# $C^2$Exchange

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Dina Tandabany – Clark Atlanta University

Ahlam Tannouri – Morgan State University

Rachel Vincent-Finley – Southern University and A&M College

# Agenda

- Intro to C²Exchange Concept
- Course Development and Implementation
  - Modeling and Simulation – UPRM
  - Computational Linear Algebra – Morgan State
- Use Cases – SUBR
- Discipline Specific Minor – CAU
- Plans v Outcomes
- Q&A

# $C^2$Exchange

The C2Exchange is an NSF-funded pilot project exploring how to create a scalable network of institutions that can collectively offer CDS minors, concentrations, or certificates with minimal investment.

| | Institution Type | Enrollment | Undergraduate STEM Enrollment |
|---|---|---|---|
| **BCU** | Private HBCU | 3,992, 78% AA/Black; 62% female | 474 |
| **CAU** | Private HBCU | 3,093, 71% female; 86% AA/Black | 646 |
| **Morgan** | Public HBCU | 7,600, 84% AA/Black; 55% female | 2074 |
| **SUBR** | Public HBCU | 6,300, 93% AA/Black; 64% female | 1199 |
| **UPRM** | Public HSI | 13,481, 100% Hispanic; 46% female | 9,254 |

Provide resources to quickly build undergraduate CDS minor programs, certificates, credential offerings

- Shared Expertise
- Shared Courses
- Shared Course Management Platform
- Collaborative development, implementation, & management
- Facilitated access to advanced computing resources for student assignments

# $C^2$Exchange Courses

- Introduction to Modeling and Simulation
- Computational Chemistry
- Computational Linear Algebra
- Data Visualization

Area 1: Simulation and Modeling

Area 2: Programming and Algorithms

Area 3: Differential Equations and Discrete Dynamical Systems

Area 4: Numerical Methods

Area 5: Optimization

Area 6: Parallel Programming

Area 7: Scientific Visualization

Competencies http://hpcuniversity.org/educators/competencies/

# Plan versus Outcomes

- Course exchange
- Collaborative course development
- Common course management platform
- Blended delivery

- Exchange materials and expertise
- Collaborative course development
- Centralized course management platform interoperable with institution platforms
- Blended delivery

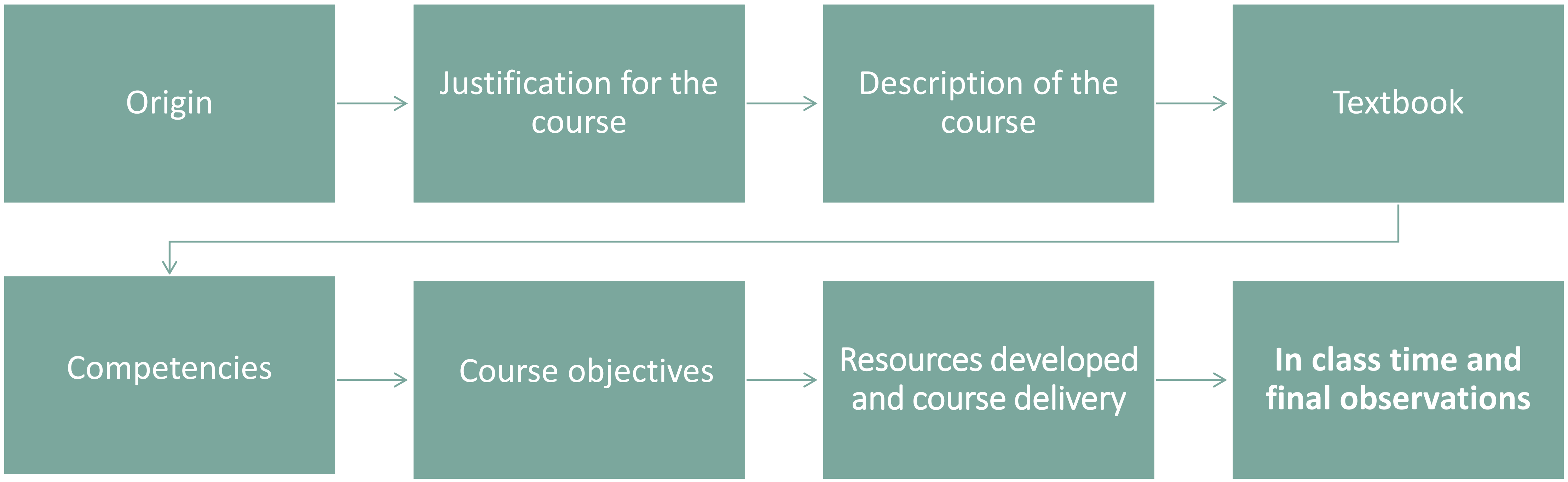
# Introductory coursein modeling, simulation, and computation

