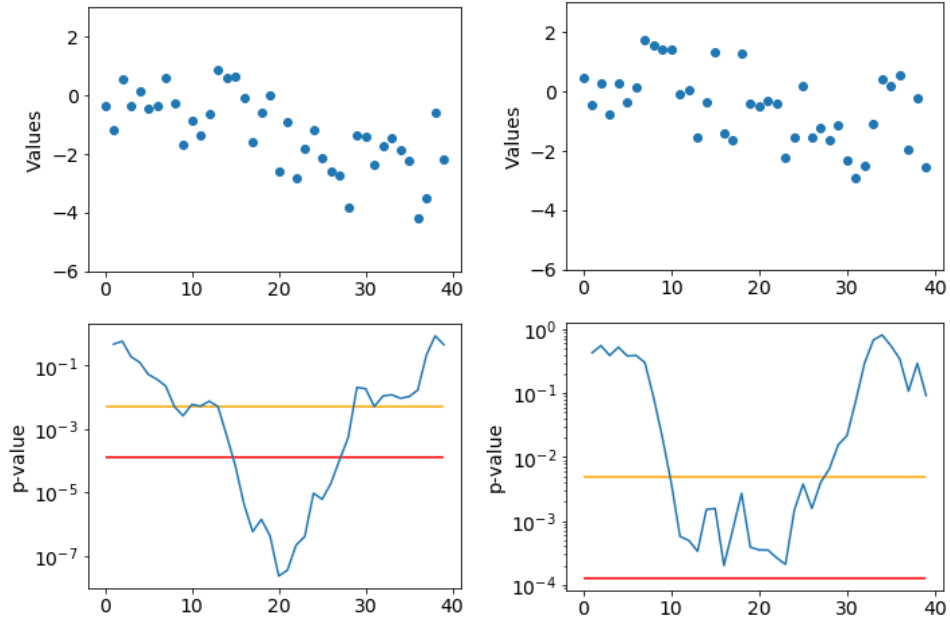


Figure 2: Simulated data (top) with the p-values resulting from our generalized likelihood ratio test (bottom). Left: the p -value for a t -test is minimized when splitting the data in the middle, passing both our original significance level of 0.5% and the Bonferroni-corrected significance level of $0.5\%/(40 - 1)$. Right: a more difficult case; none of the candidate changepoints fall below the corrected significance level.

ratio for a given candidate ν [6]. Besides evaluating a change in the mean, as in [10] [12] [6], it is also possible to test for a change in variance [7]; however, this additional testing appeared to be unhelpful for our application.

3.2 Multiple Changepoint Detection

Our time series data is likely to have multiple changepoints. A popular approach to multiple changepoint detection is to use a greedy algorithm which splits the data recursively until no more significant changepoints can be found. This approach is called binary segmentation [11], and there are various extensions to make the process more robust, such as wild binary segmentation [5]. We instead use a simpler sequential method, where we replicate the experience of recording one new observation at a time. If a changepoint is detected, we mark it as such, backtrack to immediately after the changepoint, and future analysis will disregard any data prior to that changepoint. While this process may not find the optimal changepoints, it is guaranteed not to retroactively change its decisions, which is easier to understand. Figure 3 shows an example of our method applied to simulated data, and Algorithm 2 provides pseudocode.

3.3 Robustness to Outliers

Outliers present a significant hurdle to the task of changepoint detection. Basically by definition, an outlier comes from a different distribution than the rest of the data, so changepoint models are understandably keen on detecting them. We take several steps to mitigate this effect while minimally decreasing the power of our tests.

First, in any single t -test, we first examine the data on either side of the candidate changepoint for outliers using the median absolute deviation [9], with a threshold comparable to three standard deviations, subject to removing at most one tenth of the data.

Second, we require three consecutive detections of the same changepoint before marking it as such; an outlier followed by two inliers will not yield as large of a detection.

Lastly, we limit the lookback window of our method to 30 observations. A common critique of p -values is that the smallest of changes becomes significant when samples sizes are large; setting a maximum window size helps to avoid hypersensitivity as we get further from the last detected changepoint.

