



# HPC & Data Science Summer Institute Prep Day

Tuesday, July 30, 2024

9:00 am – 11:00 am (Pacific Time)

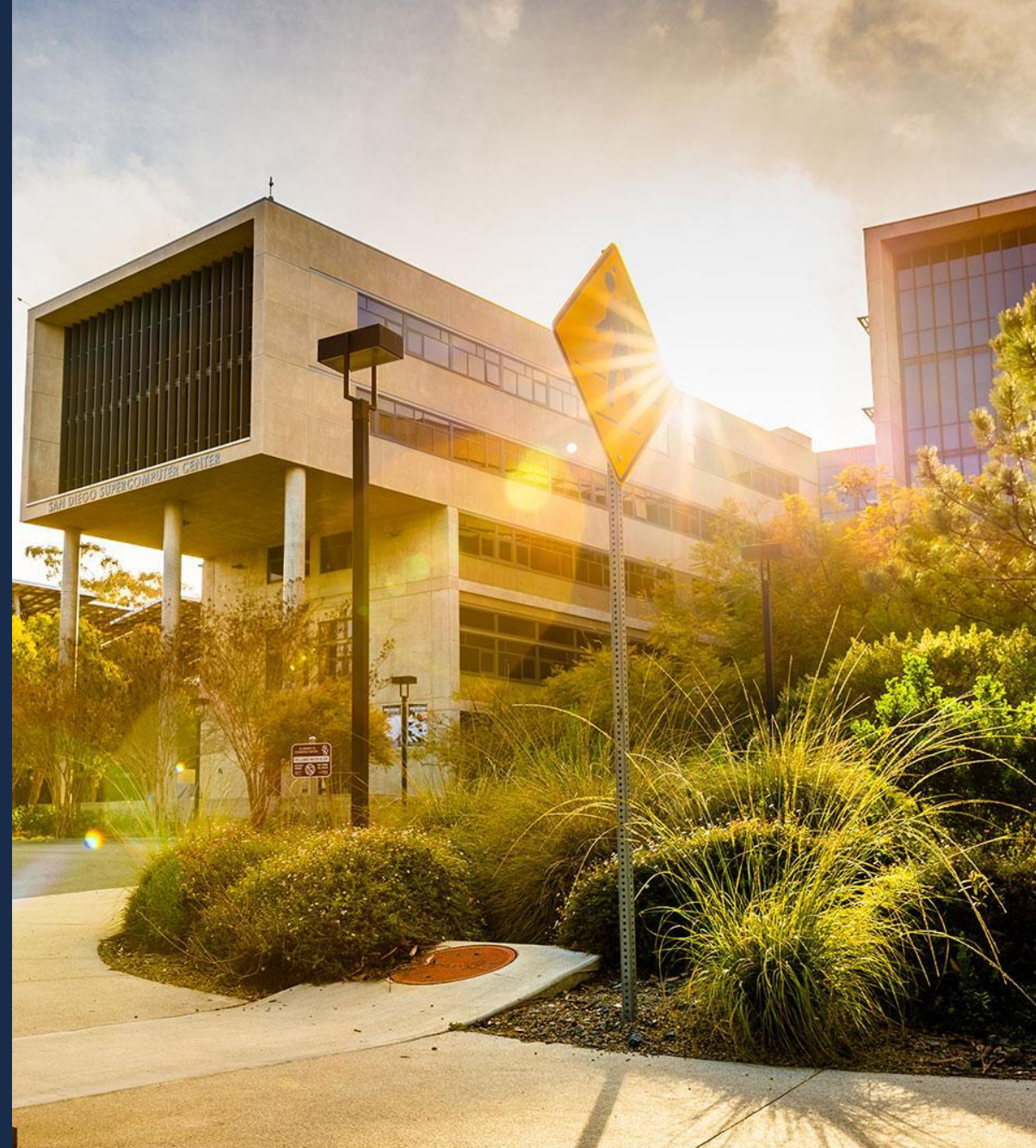
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SAN DIEGO SUPERCOMPUTER CENTER

UC San Diego

# Welcome

*Thank you for joining us today!*

- We will begin shortly after 9:00 am (Pacific Time)
- We will be tracking attendance, so please be sure your **FIRST** name, **LAST** name, and **INSTITUTION** is displayed
- Closed captioning is available. Click on the “CC” icon to enable/disable
- Prep day session will not be recorded







# HPC & Data Science Summer Institute Welcome

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# Agenda

- Can be found by navigating on the 2024 HPC and Data Science Summer Institute webpage
  - <https://na.eventscloud.com/website/70797/agenda/>
- **Session 1 (Monday-Tuesday) Non-programming skills**
  - Parallel computing concepts, intermediate Linux and bash scripting, hardware essentials, batch script execution, data management, cybersecurity, interactive computing, how to get help, code porting and installation, high throughput computing and Linux tools for file processing.
- **Session 2 (Wednesday-Friday) Programming skills**
  - Performance tuning and optimization, profiling, parallelizing software using MPI and OpenMP, Git/GitHub, GPU programming with CUDA, Python for HPC, deep learning and scalable machine learning.