Experiences creating and implementing

By: Ana Gonzalez (anacarmen.gonzalez@upr.edu)

C[2]Exchange – UPR-M

# Experiences creating and implementing an introductory course in modeling, simulation, and computation.




(anacarmen.gonzalez@upr.edu)

# Origin

The course was developed as part of the $C^2$Exchange,

- ✓ an NSF-funded pilot project
- ✓ for Computational and Data Science Literacy curriculum exchange
- ✓ UPR-M is the co-lead institution together with Southern University for developing and offering the course.

(anacarmen.gonzalez@upr.edu)

# Justification

- ✓ Is there a gap in the curriculum?

# Justification

This is a foundational course that will allow to

- ✓ to infuse fundamental competencies of Computational Science to the undergraduate curriculum
- ✓ And at the same time attract students from all majors
- ✓ To make students aware that modeling and simulation have become an essential part of the research and development process in physics, biological, and social sciences.
- ✓ To prepare students to work in undergraduate research work.

# Course Description

*Introduction* to the principles of modeling and simulation;

progressive introduction of programming principles and skills using Python;

application of programming skills to the solution of different classes of models.

✓ The pre-requisites: College algebra, no programming experience

# Textbook

**Introduction to Modeling and Simulation with Matlab and Python**
, Steven I. Gordon and Brian Guilfoos, Chapman & Hall/CRC , ISBN: 13:978-1-4987-7387-4

- ✓ its approach discussing just in time concepts of programming
- ✓ An excellent review of the history of computer computational modeling and its contribution to the advancement of science.

# Course Objectives

1. Provide a background for more advanced modeling courses.
2. Provide the students with an introduction to modeling and its importance to current practices in different subject domains, like science, social sciences, and engineering.
3. Introduce programming principles and apply them to the solution of different classes of models.
4. Provide an overview of the modeling process and the terminology associated with modeling and simulation.
5. Study the mathematical representation of different classes of models.
6. Introduce techniques for fitting a function to an experimental data set.
7. Provide the opportunity for students to document the development and implementation of a model and presenting it in oral and written from.

## Competencies

## Upon successful completion of this course, what students will be able to do

- The course content focuses on meeting a set of basic modeling and simulation competencies that were developed as part of several NSF grants:

(http://hpcuniversity.org/educators/undergradCompetencies/)

# Competencies ( 4/15)
# (learning outcomes)

Upon successful completion of this course, students will be able to :

1. Explain the role of modeling in the sciences and engineering
    a. Describe the importance of modeling to science and engineering
    b. Describe the history and need for modeling
    c. Describe the cost effectiveness of modeling
    d. Describe the time-effect of modeling
2. Explain the terms of modeling in the sciences and engineering
    a. Define modeling terms
    b. List questions that would check/validate model results
    c. Describe future trends and issues in science and engineering
    d. Identify specific examples of modeling in science and engineering
3. Create a conceptual model
    a. Utilize the Modeling Process to identify key parameters of a model
    b. Estimate model outcomes
    c. Use Python to implement the mathematical representation of the model
4. Write code in a Programming language:
    a. Understand the concept of syntax in a programming language
    b. Describe the syntax of the programming language constructs
    c. Understand the difference between a compiled and interpreted language
    d. Write and run basic programs in the language of choice
    e. Understand how to de-bug code

# Competencies ( 3/15)

| Week | Topic | Assessment Activity/Evaluation/Homework/midterm/project | Learning Outcomes |
|---|---|---|---|
| 1 | Introduction to the course | Survey, syllabus | |
| 2 | Introduction to modeling; modeling concepts and definitions | | 1a,b,c,d<br>2a,b,c,d<br>13c<br>12c |
| 3 | Introduction to the Programming Environment | | 4a,b,c,d,e<br>9c |

# Resources developed and overall format of the course

## Digital resources developed

- Videos, (each video has its corresponding script)
- Activities to practice the concepts of each module
- Walkthrough
- Multiple choice questions
- Recorded demonstrations (screen captures)

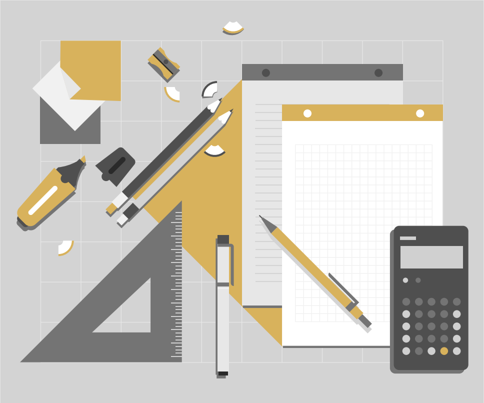
*Support of Resource Center for Distance Education*

