# A Plan for a Computational Science Program at UTK

## Intercollegiate Graduate Program in Computational Science (IGPCS)

Second meeting 2/3/06

# Possibilities Paths
## (from the last meeting on 12/7/05)

- Concentration in Computational Science
  - Original plan

- Minor in Computational Science
  - At the Graduate level
  - Modeled on: Intercollegiate Graduate Statistics Program
    - Different in the sense that there is not one department
  - Discussed courses from two groups, Level A & B

- Also considering a Certificate option Computational Science
  - Vasilios Alexiades, Math, is looking into this

- Subcommittee formed to develop details of the Minor program

# Subcommittee for Developing a Minor in Computational Science (Graduate Level)

- Jack Dongarra, Computer Science
- Christian Cardall, Physics
- Chuck Collins, Math
- Jens Gregor, Computer Science
- Robert Hinde, Chemistry
- Cynthia Peterson, Biochem, Cellular & Molecular Bio
- Peiling Wang, School of Information Sciences

# Computational Science Involves a Chain or Cycle of Linked Series of Actions

- Domain science theory
- Mathematical modeling
- Algorithm development
- Software integration
- Hardware instantiation
- Domain science integration

The minor program will be build around this cycle of activities.

# Computational Science is Interdisciplinary

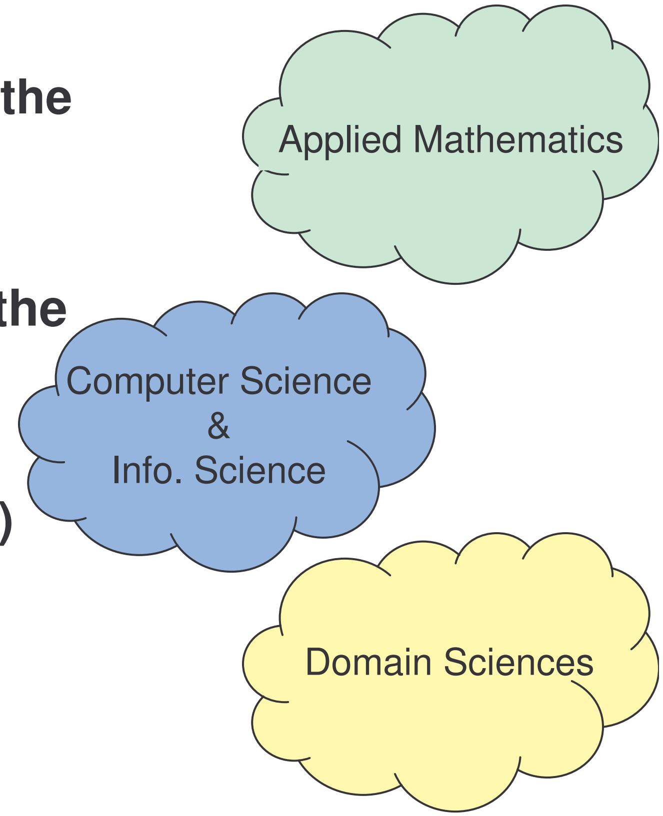
- Students in one of the three general areas in Computational Science;
  - Applied Mathematics,
  - Computer & Info. Science, or
  - a Domain Science

  will become exposed to and better versed in the other two areas that are currently outside their "home" area.

- A pool of courses which deals with each of the three main areas will be put together for students to select from.

# Requirements

- **With guidance from their home department, students will lay out a program**
  - **Choice of courses must have the approval of the IGPCS Program Committee.**
- **At the Masters level a minor in Computational Science will require 9 hours (3 courses) from the pools.**
  - **At least 6 hours (2 courses) must be taken outside the student’s home area.**
  - **Students must take at least 3 hours (1 course) from each of the 2 non-home areas**
- **At the Doctoral level a minor in computation science will require 15 hours (5 courses) from the pools.**
  - **At least 9 hours (3 courses) must be taken outside the student’s home area.**
  - **Students must take at least 3 hours (1 course) from each of the 2 non-home areas**



# Internship

- This is optional but strongly encouraged.
- Students in the program can fulfill 3 hrs. of their requirement through an Internship with researchers outside the student’s major.
- The internship may be taken offsite, e.g. ORNL, or on campus by working with a faculty member in another department.
- Internships must have the approval of the IGPCS Program Committee.

