Undergraduate Computational Science for the Quantitative Sciences

by

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Quantitative Sciences

(parts of mathematics, computer science, engineering, physics, chemistry, economics, finance, biology, …..)

All students should have at least one course that illustrates each of the three basis methods of discovery:

- **Computational Science (simulation)**
- **Inductive (laboratory)**
- **Deductive (theoretical)**

CSE Method or Process

```
Do cycle = 1 , no_money

    Call application
    Call model
    Call method
    Call computation
    Call test and assess

End do
```

Limitations from 120-credit BS

Typical math related core includes:

• CALC	12 (3 4-credits)
• ODE	3
• STAT	3
• PROG	3
	Total = 21

Need to Reorganize the Core

Three possibilities are:

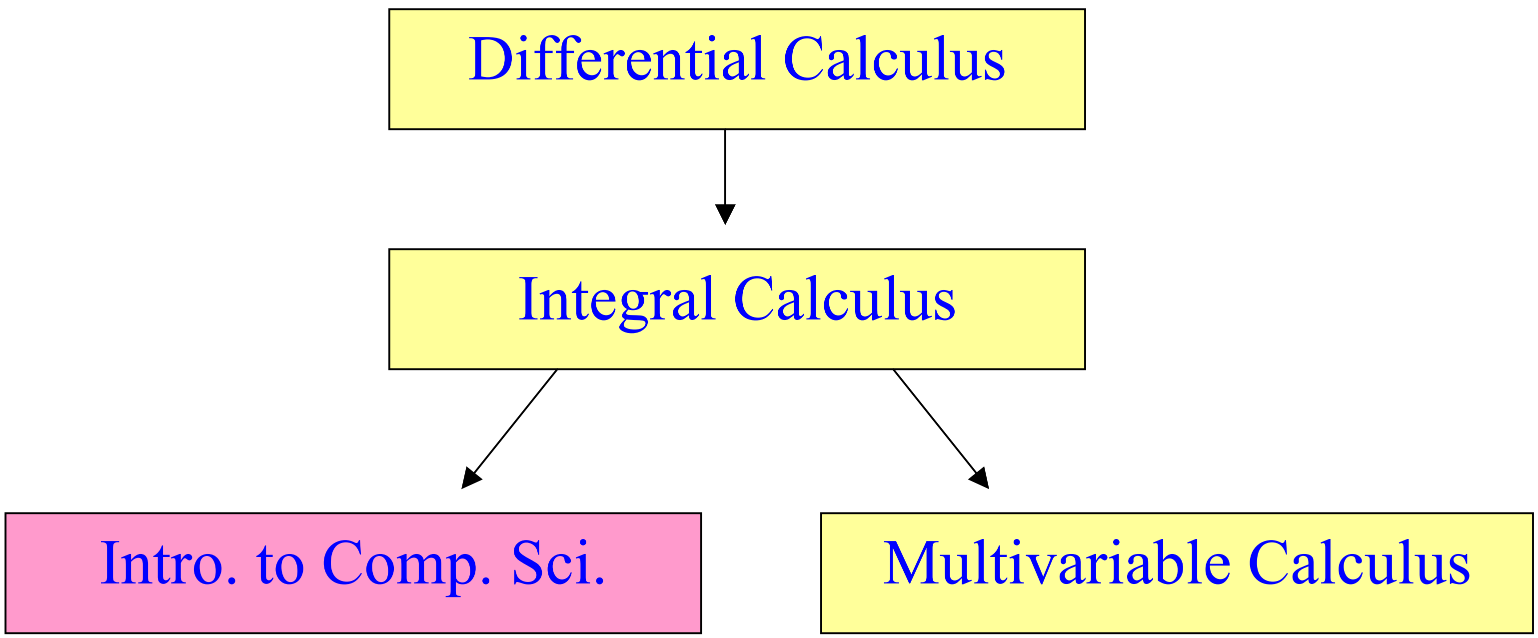
1. **Change CALC to 4 3-credit courses, and introduce a new course on computational science.**