Algorithm 3 describes our final changepoint detection model. To illustrate the effect of these modifications, Figure 4 shows how occasional outliers can trigger false detections without our adjustments, and that our adjustments allow the model to ignore these outliers.

3.4 Automated Dashboard Report

To facilitate the review of performance changes, we build a Jupyter notebook which loads `.json` files from a specified directory and runs our changepoint model. The mean and standard deviation is calculated between changepoints; this information is plotted along with the time series. Using the `Plotly` package for Python, we create interactive drop-down menus which allow selecting the test case and timer. This package also has hover-text functionality, which we use to show Git commit information. With this relatively small number of interactive features, we can export the notebook to an offline HTML document, which can be viewed on most browsers. See Figure 5 for an example of this report.

We also generate a similar notebook for comparing test cases. In addition to the time series plot, we also perform paired analysis by taking the subset of data where both test cases have timers (although the tests are all run nightly, they can occasionally fail, resulting in no timer data). We find that idiosyncrasies in cluster performance, as well as some performance changes, are highly correlated between different test cases, and a paired analysis removes some of the variation when trying to compare two time series.

Algorithm 2 The multiple changepoint detection algorithm. Parameters are the same as Algorithm 1. Returns a set \mathcal{C} of changepoints.

```

function MULTIPLECHANGEPOINT( $x_{1:n}, \alpha, k$ )
   $\mathcal{C} = []$ 
   $i = 0$ 
   $j = i + 1$ 
  while  $j \leq n$  do
     $C_j, S_j \leftarrow \text{SINGLECHANGEPOINT}(x_{i:j}, \alpha, k)$ 
    if  $C_j \neq \emptyset$  then
       $\nu^* = \arg \max_{\nu \in C_j} S_j(\nu)$ 
       $\mathcal{C} \leftarrow [\mathcal{C}, \nu^*]$ 
       $i \leftarrow \nu^*$ 
       $j \leftarrow \nu^* + 1$ 
    else
       $j \leftarrow j + 1$ 
    end if
  end while
  return  $\mathcal{C}$ 
end function

```

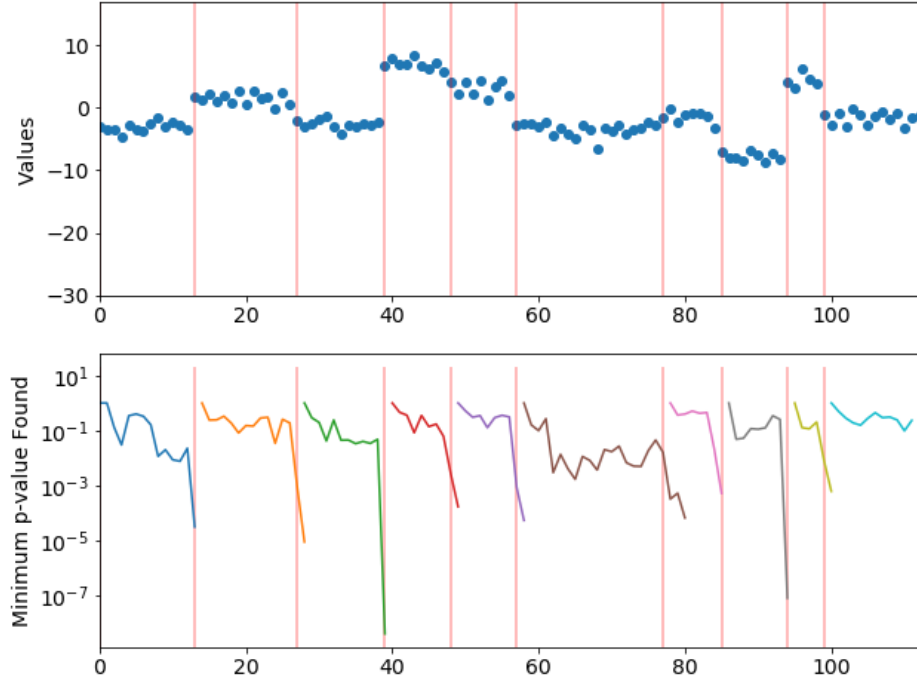


Figure 3: A multiple changepoint detection problem (top), and the p-values at the moments of detection (bottom).