- Moodle: Course Management System
- New material every Thursday
- Cycles of one week, at the end of the cycle quiz , exercise/coding, mini project ( oral presentation)

# Final Observations

- The course has been offered 2 times
  A. Blended mode
  B. online
- Plan : Develop a CDS concentration

# Next topic



- $C^2$Exchange – UPR-M

# Computational and Data Science Literacy Curriculum Exchange

C$^2$Exchange

Morgan State University

Ahlam Tannouri, PhD

Linear Algebra II-Mathematics for Machine Learning

**Collaborators: MSI**

Bethune-Cookman University

Clark Atlanta University

Morgan State University

Southern University A&M College

University of Puerto-Rico Mayaguez (UPRM)

Morgan State University is a co-educational institution and Maryland's largest HBCU. Each year, the university enrolls an average of 7,700 students in programs ranging from the baccalaureate level through the doctorate.

- Earned classification as a doctoral research institution by the Carnegie Foundation in 2007. Goal: Move from R3 (moderate research) to R2 (high research)

- Established Actuarial Science B.S. and Industrial and Computational Mathematics Ph.D. Programs in 2009

- Named a National Treasure by the National Trust for Historic Preservation in 2016
- Designated as **Maryland's *preeminent public urban research university*** in 2017

# Department of Mathematics

- Undergraduate programs leading to the following degrees:
  - Bachelor of Science (BS) in Mathematics (18): concentrations in pure mathematics and mathematics education
  - Bachelor of Science (BS) in Actuarial Science (24) **(Morgan is one of the two HBCUs in the nation and the only institution of higher education in the state of Maryland that offers the B.S. degree in ACSC**
- Graduate programs leading to the following degrees:
  - Master of Science (MS) in Mathematics
  - Master of Arts in Teaching Mathematics (3-2 program)

# Department of Mathematics (cont.)

- Graduate programs leading to the following degrees (cont.):
  - Doctor of Philosophy (Ph.D.) in Industrial and Computational Mathematics (ICM, 11) **(Morgan is one of the only three HBCUs in the nation that offers a Ph.D. degree in the mathematical sciences)**

Carnegie Hall, the oldest classroom building on campus **(Built in 1919)**

**Purpose:**

The creation of a pilot program for a curriculum exchange among five MSIs. Each institution will contribute and receive courses with the goal of providing a sequence of CDS courses that can form part of a certificate or minor program at each institution.

The exchange model facilitates the co-development of curriculum, the sharing of expertise across institutions for immediate implementation of some courses, and long-term capacity building for the implementation of CDS minors.

**Morgan State University Goal and Input for the $C^2$_Exchange**

1- Prepare the students at our institutions to become contributing members of the STEM workforce

2- Develop a Computational Linear Algebra Course to be offered locally and shared with MSI partners

3- Developing content for CDS in Data Science and Computational Mathematics.

# Linear Algebra II (Mathematics for Machine Learning)

*Catalog description:* ***Mathematics for Machine Learning and Data Science*** *- Three hours; 3 credits. Linear algebra is essential for understanding machine learning algorithms and analyzing large data sets. In this course, students will learn advanced linear algebra topics necessary for organizing information and data, and then using that information and data to solve problems.*
*Prerequisite: MATH 312 with a grade of "C" or better. (OFFERED AS NEEDED).*

Linear algebra is essential for understanding and creating machine learning algorithms and analyzing large data sets. In this course, students will acquire the linear algebra knowledge and skills necessary for organizing information and then using that information to solve problems.

Machine learning techniques required to improve the accuracy of predictive models, data science tools and libraries will be introduced. Special topics, applied and abstract are studied. Some topics include Hermitian Matrices, Quadratic Forms, Positive Definite Matrices, Canonical Forms, and Matrix decompositions. Meaningful applications will be introduced to build machine learning algorithms and predictive analytics methodologies.

# Course Goals:

1. Introduce the students to advanced topics form Computational Linear Algebra.
2. Give interpretation of matrix operations in the context of data
3. Apply Matrix decomposition algorithms to work with data
4. Provide the tools to build a broad mathematical foundation to machine learning.
5. Apply programming skills and use computational linear algebra software to analyze a real-world problem from various fields, make predictions based on data and use results for training and discovery of new results.

