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| **Research Computing Monthly Report**  **for the**  **Office of the Vice President for Research (VPR)**  **October 2021** |

**Overview**

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| For the month of October 2021, the Research Computing team saw increases in Ivy VM Projects and consulting projects.  A decrease in the number of allocation requests is due to the previous month’s high number of renewals for expired accounts. The usage of Rianna had an insignificant drop.  The decrease in new researcher accounts on Rivanna was expected because incoming faculty and students were added to Rivanna prior to October.  Furthermore, decreases in service and support requests and office hour attendees indicate that researchers encountered fewer issues with using RC services.  The remainder of this report is organized in the following main sections:   * Rivanna usage * Ivy usage * Consultations & Office Hours * Service & Support Requests * Workshops & Outreach   The following additional information is provided as attachments:   * Representative examples of Consultation projects * Planned Workshops for Fall 2021 * Research Outcomes based on allocation requests by researchers | **Monthly Trends: October 2021** |  |
| **General Support:** |  |
| 245 Service & Support Requests | 37% **↓** |
| 18 Consulting Projects | 12% **↑** |
| 45 Office Hr. & Consultations Mtgs. | 20% **↓** |
| **Rivanna:** |  |
| 34 Allocation Requests | 71% **↓** |
| 4,196,452.4 CPU Core Hours | 3% **↓** |
| 74 New Researcher Accounts | 53% **↓** |
| 5365 Total Active Researchers | 1% **↑** |
| **Ivy:** |  |
| 49 VM Projects | 17% **↑** |
| 225 Total Researchers | 4% **↑** |

**Rivanna Usage**

In October 2021, a total of 34 allocations were provisioned for a total of 3,386,000 SUs. The allocation requests included:

* 11 new standard allocations (totaling 1,100,000 SUs),
* 14 renewed standard allocations (totaling 1,310,000 SUs),
* 2 purchased allocations (totaling 501,000 SUs),
* 1 Deans' allocation (from SDS) for startup (totaling 100,000 SUs),
* 3 instructional allocations (totaling 75,000 SUs),
* 2 Capstone allocation for SDS (totaling 200,000 SUs)
* 1 condo allocation for BII (totaling 100,000 SUs)

A total of 74 new user accounts were created, bringing the total of active user accounts on Rivanna to 5365.

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**Ivy Usage**

In October 2021, there were 2 requests for new VMs. Eight new researchers were onboarded to new and existing project VMs. At the end of October, there were

* 225 individual researchers who were provisioned for one or more VMs.
* 45 active project VMs hosted on Ivy.
* 4 projects pending provisioning.

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**Consultations & Office Hours**

The consultations benefit both the researchers and the RC team members. The researchers are able to develop further their computational skills, while the team members are able to learn about the latest computational trends in various disciplines.

Office hours are held weekly on Tuesday afternoons and Thursday mornings. In addition, an “Introduction to Rivanna” session is offered each Wednesday.

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RC has been tracking the number of office hours attendees since January 2019. Although the number of attendees was down compared to last month, the number of attendees for October 2021 was higher than previous years.

**Service & Support Requests**

For the month of October 2021, Research Computing responded to 245 requests for service, training, or support. The requests, which are tracked in a ticketing system, can vary from simple questions to challenging problems that the researchers encounter.

The general types of requests can be subdivided into categories for the different platforms (e.g., Rivanna, Ivy, and Storage), as shown in the *Types of Requests* chart.

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The Level of Effort for the tickets was determined as follows:

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Moderate – the tickets required one or more RC individuals to ask up to five questions of the researcher to have sufficient information for resolving the support request.

Significant – the tickets required one or more RC individuals to work for multiple days and ask more than five questions of the researcher to resolve the support request.

**Workshops & Outreach**

For the month of October 2021, the US group members focused on their Fall workshops and the weekly “Coffee & Coding” session. While the Fall workshops provide in-depth coverage of a broad topic, the “Coffee & Coding” sessions are quick explorations of single coding topics.