# HPC & Data Science Summer Institute **Logistics**

Cindy Wong

*Events Specialist, Program & Events at SDSC*

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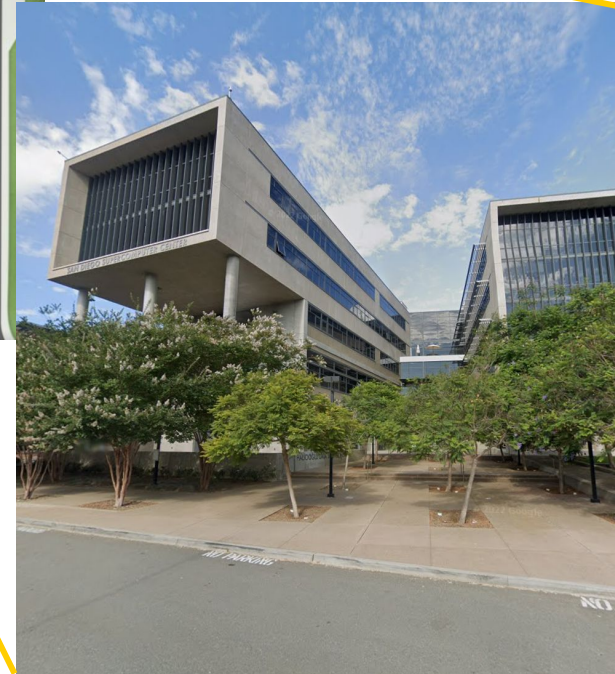
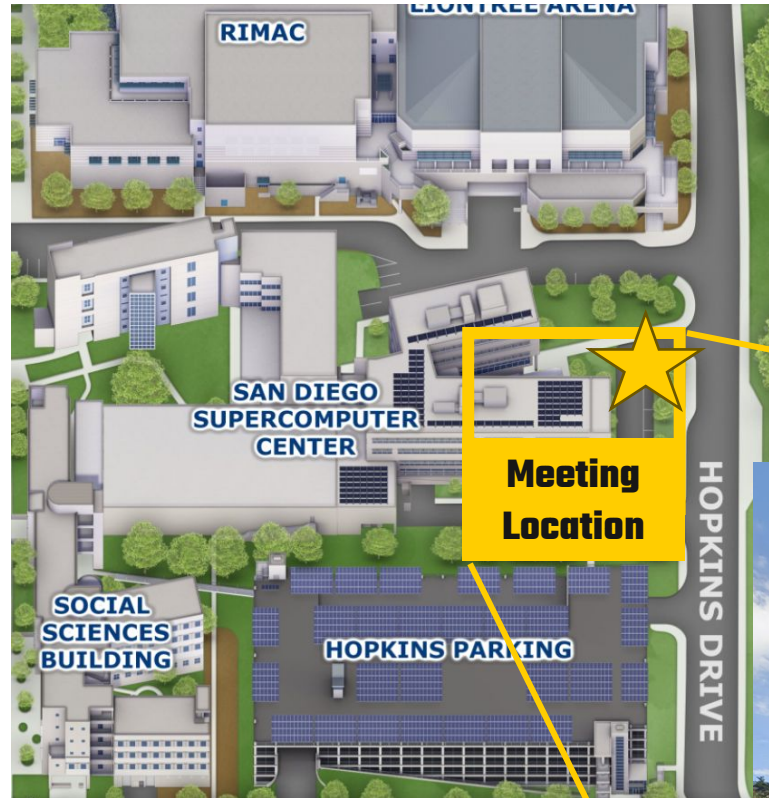
# Logistics

- **Meeting Location**
  - Parking Location
  - Meeting Entry
- **Purchasing a Parking Permit**
- **Room & Board Scholars**
  - Check-in/out location
  - Meals
  - Parking
- **GitHub & Slack**
- **Training Account**



# Meeting Location

- UC San Diego  
San Diego Supercomputer Center  
(SDSC) Auditorium
- Address: 9836 Hopkins Drive, La Jolla CA, 92093
- Google:  
<https://maps.app.goo.gl/ZeffcGEGkFQKRWCs>