# Topic list

- Quick Review of Vector Spaces, Subspaces, Linear Independence, Bases, Rank, Linear Transformations, Determinants.
- Introduction to MATLAB.
- LU decomposition and Linear system solving, basic of numerical analysis.
- Norms, Inner Products, Orthogonal Bases, Gram-Schmidt Orthogonalization, QR Factorization
- Projections, Least Squares Problems, Data Fitting/Regression
- Eigenvalues, Eigenvectors, Diagonalization, Positive Definite Matrices Range
- **Matrix Decompositions**
  - Determinant and Trace
  - Eigenvalues and Eigenvectors
  - Cholesky Decomposition
  - Eigen decomposition and Diagonalization
  - Singular Value Decomposition
  - Matrix Approximation
- Linear Regression
- Support Vector Machines
- Clustering algorithms, k-means
- Dimensionality reduction techniques, SVD/PCA, Multi-dimensional scaling
- Applications to Statistics & Data Analysis, Web Search Engines & Network problems, Information processing (signal & images, error-correcting codes), PageRank Algorithm, Recommendation Systems, identification of the foreground in a surveillance video, categorizing documents, the algorithm powering Google's search, reconstructing an image from a CT scan, cryptography, Markov decision processes and more.
- **Applications considered in this course vary based on the interests and experience of students.**

**Class Format: based on hybrid Classroom**

Under each module posted in the course site, a student will find the following items

1. What to do for this module including all deadlines
2. PPT lectures or posted notes
3. Assigned Readings
4. Videos taped by the instructor or publicly available with active links displayed
5. Assignment and project
6. Discussion Forum
7. Students will be required to do most of readings and practice exercises before the classroom meeting, and watch the videos and the PPT. During class meeting, the instructor will give an overview of the general topic, lecture on the key concept and respond to questions which students are encouraged to submit online before class, lead a discussion forum, and use the technology to highlight and visualize the concepts studied.
8. Students will be asked to prepare short oral presentation on the topic or solution to a problem to present to the class
9. Students can choose to work in small group for the mini-projects and help each other with MATLAB application.
10. Midterm exams and final exam will be supervised in class; some work on exams needs to be run on MATLAB.

# Applications:

***Culturally Responsive Teaching: CRT***

***Computational Mathematics for social justice final Projects***

**Health of Cities**

- ❖ **Analyze Quality of Life in U.S. Cities Using PCA**
  *https://www.mathworks.com/help/stats/quality-of-life-in-u-s-cities.html*

climate housing health crime transportation education arts recreation economics

- ❖ **Is Baltimore's Water Quality Really on the Decline?**

- ❖ **Baltimore's Inner Harbor pollution**
  city's streams, rivers and harbor

- **Covid -19 Spread (176 Countries): Vector Support Machine**
- **Optical Character Recognizing: ML- Cancer – Security**
- **Edge Detection: Classify Trees by the Shape of their Leaves**
- **Covid-19  Vaccine : Roll out? Hesitancy? ( Future work.)**

==============================

# Papers:

**Extracting insights from the shape of complex data using topology**

# DATA:

## $C^2$_Exchange: Implementation

1- CLA Course was developed and offered in the Fall of 2020 at Morgan state University; the course is submitted for the university final approval

2- In the development period, Several meetings were held between Southern University A&M College and the University of Puerto-Rico Mayaguez to discuss prerequisite, content and computational Platforms.

3- Modules between the three institutions were exchanged and used as units for teaching computational courses

4- Invited speakers from institutions were given opportunities to give talks based on the course content.

5- Course Sharing Technology: Moodle OSC support with a local installation.

# New Ideas
# Moving forward

# $C^2$Exchange

## Computational and Data Science (CDS)
## Curriculum Exchange

# SIGHPC Education Committee – Webinar

03/19/2021

Rachel Vincent–Finley, Ph.D.
**Southern University and A&M College**
College of Sciences and Engineering
Department of Mathematics and Physics
**Mathematics Program**

# Outline

- Overview, Southern University System
- $C^2$Exchange – Introduction to Modeling and Simulation
- $C^2$Exchange – Computational Linear Algebra
- Plans for the Future

# Overview
# Southern University System

# Southern University System

Baton Rouge – New Orleans – Shreveport
www.sus.edu

- Southern University and A&M College (SUBR)
- Southern University at New Orleans (SUNO)
- Southern University at Shreveport (SUSLA)
- Southern University Law Center (SULC)
- Southern University Agricultural Research and Extension Center (SUAgCenter)

# Southern University System

Baton Rouge
www.subr.edu

- Southern University and A&M College (SUBR)
  - College of Sciences and Engineering
    - Department of Mathematics and Physics
      - **Mathematics Program**


- Motivation for Participation in $C^2$Exchange
  - Interest in Computational Science Concentration or Certificate
    - Interest in Applied Mathematics Concentration

# Introduction to Modeling and Simulation

**Lead Developer**. Ana Gonzalez, Professor of Mathematics

University of Puerto Rico

# Introduction to Modeling and Simulation

**MATH 499**. Seminar in Mathematics – Introduction to Modeling and Simulation

**Catalog Description**. Selected topics in mathematics. The course content varies with the professor who emphasizes topics in his or her particular area. *The student may receive credit for this course for up to six hours under two different headings*.