The RC team presented the following workshops and educational sessions:

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| Date | Title | | Presenter | | Session Type/Length | | | # Registrants |
| 6, 13, 20, 27 Oct | | *Intro to Programming in Python for PhD+* | | Katherine Holcomb | | 1.5 Hour Zoom sessions | 66 | |
| 7 Oct | | *Parallel Processing with Matlab* | | Ed Hall | | Two Hour Zoom Session | 10 | |
| 12 Oct | | *Using Bioinformatics Tools on Rivanna* | | Gladys Andino (TA: Christina Gancayco ) | | Two Hour Zoom Session | 17 | |
| 14 Oct | | *Automation of Image Processing with Fiji/ImageJ* | | Karsten Siller | | Two Hour Zoom Session | 11 | |
| 15 Oct | | *Spark Training for Natasha Foutz group, McIntire School of Commerce* | | Ruoshi Sun, Christina Gancayco | | One Hour Zoom session | 12 | |
| 20 Oct | | *Introduction to Shiny* | | Christina Gancayco | | Two Hour Zoom Session | 29 | |
| 21 Oct | | *Coffee & Coding: Apply functions* | | Will Rosenow | | 30 minute Zoom Session | 5 | |
| 21 Oct | | *Scientific Image Processing with Matlab* | | Ed Hall | | Two Hour Zoom Session | 9 | |
| 25 Oct | | *Building Containers for Rivanna* | | Ruoshi Sun | | Two Hour Zoom Session | 12 | |
| 27 Oct | | *Customizing Shiny Apps* | | Christina Gancayco | | Two Hour Zoom Session | 11 | |
| 27 Oct | | *RNA-Seq Analysis Part I* | | Gladys Andino and Pankar Kumar | | Three Hour Zoom Session | 33 | |

The complete list of Fall Workshops is provided in attachment 2.  
  
  
The RC team conducted the following outreach activities:

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| **Date** | **Title/Description** | **Group/Organization** |
| 1 Oct | RC Outreach Zoom Session | McIntire School of Commerce |
| 6 Oct | Inaugural Meeting of “Virginia Women in HPC” | Led by Gladys Andino; 108 attendees from UVA, Va Tech, University of Richmond, William & Mary, George Mason, Virginia Commonwealth University, plus other locations |
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**Conclusion**

For the month of October 2021, the Research Computing team focused on consulting projects and educational programs for UVA researchers. The team handled a significant number of service and support requests from researchers.

Attachments

Table 1. Representative Examples of Consulting Projects for October 2021

Table 2 Tentative Schedule for Fall 2021 Workshops

Table 3. Highlights of Outcomes from Rivanna Allocations

**Table 1. Representative Examples of Consulting Projects for October 2021**

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| **Client** | **Problem** | **Solution** |
| **Anupreet Kour**    **Dept**: Cardiovascular Research Center | Anupreet Kour requested assistance with running algorithms on Rivanna to search for MicroRNA’s | RC staff created and troubleshot an R script to use BiomaRt for extracting genes given genomic coordinate locations. |
| **Anna Sviripa**  **Dept:** Chemical Engineering | Anna Sviripa wanted to compile custom versions of LAMMPS, a molecular dynamics simulation software package, with two different plugins, MGP and Flare++. | RC added the MGP plugin by following the documentation. No documentation is provided for the Flare++ plugin but RC was able to install that as well. RC provided the steps to the client. |
| **Chris Maurer**  **Dept:** Commerce | Chris Maurer wanted to set up an environment for his spring course GCOM 7260. | RC installed the packages in the instructional project storage so that students do not need to do their own installations. RC prepared a launch script and gave the instructions to the client. |
| **Elizabeth Godschall**  **Dept:** Electrical Engineering | Elizabeth Godschall was getting an out-of-memory error using the software Cite-seq-Count. | RC Staff ran the “top monitor” script, developed by RC staff member Ed Hall, on Elizabeth’s code and determined the optimal number of cores and memory she needed to run the code. After determining the optimal resources need, we provided Elizabeth with an updated slurm script to use. The script was passed to a colleague of hers, who encountered the same errors. |
| **Jaya Lakshmi**  **Dept:** Biology | Jaya Lakshmi asked for assistance to parallelize her Matlab code so that it could run efficiently on Rivanna. | RC Staff has ensured that Jaya received proper training on Rivanna by having her attend the Intro to Rivanna session and the Parallel Computing in Matlab workshop. We are working with her to determine the optimal placement of a parallel for loop (a “parfor” loop) in the code and the necessary resource parameters for her SLURM job script. |

