

From Calculus to a Course on An Introduction to Parallel Computing

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Attributes of Computation Science

- *Cross disciplines:*
applications, mathematics and computing
- *Illustrate the process:*
application, model, method, computation and assessment
- *Model types:*
deterministic/statistical, continuous/discrete, simplistic/complex

Three "Computation Science" Courses

- **Introduction to Applied Mathematics (second year)**
- **Computational Modeling (third year)**
- **Introduction to Parallel Computing (fourth year)**

Introduction to Applied Mathematics (MA 325)

- **A survey of applications of mathematics**
- **Suitable for students who have taken multivariable calculus**
- **Student to formulate a cohesive plan of study for the third and fourth years**
- **Five three-week modules on variety of applications**

Module on Heat and Mass Transfer

- **Newton cooling and stability**
- **Discrete versus continuous models**
- **Analysis of discretization error**
- **Diffusion in a wire**
- **Analysis of stability**
- **Diffusion in a cooling fin**
- **Pollutant transfer in a stream**
- **Pollutant transfer in a lake**
- **Analysis of von Neumann series**

R. E. White

Module on Acoustic Waves and Boundary Conditions

- **Development of the wave equation from first principles**
- **Development continued**
- **Development of several types of boundary conditions**
- **Discuss experimental procedures and data collection**
- **Formulate the least square problem for parameter estimation**
- **Visit to the CRSC/Math laboratory for data collection**
- **Analysis of data**
- **Analysis continued**

H. T. Tran

Module on Cryptography

- **Some elementary cryptosystems.**
- **The Hill cryptosystems.**
- **The Hill cryptosystem with Maple.**
- **Generalizations of the Hill cryptosystem.**
- **The two-message problem.**
- **Mathematical prerequisites for the RSA encryption**
- **The RSA encryption and decryption.**
- **The RSA cryptosystem and Maple.**

E. L. Stitzinger

Module on Modeling of Random Phenomena

- **Basic concepts in Probability. Bayes formula and decision examples.**
- **Bernoulli model. Examples of queuing systems. Markov chains and equilibrium.**
- **Random walks. A probabilistic approach to heat diffusion. Monte Carlo simulations.**
- **Law of Large Numbers. Example of a particle moving in a random medium.**
- **Central Limit Theorem. Estimation from large samples.**
- **Financial Mathematics. An introduction to the problem of pricing and hedging financial derivatives. The one-period model.**
- **Multi-period model and binomial trees. Examples of American and exotic options.**
- **Black-Scholes formula from discrete to continuous time models. Brownian motion.**

Jean-Pierre Fouque

Module on Biological Modeling

- **Compartmental models. How is alcohol different from Prozac?**
- **Disease transmission. How does an epidemic happen? What happens when you vaccinate some of the population?**
- **Human population growth. When will Raleigh have 1 million people? How many people will the world have in the long run?**

S. R. Lubkin

Computational Modeling (MA 402)

- **For students in the sciences or engineering who use PDEs**
- **Often there is a BIG gap going from the basic ODE to senior year work**
- **Applications driven with Matlab computations and**
- **Topics as needed in matrix algebra, numerical PDE models and numerical methods**

Time Dependent Matrix Models: $u^+ = Au + d$

Newton Cooling Models

Heat Diffusion in a Wire

Heat Diffusion in a Wire with Little Insulation

Flow and Decay of a Pollutant in a Stream

Convergence Analysis for Euler Method

Convergence Analysis for Heat and Mass Transfer

High Performance Computing

Vector Pipeline Computer and Matrix Products

Vector Computations for Heat Diffusion in Two Directions

Multiprocessing Computers and Mass Transfer in Two Directions

MPI and IBM/SP

MPI and Matrix Products

MPI and 2D Models

Steady State Matrix Models: $u = Au + d$

Steady State and Triangular Solves

Heat Diffusion and Gaussian Elimination

Cooling Fin and Tridiagonal Matrices

Schur Complement and Domain Decomposition

Convergence to Steady State

Convergence to Continuous Model

Poisson Equation Models: $-\Delta u = f$

Steady State and Iterative Methods

Heat Transfer in 2D Fin and SOR

Fluid Flow in a 2D Porous Medium

Ideal Fluid Flow

Deformed Membrane and Steepest Descent Method

Conjugate Gradient Method

Nonlinear and 3D Models

Nonlinear Problems in One Variable

Nonlinear Heat Transfer in Wire

Nonlinear Heat Transfer in 2D

Steady State 3D Heat Diffusion

Time Dependent 3D Diffusion

High Performance Computations in 3D

Introduction to Parallel Computing (MA/CSC 583)

- **Computational science has filtered into the undergraduate programs**
- **Message passing interface (MPI) has evolved for distributed multiprocessors or networked computers**
- **"Parallel Programming with MPI" by Peter Pacheco**
 - **introduces MPI**
 - **additional demo MPI codes to be used**
- **"Computational Modeling with Methods and Analysis" by R. E. White**
 - **more advanced applications of MPI**
 - **domain decomposition, CG and GMRES**
- **Flexible prerequisites include some understanding in each, with expertise in one, of applications, matrix algebra and computer science**

High Performance Computing

Vector Pipeline Computer and Matrix Products

Vector Computations for Heat Diffusion in Two Directions

Multiprocessing Computers and Mass Transfer in Two Directions

MPI and IBM/SP

MPI and Matrix Products

MPI and 2D Models

Message Passing Interface

Basic MPI Subroutines

Reduce and Broadcast

Gather and Scatter

Derived Data Types

Communicators

Application to Fox's Algorithm

Classical Methods for $Ax = d$

Gaussian Elimination and LAPACK

Schur Complement and SPD

Domain Decomposition and MPI

SOR and P-regular Splittings

SOR, Domain Decomposition and MPI

ADI and MPI

Krylov Methods for $Ax = d$

Krylov Space of Vectors

Conjugate Gradient and Classical Preconditioners

PCG and MPI

Hessenburg Matrix and Least Squares

GMRES and Parallel Preconditioners

GMRES and MPI

