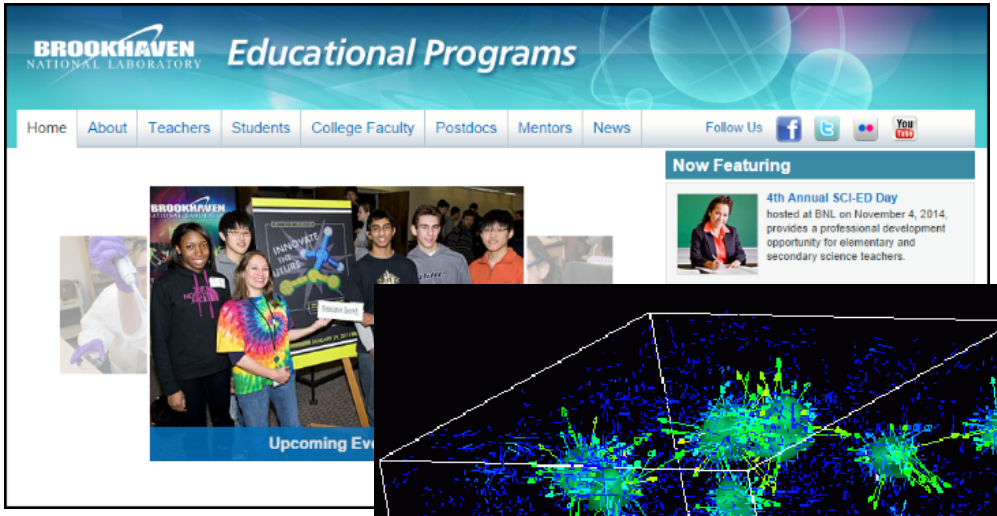
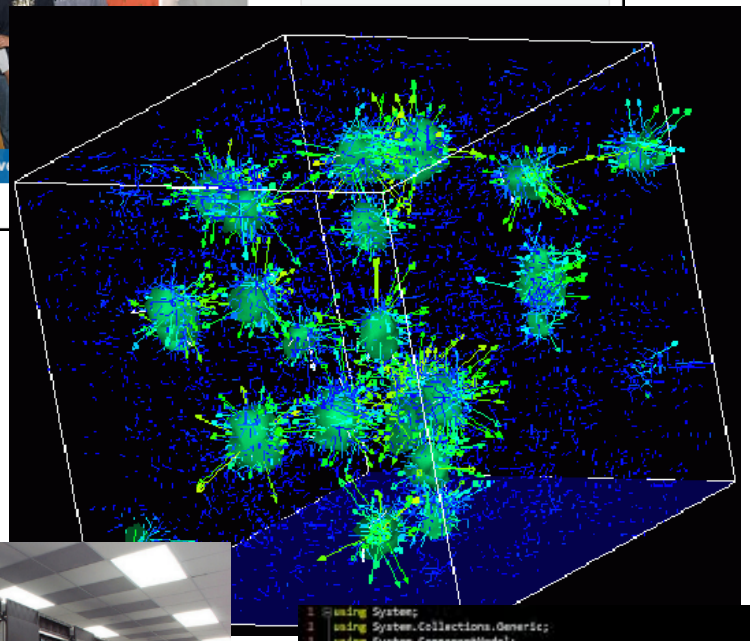
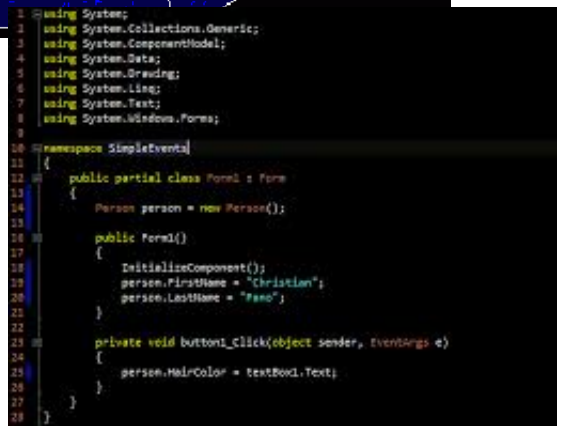






Survey of Scientific Computing (SciComp)

Unit 1

Course Overview,
Hello Problems

About Brookhaven National Laboratory

Who We Are

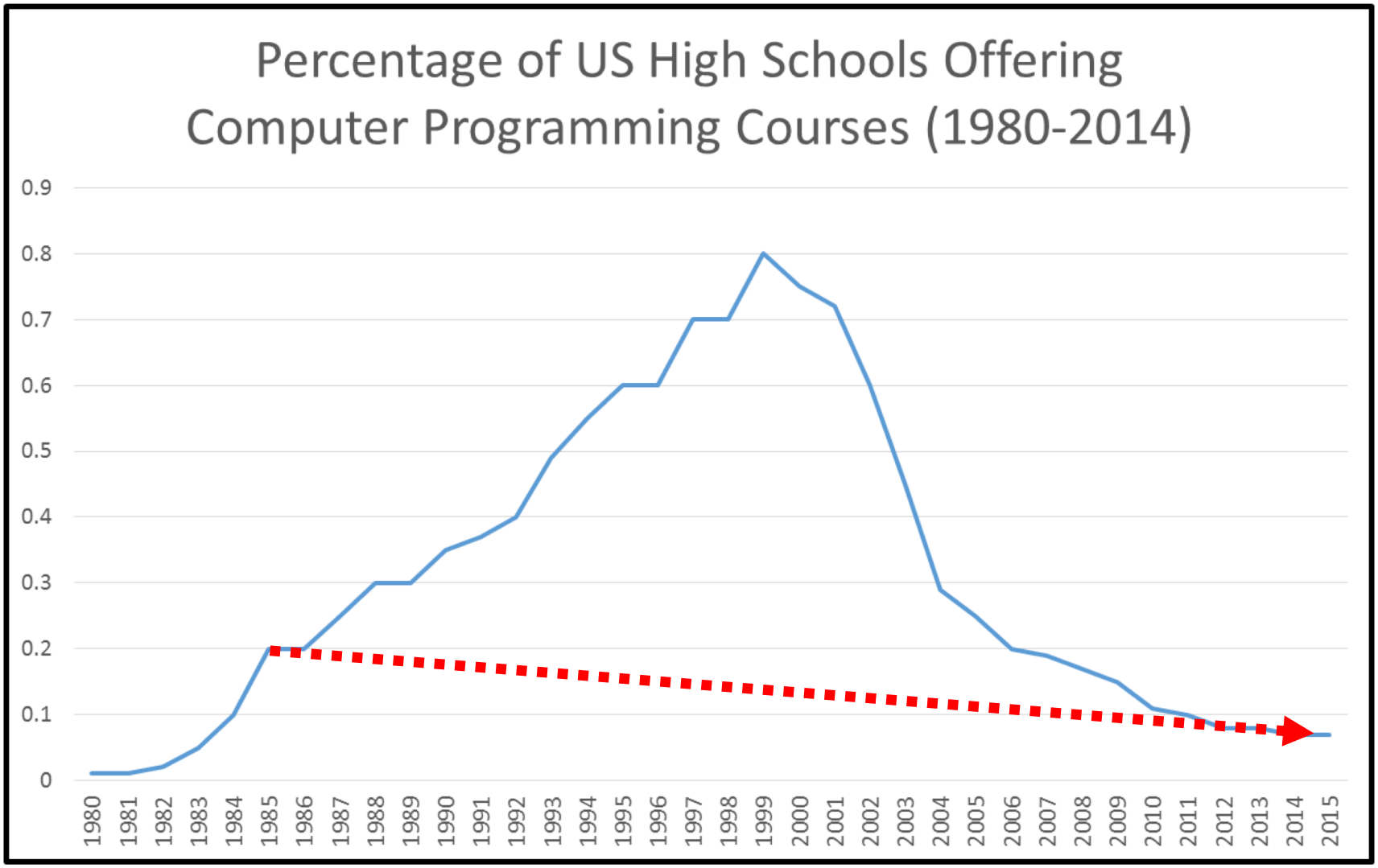
Brookhaven National Laboratory is a multipurpose research institution funded primarily by the U.S. Department of Energy's Office of Science. Located on the center of Long Island, New York, Brookhaven Lab brings world-class facilities and expertise to the most exciting and important questions in basic and applied science—from the birth of our universe to the sustainable energy technology of tomorrow.

We operate cutting-edge large-scale facilities for studies in physics, chemistry, biology, medicine, applied science, and a wide range of advanced technologies. The Laboratory's almost 3,000 scientists, engineers, and support staff are joined each year by more than 4,000 visiting researchers from around the world. Our award-winning history stretches back to 1947, and we continue to unravel mysteries from the nanoscale to the cosmic scale, and everything in between.

Agenda

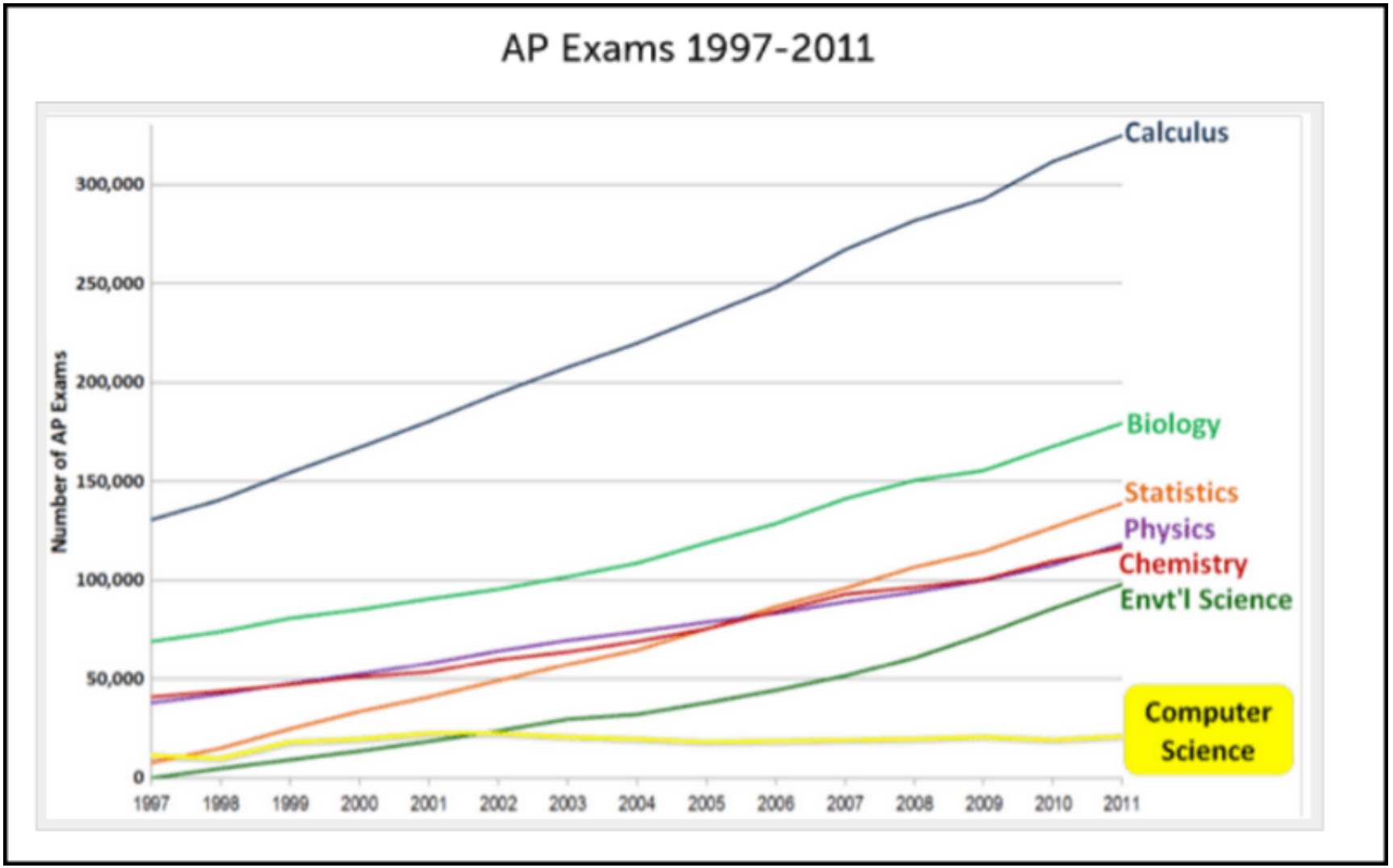
- The Growing Need for Scientific Computing
- Differentiating CompSci vs. **SciComp**
- Scientific Computing is ***the*** Pathway for STEM
- SciComp as a **Translational** Science
- Detailed Course Syllabus
- Motivation for learning C++
- Reasonable Course Expectations
- Getting a Degree in Scientific Computing