Algorithm 3 The robust multiple changepoint detection algorithm. In addition to the parameters of Algorithm 2, we also define the minimum number of consecutive detections, m , and the maximum lookback window, w . We call a modified version of the single changepoint algorithm, `SINGLECHANGEPOINREMOVEOUTLIERS`, which removes outliers from each sample prior to performing a t -test. Returns a set \mathcal{C} of changepoints.

```

function ROBUSTMULTIPLECHANGEPPOINT( $x_{1:n}, \alpha, k, m, w$ )
   $\mathcal{C} = []$ 
   $i = 0$ 
   $j = i + 1$ 
  while  $j \leq n$  do
     $C_j, S_j \leftarrow \text{SINGLECHANGEPPOINTREMOVEOUTLIERS}(x_{i:j}, \alpha, k)$ 
     $\mathcal{V} = C_{j-m+1} \cap C_{j-m+2} \cap \dots \cap C_j$ 
    if  $\mathcal{V} \neq \emptyset$  then
       $\nu^* = \arg \max_{\nu \in \mathcal{V}} \left( \sum_{\ell=j-m+1}^j S_\ell(\nu) \right)$ 
       $\mathcal{C} \leftarrow [\mathcal{C}, \nu^*]$ 
       $i \leftarrow \nu^*$ 
       $j \leftarrow \nu^* + 1$ 
    else
       $j \leftarrow j + 1$ 
       $i \leftarrow \max(i, j - w)$ 
    end if
  end while
  return  $\mathcal{C}$ 
end function

```

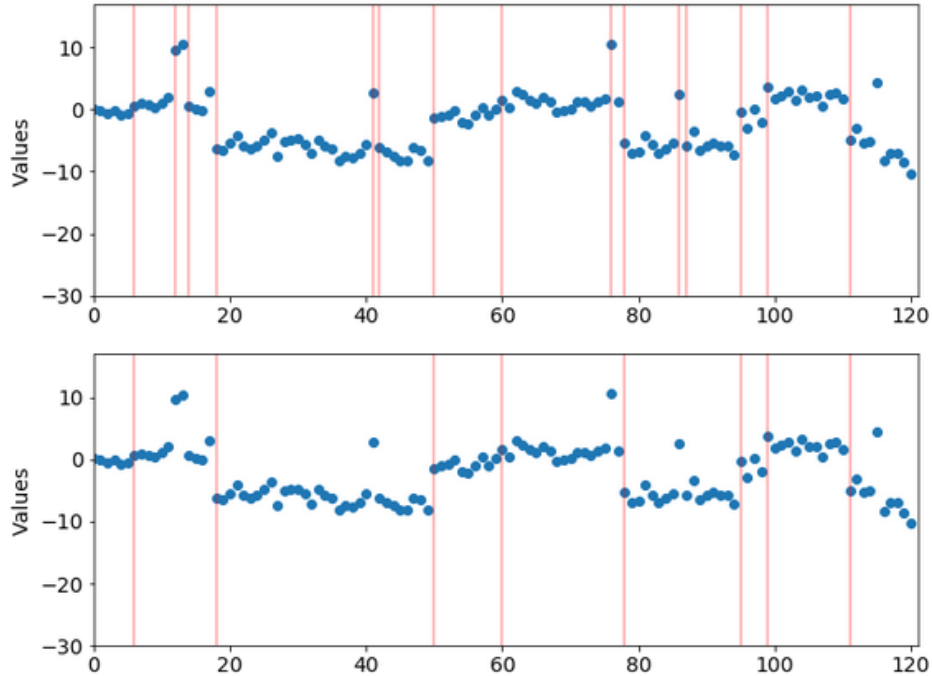


Figure 4: Our multiple changepoint detection algorithm without (top) and with (bottom) the tweaks for robustness against outliers.