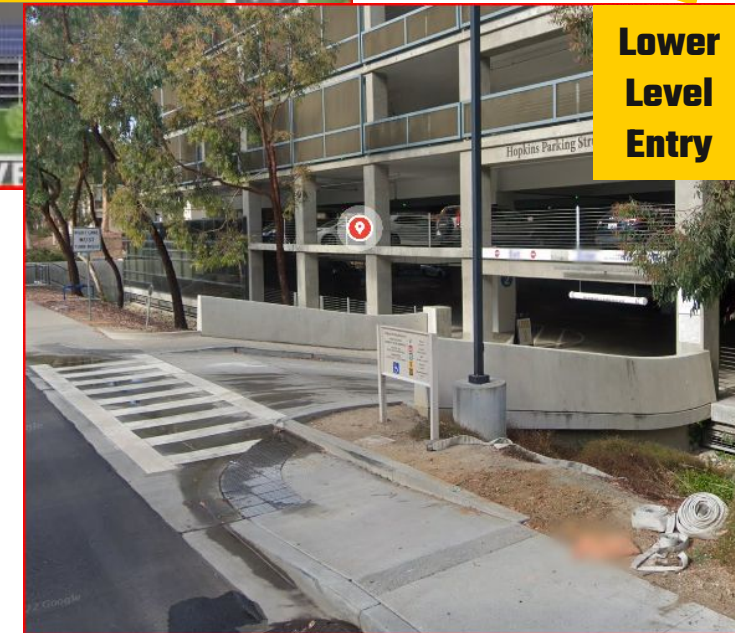


# Parking

- Closest: Hopkins Parking Structure

<https://goo.gl/maps/L4A4Ufwxosx9XXNZ7>

- Parking permit required





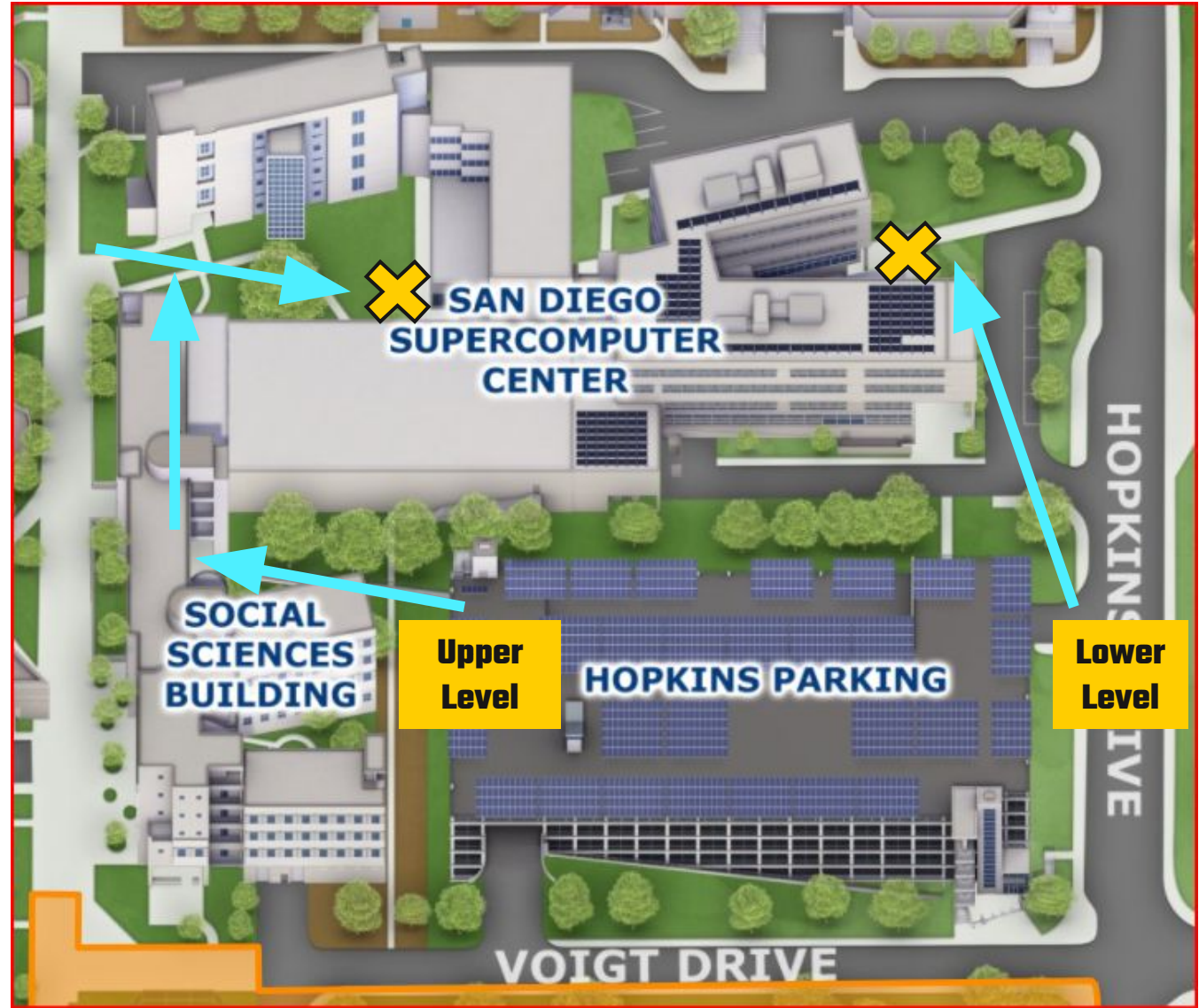
# Parking – Alternate Location

- Alternate: Pangea Parking Structure  
<https://goo.gl/maps/aJnWNCUMzb5kuB696>
- Parking permit required



# Meeting Entrance

- SDSC Auditorium located on the UC San Diego campus
- Address: 9836 Hopkins Drive, La Jolla CA 92093-0505
- Location:  
<https://goo.gl/maps/tGtzXfVrLEsky5uJ7>
- Directional signage will be posted closer to meeting location







# **HPC & Data Science Summer Institute** **Purchasing a Parking Permit**

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# Parking Permit

- Purchase your permit through the **ParkMobile App**
- Details:  
<https://transportation.ucsd.edu/visit/visitor/conference.html>
- Rates:
  - 1-day “B” space: \$8/day (#47800)
  - 7-day “B” space: \$42
    - *Available via online portal only*

## Parking for Campus Conference Attendees

If you are attending a conference on the UC San Diego campus, you can choose from these parking options. Online permits are available June 17 through Sept. 9, 2024.

### Pay with the ParkMobile App

#### 1-Day B

- Rate: \$8/day
- Valid in these spaces: **S** and **B**, 7 a.m. – 11 p.m.

### Access Your ParkMobile Account

Most people prefer to access ParkMobile using their mobile app; however, you can also manage your ParkMobile account or pay for parking on the ParkMobile website. Log into your [ParkMobile account](#).

### Get the ParkMobile App



### How to Pay

- Conference Services guests park in any **B** or **S** parking space in a campus parking lot.
- Enter zone number 47800.
- Confirm your information, including location, license plate, time and cost.

### Other Payment Options

We recommend using the ParkMobile app for the best virtual access experience. If you are unable to use the app, you can use this [web option](#).