A National Challenge



2015 - National Center for Education Statistics, Dept. of Education

A National Challenge



The Challenge to DOE

- Scientists across DOE have noted a dramatic rise in the **startup latency** of interns who do not possess foundational programming skills
- This latency means that for the ***initial 6-8 weeks of their assignment***, the interns are essentially unproductive as they must first acquire basic knowledge of how to write software
- Instead of learning key scientific principles from their mentor, the interns are spending their precious lab time **often working alone**, figuring out how to instruct the computer to perform rudimentary data processing tasks
- From the perspective of DOE scientists, **the need to adeptly wield software tools has never been as urgent as it is today**

The Hype

Kevin's Story

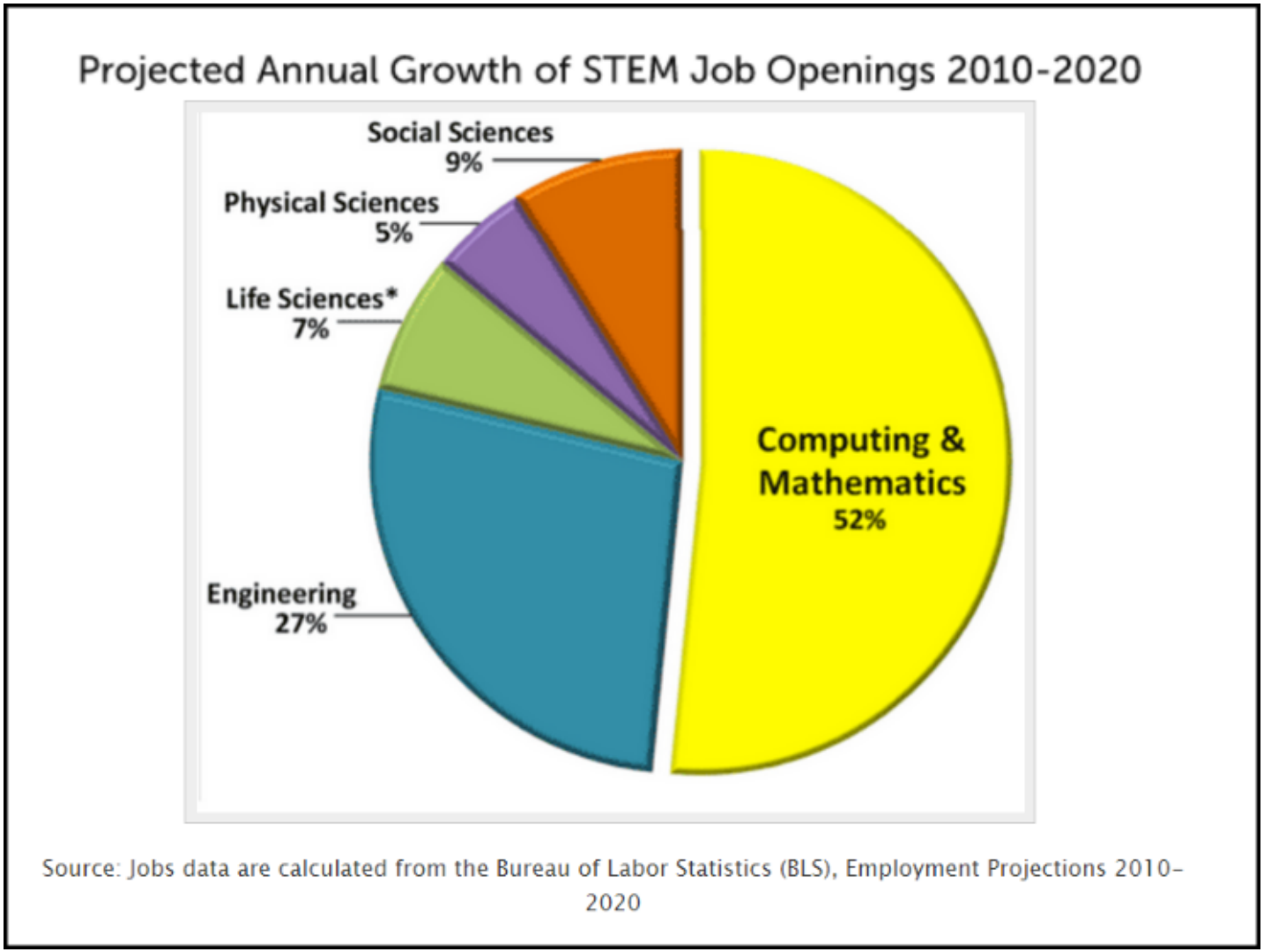
Modern-day scientists and engineers are spending more and more of their work days in front of the computer. As an example, consider my friend Kevin, who works in oceanography and mechanical engineering. Whoa, sounds like he's probably spending all day out on high-tech boats rigging together mechanical devices like MacGyver and collecting data from underwater sensors, right? This must be his typical work day -- hard hats and heavy-duty work gloves.

The Reality

Actually, Kevin spends less than 5% of his time out on the ocean; the other 95% of the time, he's sitting in front of the computer writing programs to clean up, transform, process, and extract insights from data collected out in the field. This is what Kevin looks like at work on most days:

The same story plays out for scientists and engineers in all sorts of fields: astronomers, biologists, physicists, aerospace engineers, economists, geneticists, ecologists, environmental engineers, neuroscientists ... the list goes on and on. Modern-day science and engineering is all about processing, analyzing, and extracting insights from data.

The Irony


Projected Annual Growth of STEM Job Openings 2010-2020
Social Sciences
9%
Physical Sciences
5%
Life Sciences*
7%
Engineering
27%
Computing &
Mathematics
52%
Source: Jobs data are calculated from the Bureau of Labor Statistics (BLS), Employment Projections 2010–2020

US Department of Labor - 2019

Robotics Engineering Careers

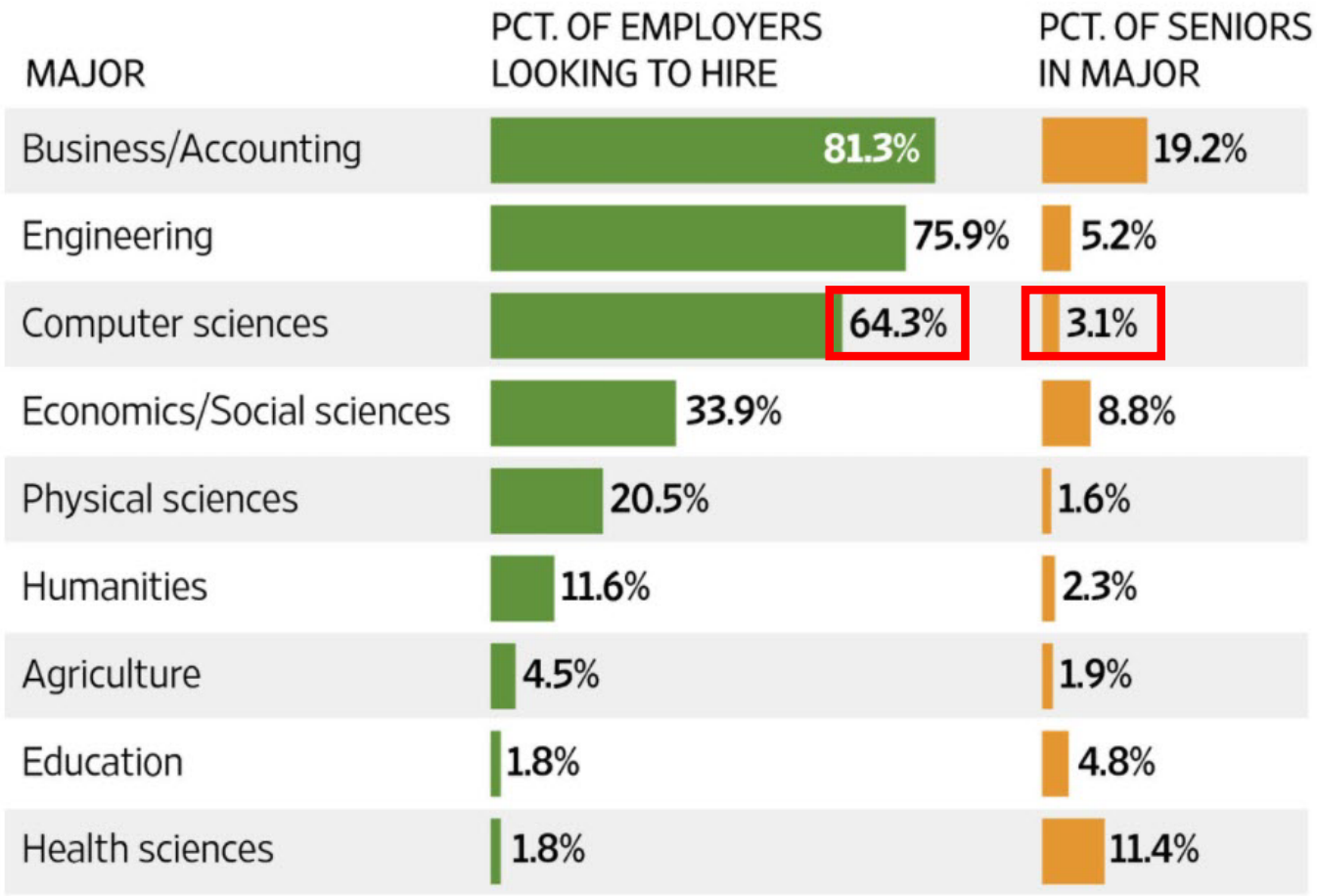
Quick Facts: Electro-mechanical Technicians	
2018 Median Pay	$57,790 per year $27.78 per hour
Typical Entry-Level Education	Associate's degree
Work Experience in a Related Occupation	None
On-the-job Training	None
Number of Jobs, 2016	13,800
Job Outlook, 2016-26	4% (Slower than average)
Employment Change, 2016-26	500