# How It Might Work For Students

| Degree Program | Recognition Sought | Requirements |
|---|---|---|
| Master's in Home Dept. | Minor in Computational Science | 9 hrs: 0-3 hrs in Dept.<br>6 hrs Outside Dept. |
| Doctorate in Home Dept. | Minor in Computational Science | 15 hrs: 0-6 hrs in Dept.<br>9 hrs Outside Dept. |

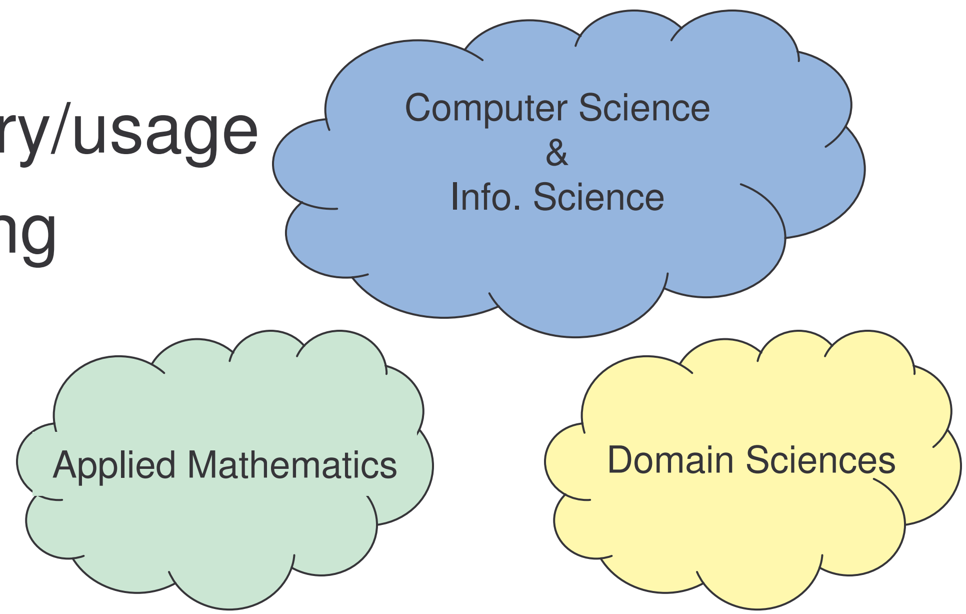
- Open to all students in departments with approved minor
- IGPCS Program Committee establishes an approved program/list of courses
- Home dept. must verify fulfillment of non-Computational Science degree requirements
- ORNL or other internship strongly encouraged

# Additional Hours?

- To fulfill the requirements for the minor a student may be required to take additional hours above the normal hours requires for the graduate degree.

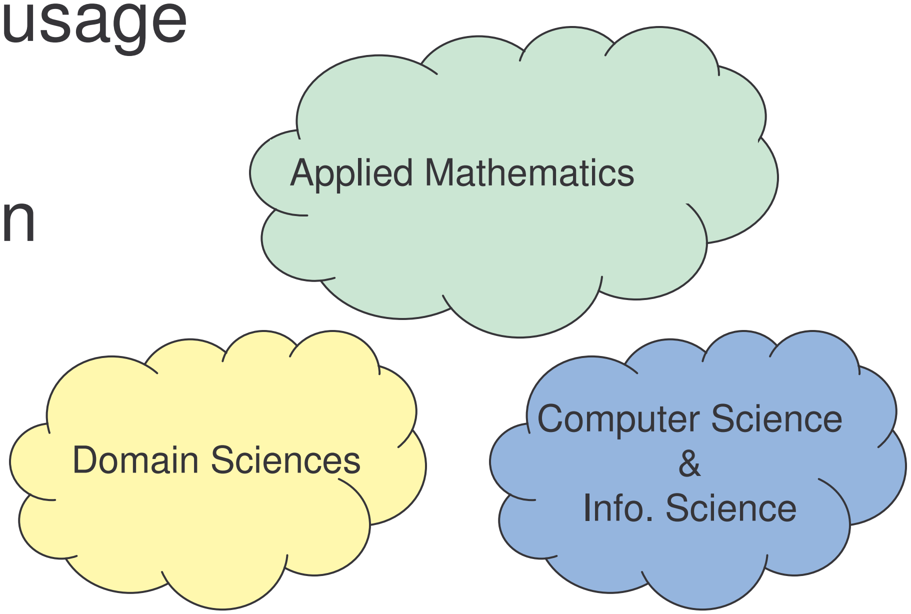
# Example

- A student pursuing a minor at the MS level in, say, Computer Science would be required to take 6 hours from the pools of courses dealing with:
  - Domain science theory/usage
  - Mathematical modeling