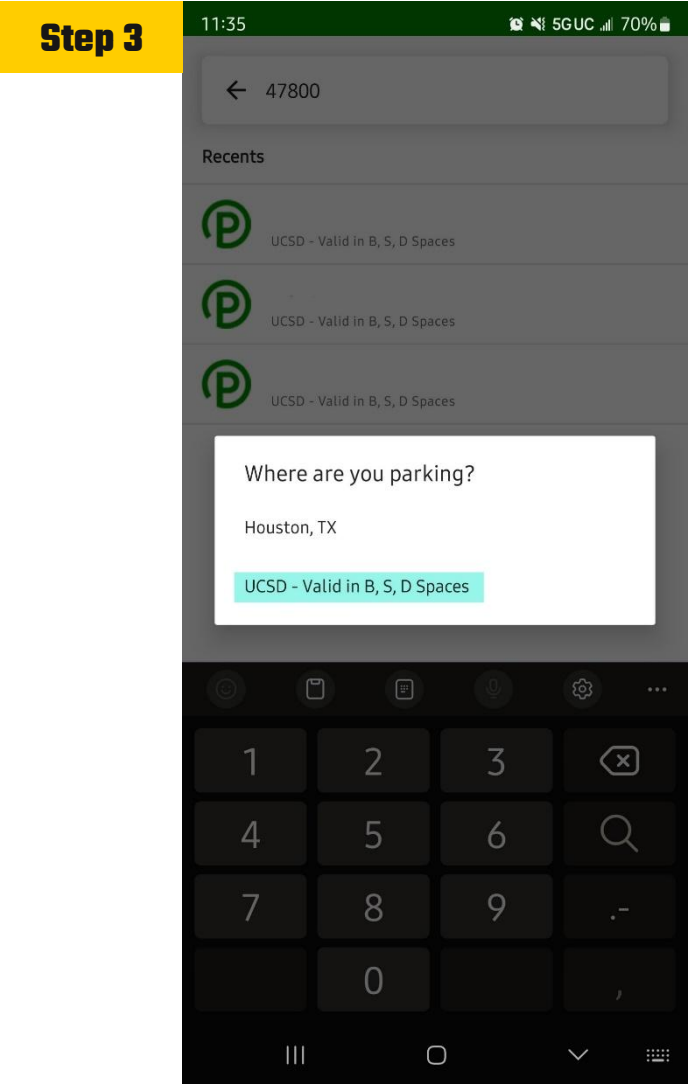
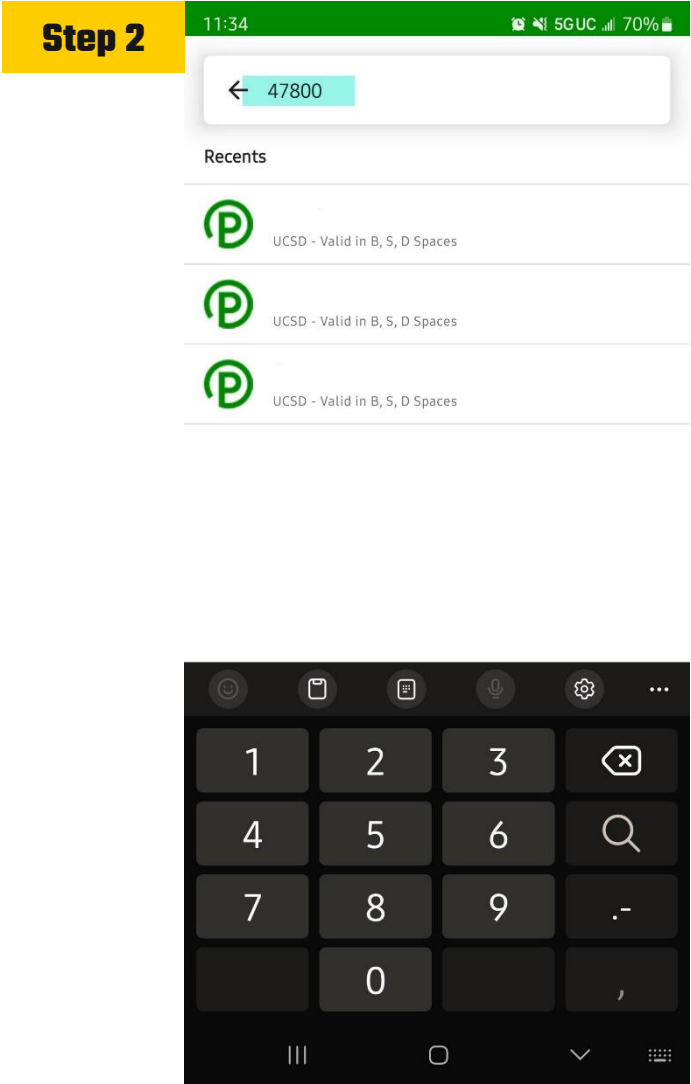
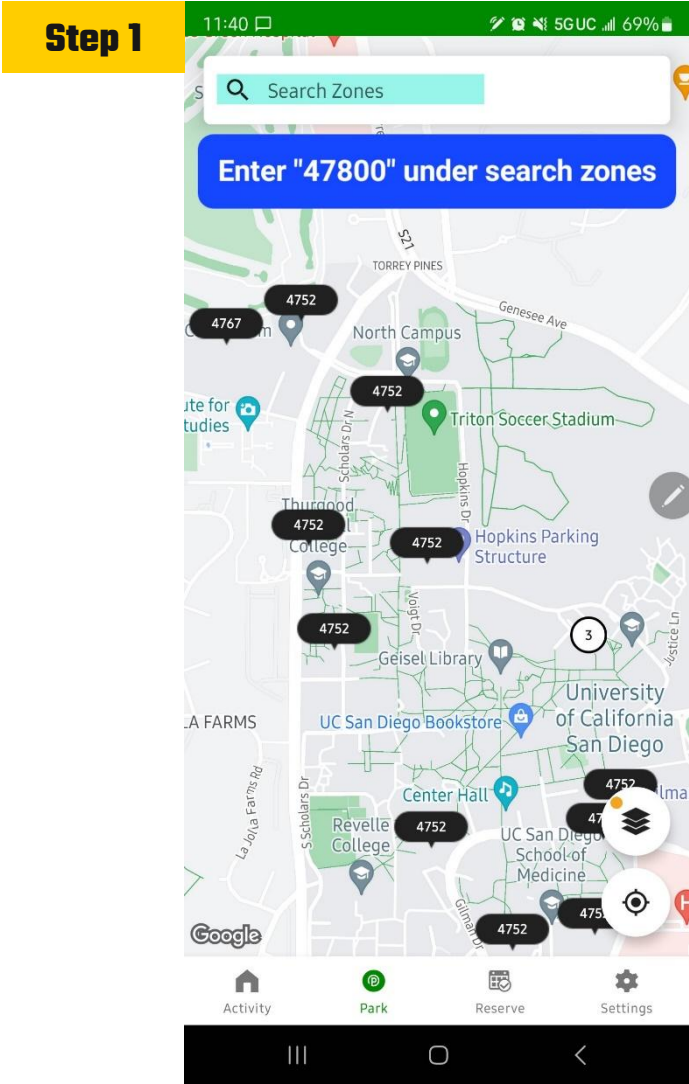
### Online Parking Permits

#### 1-Day B

- Rate: \$8/day
- Valid in these spaces: **S** and **B**, 7 a.m. – 11 p.m.