Scientific Computing Careers

Quick Facts: Computer and Information Research Scientists	
2018 Median Pay	$118,370 per year $56.91 per hour
Typical Entry-Level Education	Master's degree
Work Experience in a Related Occupation	None
On-the-job Training	None
Number of Jobs, 2016	27,900
Job Outlook, 2016-26	19% (Much faster than average)
Employment Change, 2016-26	5,400

The College Majors Employers Want

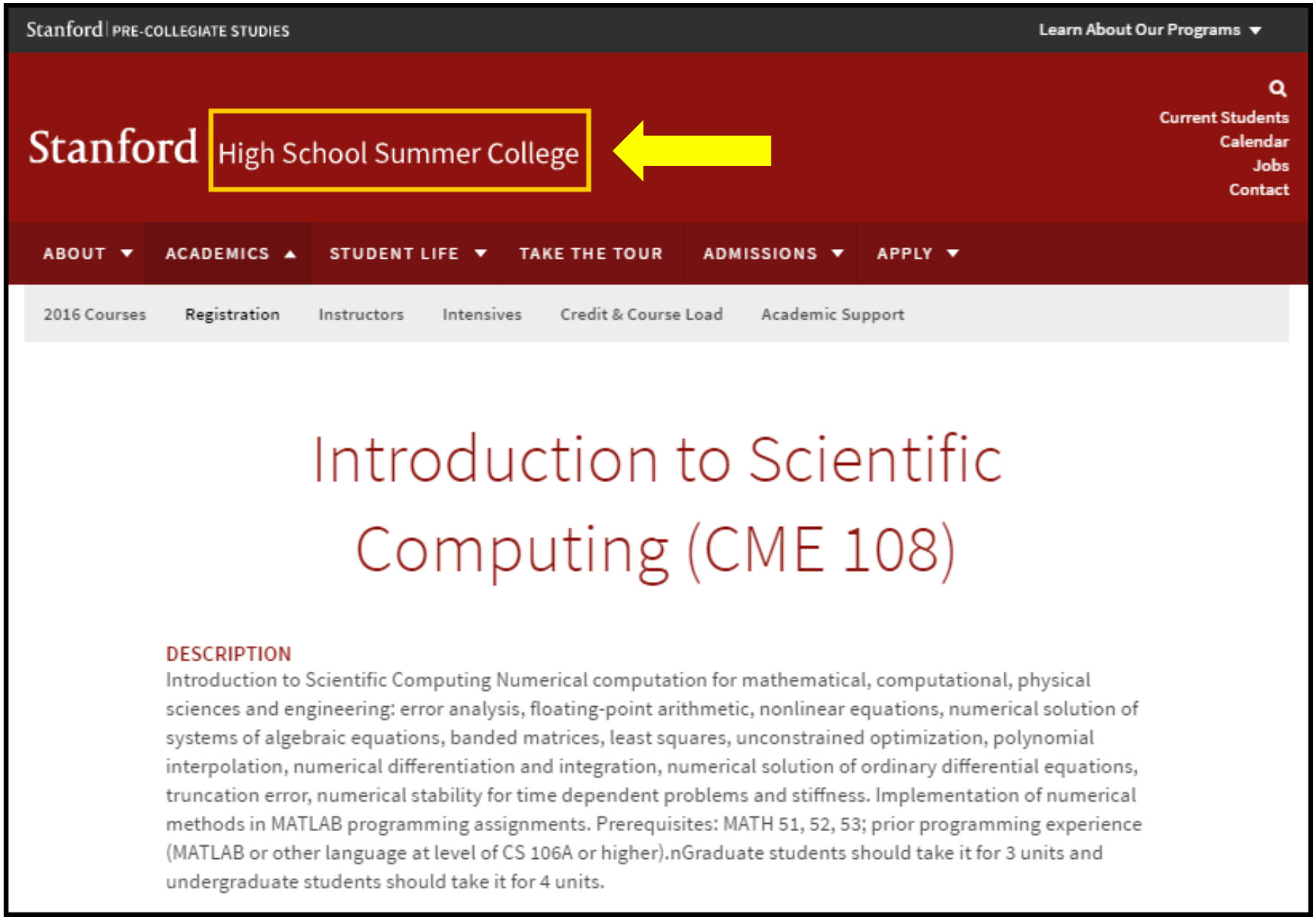
Employers are on the hunt for engineering, business and computer-science graduates; here's how popular those majors are among college seniors.



Note: Current hiring plans compared with degrees conferred in 2015

Sources: National Association of Colleges and Employers; National Center for Education Statistics

THE WALL STREET JOURNAL.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Introduction to Scientific Computing (CME 108)
DESCRIPTION
Introduction to Scientific Computing Numerical computation for mathematical, computational, physical sciences and engineering: error analysis, floating-point arithmetic, nonlinear equations, numerical solution of systems of algebraic equations, banded matrices, least squares, unconstrained optimization, polynomial interpolation, numerical differentiation and integration, numerical solution of ordinary differential equations, truncation error, numerical stability for time dependent problems and stiffness. Implementation of numerical methods in MATLAB programming assignments. Prerequisites: MATH 51, 52, 53; prior programming experience (MATLAB or other language at level of CS 106A or higher).nGraduate students should take it for 3 units and undergraduate students should take it for 4 units.

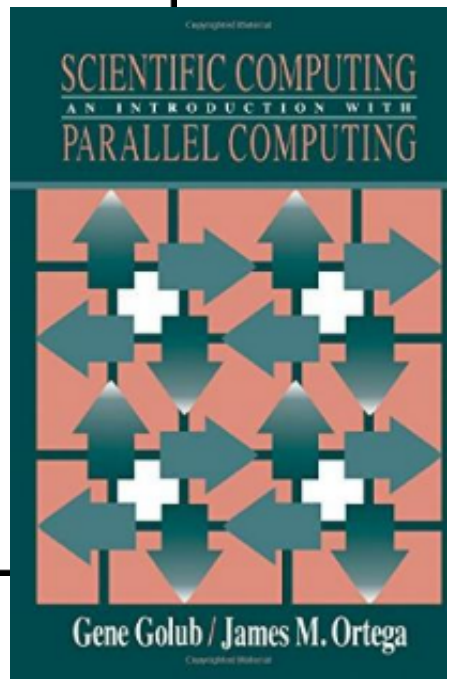
What is Scientific Computing?

Golub and Ortega: *"Scientific computing is the collection of tools, techniques and theories required to solve on a computer mathematical models of problems in science and engineering."*

Or a more narrow definition: *"Development and use of numerical methods and mathematical models to solve real-world problems efficiently on computers."*

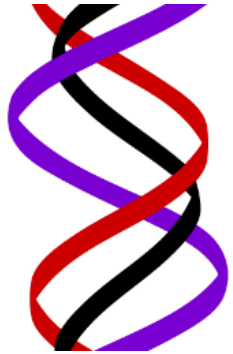
Interdisciplinary field requiring:

- knowledge about the underlying (physical) problem,
- ability to formulate a mathematical model,
- stable & accurate numerical schemes,
- efficient implementation on high performance computers.



What is Scientific Computing?

- Scientific computing problems **cannot be solved** using a graphing calculator or with Microsoft Excel
  - The computer should not been seen as just another closed form tool like an scientific instrument
  - SciComp does not require writing thousands of lines of code to answer problems – complete code usually fits on **one** slide!
- SciComp is **applied** computer science
  - The first name of CompSci is *computer*
  - The first name of SciComp is **science**
  - A **triple helix** of math, science, and computing



SciComp vs CompSci

Scientific Computing

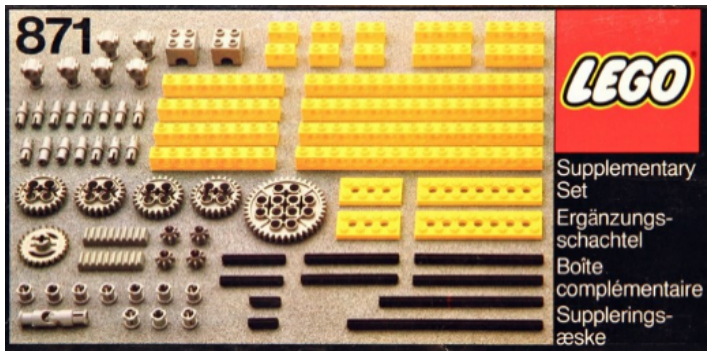
- Probability and Statistics
- Simulation and Modelling
- Data Visualization
- Storing and Analyzing Very Large Datasets
- Parallel & Distributed Algorithms
- Speed and Accuracy Paramount
- Functional Languages
- Open-Ended Problems with Unknown Solutions

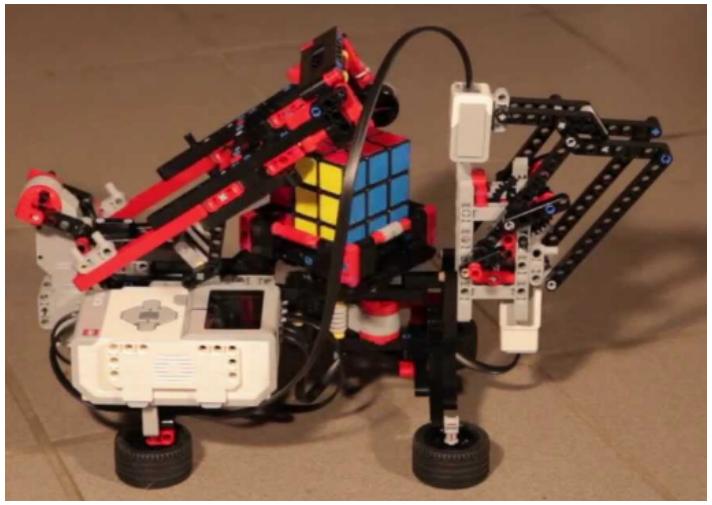
Computer Science

- General Data Structures
- Design Methodologies
- Procedural Languages
- Stand-Alone Programs
- Emphasis on Object-Orientation
- Simple Data Models
- Sequential Algorithms
- Less Graphics Intensive
- Directed Closed-Form Problems with Known Solutions