- **Prerequisite**: SMAT 212B – Calculus II with a grade of "C" **or** better *or* consent of the professor.
- **Course Credit**: 3 credit hours

- **Topic**. ***$C^2$Exchange***. *Introduction to the principles of modeling and simulation*. A progressive introduction of programming principles and skills using Python. Application of programming skills to the solution of different classes of models will be discussed and implemented.
  - **Course Textbook**: *Introduction to Modeling and Simulation with MATLAB® and Python*, Steven I. Gordon and Brian Guilfoos, CRC Press, 2017.

# Introduction to Modeling and Simulation

**MATH 499**. Seminar in Mathematics – Introduction to Modeling and Simulation

- **Fall 2019**
  - **Enrollment**. 2 mathematics majors
  - Project based
    - Student 1. Moose and Wolves Population
    - Student 2. Stochastic Model for Traffic from Home to Work
- **Spring 2021** (synchronous remote, independent study)
  - **Enrollment**. 1 mathematics major
  - Project based

# Computational Linear Algebra

**Lead Developer**. Ahlam Tannouri, Lecturer, Department of Mathematics, Morgan State University

# Computational Linear Algebra

**MATH 433**. Linear Algebra

**Catalog Description**. An advanced study of vector spaces, subspaces and dimension; inner products; elementary matrices, the inverse of a matrix and rank of a matrix; linear transformations; rank, nullity, and inverse of a linear transformation; eigenvalues and eigenvectors; similarity: and Cayley-Hamilton Theorem. **A good mixture of proofs and computations is given**.

- **Prerequisite**: MATH 233 – Introduction to Linear Algebra with a grade of "C" **or** better *or* consent of the professor.
- **Course hours**: 3 credit hours
- **Course References**:
  - *Linear Algebra with Applications*, W. Keith Nicholson, 2021.
    - https://open.umn.edu/opentextbooks/textbooks/linear-algebra-with-applications
  - *A First Course in Linear Algebra*, Robert Beezer, 2015.
    - https://open.umn.edu/opentextbooks/textbooks/a-first-course-in-linear-algebra
  - *A First Course in Linear Algebra*, Ken Kuttler, 2017.
    - https://open.umn.edu/opentextbooks/textbooks/a-first-course-in-linear-algebra-2017
  - *A Gentle Introduction to the Art of Mathematics*, Joseph Fields.
    - https://open.umn.edu/opentextbooks/textbooks/a-gentle-introduction-to-the-art-of-mathematics-177
  - *Mathematics for Machine Learning*, Marc Peter Deisenroth, A. Aldo Faisal, Cheng Soon Ong, April 2020, Cambridge University Press, April 2020, ISBN: 9781108455145

# Computational Linear Algebra

**MATH 433**. Linear Algebra

- **Spring 2021**
  - **Enrollment**. 2 mathematics majors
  - Project based
    - Students will use Matlab to explore applications.
    - https://matlabacademy.mathworks.com
      - Getting started. MATLAB Onramp

# Plans for the Future

# Plans for the Future

- Motivation for Participation in $C^2$Exchange
  - Interest in Computational Science Concentration or Certificate
  - Interest in Applied Mathematics Concentration
    - College of Sciences and Engineering
      - **Department of Mathematics and Physics**
        - **Mathematics Program**
        - Physics Program
      - Department of Biological Sciences and Chemistry
        - Biology Program
        - Chemistry Program
      - Department of Computer Science
      - Department of Civil Engineering
      - Department of Electrical Engineering
      - Department of Mechanical Engineering

- Offer Modules to support Honors College Thesis

- Offer Modules to support REU professional development

- Share courses across the Southern University System

# Acknowledgements

- This work is supported by the National Science Foundation.
  - Title: CyberTraining:CIU:Computational and Data Science Literacy Curriculum Exchange
  - NSF Award # 1829717
- Partner Institutions
  - Ohio Supercomputer Center (OSC)
  - Bethune Cookman University (BCU)
  - Clark Atlanta University (CAU)
  - Morgan State University (Morgan)
  - Southeastern Universities Research Association (SURA)
  - Southern University and A&M College (SUBR)
  - University of Puerto Rico at Mayaguez (UPRM)