# Purchasing permit Park Mobile App



## Step 4

11:35 5G UC 70%

←

Zone #  
**47800**  
UCSD - Valid in B, S, D Spaces

Accepted Payment Methods

AM EX VISA DISCOVER UCB PayPal G Pay

Parking Duration

**i Flat Rate Pricing In Effect**  
There is currently one rate available for this location.  
You may park your vehicle for 12hrs 25m until 12:00 AM, Aug 02.

Select Duration

Your Vehicle + Add New

Choose a Parking Rate

Maximum parking time

## Step 5

11:35 5G UC 70%

← Zone # 47800

Zone #  
**47800**  
UCSD - Valid in B, S, D Spaces

Accepted Payment Methods

AM EX VISA DISCOVER UCB PayPal G Pay

Parking Duration **\$8.00**

**i Flat Rate Pricing In Effect**  
There is currently one rate available for this location.  
You may park your vehicle for 12hrs 25m until 12:00 AM, Aug 02.

**12 25**  
Hours Minutes

Your Vehicle + Add New

**Proceed To Checkout - \$8.00**

## Step 6

11:40 5G UC 69%

← Confirm and Pay

**Location Details**

Zone  
# 47800 (UCSD - Valid in B, S, D Spaces)

**Vehicles**

License Plate Number  
Double check this!

**Duration**

Total Time  
12 Hours 19 Minutes

End Time  
Aug 1, 11:59 PM

**Payment Method**

G Pay Google Pay

**Price Details**

Parking Subtotal \$8.00  
Total Cost **\$8.00**

**Buy with G Pay**





# **HPC & Data Science Summer Institute** **Room & Board Scholars**

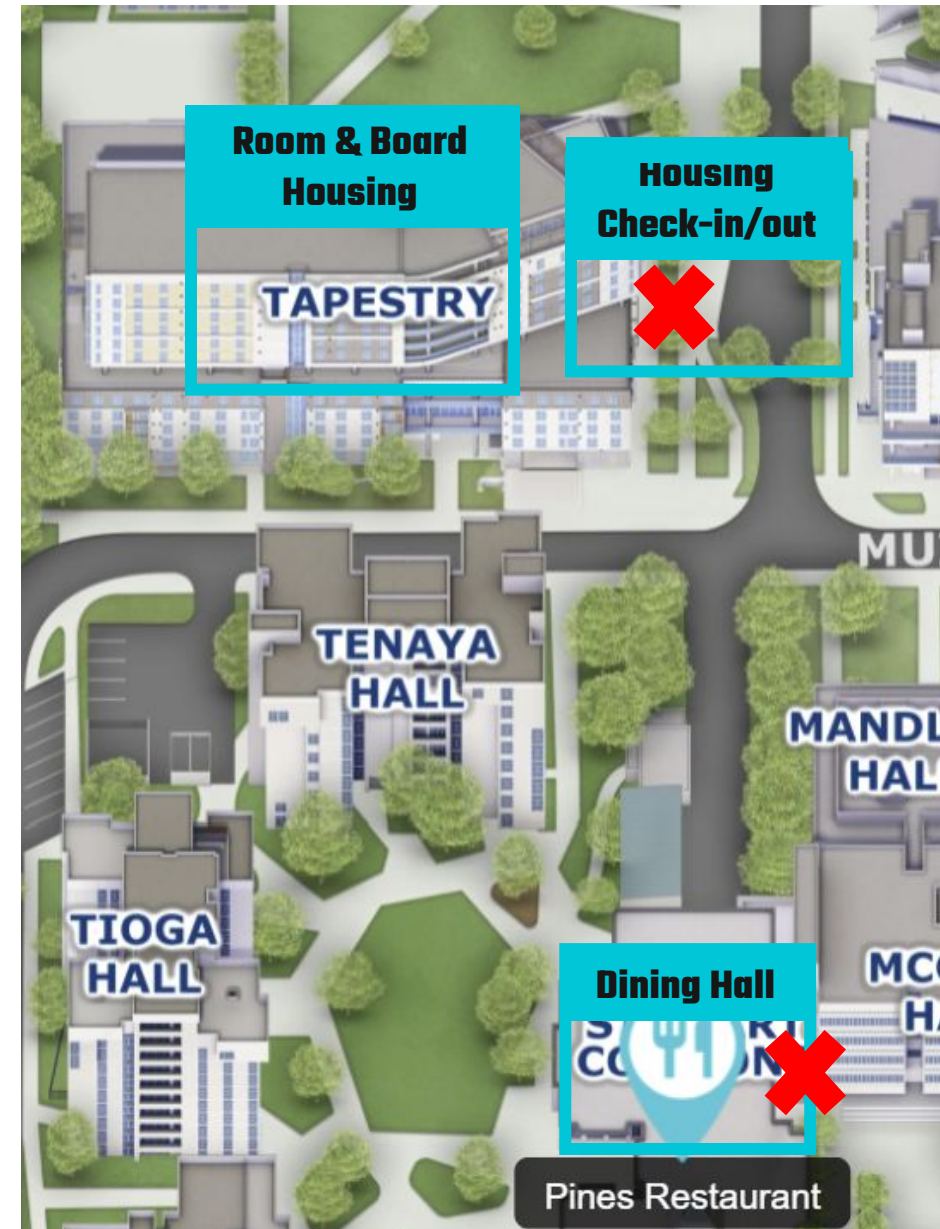
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# Room & Board Housing and Check In/Out

- Tapestry, Sixth College, North Torrey Pines Living Learning Neighborhood
  - Address: [9610 Scholars Drive North](#)
- *The Hospitality Information Desk is located on the Southeast corner of the Tapestry Building, across from Sixth Market.*

- Check-in Date and Time:
  - Sunday, Aug 4, between noon - 8pm (Pacific Time)
- Check-out Date and Time:
  - Friday, Aug 9, by 11:00 am (Pacific Time)



