Some Thoughts on Computational and Applied Mathematics, and Their Role in Interdisciplinary Research

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Computers have changed the way we live, and the way we think, and the way we do research

- Increased computational ability.
- Ability to collect and analyze massive data.
- Ability to access information, cross disciplinary boundaries.

Increased computational ability: What if Newton had access to the computational power we have now?

- Example: Computing the volume of an object
  1. Before calculus
  2. After calculus but before computers
  3. After computers
- Physics:
  1. "Back of the envelop" calculations no longer imperative (still helpful)
  2. Can handle complex realistic models directly, no need to make drastic simplifications
- Chemistry
  1. Theoretical chemistry requires solving Schrodinger equations
  2. Computation is the main tool

Fundamental first principles are largely understood

What remains is largely a mathematical problem

Example: Fluid dynamics

- Fundamental equations (Navier-Stokes) were understood more than 150 years ago (as a physics problem, it was considered understood).
- As a mathematical problem, it is very complex.
- Engineers avoided using the Navier-Stokes equations for a long time, making predictions based on experience and intuitions, but not any more.

Before we had the computational power

Simplify, simplify, simplify!!!

Intuitions and experiences are crucial.

"Sweeping things under the rug" is necessary.

Now that we do have the computational power

- Computational modeling is becoming a popular tool in many different disciplines.
- Computers only understand mathematical models. The process of "mathematicalization" has become a much more important part of research.
- Can handle very complex, realistic models.

It does not come free!

1. Well, to begin with, what are good problems to study?
2. Algorithms are needed.
3. How do we understand the results?
   "Your computer may have understood the problem, but you don't."

Summary: Mathematics – Unprecedented opportunity, unprecedented challenge

Unprecedented opportunity

The role of mathematics in science, engineering and technology has changed: It is no longer just a "helper"', it is in the "driver's seat."

In many problems at the frontier of science, the main bottleneck is the mathematics.

Conclusion: The link between math and science, engineering and technology is now much closer.

Example: The Moving Contact Line Problem

Unprecedented challenge

Mathematics, particularly applied and computational mathematics, is done in many disciplines. Mathematics community might lose its advantage.

Do we always want to limit our roles to: “dot the i’s, dash the t’s”?

Example: Computational Chemistry

- What was theoretical chemistry like before computations? Example: The periodic table.
- Nobel prize to Kohn and Pople in 1998.
- The problems are very much like the problems in computational mathematics
- The area is developed with little paricipation from applied mathematics. For example, spectral methods, optimization methods, conjugae gradient methods.
- Chemists developed their own methodology and terminology, e.g.
    1. Fourier method – plane wave methods
    2. Finite difference and finite element – real space methods

The implications for not having mathematicans involved

- Slowed down science
- Lost opportunity for computational/applied math
- Lost resources for math

If this trend continues, math and applied math will be **marginalized**.

Example: Complex networks

- internet network, the world wide web
- power grid
- social networks
- biological networks
- communication networks
- ....

Issues:

1. Network security, stability and efficiency.
2. Interplay between their topology, algebraic structure, and dynamics.

Physicists/computer scientists are dominating the field right now.

Why is it?

- Mathematics, including applied and computational mathematics has the tendency of becoming a closed subject.

- Not only in research, but also in education.

The dilemma facing mathematics community

On one hand, mathematics is becoming an essential tool for many exciting areas of science/engineering/technology.

On the other hand, mathematics community is not involved, and poorly prepared.

What should we do?

1. Encouraging interdisciplinary exchange
2. Education: How can we learn both math and the necessary science?

What about teaching (pure) mathematics?

New connections with mathematics:

- mathematical physics
- probability theory and stochastic process
- dynamical systems
- ......

Mathematical thinking: Bottom up (deductive)

Mathematics is not just a collection of subject matter, it is a way of thinking.

1. Concrete – abstract
2. Intuition – rigor (precision)

This kind of thinking is needed in many other disciplines.

- Currently, the teaching of pure math is aimed at experts only.
- We need to teach both mathematical thinking, and techniques.
- Applied math students need to learn more **math thinking.**

What about other sciences?

Chemistry, biology, material science ....

Too much to learn!!

Most important is to **teach the students the ability to teach themselves.**

Understanding basic physics is the key.

Undergraduate curriculum:

1. Simplify existing courses, restore elegance
2. For numerical methods course, stress applications
3. Add new courses
   3.1 Computational introduction to physics
   3.2 New numerical methods course (application oriented, with labs sessions)
   3.3 Mathematical biology (emphasize cell biology, but also some aspects of physiology, ecology)
   3.4 Nonlinear dynamics (dynamical systems, bifurcation theory, pattern formation, chaos)
   3.5 Applied stochastic analysis (Markov chains, Monte Carlo methods, etc)

Graduate curriculum: Summer School in Applied Math/Computational Science

1. Mathematical introduction to physics (continuum, statistical, quantum mechanics)
2. Applied stochastic analysis
3. Introduction to atomistic modeling
4. Applied partial differential equations

Some thoughts about interdisciplinary research

Why "interdisciplinary"?

- Disciplinary research has become more mature.
- Biology, chemistry, material science, ... require tools and principles from physics and mathematics

A basic problem we are facing in the new century: Conflict between our educational system and the frontier of research.

A new model:

- Foundational:
  1. Mathematics: Mathematical thinking (concrete and abstract, intuition and rigor); mathematical language (algebra, geometry, analysis); tools (computation, statistics).
  2. Physics: Quantum physics, statistical physics, electromagnetism (how do we become a professional modeller?).
- Applicational:
  1. Biological science
  2. Material science
  3. Enviornmental science
  4. New technology
  5. ....

Will the value and integrity of mathematics be preserved?

No, mathematics will not be broken into little sub-areas of other sciences.

To the contrary, it will help to unify other areas.

Fluid mechanics serves as a good example.

Summary: Looking beyond traditional boundaries of mathematics

- Unprecedented opportunity, unprecedented challenge
    1. Main challenges in many scientific areas have become mathematical in nature
    2. Our community is not well-prepared, and our system is not set-up to take advantage of this opportunity

- Education is the key
- Whoever solves the education problem first will lead applied/computational math

Chairman Mao said:

Though the path in front of us is wavy, the future is bright!!

We can always say:

"Mathematics is the language of science".

But, ...

L. Carlesson's analogy with Latin.