Performance Timelines

Events in the most recent 10 days:

```
02/26/2020:
  ant-2-20km_mu_dls_np384: Total Time
                           NOX Total Preconditioner Construction
                           NOX Total Linear Solve
  green-1-7km_fea_lws_np8: Residual Fill Evaluate
02/27/2020:
  green-1-7km_fea_mem_np8: Residual Fill
02/29/2020:
  green-1-7km_fea_lws_np8: Jacobian Fill Export
  green-1-7km_fea_mem_np8: Total Time
                           Total Fill Time
                           Jacobian Fill
                           NOX Total Linear Solve
03/03/2020:
  ant-2-20km_mu_dls_np384: Jacobian Fill
```

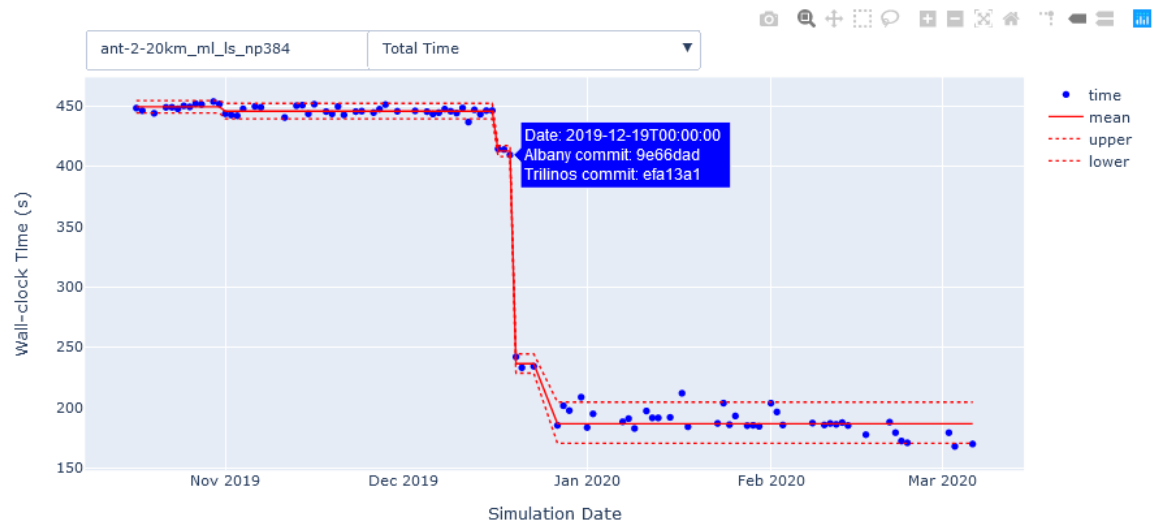


Figure 5: An example of the offline HTML report, with interactive drop-down menus and hover text.