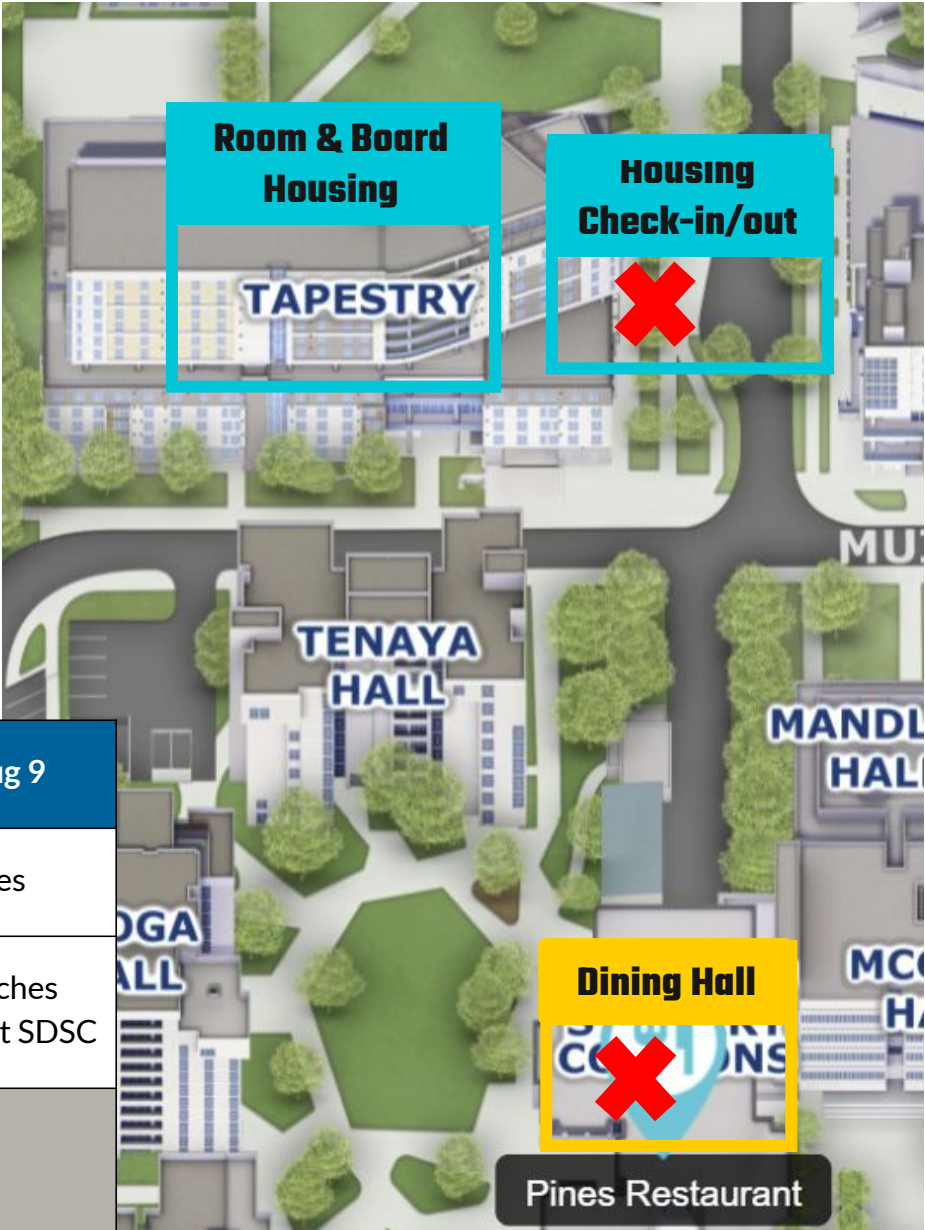


# Room & Board

## Dining Location & Schedule

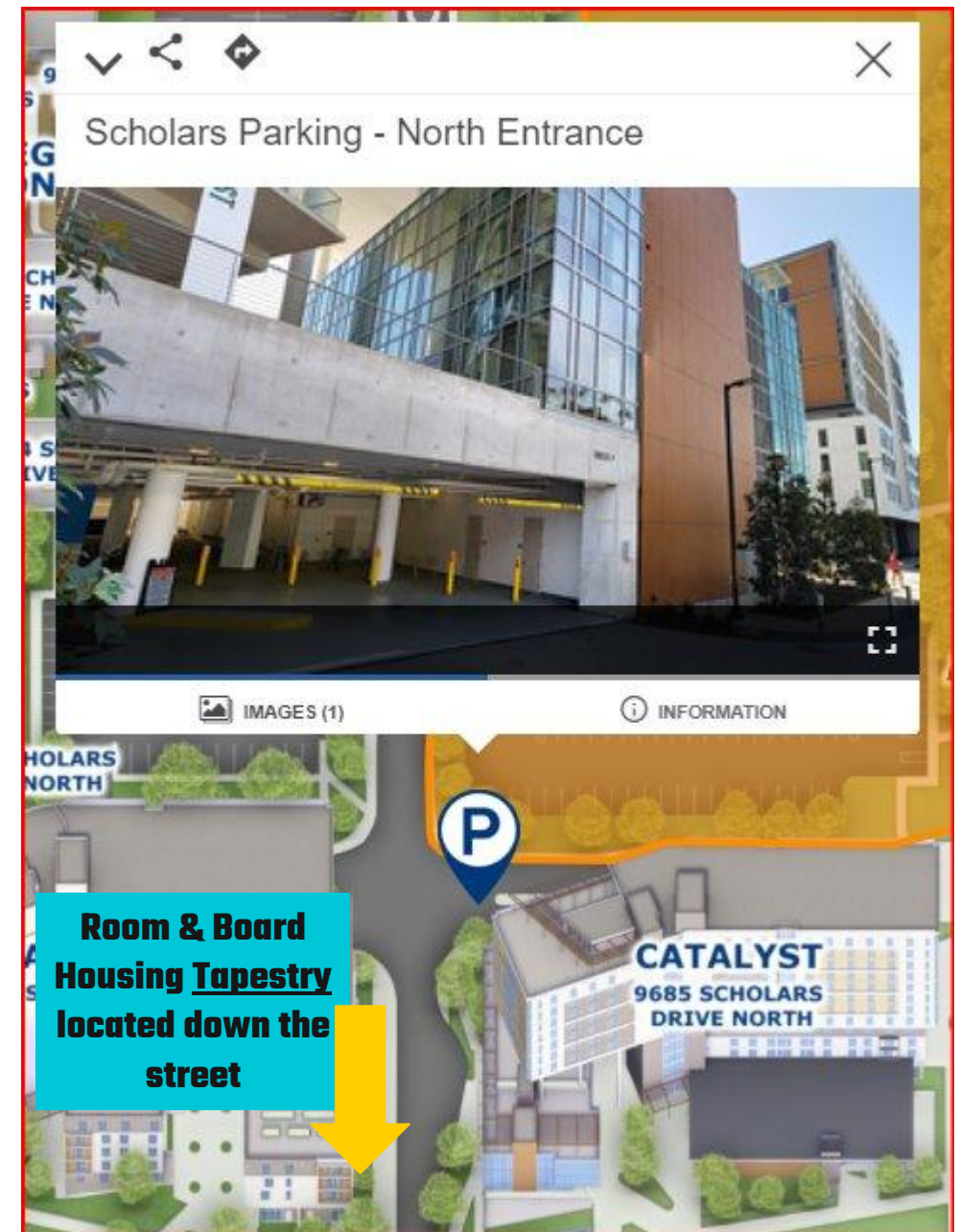
- Pines at Muir College
  - Address: [9545 Scholars Drive North](#)
- Meal Hours:
  - Breakfast Time(s): 7:15 am - 8:00 am
  - Lunch Time(s): 12:30 pm - 1:15 pm (except when with the HPC & DS Group)
  - Dinner Time(s): 6:15 pm - 7:00 pm