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# Introduction to Computational Chemistry and Molecular Modeling @ $C^2$Exchange

Dinadayalane Tandabany, Ph.D. (Dina)
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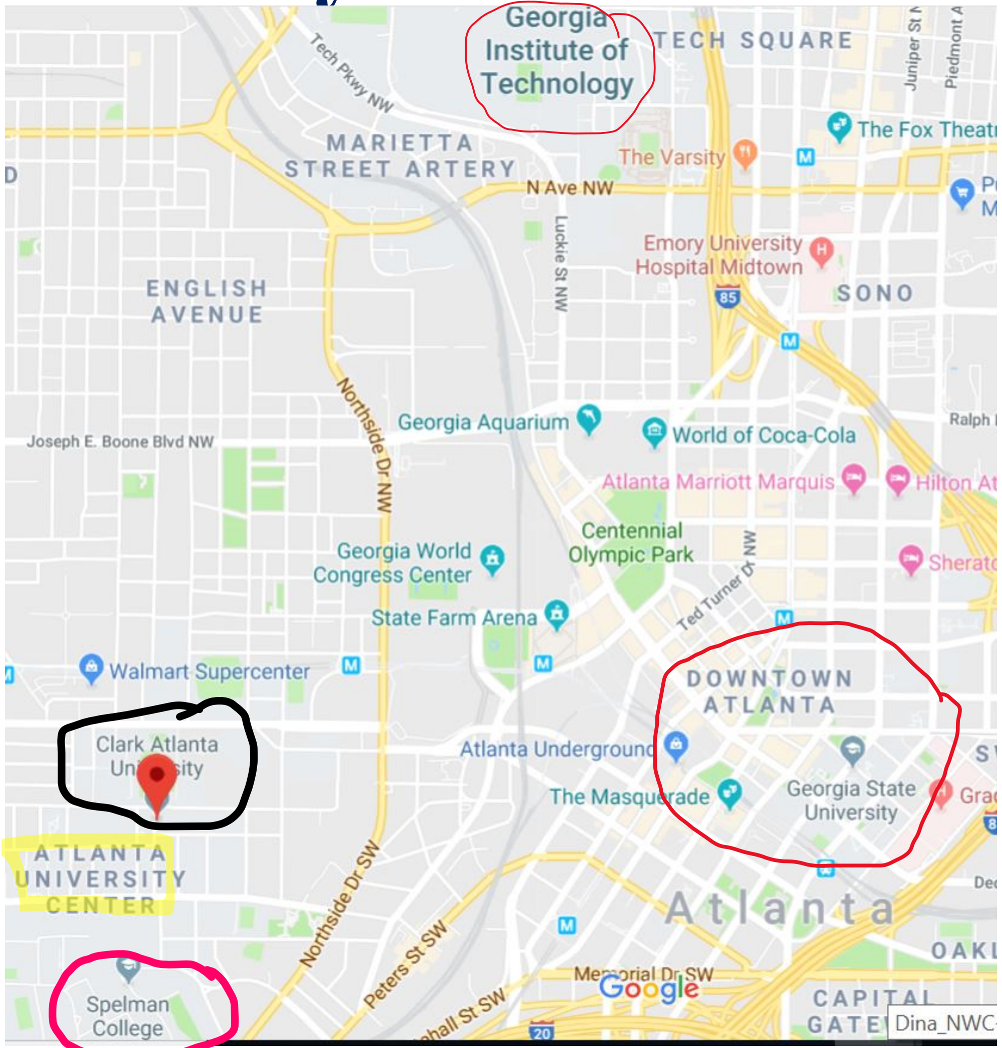
# Clark Atlanta University

- Non-profit, private HBCU
  (Bachelors, Masters and doctoral programs)
(Approx. **3800** students)
- **Established in 1988 by merging of two intuitions:** Atlanta University (1865) & Clark College (1869)

**School of Arts and Sciences:** Approx. **2400** UG students (include 700 students in STEM)




CAU is the only university in the historic Atlanta University Center (**AUC**), a consortium of 8,000 primarily African-American scholars.

# Introduction

- An improved curriculum, better use of technology in content delivery, effective academic support and student success are essential for increasing the number of undergraduate minority students in STEM.
- **Computation** is now regarded as an equal and essential element along with theory and experiment in the advancement of scientific knowledge and engineering practice.
- It is important to educate the next generation of undergraduate students to confront the challenges in computational and data-enabled science.

