RexDash: A Comprehensive Dashboard for Analyzing REMD Simulation Performance

Soham Jain, Christopher Lockhart
School of Systems Biology, College of Science, George Mason University

Aspiring Scientists Summer Internship Program

Abstract

Replica exchange molecular dynamics (REMD) simulations have emerged as an effective tool to explore the conformational ensemble of **biomolecular systems**. By initiating several molecular dynamics simulations under different conditions and periodically swapping structures generated from adjacent conditions, REMD **enhances sampling** from simulations and **facilitates the computation of thermodynamic properties**. However, despite REMD's advantages, there is neither a standardized technique nor a widely adopted toolkit to ensure that REMD simulations are performing as expected. We address these limitations by developing **RexDash**, an extensive **dashboard** that features various metrics for assessing the **technical performance** of REMD simulations. Currently, the dashboard implements **Python** as the front-end framework to display plots for exchange rates, replica mixing parameters, replica trajectories, and potential energy distributions. RexDash utilizes the **Plotly** graphing library to render these metrics for REMD data supplied by the user in **comma-separated value** format. In addition, RexDash employs **HTML** and **Flask**, a backend web framework that enables visualization of REMD simulation results by deploying the webpage as an **online server**. To validate and test metrics generated by the dashboard, we conducted REMD simulations of **alanine dipeptide**, a standard model system for molecular simulations. RexDash will provide future researchers and simulation practitioners with a readily available resource to analyze the technical setup of their REMD simulations and, therefore, is an important first step in the **standardization** of REMD results.

Materials and Methods

- Microsoft **Visual Studio Code** is the source-code editor used for programming and debugging RexDash.
- RexDash employs **Plotly**, a **Python** graphing library to render replica exchange metrics on the dashboard. The figures provide comprehensive data to assess the simulation's technical performance.
- **HTML** and **Flask** were implemented as backend web frameworks to deploy the webpage as an online server. Currently, the server can be accessed via local host.
- The dashboard was tested and validated using **comma-separated-value data** of REMD simulations on **alanine dipeptide**, a conventional model system for molecular dynamics simulations.

Results

RexDash features **five metrics** for assessing the technical performance of REMD simulations. The plots display data for **exchange rates**, **replica mixing parameters**, **replica trajectories**, and **potential energy distributions**.

