

# Interoperable Workflows Using Workflow Management Systems and Singularity Containers

Wednesday, October 4, 2023, 11 am – 5 pm Eastern time

Oct 2, 2023

## General Information

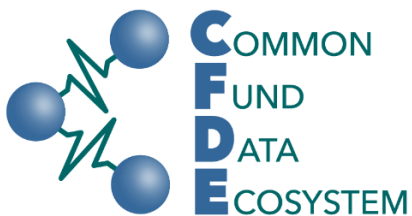
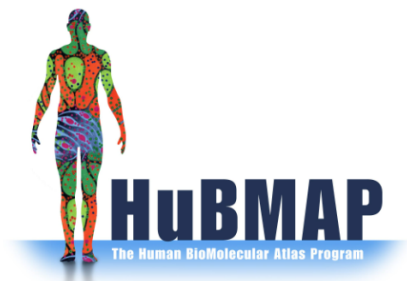
- ★ We will use this Google Document to share information with you. This document is not static and will be updated as needed.
- ★ **Register on the Slack workspace as soon as possible.** To register, click [here](#). When joining the Slack channel use the full name you used to register for the workshop.
- ★ Materials and lectures will be added to the document.
- ★ If you don't have an **ACCESS/XSEDE** account, please follow the instructions in this link <https://identity.access-ci.org/new-user> and get an account and share your username with us using this form: <https://forms.gle/eD3HkbcXDd9dKQqHA> by the end of today as we need this information to activate your account for the workshop.
- ★ We will be using Zoom for video conferencing.
- ★ We will be available on Slack to chat with attendees. Please feel free to use this workspace to leave comments, ask questions or just to say hi.
- ★ Zoom meetings are going to be recorded and will become available on YouTube after the workshop.
- ★ **Please fill out this survey: <https://forms.gle/tw5PahwgiE4siLNM9>**  
It takes only a few minutes and will help us improve our next workshop.
- ★ If you have any problems with anything at all during the meeting, please leave a message in the #general channel on Slack
- ★ For more details see:  
<https://www.psc.edu/events/workshop-interoperable-workflows-using-cwl/>

## Instructor

[Iván E. Cao-Berg](#)

Ivan is a Research Software Specialist in the Biomedical Applications Group





## Agenda

Schedule is in Eastern Time (EDT).

| Time (EDT)* | Topic                                                                                                                                                                                                                                                                                                | Materials                                                                                  | Zoom Link                                                                                                                                                                           |
|-------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 11:00-12:30 | <b>Part 1: Elevating Scientific Computing with Singularity Containers</b> <ul style="list-style-type: none"><li>• Overview of Singularity Containers</li><li>• Singularity Container Sharing on Sylabs.io</li><li>• Container Creation and Building</li></ul>                                        | <a href="#">Slides</a><br><a href="#">Exercises</a><br><a href="#">Meeting recordings:</a> | <a href="https://cmu.zoom.us/j/99358430599?pwd=UG1YdDNXZEJkTmh1em1McDJNLzZNdz09">https://cmu.zoom.us/j/99358430599?pwd=UG1YdDNXZEJkTmh1em1McDJNLzZNdz09</a><br><br>Passcode: 111428 |
| 12:30-1:30  | Break                                                                                                                                                                                                                                                                                                |                                                                                            |                                                                                                                                                                                     |
| 1:30-2:45   | <b>Part 2: Streamlining Reproducible Data Analysis using Workflow Management Systems and Singularity Containers</b> <ul style="list-style-type: none"><li>• Introduction to Workflow Management Systems (WMS)</li><li>• Dive into Nextflow</li><li>• Dive into Snakemake</li><li>• Q&amp;A</li></ul> | <a href="#">Slides</a><br><a href="#">Exercises</a><br><b>Meeting Recording:</b>           |                                                                                                                                                                                     |
| 2:50-3:05   | Break                                                                                                                                                                                                                                                                                                |                                                                                            |                                                                                                                                                                                     |
| 3:05-5:00   | <b>Part 2: continued...</b> <ul style="list-style-type: none"><li>• Introduction to Common Workflow Language (CWL)</li><li>• Singularity Containers for Reproducibility</li><li>• Integrating CWL with Singularity Containers</li><li>• Q&amp;A</li></ul>                                            | <a href="#">Slides</a><br><a href="#">Exercises</a><br><b>Meeting Recording:</b>           |                                                                                                                                                                                     |