By the support of NSF, Dr. Tandabany **developed and implemented** Junior/Senior level undergraduate course at Clark Atlanta University (CAU):

- "*Introduction to Computational Chemistry and Molecular Modeling*" in Department of Chemistry

Through the NSF **C²Exchange** grant, this course is available to exchange with partner institutions of other minority serving institutions (MSIs) – Full course or selected modules.

# CCHE 445 - Introduction to Computational Chemistry and Molecular Modeling

**Number of credit hours: 4**

**Brief Description**:

- This course has the lecture and lab to introduce the concepts of computational chemistry and molecular modeling and their applications in chemistry and biology.
- The main purpose of this course is to introduce some of the techniques used in computational chemistry and molecular modeling and to demonstrate how these techniques can be used to study physical, chemical and biological phenomena.
- This course is intended to prepare undergraduate students for higher education on computational-based research in chemistry, biology or engineering by introducing the concepts and techniques used in computational chemistry and molecular modeling.

## **Prerequisites**:

General Chemistry I and II (CHE 111 & 112); General Biology I and II (BIO 111 & 112); Organic Chemistry I and II (CHE 231 & 232); Calculus I (MAT 111).

**Learning Outcomes:**

Upon successful completion of this course, students will be able to

(1) Employ the concepts and techniques used in computational chemistry and molecular modeling.

(2) Apply semi-empirical, *ab initio* and density functional theory (DFT) methods for calculations of molecular structures, energetics and electronic properties of chemical and biological systems.

(3) Perform calculations for small molecules, the intermolecular interactions, conformational analyses of acyclic molecules and build polypeptides.

(4) Report and analyze results of their calculations.

(5) Apply self-confidently for higher education on computational-based research in science or engineering fields, data science and be ready for the advanced level courses related to Computational Chemistry and Molecular Modeling.

**Required Text:**

**Molecular Modelling: Principles and Applications**, Andrew R. Leach, **Second Edition**, Pearson, England. (ISBN: 0-582-38210-6)

# C²Exchange grant

- This course can be implemented by partner institutions as such or with modifications or partly.
- Physical Chemistry course at undergraduate level chemistry program include quantum mechanics and its applications.
- The **selected modules** of ***Introduction to Computational Chemistry and Molecular Modeling*** were adapted to the Physical Chemistry course at Bethune-Cookman University.
- This course has laboratory with lectures. Students enjoyed doing computational labs.


National Science Foundation
Funding through HBCU-UP TIP Grant (HRD-1623287)

# SEAGrid Science Gateway

- Web Portal Interface & Desktop Client
- Simplifies access to HPC resources on behalf of a wide variety of research communities and broad Science and Engineering domains
- In operation since 2005, serves more than 600 scientists and students under 320 projects
- **Easy job submission and project file management**
- Built in molecular editors and input file creation – Desktop Client
- Student experience:
  - Easily accessible – one stop dashboard to handle multiple applications, projects, allocations, and compute resources – Highly Recommended

- SEAGrid Data Catalog
  - Easy viewing of initial job collection, summary, metadata, and visualization

SEAGrid Data Catalog | Search | Directory Browser

N.B: This data is automatically extracted using set of configured parser and may contain errors. Please report any issues in the issue tracker

| Calculation | |
|---|---|
| Package | Gaussian 09, Revision E.01 |
| Calculation Type | FOpt; Freq |
| Methods | RB3LYP; RB3LYP |
| Basis Set | 6-31G(d,p) |
| Number of Basis Functions | 760 |
| Number of Molecular Orbitals in the Calculation | 760 |
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| Job Status | CalcDone |
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| Energy (au) | -1616.0971637 |
| Dipole (debye) | -0.0328227,-0.1402467,0.0158595 |
| HF (au) | -1616.0971637 |
| Homos | 138 |
| Homo Eigenvalue (ev) | -5.340506429913 |
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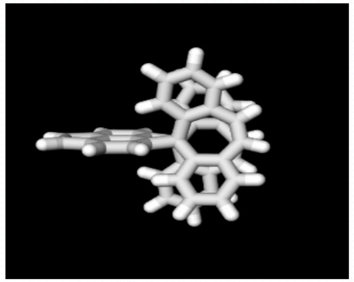
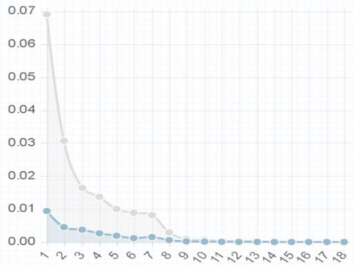