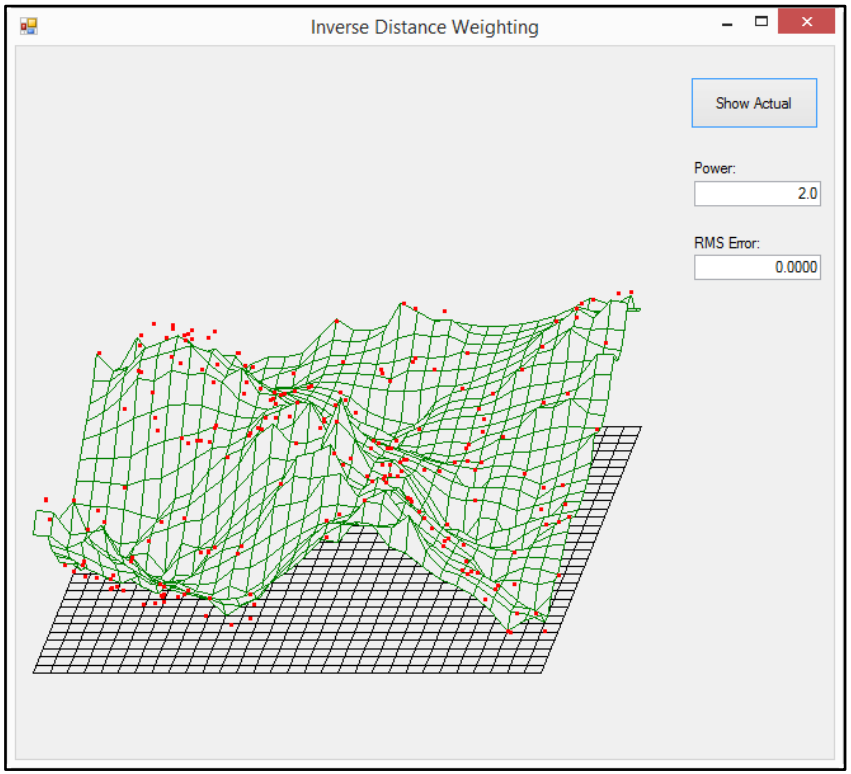
SciComp = **Just Enough** CompSci

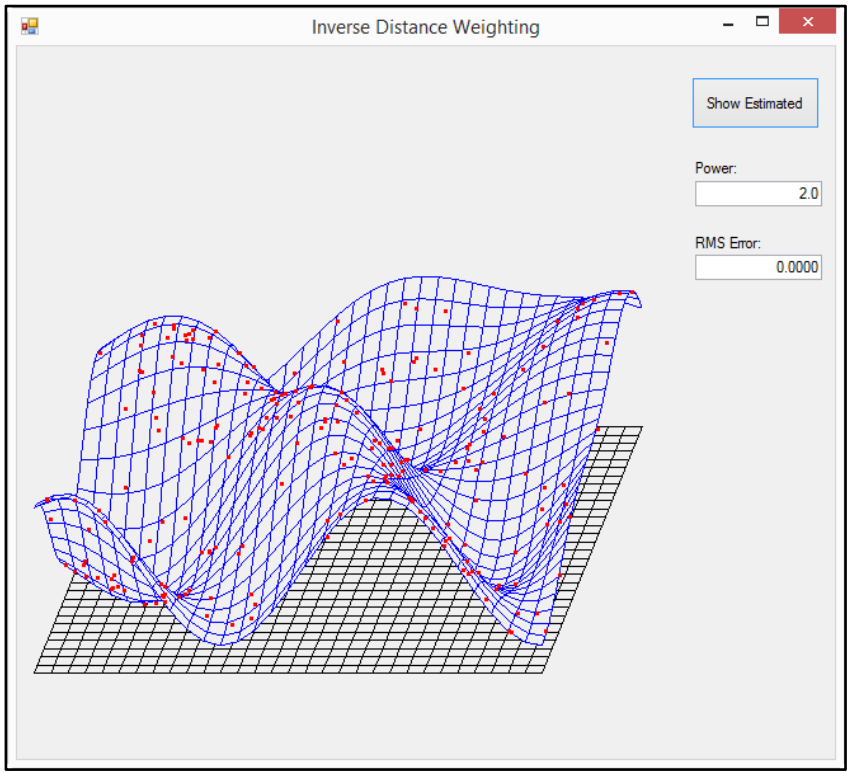
- Data **types**: **int, double, bool, string**
- Data **structures**: pointers, vectors, streams, classes
- **Statements**: **for(), while(), if(), return**
- **Patterns**: brute force, recursion, divide & conquer, map-reduce
- **Algorithms**: GCD, mean/variance, sorting, searching
- **Helpers**: **Random**, mod %, Stopwatch, **Allegro, ROOT**





Example SciComp Topic
Multidimensional Interpolation





A first order approximation having only 24%
of the world sampled (220 of 900 actual points)

SciComp As Translational Science

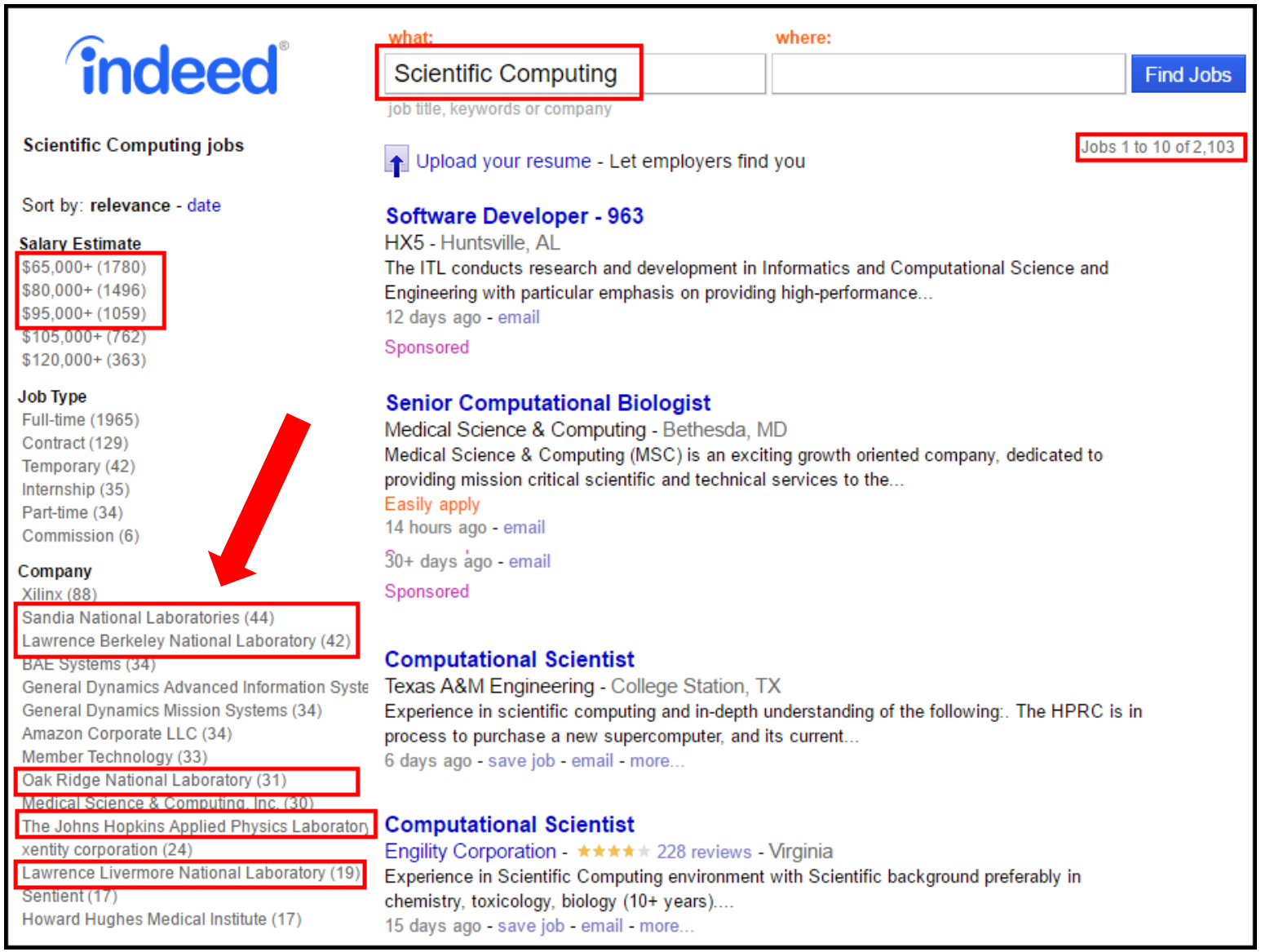
$$u(\mathbf{x}) = \begin{cases} \dfrac{\sum_{i=1}^{N} w_i(\mathbf{x}) u_i}{\sum_{i=1}^{N} w_i(\mathbf{x})}, & \text{if } d(\mathbf{x}, \mathbf{x}_i) \neq 0 \text{ for all } i \\ u_i, & \text{if } d(\mathbf{x}, \mathbf{x}_i) = 0 \text{ for some } i \end{cases}$$