Meal Type	Sun., Aug 4	Mon., Aug 5	Tues., Aug 6	Wed., Aug 7	Thurs., Aug 8	Fri., Aug 9
Breakfast	No	@Pines	@Pines	@Pines	@Pines	@Pines
Lunch	No	@Pines as a Group	@Pines as a Group	@Pines as a Group	@Pines as a Group	Box lunches provided at SDSC
Dinner	@Pines	@Cutwater Tasting Room	@Pines	@Pines	@15th Floor (on-campus)	No



# Parking for R&B

- Closest: Scholars Parking – North Entrance  
<https://goo.gl/maps/cGSdwCf75hp8igsy9>
- Parking Permit Required





A nighttime photograph of the San Diego Supercomputer Center building, a modern multi-story structure with large glass windows and concrete pillars. The building is illuminated by streetlights, and the sky is dark blue. The text "HPC & Data Science Summer Institute" is in white, and "GitHub & Slack" is in yellow, both in a bold sans-serif font.

# HPC & Data Science Summer Institute

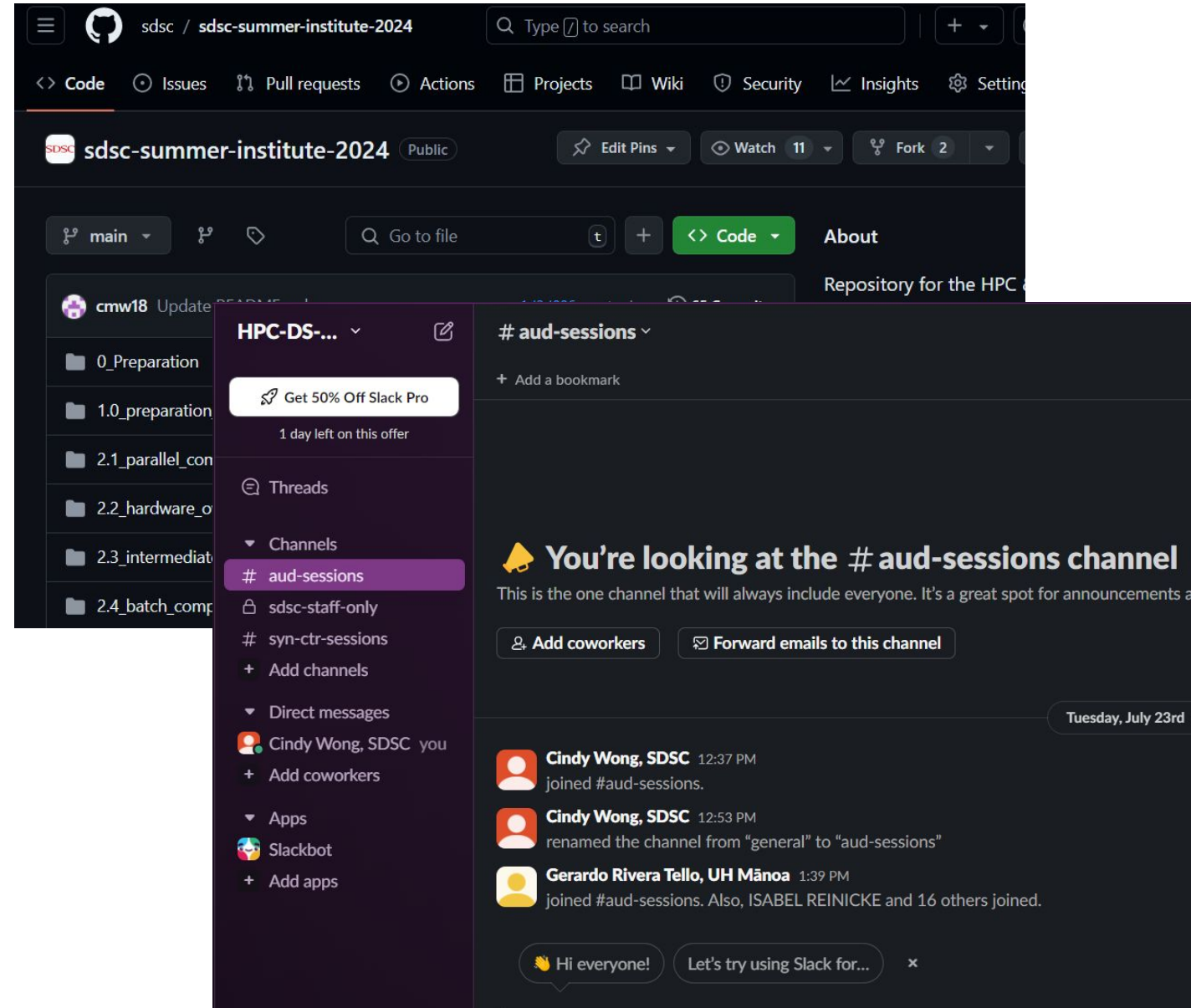
# GitHub & Slack

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# GitHub & Slack

- **GitHub:**  
<https://github.com/sdsc/sdsc-summer-institute-2024>
  - Make sure you review 0\_Preparation
- **Slack:** Join the HPC-DS-SDSC-2024 workspace
  - Channels
    - aud-sessions
    - syn-ctr-sessions







# HPC & Data Science Summer Institute Training Account

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UC San Diego

# Training Account

## HPC & DS 2024 Summer Institute: Account Set-Up



consult@sdsc.edu

To Wong, Cindy



Reply



Reply All



Forward



Mon 7/29/2024 12:15 PM

Your personalized account information is given below.

Your password is made available through a one-time URL. Be sure to securely record your password immediately since you will not be able to access the URL a third time.

The one-time URL will expire after 14 days, or after 2 viewings, whichever comes first.

Username:



URL to retrieve password:



As a reminder, we are asking all attendees to use the training accounts that we are providing, even if you already have your own account. This will minimize problems related to custom configurations (e.g. environment variables, choice of shell, etc.) that may cause some of the hands-on examples to break.

This training account may be used:

- \* Via SSH directly to login.expense.sdsc.edu
- \* Via a special page on the Expanse Portal: <https://portal.expense.sdsc.edu/training>

For any account user issues/questions, contact [consult@sdsc.edu](mailto:consult@sdsc.edu).





# Questions?

- Contact [events@sdsc.edu](mailto:events@sdsc.edu) for any logistical related questions.
- Contact [consult@sdsc.edu](mailto:consult@sdsc.edu) for training account related questions

**Stop here**



# Don't forget to pay for parking!

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<https://transportation.ucsd.edu/visit/visitor/conference.html>
- Rates:
  - 1-day “B” space: \$8/day
  - *Overnight: check with Housing Front Desk*

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# SDSC CIML Instructors



**Andreas Goetz Ph.D.**  
Research Scientist, Principal  
Investigator



**Mai Nguyen Ph.D.**  
Lead for Data Analytics