Final Molecular Structure




Gradient vs Iteration

# Access to Supercomputers

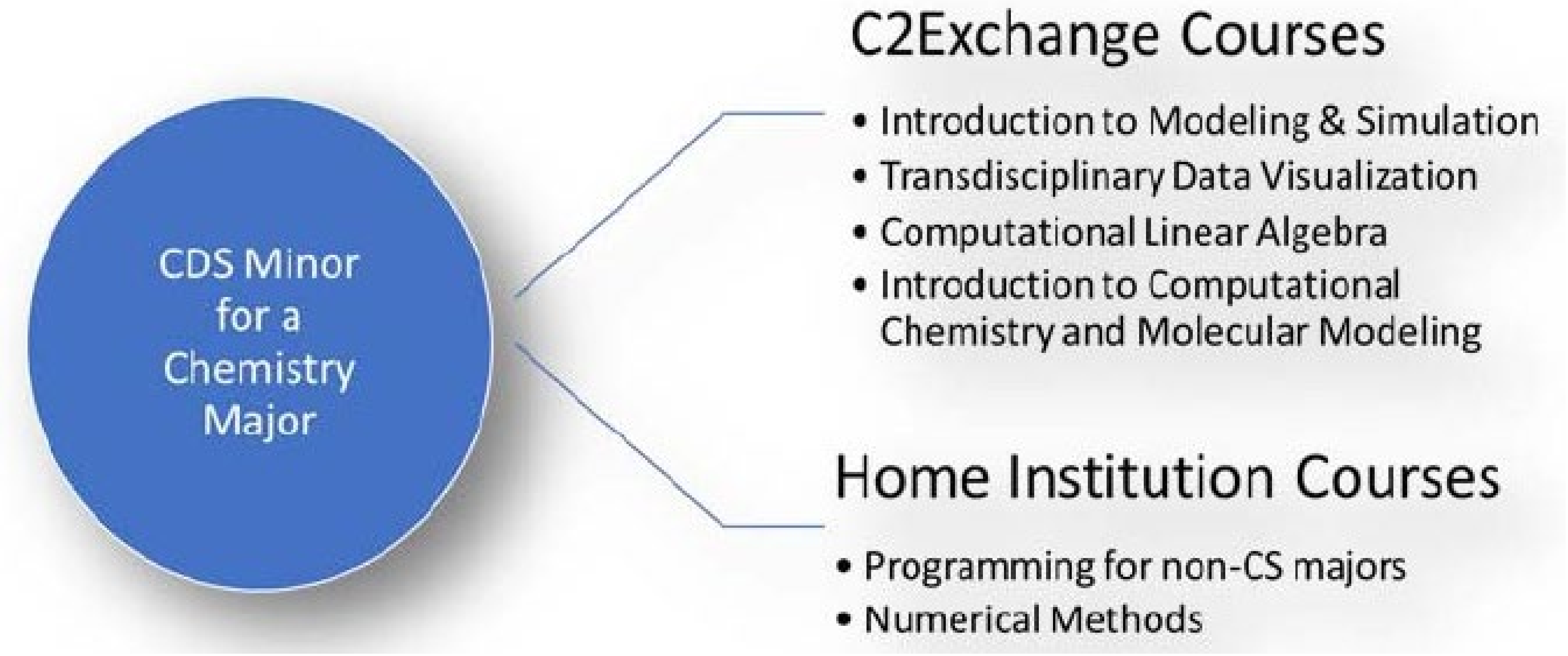
## Students accessed to XSEDE (Extreme Science and Engineering Discovery Environment) Supercomputers for the Laboratory and Undergraduate Research via SEAGRID Science Gateway


- **Bridges** – Pittsburgh Supercomputing Center (PSC)
  - Petascale resource for empowering diverse communities by bringing together HPC, AI and Big Data
  - Regular, Large, and Extreme Shared Memory nodes – 128GB, 3TB, and 12TB memory
  - GPU nodes – Tesla K80 and P100 GPUs, 128GB RAM each

- **Comet** – San Diego Supercomputer Center (SDSC)
  - Standard Compute nodes – 128 GB memory and 24 cores
  - Large Memory nodes – 1.5 TB memory and 64 cores
  - GPU nodes - NVIDIA K80 and P100 GPUs

# Building capacity for Computational and Data Science (CDS) Minor at MSIs

Pathway to **minor** for a chemistry or biology or physics major at CAU



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- The Extreme Science and Engineering Discovery Environment (XSEDE) for computational resources
- SEAGRID Science Gateway from Indiana University
- Ohio Supercomputer Center

# Questions?