where

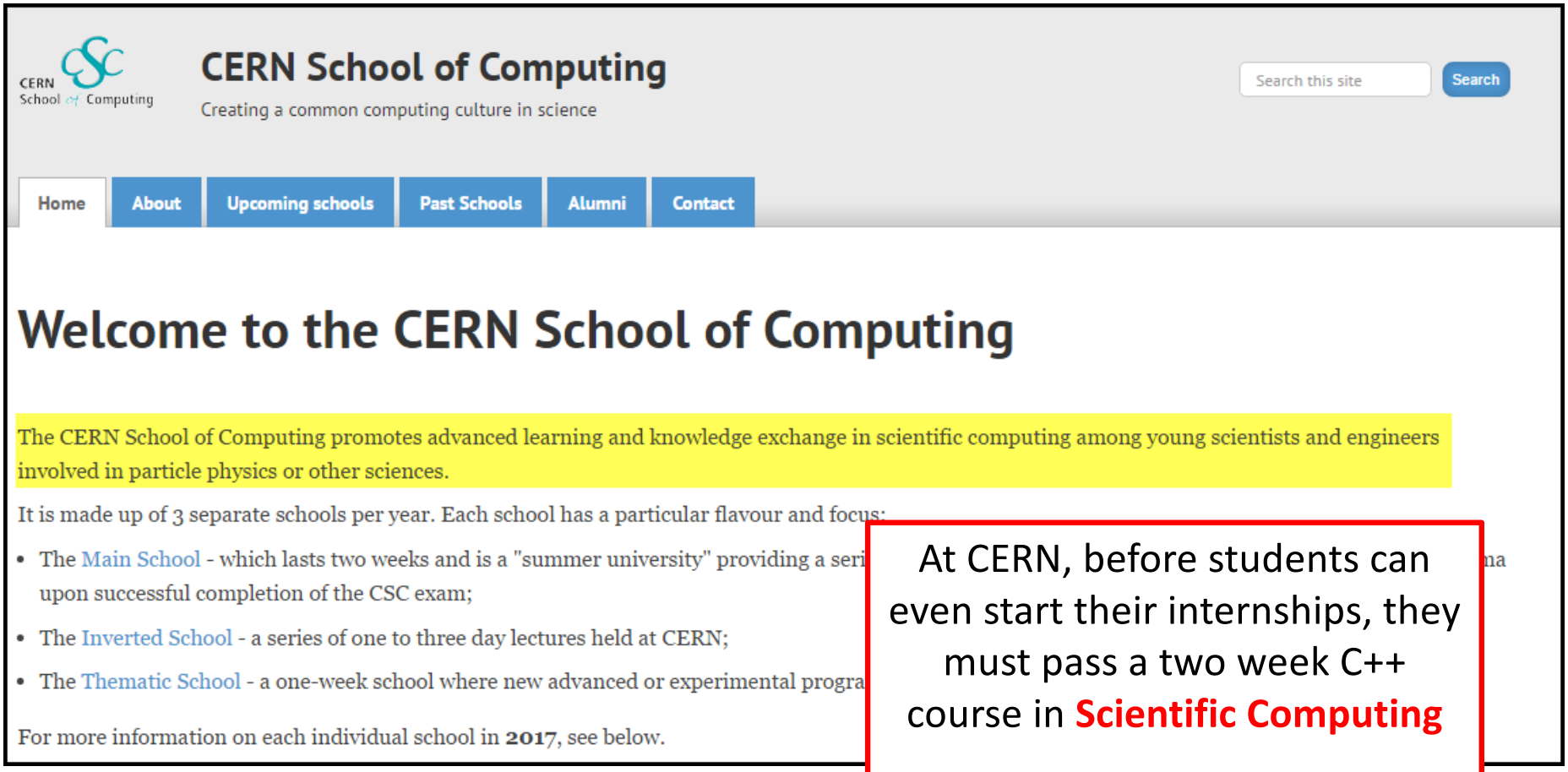
$$w_i(\mathbf{x}) = \frac{1}{d(\mathbf{x}, \mathbf{x}_i)^p}$$

```
double GetEstHeight(double x, double z)
{
    double sumWeight = 0;
    double sumHeightWeight = 0;

    for (size_t n{}; n < numSamples; ++n) {
        double distance = sqrt(pow(x - samples[n].x, 2)
            + pow(z - samples[n].z, 2));

        if (distance == 0) return samples[n].y;

        double weight = 1 / pow(distance, p);

        sumWeight += weight;
        sumHeightWeight += samples[n].y * weight;
    }

    double height = sumHeightWeight / sumWeight;

    return height;
}
```

SciComp = The Pathway to Internships



SciComp = The Pathway to Internships



CERN School of Computing

Creating a common computing culture in science

Search this site | Search

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Welcome to the CERN School of Computing

The CERN School of Computing promotes advanced learning and knowledge exchange in scientific computing among young scientists and engineers involved in particle physics or other sciences.

It is made up of 3 separate schools per year. Each school has a particular flavour and focus:

- The Main School - which lasts two weeks and is a "summer university" providing a seri… upon successful completion of the CSC exam;
- The Inverted School - a series of one to three day lectures held at CERN;
- The Thematic School - a one-week school where new advanced or experimental progra…

For more information on each individual school in **2017**, see below.

At CERN, before students can even start their internships, they must pass a two week C++ course in **Scientific Computing**

That is how important CERN views these skills!

BROOKHAVEN NATIONAL LABORATORY **Educational Programs**

Home | About | Teachers | Students | College Faculty | Postdocs | Mentors | News | Follow Us

(HSRP - Research) High School Research Program

The High School Research Program (HSRP) is a highly competitive six week educational program for students interested in pursuing science, technology, engineering and mathematics (STEM) studies. Selected students, together with Brookhaven National Laboratory (BNL) scientific staff collaborate on projects that support BNL and the Department of Energy mission.

HSRP is a commuter program. BNL does not provide housing or transportation to and from the Laboratory.

Audience for This Program

Recommended for students that have completed 11th grade. Due to BNL safety regulations students under the age of 18 may not be allowed to perform certain tasks.

Rules & Eligibility Criteria

1. Must be available for the entire duration of the program, Monday to Friday 8:30 a.m. to 5:00 p.m.
2. Transportation and housing is not provided.
3. Must be a United States Citizen or Permanent Resident Alien (PRA) at the time of applying. PRA must hold an active United States Permanent Resident Card.
4. Recommended for students that have completed the 11th grade and not be younger than 15 years of age at the start of the program.

The High School Research Program (HSRP) is an advanced high school program in which students are paired with a BNL scientist.

Important Dates

Registration Opens:
Wednesday, December 19, 2018, at 9:00 a.m.

Registration Closes:
Friday, March 22, 2019, at 5:00 p.m.

Program Starts:
Monday, July 8, 2019, at 9:00 a.m.

Program Ends:
Friday, August 16, 2019, at 5:00 p.m.

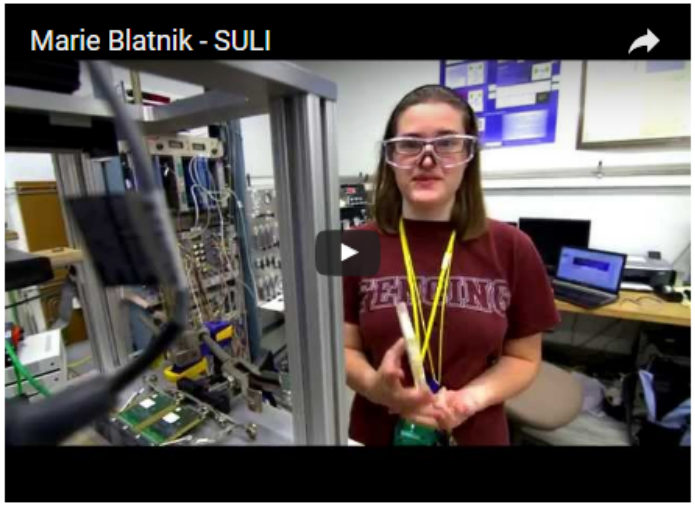
Application Deadline:
Friday, March 22, 2019, at 5:00 p.m.

All notifications send by:
Friday, May 17, 2019, at 5:00 p.m.

Contact Information

For more information about this program

(Internship - SULI) Science Undergraduate Laboratory Internship



SULI Intern Interview: Studies in calorimetry using silicon photomultipliers and tracking using gas electron multipliers for the super-PHENIX upgrade Experiment

The United States Department of Energy (DOE) has established undergraduate research internships at national laboratories across the country. These internships are run for 10 weeks during the summer and for 16 weeks during the fall and spring semesters. Internships are offered in areas such as physics, biology, chemistry, environmental and atmospheric sciences, engineering, computers applied mathematics and nuclear science.

The U.S. Department of Energy (DOE) has established a national program to give research experience in areas of chemistry, physics, engineering, biology, nuclear medicine, applied mathematics, high- and low-energy.

Brookhaven National Laboratory (BNL) offers student appointments though a national program titled the Science Undergraduate Laboratory Internship (SULI) developed through DOE. Participants will be placed with members of the scientific and professional staff in an educational program developed to give research experience in areas such as chemistry, high- and low-energy physics, engineering, biology, nuclear medicine, applied mathematics.

At BNL, a SULI appointment will include features which have been the mainstay of our undergraduate Student Program since 1952:

Important Dates

Program Starts:
Monday, January 9, 2017, at 8:00 a.m.

Program Ends:
Friday, April 28, 2017, at 5:00 p.m.

Spring Application Due:
Friday, October 7, 2016, at 5:00 p.m.

Contact Information

For more information about this program, contact:

Dr. Mel Morris
Brookhaven National Laboratory
Bldg.438 – P.O. Box 5000
Upton, NY 11973-5000
631-344-5963 (phone)
631-344-5832 (fax)
mmorris@bnl.gov

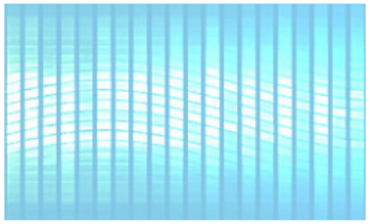
• You will participate in a cutting-edge scientific research program, directed by a BNL staff member. The nature of your research assignment will be determined after a review of your background and interests by our staff, relative to their current research activities.

BROOKHAVEN NATIONAL LABORATORY

Computational Science Initiative

U.S. DEPARTMENT OF ENERGY

CSI Home | Components of the Initiative | People | Org Chart | News



Computer Science & Mathematics

Scientific Data & Computing Center

Center for Data-Driven Discovery

Computational Science Lab

About Us

Building on its capabilities in data-intensive computing and computational science, Brookhaven National Laboratory is embarking upon a major new Computational Science Initiative.

Advances in computational science, data management and analysis have been a key factor in the success of Brookhaven Lab's scientific programs at the Relativistic Heavy Ion Collider (RHIC), the National Synchrotron Light Source (NSLS), the Center for Functional Nanomaterials (CFN), and in biological, atmospheric, and energy systems science, as well as our collaborative participation in international research endeavors, such as the ATLAS experiment at Europe's Large Hadron Collider.

The Computational Science Initiative (CSI) brings together under one umbrella the expertise that has driven this success to foster cross-disciplinary collaborations to address the next generation of scientific challenges posed by facilities such as the new National Synchrotron Light Source II (NSLS II). A particular focus of CSI's work will be the research, development and deployment of novel methods and algorithms for the timely analysis and interpretation of high volume, high velocity, heterogeneous scientific data created by experimental, observational and computational facilities to accelerate and advance scientific discovery. CSI is hereby taking an integrated approach, providing capabilities from leading edge research to multi-disciplinary teams that deliver operational data analysis capabilities to the scientific user communities.