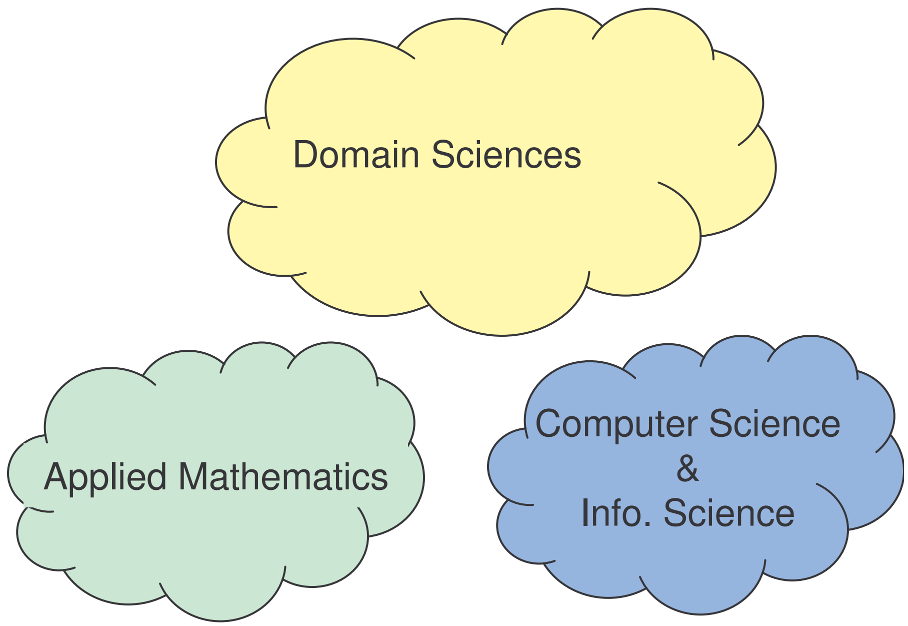
# Example

- A student pursuing a minor at the MS level in Mathematics would be required to take 6 hours from the pools of courses dealing with:
  - Domain science theory/usage
  - Algorithm development
  - Software implementation
  - Hardware instantiation



# Example

- A student pursuing a minor at the MS level in Physics would be required to take 6 hours from the pools of courses dealing with:
  - Mathematical modeling
  - Algorithm development
  - Software implementation
  - Hardware instantiation



# Pool of Courses

## Applied Mathematics and Mathematical Modeling

- Chem Eng 507 Application of Linear Algebra in Eng. Systems
- Math 512 Methods in Applied Mathematics II
- Math/CS 571-572 Numerical Mathematics
- Math/CS 574 Finite Element Method
- Math/CS 575 Matrix Theory and Techniques in Num Analysis
- Math 577 Optimization
- Math 578 Numerical Solution of PDEs
- Math 581-582 Mathematical Ecology 1 & 2
- ECE 503 Modern Transform Methods
- ESci 539 Continuum Mechanics
- Phys 531 Classical Mechanics
- Phys 571-572 Mathematical Methods in Physics 1 and 2

## Computer & Info. Science (software, hardware, algorithms)

- CS 525 Software Engineering
- CS 530 Computer Systems Organization
- CS 551 Pattern Analysis
- CS 552 Image Analysis
- CS 576 Sparse Matrix Computations
- CS 594 Special Topics (on a case-by-case basis)
- ESci 551 Finite Elements for Engineering Applications
- ESci 577 Neural Networks in Engineering
- ECE 557 Computer Architecture and Design
- IS 565 Digital Libraries
- IS 584 Database Management Systems
- IS 588 Human-Computer Interaction
- IS 585 Information Technologies
- IS 589 Information Networking Technologies

## Domain Science (more to come)

- Geology 401 Quantitative Methods in Geology
- Geology 501 Fractal Models in Earth Sciences
- Geography 510 Geographic Software Design
- Phys 511-512 Theoretical Physics 1 and 2
- Stat 574 Data Mining Methods and Applications
- Phys 573 Numerical Methods in Physics
- BCBM 615 Special Topics in Biochemistry, Cellular and Molecular Biology
- LS 507 Bioinformatics and Computational Biology
- BCMB 511 and 512 Protein Chemistry and Molecular Biology, respectively
- MS&E 511 and 512

# Internship in Computational Science

- 5xx Practicum: Opportunity to translate theory into practice under guidance of qualified instructor. (Is normally performed outside the University, e.g. ORNL.)
  - May be used toward requirements for graduate degree in the students home department.

- 5xx Practicum: Experience using techniques of computational science to address research problems in chemistry, supervised by departmental faculty.
  - May not be used toward requirements for graduate degree in the students home department.