**Robert Sinkovits Ph.D.**  
Director of Education and  
Training



**Paul Rodriguez Ph.D.**  
Computational Data Scientist



**Marty Kandes Ph.D.**  
Computational and Data Science  
Research Specialist



**Peter Rose Ph.D.**  
Director for Structural Bioinformatics  
Laboratory



**Mary Thomas Ph.D.**  
Computational Data Scientist and  
HPC Trainer



# Agenda – Day 1 AM

8:00 am - 8:30 am	<b>Light Breakfast &amp; Check-in</b> Location: SDSC Auditorium
8:30 am - 9:30 am	<b>2.1 Welcome and Introductions</b> Mary Thomas, Computational Data Scientist & Director of the CIML Summer Institute
9:30 am - 10:15 am	<b>2.2 Parallel Computing Concepts</b> Robert Sinkovits, Director of Education and Training <i>We will cover supercomputer architectures, the differences between threads and processes, implementations of parallelism (e.g., OpenMP and MPI), strong and weak scaling, limitations on scalability (Amdahl's and Gustafson's Laws) and benchmarking.</i>
10:15 am - 10:30 am	<b>Break</b>
10:30 am - 11:15 am	<b>2.3 Getting Started with Batch Job Scheduling</b> Marty Kandes, Computational and Data Science Research Specialist <i>Batch job schedulers are used to manage and fairly distribute the shared resources of high-performance computing (HPC) systems. Learning how to interact with them and compose your work into batch jobs is essential to becoming an effective HPC user.</i>
11:15 am - 12:30 pm	<b>2.4 Data Management and File Systems</b> Marty Kandes, Computational and Data Science Research Specialist <i>Managing data efficiently on a supercomputer is important from both users' and system's perspectives. We will cover a few basic data management techniques and I/O best practices in the context of the Expanse system at SDSC.</i>
<b>12:30 pm - 1:30 pm</b> <b>Lunch @ Cafe Ventanas</b>	

# Agenda – Day 1 PM

1:30 pm - 3:00 pm	<b>2.5 GPU Computing - Hardware architecture and software infrastructure</b> Andreas Goetz, Research Scientist & Principal Investigator <i>Brief overview of the massively parallel GPU architecture that enables large-scale deep learning applications, access and use of GPUs on SDSC Expanse for ML applications</i>
3:00 pm - 3:15 pm	<b>Break</b>
3:15 pm - 4:45 pm	<b>2.6 Software Containers for Scientific and High-Performance Computing</b> Marty Kandes, Computational and Data Science Research Specialist <i>Singularity is an open-source container engine designed to bring operating system-level virtualization to scientific and high-performance computing. With Singularity you can package complex computational workflows --- software applications, libraries, and data --- in a simple, portable, and reproducible way, which can then be run almost anywhere.</i>
4:45 pm - 5:00 pm	<b>Q&amp;A, Wrap-up</b>
5:00 pm - 5:30 pm	<b>SDSC Data Center Tour</b>
<b>5:30 pm - 7:30 pm</b> <b>Evening Reception - UC San Diego, Seventh College, 15th Floor</b>	





# Questions?

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- Contact [consult@sdsc.edu](mailto:consult@sdsc.edu) for training account related questions