

# Introduction to Scientific and Technical Computing

## SDS 335/394

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### **Lecture 1: Introduction to Course**

- We tell you about the class (go over syllabus)
- Set-up TACC accounts, access canvas, piazza
- You tell us about yourselves, ask us questions

# Instructors:

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## **Dr. Damon McDougall**

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Office hours: After/before each class at FAC or by appointment.

## **Dr. Anne Bowen**

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Teaching Assistant:

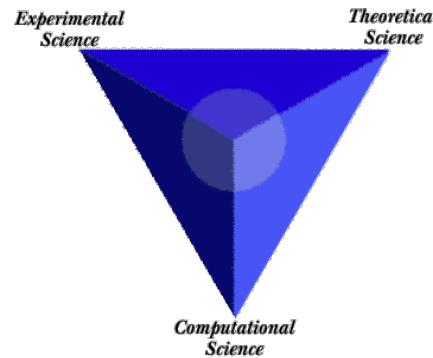
## **Udaivir Yadav**

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Office hours: TBD

# Scientific and Technical Computing (STC)

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- Computing is the third pillar of science, complementing both experiment and theory. The modern scientist is required to use programs effectively. STC is an introduction to techniques and practices of scientific and technical computing.
- This course is NOT:
  - Computer Science class, Mathematics class, Programming Language class, Numerical Methods class

# Specific Learning Objectives

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- Lecture sessions will cover computer architecture including parallel architectures, machine arithmetic, the sources or large computational problems and the techniques for solving them efficiently.
- Practical topics covered will concern the development and maintenance of scientific software. We also include lectures of scientific libraries and analysis, post-processing and visualization tools and data analysis.

# Course Assumptions/Prerequisites

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- Students will be expected to have mastered the material taught in SSC 222/292 (ie we don't teach any programming skills, but assume you have some experience coding) and Mathematics 408D or 408M (ie we will apply numerical methods that assume you are familiar with the theory) these courses are listed as requirements but they have not been enforced during the registration process.

A partial list of these skills include:

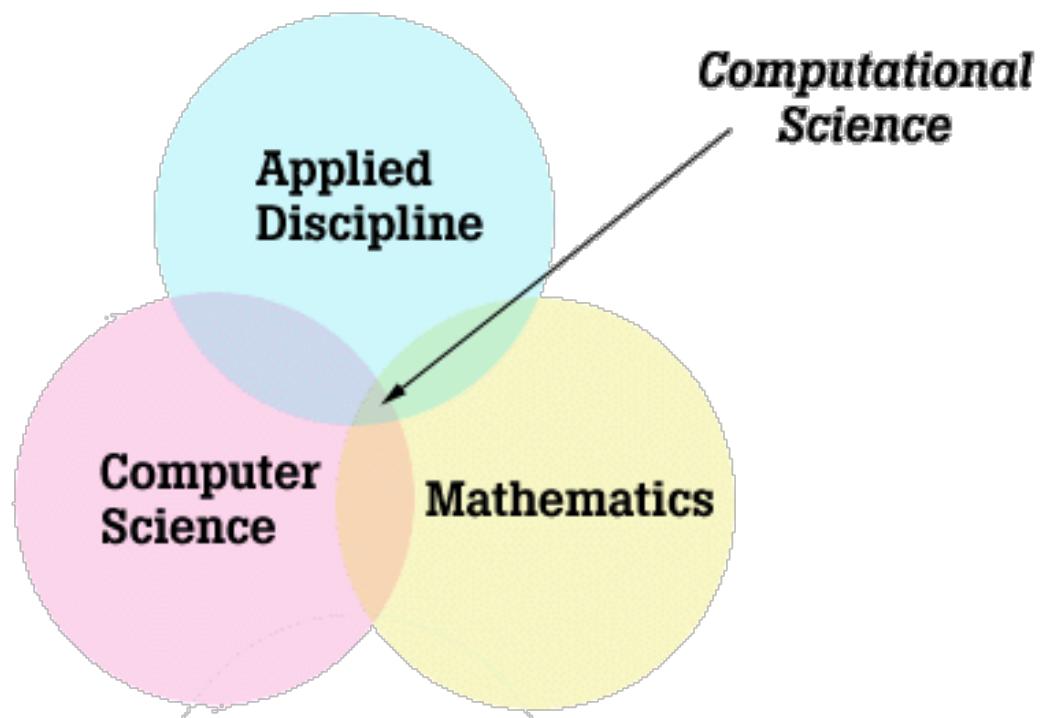
- Programming experience, working understanding of C/C++ or Fortran, knowledge of common data types and structures, control structures, algorithms.
- An understanding of multivariate calculus and matrix operations, Parametric equations, sequences, functions of several variables, Infinite series, power series, Vectors, vector calculus, Partial derivatives, gradients, and multiple integrals.

Missing any of the prerequisites above is not a reason to drop the course, but please plan on allocating time to catch up on these topics.