- Prereq: Consent of instructor.
- Graded: A/B/C/D/F or P/F?

# Program Administration

- IGPCS Program Committee (6 to 8 people)
  - Subset of the Program Faculty
  - 1-2 representatives from each of the colleges involved, appointed by the Dean of that college
  - Renewable 2 year terms
  - Responsible for oversight: program requirements, approving courses and department programs, student course selection, etc.
- IGPCS Program Faculty
  - Any faculty member, assistant professor or above in rank, nominated by department head and approved by program committee
  - Responsible for teaching program courses, directing student research, serving on student committees

# Steps to Implement this Model

- IGPCS Subcommittee to develop a plan
- Participating departments put forward some possible courses/descriptions for the minor
- Initial IGPCS Program Committee is formed
- Program committee works with other IGPCS faculty to evaluate courses and identify relevant sequences among them
- Departments propose a program (course options, suitably sequenced) for their students
- Program Committee reviews and either accepts or returns for modification

# Roadmap

- <u>December 2005 – February 2006</u>
  - Group meets and agrees on some initial version of the plan
  - Group members take the initial draft back to departments; iterate on the plan via e-mail <u>early February 2006</u>
  - Updated version of the plan is presented to the Chancellor, Dean's meeting, and/or the Graduate Council
  - Group meets to finalize the plan
  - Overall program plan is presented in a letter to Chancellor/Chancellor's staff for approval. That approval would transform our working group, or some subset of it into the initial Program Committee for the new Computational Science Program.
- <u>March – April 2006</u>
  - Catalogue copy for new courses is developed by each department that wants to offer Computational Science Minor
  - Departmental program plans are reviewed and approved by the Computational Science Program Committee as meeting program requirements
  - Catalogue copy is submitted to each department. At this point, the catalogue copy would begin the normal process up the hierarchy in order to be approved and included in the catalogue for 07-08.

# Applied Math Pool of Courses

**Mathematics for Modeling**

- Math 453 Matrix Algebra II (3, every semester + summer)
  - Basic matrix theory. Amount of application varies with instructor
- Math 512 Methods in Applied Mathematics II (3, Spring)
  - Surveys the material from Math 431 Differential Equations II & Math 435 Partial Differential Equations with more emphasis on modeling and qualitative solution methods

**Mathematical Modeling**

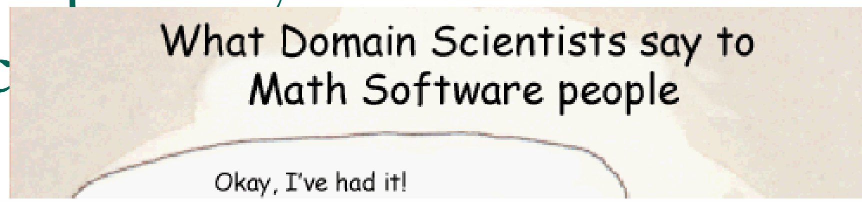
- Math 411 Mathematical Modeling (3, Fall)
  - Basics of mathematical modeling covering continuous and discrete (in time) models and stochastic models. Emphasis on the modeling cycle and projects. The basic mathematics is covered as needed.
- Math 475 Industrial Mathematics (3, Spring)
  - Focuses on a handful of specific projects going from the development of the model, to the mathematical analysis of the model, to the numerical solution of the model. Prereq: Some programming skill