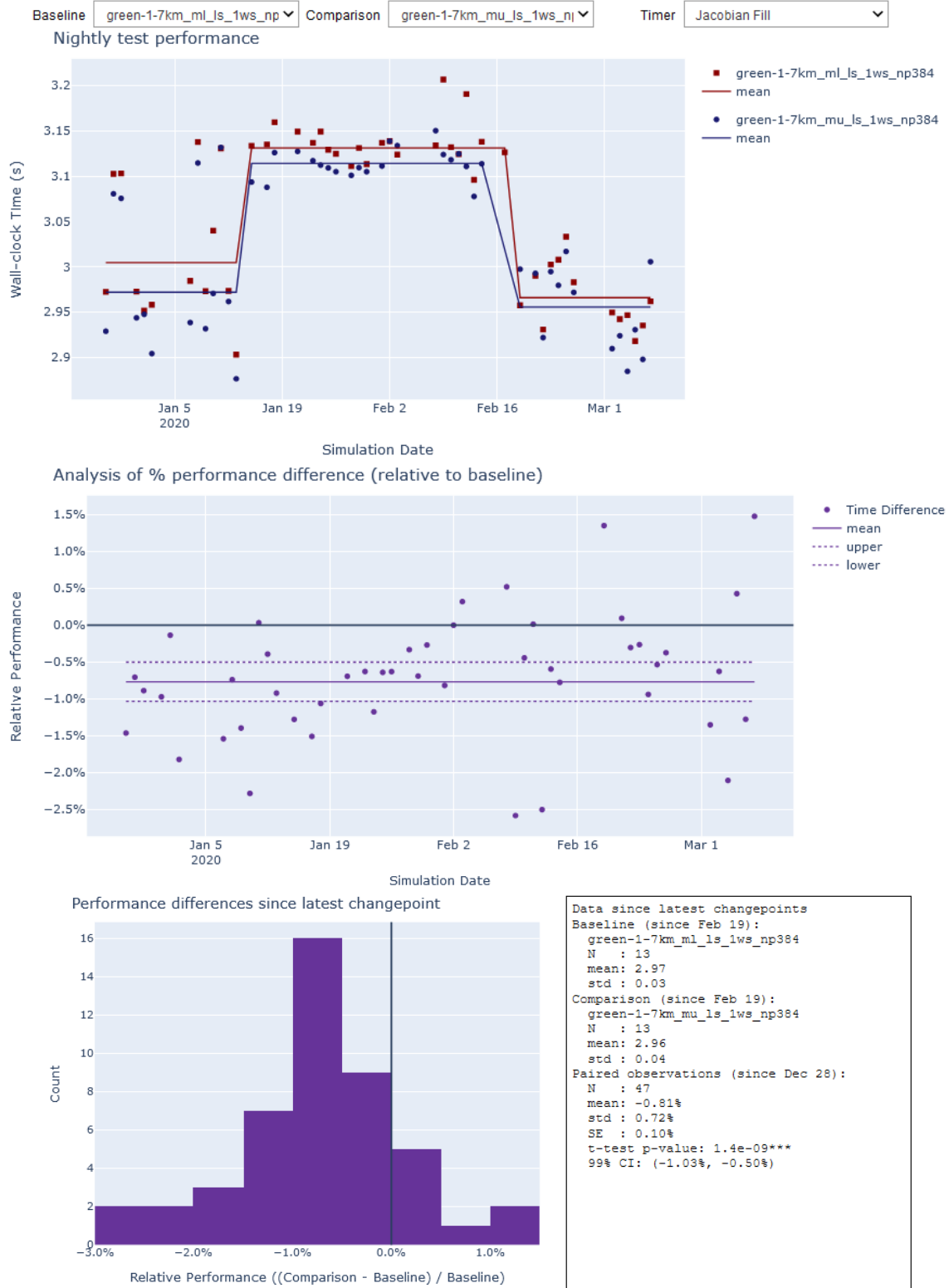


Figure 6: An example of the comparison notebook, with paired analysis of the two test cases.

For our paired analysis, we take the difference between the log-transformed timers for two test cases, and take the exponent minus one, yielding a relative performance difference between one test case (the Baseline) and another (the Comparison). We use our changepoint analysis on the log data, and show the mean between changepoints and a 99% confidence interval for the mean. Furthermore, we include a histogram of the relative differences since the last changepoint, and summary statistics including the significance of a t -test for the mean relative difference. Due to the additional computations that require a Python backend, this notebook must have a Python kernel to use the drop-down menus, and the interactivity cannot be used in an exported HTML file. See Figure 6

4 Results

Since we have very few cases of confirmed performance changes, our performance analysis relies mostly on human judgment. In Section 3, we showcased our model on simulated examples, which generally worked well. When used on actual data, we are generally happy with the results, but outliers continue to be an issue at times. This is best shown by example; see Figure 7 below. In particular, the middle panel suggests that there is room for improvement. The data contains several large outliers in every regime; an ideal model would identify these outliers and focus on the small range of variation when they are excluded. When a fifth of the data are outliers, though, the task becomes understandably difficult.

5 Conclusion and Future Work

In this project, we implemented a relatively simple changepoint detection method, with several modifications to improve robustness with our dataset. Our Jupyter notebooks are intended to showcase the changepoint model, and also demonstrate the utility of automatically-generated, interactive reports. We are pleased to have received positive feedback on these notebooks, which should serve as an upgrade for the automatically-generated notebooks currently being used at Sandia. Our changepoint model is also being integrated into email summaries of nightly test data.

5.1 Future Work

There is room for future improvement in both the changepoint model and the visualization tools.