# By the end of this course, students will:

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- Understand the **architecture** of the most common research compute clusters.
- Be familiar with programming techniques and tools in a **scientific computing** environment.
- Be able to utilize **numerical scientific libraries** in applications and an awareness of coding practices that affect **performance**.
- Be able to **analyze and visualize scientific data** and understand data intensive computing.



# weeks 1-7: programming techniques and tools in a **scientific** **computing** **environment**

- Schedule

Week	Main Topics	Description
1, Th	Introduction to course	Syllabus, TACC account, canvas and piazza account
2, T	Types of computers	Architectures (laptop, cluster, supercomputer). What computers look like and how the pieces interact
2, Th	Unix tools and environment, part 1	How to interact with a linux box and edit files
3, T	Unix tools and environment, part 2	Using TACC systems. ssh and remote access. How to transfer files and manipulate a machine remotely
3, Th	Unix tools and environment, part 3	Advanced Unix, tips and tricks
4, T	Version control	Overview of version control systems, Using Git
4, Th	Version control	
5, T	Representation of numbers	Floating point error and related numerical representation issues with computers
5, Th	Computing environments	Machines, operating systems, tools, differences
6, T	Compilers	What they are, how they work, and why we need them, how to use them
6, Th	Compilers	
7, T	Make	An introduction to build automation tools and how to use them

- Schedule

weeks 8-12:

**numerical scientific libraries** in applications and an awareness of coding practices that affect performance

7, Th	Scientific libraries	BLAS, LAPACK and FFTW
8, T	Scientific libraries	
8, Th	Debugging	How to find bugs, and software to use for doing this
9, T	Performance analysis	How to find performance bottlenecks and bugs, and software to use for doing this
9, Th	Software testing/documentation	Best practices in software testing and documentation
10, T	Software testing/documentation	Best practices in software testing and documentation Overview, MPI, OpenMP
10, Th	Intro to parallel computing	
11, T	Intro to parallel computing	Overview, MPI, OpenMP
11, Th	Scientific Data	What file formats are available, what metadata is, best practices for I/O on HPC systems
12, T	Computer graphics	Graphics pipeline, rendering, openGL and Matrix Transforms and Operations
12, Th	Numerical Linear algebra	Intro to Interactive Methods
13, T	Numerical Linear algebra	Intro to Interactive Methods

- Schedule

weeks 14,15:

**analyze and  
visualize scientific  
data** and understand  
data intensive  
computing

13, Th	No Class Thanksgiving Holiday (Thursday Nov 23)	
14, T	Intro to Sci Vis	Introduction to Data Vis, Sci Vis and Paraview
14, Th	Intro to Sci Vis	
15, T	Data analysis/vis tools	Introduction to Info Vis tools (python/matplotlib, RShiny, d3)
15, Th	Immersive/Interactive visualisation	Tools/Libraries for data explorations with VR/AR

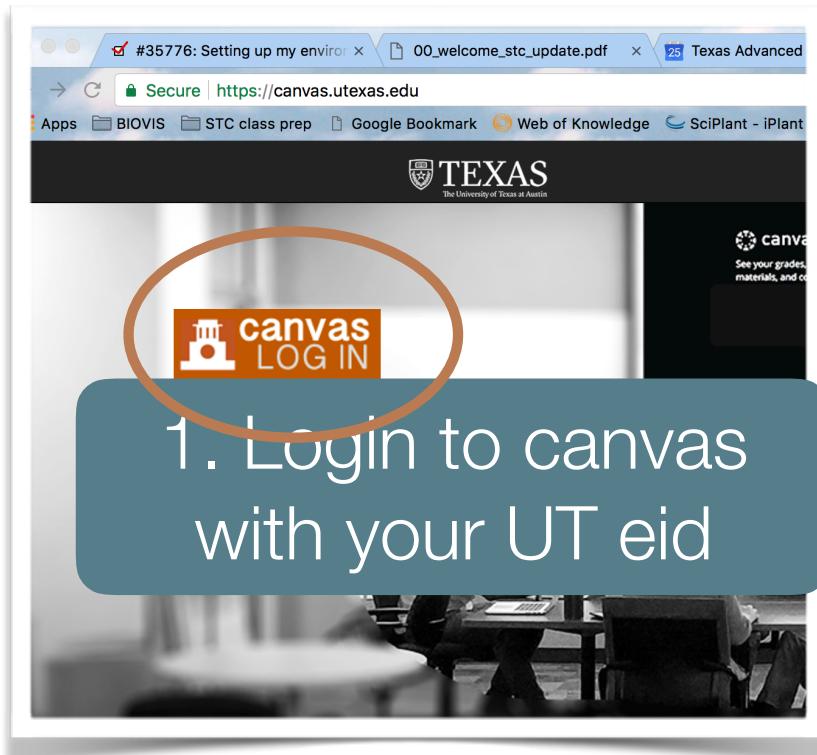
# Grading/Class Format

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- A class will consist of a lecture and often some time for lab tutorials. 5 assignments will be given at the end of topics, and will be due at assigned times. All assignment will be assessed a 1 point penalty for each hour late. 5 quizzes will be given on assigned days (in syllabus and on canvas)
- 20% Quizzes
- 50% Homework
- 30% Final project
- We reserve the right to curve the grades to the benefit of the student. Final grade will be given according to the scale of
  - A: [1000, 900], B: [800,900], C: [700,800], D: [600,700], F: below 600