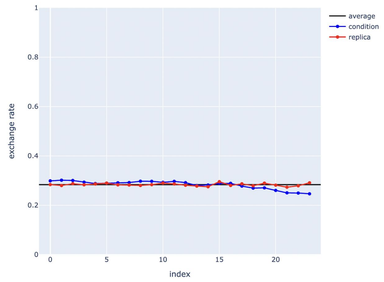

Figure 1. Replica Exchange Rate Plot

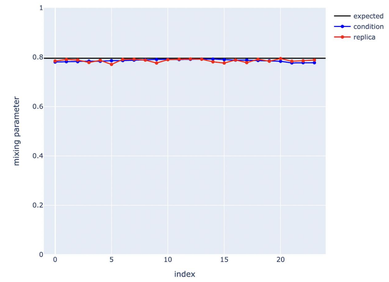

Figure 2. Replica Mixing Parameters Plot

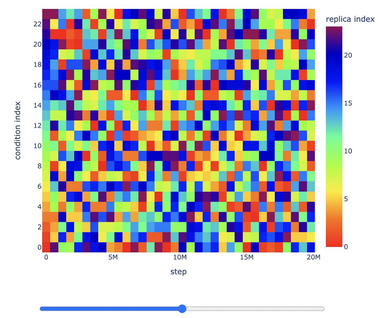

Figure 3. Dynamic Replica Trajectories Mosaic Plot

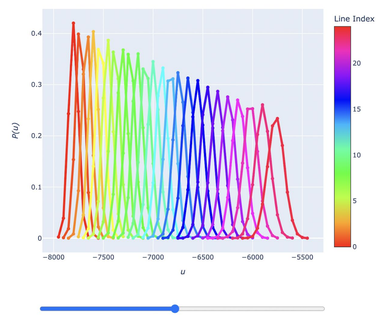

Figure 4. Dynamic Potential Energy Distributions Plot

Partner Replica

Replica	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23
0	0.000	0.257	0.297	0.282	0.308	0.278	0.297	0.266	0.296	0.256	0.300	0.317	0.291	0.261	0.279	0.272	0.257	0.330	0.306	0.315	0.288	0.256	0.270	0.268
1	0.257	0.000	0.294	0.265	0.316	0.311	0.259	0.262	0.267	0.302	0.280	0.294	0.252	0.262	0.262	0.298	0.291	0.266	0.296	0.277	0.275	0.262	0.281	0.301
2	0.297	0.294	0.000	0.278	0.298	0.307	0.271	0.298	0.282	0.257	0.317	0.274	0.311	0.308	0.232	0.320	0.270	0.246	0.261	0.330	0.243	0.274	0.326	0.337
3	0.282	0.265	0.278	0.000	0.297	0.301	0.295	0.302	0.279	0.243	0.273	0.307	0.305	0.249	0.244	0.280	0.282	0.281	0.273	0.312	0.311	0.248	0.247	0.314
4	0.308	0.316	0.298	0.297	0.000	0.304	0.226	0.274	0.285	0.295	0.284	0.271	0.292	0.279	0.261	0.256	0.272	0.293	0.237	0.316	0.319	0.262	0.292	0.320
5	0.278	0.311	0.307	0.301	0.304	0.000	0.305	0.322	0.320	0.273	0.295	0.292	0.315	0.296	0.252	0.280	0.288	0.268	0.275	0.310	0.285	0.267	0.288	0.243
6	0.297	0.259	0.271	0.295	0.226	0.305	0.000	0.291	0.257	0.313	0.294	0.309	0.282	0.289	0.296	0.263	0.281	0.311	0.266	0.327	0.282	0.257	0.281	0.256
7	0.266	0.262	0.298	0.302	0.274	0.322	0.291	0.000	0.290	0.271	0.269	0.321	0.285	0.266	0.288	0.309	0.288	0.281	0.287	0.291	0.241	0.255	0.274	0.273
8	0.296	0.267	0.282	0.279	0.285	0.320	0.257	0.290	0.000	0.294	0.319	0.259	0.248	0.302	0.259	0.309	0.249	0.281	0.261	0.288	0.271	0.320	0.254	0.273
9	0.256	0.302	0.257	0.243	0.295	0.273	0.313	0.271	0.294	0.000	0.282	0.260	0.284	0.287	0.300	0.340	0.287	0.306	0.286	0.277	0.292	0.288	0.260	0.302
10	0.300	0.280	0.317	0.273	0.284	0.295	0.294	0.269	0.319	0.282	0.000	0.293	0.288	0.320	0.276	0.271	0.268	0.322	0.269	0.300	0.278	0.273	0.278	0.336
11	0.317	0.294	0.274	0.307	0.271	0.292	0.309	0.321	0.259	0.260	0.293	0.000	0.266	0.252	0.259	0.373	0.248	0.296	0.282	0.274	0.282	0.283	0.302	0.319
12	0.291	0.252	0.311	0.305	0.292	0.315	0.282	0.285	0.248	0.284	0.288	0.266	0.000	0.256	0.253	0.311	0.277	0.277	0.234	0.299	0.259	0.307	0.300	0.279
13	0.261	0.262	0.308	0.249	0.279	0.296	0.289	0.266	0.302	0.287	0.320	0.252	0.256	0.000	0.274	0.292	0.260	0.311	0.295	0.254	0.297	0.279	0.250	0.284
14	0.279	0.262	0.232	0.244	0.261	0.252	0.296	0.288	0.259	0.300	0.276	0.259	0.253	0.274	0.000	0.304	0.297	0.303	0.273	0.269	0.279	0.281	0.288	0.293
15	0.272	0.298	0.320	0.280	0.256	0.280	0.263	0.309	0.309	0.340	0.271	0.373	0.311	0.292	0.304	0.000	0.261	0.301	0.320	0.268	0.286	0.302	0.301	0.323
16	0.257	0.291	0.270	0.282	0.272	0.288	0.281	0.288	0.249	0.287	0.268	0.248	0.277	0.260	0.297	0.261	0.000	0.276	0.288	0.307	0.301	0.271	0.296	0.334
17	0.330	0.266	0.246	0.281	0.293	0.268	0.311	0.281	0.281	0.306	0.322	0.296	0.277	0.311	0.303	0.301	0.276	0.000	0.296	0.318	0.295	0.260	0.281	0.251
18	0.306	0.296	0.261	0.273	0.237	0.275	0.266	0.287	0.261	0.286	0.269	0.282	0.234	0.295	0.273	0.320	0.288	0.296	0.000	0.305	0.278	0.243	0.289	0.277
19	0.315	0.277	0.330	0.312	0.316	0.310	0.327	0.291	0.288	0.277	0.300	0.274	0.299	0.254	0.269	0.268	0.307	0.318	0.305	0.000	0.249	0.304	0.270	0.265
20	0.288	0.275	0.243	0.311	0.319	0.285	0.282	0.241	0.271	0.292	0.278	0.282	0.259	0.297	0.279	0.286	0.301	0.295	0.278	0.249	0.000	0.276	0.256	0.298
21	0.256	0.262	0.274	0.248	0.262	0.267	0.257	0.255	0.320	0.288	0.273	0.283	0.307	0.279	0.281	0.302	0.271	0.260	0.243	0.304	0.276	0.000	0.274	0.269
22	0.270	0.281	0.326	0.247	0.292	0.288	0.281	0.274	0.254	0.260	0.278	0.302	0.300	0.250	0.288	0.301	0.296	0.281	0.289	0.270	0.256	0.274	0.000	0.276
23	0.268	0.301	0.337	0.314	0.320	0.243	0.256	0.273	0.273	0.302	0.336	0.319	0.279	0.284	0.293	0.323	0.334	0.251	0.277	0.265	0.298	0.269	0.276	0.000

Figure 5. Replica and Partner Replica Exchange Rate Table

Conclusions and Future Research

In this study, we created an **online dashboard** that displays metrics for assessing the technical performance of replica exchange molecular dynamics simulations.

Our research is the first step in the **standardization** of REMD results. RexDash streamlines the process of data submission by ensuring that users upload their REMD simulation results in a **consistent** and **uniform** format. The specific structure for **comma-separated-value** (CSV) data guarantees accurate generation of five standard metrics (see Figures 1-5).

Through generating these metrics, RexDash offers future **simulation practitioners** and **researchers** with a convenient tool to analyze their simulation's technical setup. The dashboard incorporates **interactive plots** for all five metrics and **dynamic rescaling** for replica trajectories and potential energy distributions, which allow users to visualize and analyze data more effectively.

Although RexDash is currently accessible on a **local host** server, we intend to host the dashboard on a **public domain** in future research.

References

A description of RexDash metrics are available in:

Smith, A. K., Lockhart, C., & Klimov, D. K. (2016). Does Replica Exchange with Solute Tempering Efficiently Sample Aβ Peptide Conformational Ensembles? *J. Chem. Theory Comput.* 12(10): 5201–5214.

Acknowledgements

This research was made possible through the support of George Mason University's College of Science, which supports the ASSIP Program.