Our changepoint model does not always make the judgements we expect, particularly when outliers are involved. While we tried a few modifications to reduce the effect of outliers, there are more options that could be useful. We noted previously that an outlier is effectively a changepoint, but not one we're typically interested in. If multiple changepoints are detected in a short period of time, then we could test whether the data has reverted to a previous distribution, thereby acknowledging potential outliers while not letting them affect future decisions.

Another option would be to run test cases multiple times a day. This would allow the effects of outliers to be diluted by non-outliers. However, the current code would need to be modified to recognize that changepoints can only occur between days. As mentioned in Section 3, using Welch's t -test may also yield better results, although some brief testing did not show it helping with outliers.

Other options to improve the model include using more sophisticated methods, such as nonparametric methods. Given the almost-normality of most of our data, this seemed less likely to help, particularly within the constraint of a ten-week quarter.

In creating the notebooks, we focused on providing useful information, but as a result they could use additional polish. If the time comes to upgrade these notebooks, switching to a server-hosted Python app would leave the most room for improvement. For example, while the single-test-case notebook can be exported to HTML, it has limited flexibility in the type of information shown; two drop-downs is the limit for this method. With the recent popularity of data science, there exist many packages focused on enabling (relatively) novice programmers to create dashboards with a wide

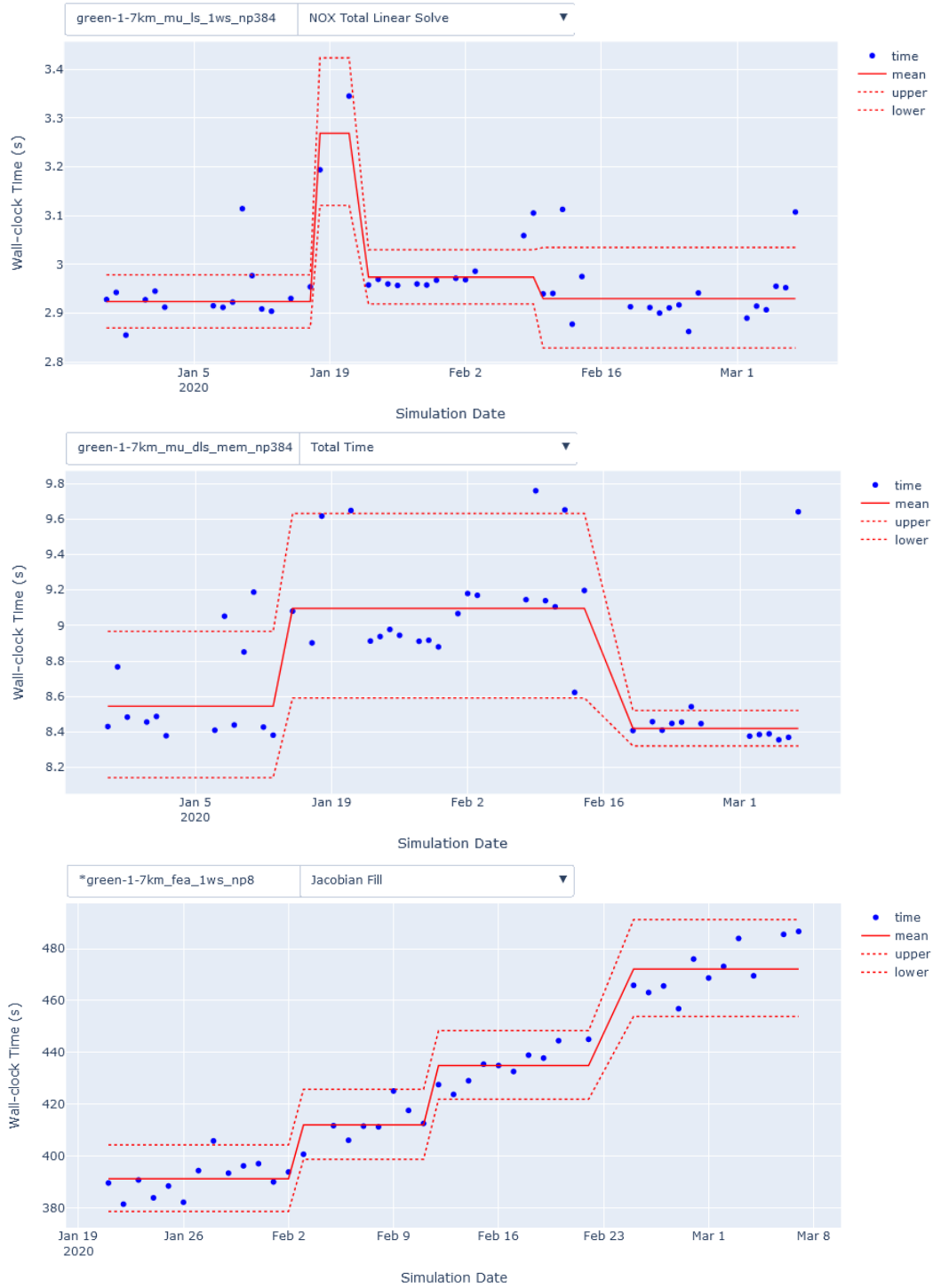


Figure 7: Several examples of the changepoint model's results. In the top panel, the model identifies two outliers as a changepoint. In the middle panel, performance seems reasonable, but perhaps Feb 1 should be a changepoint. In the bottom panel, simulation times are creeping up, and the model detects multiple changepoints at somewhat arbitrary locations.