Job Opportunities

- Director of the Center for Data Driven Discovery (C3D)
- Software Engineers

Contacts

Kerstin Kleese van Dam
Director, Computational Sciences Initiative and Chair of the Center for Data-Driven Discovery
631.344.6019

Robert Harrison
Chief Scientist

Lauri Peragine
Administrative Specialist, 631.344.7090

Events

Brookhaven Lab Advances its Computational Science and Data Analysis Capabilities

Using leading-edge computer systems and participating in computing standardization groups, Brookhaven will enhance its ability to support data-driven scientific discoveries

November 18, 2016

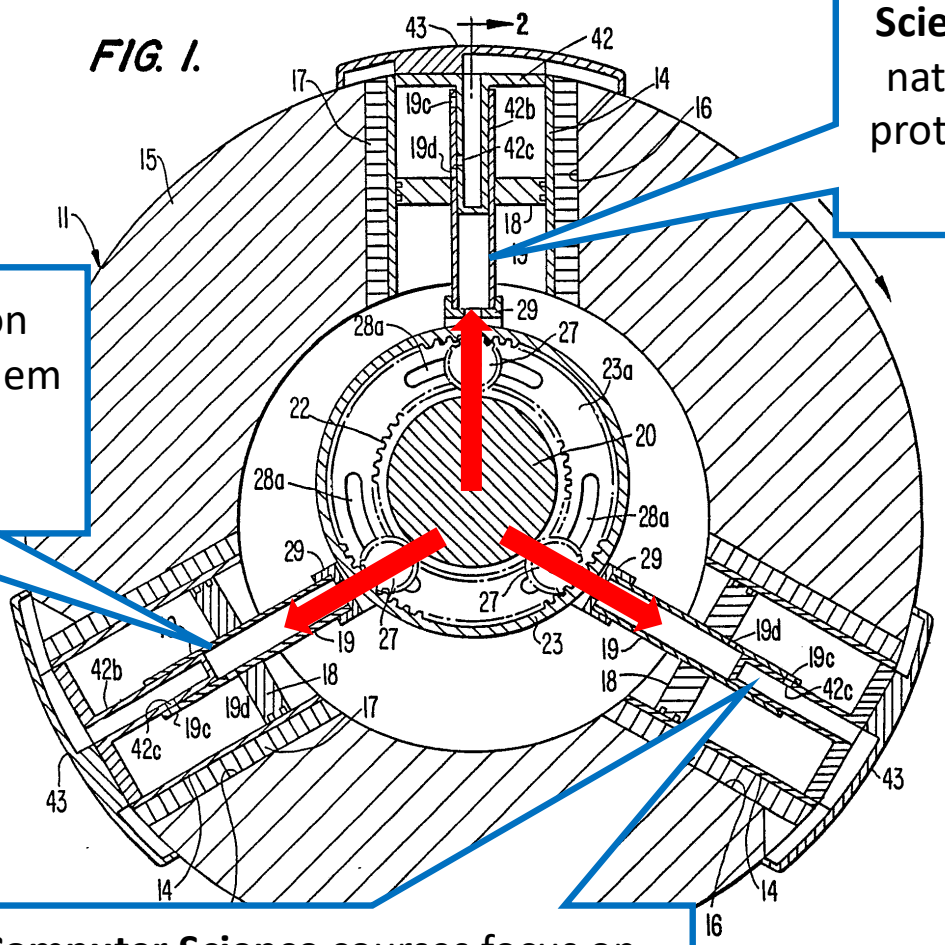
Members of the commissioning team—(from left to right) Imran Latif, David Free, Mark Lukasczyk, Shigeki Misawa, Tejas Rao, Frank Burstein, and Costin Caramarcu—in front of the newly installed institutional computing cluster at Brookhaven Lab's Scientific Data and Computing Center. +ENLARGE

At the U.S. Department of Energy's (DOE) Brookhaven National Laboratory, scientists are producing vast amounts of scientific data. To rapidly process and interpret these data, scientists require advanced computing capabilities—programming tools, numerical models, data-mining algorithms—as well as a state-of-the-art data, computing, and networking infrastructure.

The Challenge Facing Educators

- How to introduce SciComp into a tightly controlled preexisting **science** curriculum?
- How to control compute resources normally owned by the Math, Engineering, or Business departments?
- How to demonstrate solving **science problems** using code *before* students complete their first CompSci course?
- How to address worries that writing code impairs scientific intuition or reduces the time for hands-on experiences?
- How to raise the comfort level of science educators who have not written computer code **in years**?

SciComp Is Getting Lost in the Middle

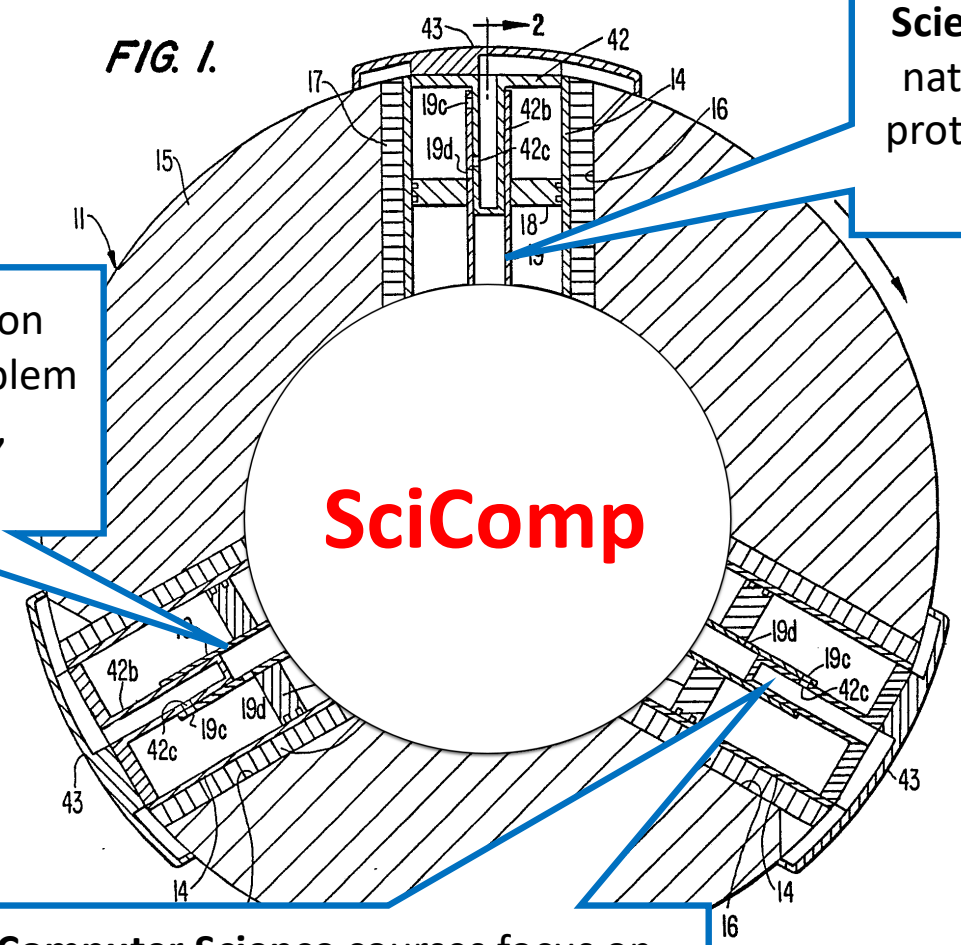


Science courses focus on natural laws, laboratory protocols, physical device manipulation

Math courses focus on formulae, proofs, problem solving mechanics, abstract tasks

Computer Science courses focus on theory, platforms, tools, languages, business information systems

SciComp Is Getting Lost in the Middle



Science courses focus on natural laws, laboratory protocols, physical device manipulation

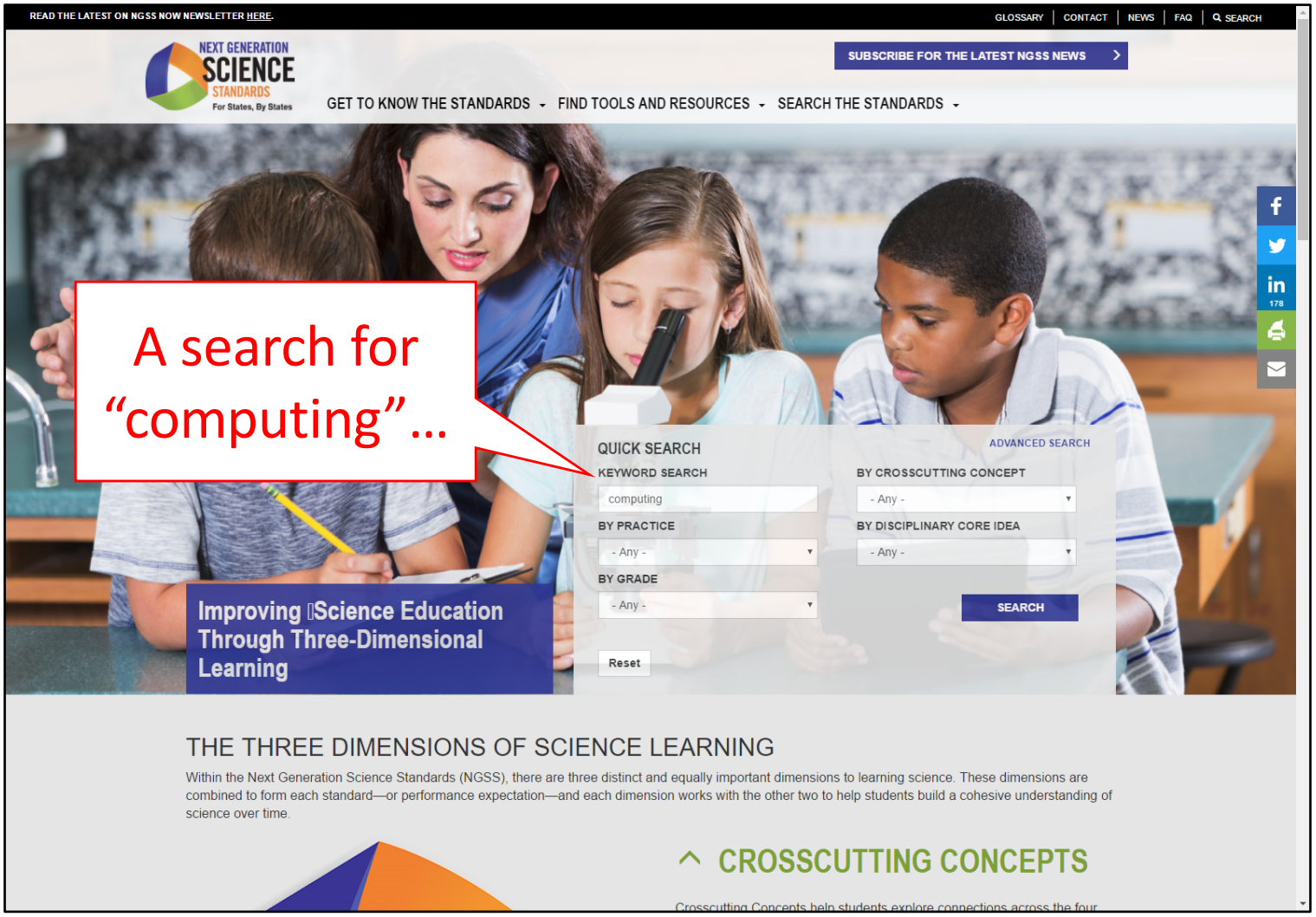
Math courses focus on formulae, proofs, problem solving mechanics, abstract tasks