# Canvas

<http://canvas.utexas.edu>



<http://canvas.utexas.edu>

A screenshot of a web browser window showing a Canvas course page. The left sidebar has icons for canvas, user profile, clock, and help. The main content area displays a message "New Canvas Workshops!!" addressed to "UT Faculty and TAs," with a link to "New workshops and additional office hours here." A large blue callout bubble with a downward arrow points to the course list. Inside the bubble, the text reads "2. If you are enrolled, you should see the class listed." Below the bubble, a green course card is visible with the title "Fa17 - SCIENTIF & TECHNICAL C..." and "SDS 335 Fall 2017" along with edit and message icons.

# Set up your TACC account

- Right now:
  - ✓ Go to [portal.tacc.utexas.edu](http://portal.tacc.utexas.edu)
  - ✓ click “create a TACC Account”
  - ✓ fill out form
  - ✓ respond to e-mail verification request
  - ✓ Send email with your name, eid and TACC username to [damon@tacc.utexas.edu](mailto:damon@tacc.utexas.edu)
- We will then add your account to the project of this course, so you can login to TACC systems

The screenshot shows a web browser window with several tabs open at the top. The active tab is 'Calendar - adb@tacc.utexas.edu'. Other tabs include 'Cornell Virtual Workshop' and 'Shared with me - Google D...'. Below the tabs, there's a toolbar with links to NPR, KUT, BBC News, Good News, Inspiring..., How to Cook Everything, KXAN, and a checked item '#35776: Setting'. The main content area has a blue header with the word 'TAC' partially visible. A navigation bar below it includes 'STATION', 'TRAINING', 'CONSULTING', and 'ABOUT'. To the right of the navigation bar is a 'Sign In' link. The main body of the page features a section titled 'Log in to the TACC User Portal' with two buttons: 'Log in with TACC Account' (green) and 'Log in with UT System / UT EID' (blue). Below this is a section for users without accounts, with a link to 'Create an account with their UT System Institution credentials'. A call-to-action button 'Create a TACC Account' is highlighted with a red oval. At the bottom, a large teal callout box contains the text: 'Note: The TACC User Portal is a centralized account for all systems: Portal and system username/password are the same.'

# piazza

The screenshot shows a web browser window with multiple tabs open. The active tab is for the Piazza platform at <https://piazza.com/utexas/fall2017/sds335394>. The browser's address bar also displays the URL. The Piazza page header includes the university name "The University of Texas at Austin". Below the header, there is a section for joining classes, specifically for "Fall 2017". It shows one class listed: "Class 1: SDS 335/394: STC 335/394 (edit)" with "Instructors: Damon, Anne Bowen - 2 Enrolled". A radio button labeled "Student" is selected, with a note stating "Instructor self-enrollment has been disabled for this class". There are also fields for "Class 2:" and "Class 3:", each with a delete icon. At the bottom of this section are buttons for "Add Another Class" and "Join Classes".

1. Go to (and bookmark): [piazza.com/utexas/fall2017/sds335394](https://piazza.com/utexas/fall2017/sds335394)
2. Join as: Student, Click “Add Class”
3. Activate and supply password
4. Read Welcome to Piazza

# Please Introduce yourself in the discussion form

- Click on “polls” in the upper right
- Please “read the question
- “New Post” and use your name as the “Summary” field

The screenshot shows a classroom discussion forum interface. At the top, there are navigation links: SDS 335/394, Q & A, Resources, Statistics, and Manage Class. Below this, a header bar includes a folder icon labeled "polls", tabs for "hw", "hw2", "hw3", and "hw4", and status indicators for "Unread", "Updated", "Unresolved", and "Following". A "New Post" button is highlighted with an orange circle. A search bar contains the placeholder "Search or add a post...". A filtering option "Filtering by: polls" is shown with a close button. The main content area displays a post from "Instr" titled "Introductions. Please post a ...". The post text reads: "Let's get to know one another in the discussion forum. It would be helpful to include a picture! What is your name". The timestamp "9:07 AM" and a reply icon are next to the post. To the right, there is a sidebar for "Class Signup Link" with an input field containing "john@email.com". Below the sidebar, sections for "Student Enrollment" show "0 enrolled" and "After you enter y".

# Introductions (please post on piazza)

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- What is your name?
- What is your major?
- What year are you in?
- What is your current research interest if any?
- What do you hope to take away from the class

- Introduction to piazza (tips)
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- Please use piazza for posting questions, and soliciting responses from other students, TA and Instructors.
    - organized in time
    - o in the left-hand side means you have not read the question/note/etc.
    - Use TAG (#...) to provide good searches
    - Create a hyperlink to another post by typing the “@“ symbol followed by that post’s number (e.g. @109)
    - Find a post’s number by looking in the URL, or by hovering over the arrow to the left of the question’s title in the question feed.

Any questions?