**Table 2. Schedule for Fall 2021 Workshops**

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| DATE | WORKSHOP | INSTRUCTOR |
| 22 Sept 2021 | *Using Rivanna from the Command Line* | Gladys Andino |
| 30 Sept 2021 | *Sentiment Analysis with Python* | Jacalyn Huband |
| 7 Oct 2021 | *Parallel Processing with Matlab* | Ed Hall |
| 12 Oct 2021 | *Using Bioinformatics Tools on Rivanna* | Gladys Andino |
| 14 Oct 2021 | *Automation of Image Processing with Fiji/ImageJ* | Karsten Siller |
| 20 Oct 2021 | *Introduction to Shiny* | Christina Gancayco |
| 21 Oct 2021 | *Scientific Image Processing with Matlab* | Ed Hall |
| 25 Oct 2021 | *Building Containers for Rivanna* | Ruoshi Sun |
| 27 Oct 2021 | *Customizing Shiny Apps* | Christina Gancayco |
| 27 Oct 2021 | *RNA-Seq Analysis Part I* | Gladys Andino |
| 3 Nov 2021 | *RNA-Seq Analysis Part II* | Gladys Andino |
| 4 Nov 2021 | *Scientific Image Processing with Python* | Karsten Siller |
| 4 Nov 2021 | *Scientific Computing with Julia on Rivanna* | Ed Hall |
| 8 Nov 2021 | *Accelerate Python with RAPIDS* | Ruoshi Sun |

**Table 3. Highlights of Outcomes from Rivanna Allocations**

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| PI/Dept | Project Description |
| Bicheng Zhou  Dept: Materials Science & Engineering | “This request is to renew the standard allocation to support the computational materials science research in the research group, the Computational Thermodynamics and Kinetics Group (4 PhDs, 1 Postdoc) led by Prof. Bi-Cheng Zhou. . . .  The **research works are supported by the following federal grants**:  DOD: 161307 EN-MSE-Zhou-Design of UHTC “Design of UHTC for Oxidation Resistance”  NSF: 163836 EN-MSE GPzonesZhou: “DMREF: Collaborative Research: Low cost, high strength and ductile Mg alloys”  NSF: 166661 EN-MSE ZhouCAREER: Novel Comp: “CAREER: A Novel Computational Thermodynamics Framework with Intrinsic Chemical Short-Range Order”  DOE: 167420 EN-MSE HERO-Zhou: “High Entropy Rare-earth Oxide (HERO) Coatings for Refractory Alloys”  DOE: 168338-101- GQ10081-31345: “Development of Industrial Scale Rare Earth Master Alloys from Their Native Oxides for Magnet Production”  **Publications supported by Rivanna**:  K Wang, D Cheng, CL Fu, BC Zhou, “First-principles investigation of the phase stability and early stages of precipitation in Mg-Sn alloys” Physical Review Materials 4 (1), 2020, 013606  D Cheng, K Wang, BC Zhou, "First-principles investigation of early-stage precipitation in Mg-Sn and Mg-Zn alloys" Magnesium Technology 2022 Conference Proceeding (Accepted)” |
| Francine Garrett-Bakelman  Dept: Medicine | “… The research projects performed which utilize research computing services and resources on Rivanna have included the study of pathogenesis in Acute Myeloid Leukemia (AML) relapse **(PMID: 33500244**; **PMID: 33580203; poster presentation at the FASEB hematological malignancies meeting 7/2021**; **grant proposals to Pew Foundation** that was funded).  We have also been analyzing data for a project assessing pathogenesis and risk classification development for AML patients over the age of 60 (**Poster presentation at the FASEB hematological malignancies meeting 7/2021**; **grant proposal to NIH**). All projects utilize de-identified data files and no HIPAA sensitive information is stored on Rivanna” |