SciComp

Computer Science courses focus on theory, platforms, tools, languages, business information systems

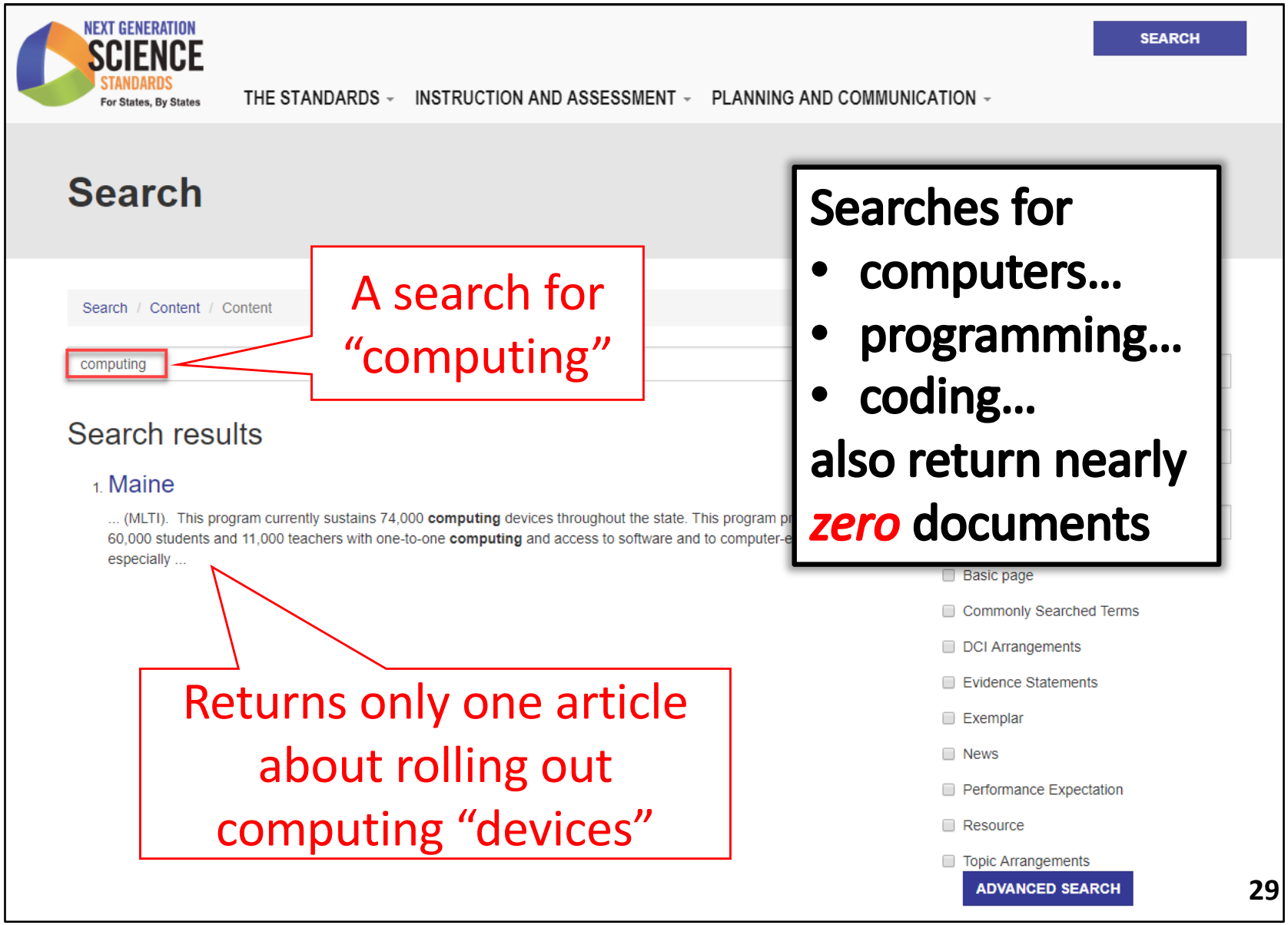
1. **Historical Departmental Silos**
2. **Organizational Inertia**
3. **Instructor Readiness**

The Challenge Facing Educators

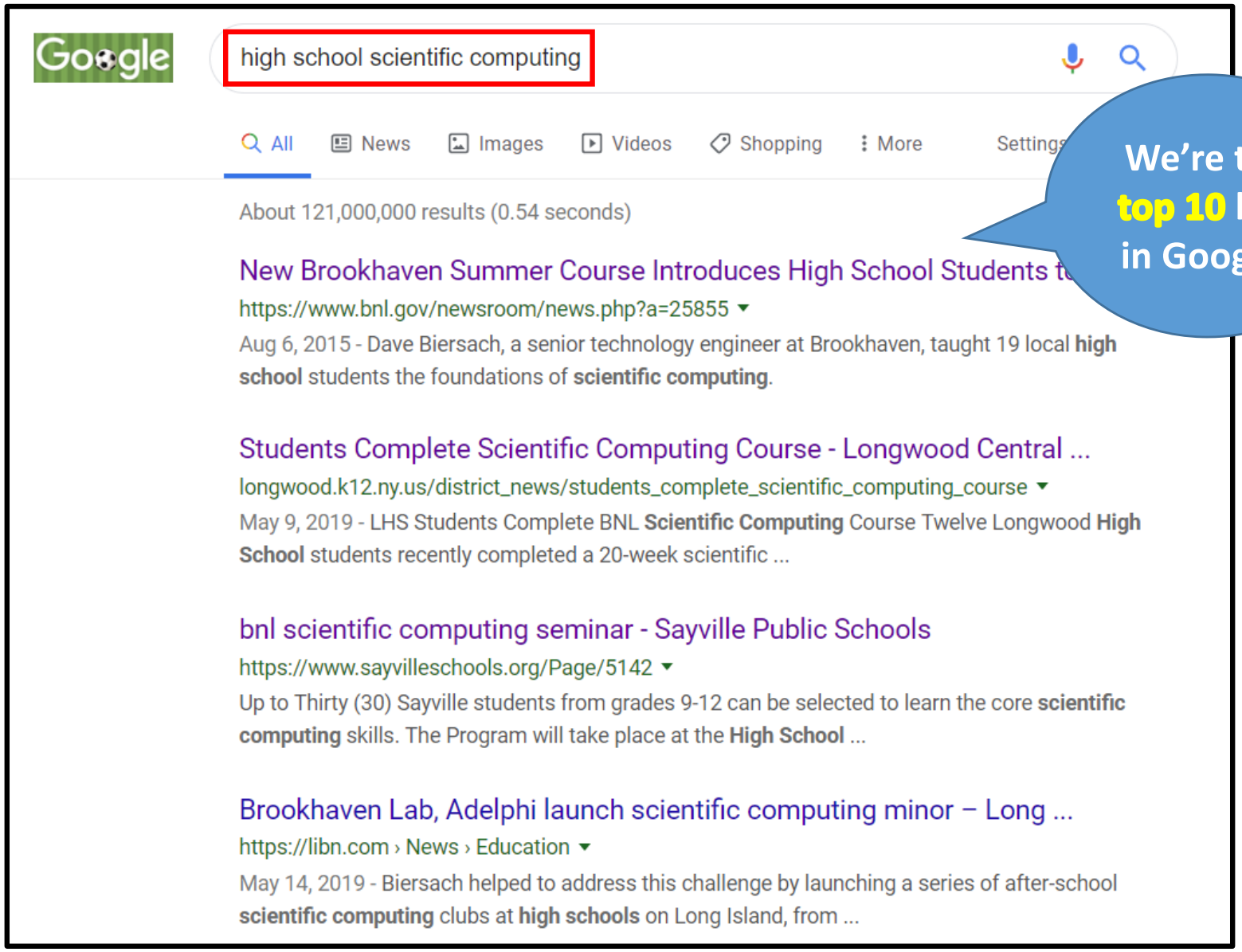


https://www.nextgenscience.org

The Challenge Facing Educators



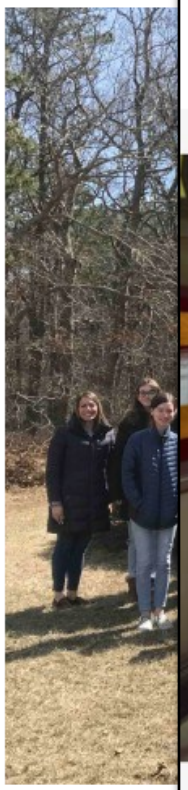
Yet you are Leading the World!



RIVERHEAD MIDDLE SCHOOL

Riverhead computing students visit Brook

By RiverheadLOCAL



Riverhead mi
Elementary S
Program visit
see how com

Coding Enrichment Program For Budding Scientists

Smithtown High School East is offering an enrichment program open to all interested 10th -12th grade students

SMITHT
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Longwood Central School District » District News » **Students Complete Scientific Computing Course**

STUDENTS COMPLETE SCIENTIFIC COMPUTING COURSE

LHS Students Complete BNL Scientific Computing Course

Posted on 05/09/2019

Twelve Longwood High School students recently completed a 20-week scientific computing course designed to spark an interest in computer-literate researchers of tomorrow.