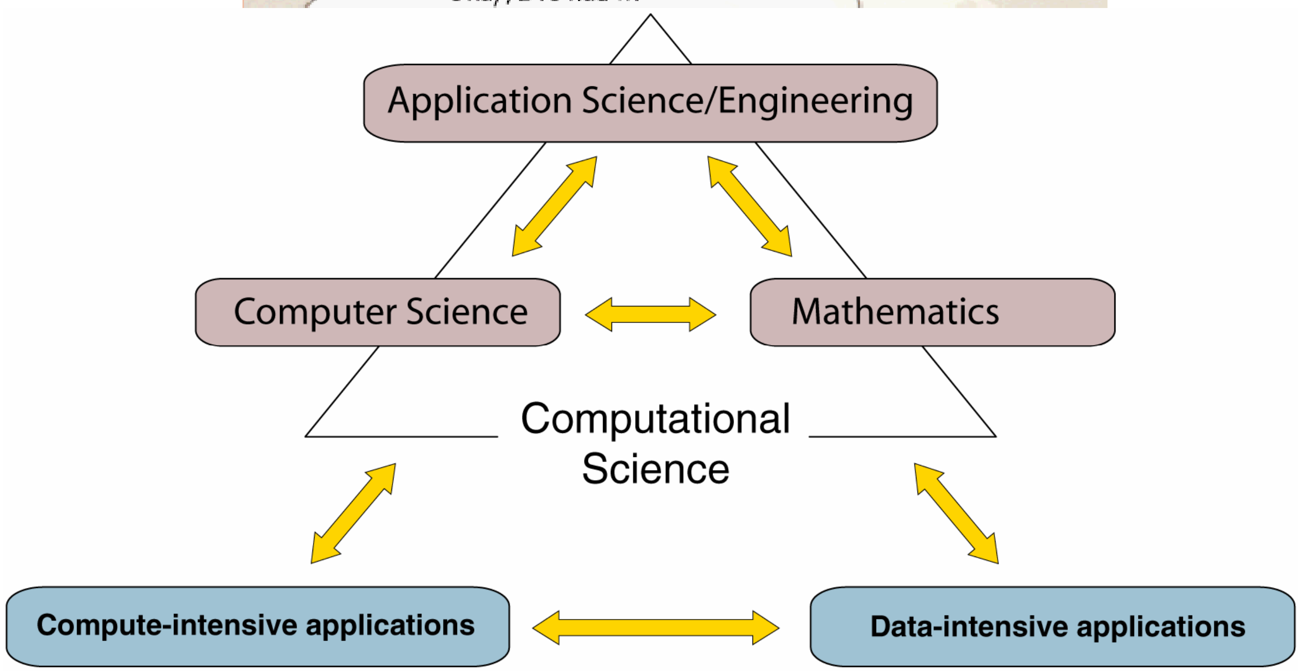
**Numerical Analysis**

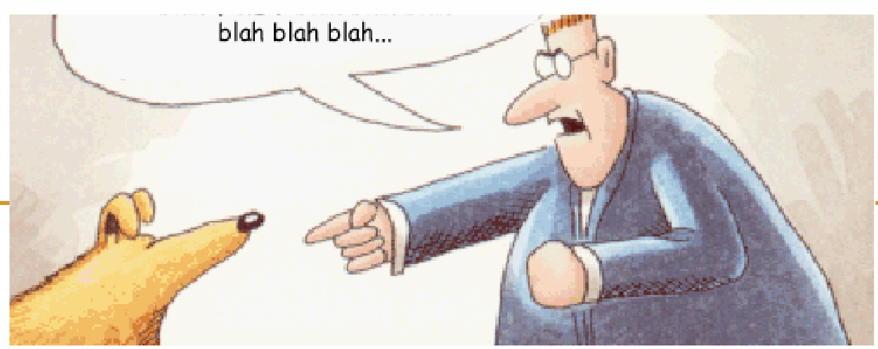
- Math/CS 471 Numerical Analysis (3, Fall)
  - Covers interpolation and approximation by polynomials & splines, numerical integration and numerical solution of ODEs
- Math/CS 472 Numerical Algebra (3, Spring)
  - Covers direct and iterative methods for solving linear systems, methods for finding eigenvalues, and methods for solving nonlinear systems of equations.
- Math 577 Optimization (3, Fall/Alt w/578)
  - Covers the basic methods for unconstrained and constrained optimization. Emphasis is more on theory than on practical issues.
- Math 578 Numerical Solution of PDEs (3, Fall/Alt w/577)
  - Covers numerical approximation of PDEs, especially conservation laws, and the methods used to solve the approximation. Includes some discussion of modeling and implementation. Requires a course in PDEs (435 or 512) and a basic numerics course (371)
- Math/CS 571-572 Numerical Mathematics (3,3)
  - 571 covers the topics of 472 at a greater depth, with the theory behind the methods. 572 covers the topics of 471 as well as basic methods for numerical solution of PDEs, at a greater depth. This is a prelim sequence in the Math Ph.D. program so the theory is the emphasis. Requires some analysis background (proofs)
- Math/CS 574 Finite Element Method (3, Irr)
  - Covers the theory of the finite element method for the solution of PDEs. Includes some discussion of implementation. Requires a course in PDEs (435 or 512) and a basic numerics course. More theoretical than 578
- Math/CS 575 Matrix Theory and Techniques in Numerical Analysis (3, Irr)
  - Advanced topics related to numerical linear algebra. Requires 400-level numerical analysis or higher.

# At the Turn of the Century - Collaborative Interdisciplinary Science Is The Thing;

Domain Sc … maticians




With Apologies to
Gary Larson