2. **Keep CALC as 3 4-credit courses, but insert "9" 2-lecture modules illustrating computational science.**

3. **Modify PROG, the basic computer programming course, to include more computational science and current computing tools.**

Option 1: CALC becomes 4 3-credit courses

New Course on "Computational" Calculus or Introduction to Computational Science



Option 1: CALC becomes 4 3-credit courses

An Introduction to Computational Science
(application driven, Matlab and visualization)

1. **Symbolic**
2. **Numeric and Basic Programming**
3. **Numerical Differential Equations**
4. **Matrices and Arrays**
5. **Fortran or C**

Option 2: CALC is 3 4-credit courses with CSE modules

Module 1: Falling Mass and Derivatives

Cycle 1: no air resistance, forward finite difference

Cycle 2: no air resistance, centered finite difference

Cycle 3: air resistance

Option 2: CALC is 3 4-credit courses with CSE modules

Module 2: Optimization and Display Area

Cycle 1: graphical

Cycle 2: derivative

Cycle 3: constraints on x and y lengths

Option 2: CALC is 3 4-credit courses with CSE modules

Module 3: Optimization and Roots

Cycle 1: bisection and sqrt(x)

Cycle 2: Newton's method

Cycle 3: cost of a box with materials and labor

Option 2: CALC is 3 4-credit courses with CSE modules

Module 4: Integrals and Work

Cycle 1: rectangles

Cycle 2: trapezoids

Cycle 3: Simpson's rule

Option 2: CALC is 3 4-credit courses with CSE modules

Module 5: Cooling and ODE

Cycle 1: Euler

Cycle 2: Improved Euler

Cycle 3: Surrounding temperature varies with time

Option 2: CALC is 3 4-credit courses with CSE modules

Module 6: Mass-Spring and ODE

Cycle 1: no damping

Cycle 2: damping

Cycle 3: resonance

Option 2: CALC is 3 4-credit courses with CSE modules

Module 7: Trajectories

- Cycle 1: no air resistance in 2D
- Cycle 2: no air resistance in 3D
- Cycle 3: air resistance

Option 2: CALC is 3 4-credit courses with CSE modules

Module 8: Parameter Identification

Cycle 1: economy of scale and price

Cycle 2: partial derivatives

Cycle 3: normal equations

Option 2: CALC is 3 4-credit courses with CSE modules

Module 9: Mass and Double-Triple Integrals

Cycle 1: summations

Cycle 2: nested loops

Cycle 3: change of coordinates

Option 3: Modify PROG to include basic CSE

- **Many CSC departments have gone to JAVA for the base CSC major programming course.**
- **This is more applicable to IT than CSE, and this presents an obstacle to higher level CSC courses.**
- **Part time instructors are teaching many sections of Fortran and C.**
- **Many applied departments are using Matlab in their upper level courses.**

Option 3: Modify PROG to included basic CSE

Fortran uses one semester of calculus for a prerequisite and often has topics on:

- **Computing history**
- **Code and structure**
- **Loops and branching**
- **Input-output**
- **Arrays**
- **Functions, subroutines and modules.**

Often applications are not stressed.

Option 3: Modify PROG to included basic CSE

A more useful alternative may be to use Matlab as a first programming course for the quantitative science students.

- **One could include more applications.**
- **Illustrate the computational science method.**
- **Give the student tools that will be used in their area of study.**

Concluding Remarks

- **“I do not know what you are going to do about technology”**

  from retiring professor of math.

- **“Calculus is a nice historical perspective”**

  from current professor of math.

- **“How do you teach whether or not the computer is giving the correct answer?”**

  from former college Dean.

In other words,

Computers are being used by a larger segment of society and scientist and will not go away.

Discrete models have replaced many traditional continuum models.

The mathematical questions about approximation and accuracy of the models are even more a concern with the use of computers.

It is not sufficient to learn to operate a computer, but one must learn how to utilize a computer.