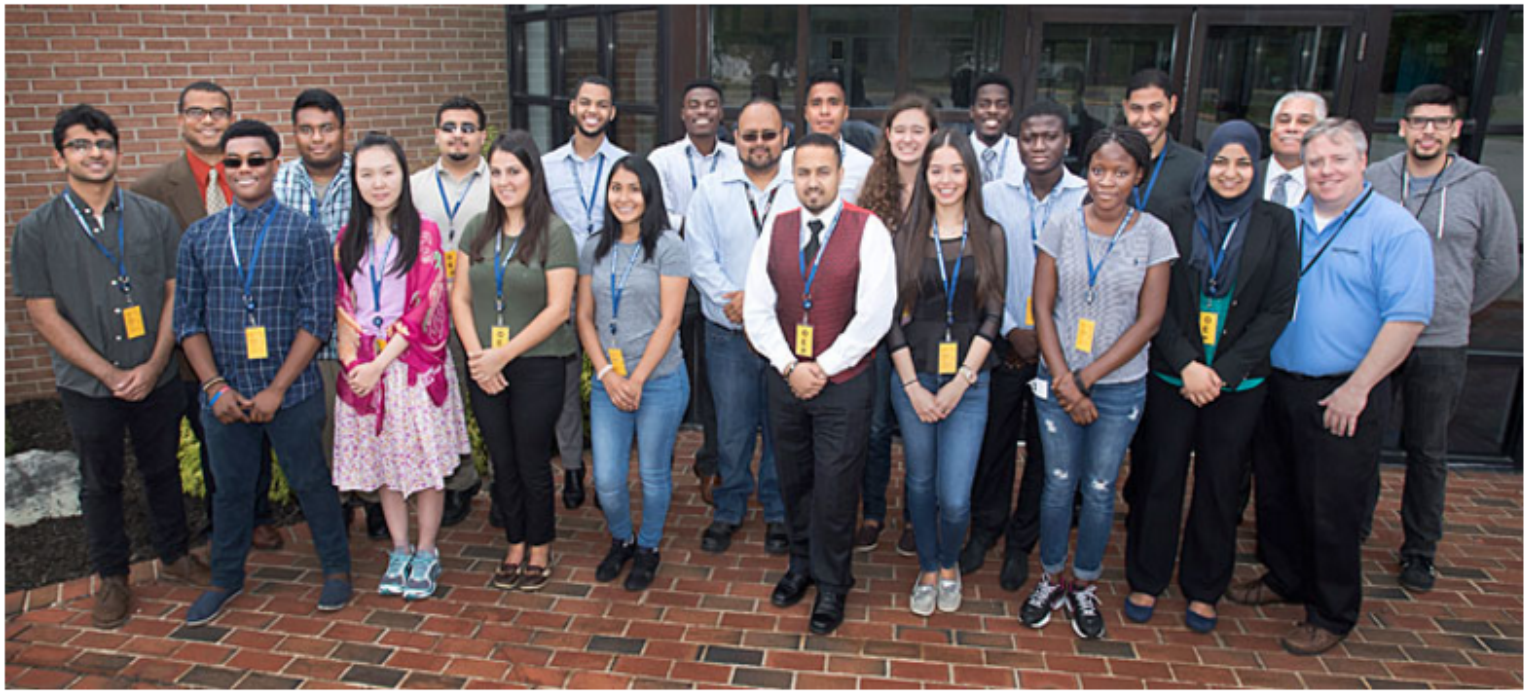
Sponsored by Brookhaven National Laboratory and developed by instructor and technology architect David Biersach, the course introduced the students to modern coding techniques to address data analysis challenges in sciences. Additionally, students had access to Wolfram Mathematica software as well as cloud computing to complete lab exercises designed to introduce 11 fundamental techniques of analysis and presentation of scientific data.

"The Scientific Computing Course gave me the knowledge to work through difficult problems in my future career," said sophomore Jack Mendes.

The students met once a week at the high school and completed 45 hands-on programming labs. The course also provided an introduction of internship and research opportunities offered by Brookhaven National Laboratory.

Developing Scientific Computing Capabilities for the Workforce of Tomorrow

This summer's Scientific Computing 102 internship prepared college students for the big data challenges facing researchers in science, technology, engineering, and mathematics (STEM)



+ ENLARGE The 2016 Scientific Computing 102 students with their instructor, David Biersach (first from the right, front row) and the Office of Educational Programming team.

For young scientists joining a research project for a summer, every minute of the experience is precious. In addition to reading previous publications and learning the scientific vernacular, many of the students coming to the U.S. Department of Energy's (DOE) Brookhaven National Laboratory for summer research internships must scramble to teach themselves how to code so they can work with their data.

"If six out of their ten weeks here are spent just learning the basics of computer programming, those undergraduates will have a reduced opportunity to acquire true expertise in their field," noted David Biersach, a technology architect at Brookhaven Lab. "I work with the Information Technology Division [ITD], so I get to see what scientists across the lab are doing with custom coding solutions and where a lot of the interns are struggling."

Writing Code for a More Skilled and Diverse STEM Workforce

Twenty science, technology, engi
undergraduates funded by the N
Alliances for Minority Participatio
summer for a new three-week wo
skills

September 6, 2018

Working with Brookhaven Lab, Adelphi Offers First Scientific Computing Minor in New York State

An introductory scientific computing course that started out in 2015 as a weekly high-school after-school program developed by Brookhaven Lab is now part of the curriculum for a new scientific computing minor offered at Adelphi University.

SciComp
Survey of Scientific Computing

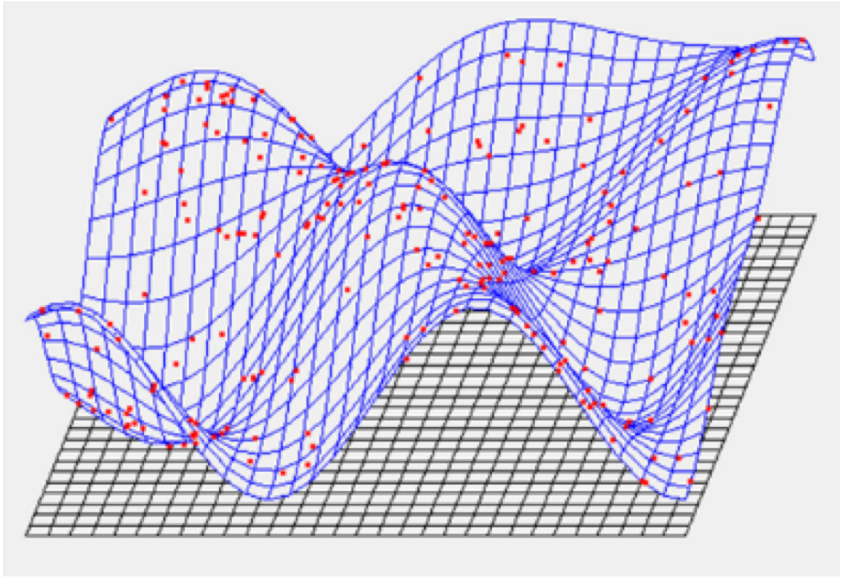
- Objectives
  - Provide patterns for solving real-world **science problems** by writing custom software
  - Demonstrate how **scientific computing impacts all science disciplines**
  - Enable students to **translate scientific formulas into correct and efficient code**
  - Review techniques for the **effective visualization** of complex data
  - Show optimal methods to store and analyze very large data sets
  - **Prepare students to conduct interdisciplinary research at world-class institutions**

Mathematical Concepts

- Systems of Equations
- Probability Distributions
- Combinatorics
- Simulation & Modeling
- Monte Carlo Integration
- Polar & Spherical Coordinates
- Dynamical Systems
- Mesh Interpolation
- 2D Affine Transformations
- Vector & Complex Algebra
- Signals Analysis

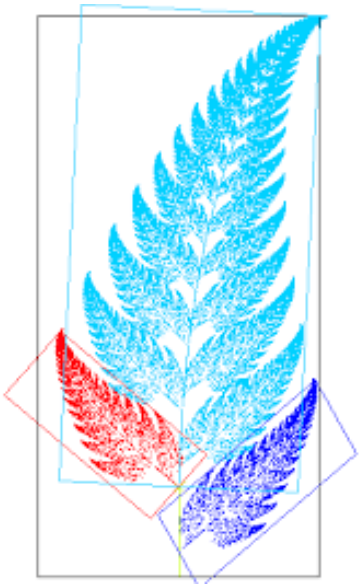
$$\varphi = [1; \{1\}]$$

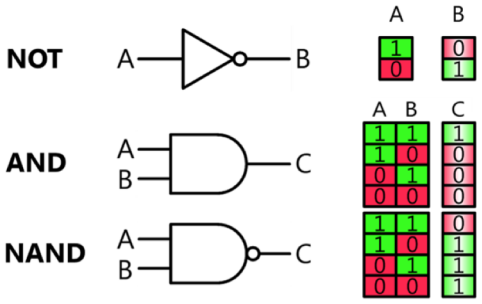
$$\sum_{n=1}^{\infty} \frac{1}{n^2} = 1 + \frac{1}{4} + \frac{1}{9} + \frac{1}{16} + \frac{1}{25} + \cdots = \frac{\pi^2}{6}$$



Computer Science Concepts

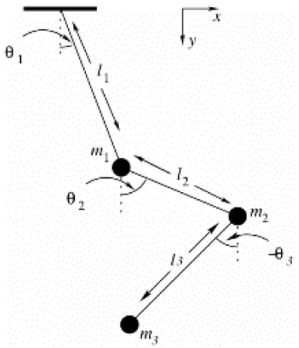
- Representations and Encodings
- Random Number Generation
- Strings, Arrays, Operators
- Loops, Functions, Recursion
- Searching & Sorting
- 2D and 2.5D Graphics (Oblique Projection)
- Boolean Algebra, Digital Logic Circuits
- Runtime Complexity
- File I/O (CSV)
- CERN ROOT

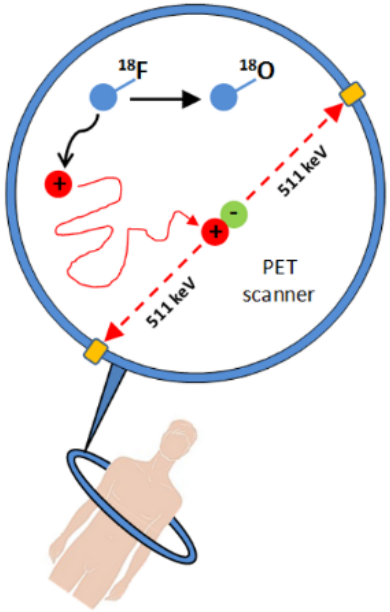




Science Concepts

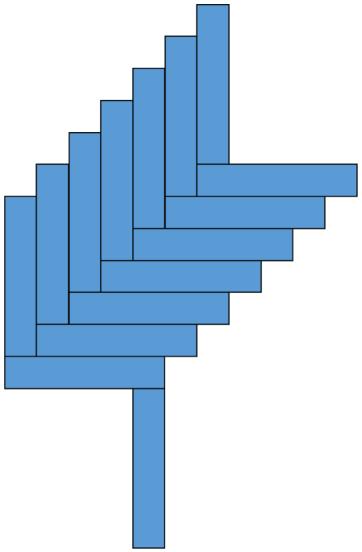
- Mechanics and Kinematics
- Waves (Fourier Analysis)
- Unit Conversion
- Genetic Sequence Analysis
- Balancing Ionic Equations
- Projectile Motion
- Equilibrium & Thermodynamics
- Radioactive Decay





$$\mathbf{10}P_2I_4 + \mathbf{13}P_4 + \mathbf{128}H_2O \rightarrow \mathbf{40}PH_4I + \mathbf{32}H_3PO_4$$

Phosphonium iodide



sorted suffixes

0	aacaagtttacaagc
11	aagc
3	aagtttacaagc
9	acaagc
1	acaagtttacaagc
12	agc
4	agtttacaagc
14	c
10	caagc
2	caagtttacaagc
13	gc
5	gtttacaagc
8	tacaagc
7	ttacaagc
6	tttacaagc