range of interaction and plotting options, which can be viewed in both desktop and mobile browsers. Budget is the main concern here, although it may be possible to host an app locally, such that it can be accessed by other devices on the same network.

References

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Appendix

Case Name	Processes	Description
ant-2-20km_ml_ls	384	Unstructured 2-20km AIS, ML w/ line smoothing
ant-2-20km_mu_ls	384	Unstructured 2-20km AIS, MueLu w/ line smoothing
ant-2-20km_mu_dls	384	Unstructured 2-20km AIS, MueLu w/ decoupled line smoothing
greenland-1-7km_fea_1ws	384	Unstructured 1-7km GIS, finite element assembly only, single workset
greenland-1-7km_ml_ls_1ws	384	Unstructured 1-7km GIS, ML w/ line smoothing, single workset
greenland-1-7km_mu_ls_1ws	384	Unstructured 1-7km GIS, MueLu w/ line smoothing, single workset
greenland-1-7km_mu_dls_1ws	384	Unstructured 1-7km GIS, MueLu w/ decoupled line smoothing, single workset
greenland-1-7km_fea_mem	384	Unstructured 1-7km GIS, finite element assembly only, memoization
greenland-1-7km_ml_ls_mem	384	Unstructured 1-7km GIS, ML w/ line smoothing, memoization
greenland-1-7km_mu_ls_mem	384	Unstructured 1-7km GIS, MueLu w/ line smoothing, memoization
greenland-1-7km_mu_dls_mem	384	Unstructured 1-7km GIS, MueLu w/ decoupled line smoothing, memoization

Figure A.1: Test cases on Blake test bed

Case Name	Processes	Description
greenland-1-7km_fea_1ws	8	Unstructured 1-7km GIS, finite element assembly only, single workset
greenland-1-7km_fea_mem	8	Unstructured 1-7km GIS, finite element assembly only, memoization

Figure A.2: Test cases on Waterman test bed

Timer Name	Level	Description
Albany Total Time	0	Total wall-clock time of simulation
Albany: Setup Time	1	Preprocess
Albany: Total Fill Time	1	Finite element assembly
Albany Fill: Residual	2	Residual assembly
Albany Residual Fill: Evaluate	3	Compute the residual, local/global assembly
Albany Residual Fill: Export	3	Update global residual across MPI ranks
Albany Fill: Jacobian	2	Jacobian assembly
Albany Jacobian Fill: Evaluate	3	Compute the Jacobian, local/global assembly
Albany Jacobian Fill: Export	3	Update global Jacobian across MPI ranks
NOX Total Preconditioner Construction	1	Construct Preconditioner
NOX Total Linear Solve	1	Linear Solve

Figure A.3: Timer hierarchy for nightly test runs