# Department of Computational Mathematics, Science, and Engineering*

*A proposal to the MSU Board of Trustees
during the 2014-15 Academic Year.
Information in these slides is subject to revision.

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# Motivations

- Computation is an essential and cross-cutting element of all STEM disciplines.
- Computational science has developed into a discipline of its own right.
- Students at both undergraduate and graduate level are unprepared to use computational modeling, data science, and high performance computing – **skills valued by a broad range of employers.**

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# Focus of New Department

**Computational science:** **When pen and paper is no longer enough, one resorts to approximation via computation.**

**Foundation:**

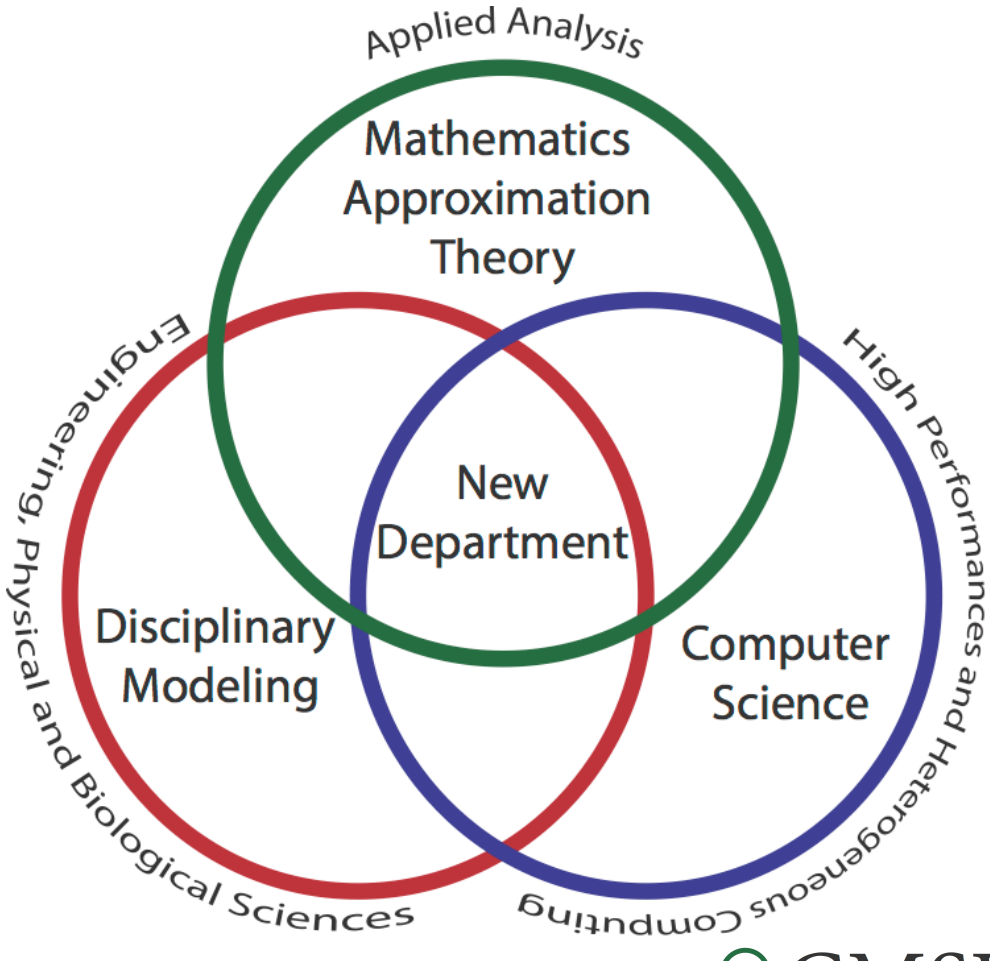
Discipline leverages:

1. Application knowledge
2. Computer science
3. Mathematics

To develop new methods for investigating complex problems through computation.

**Impact:**

Analysis of complex exterminates;
virtual prototyping;
virtual laboratory;
etc…

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# Goals

- Position MSU as a leader in computational science by recruiting faculty whose expertise pertains to large-scale computing and mathematical foundations of data science - both generalists (algorithm/tool developers) and specialists (focused on specific disciplines).
- Develop a comprehensive set of courses and degree programs at both the undergraduate and graduate levels, including minors and graduate certificates, that will give **students across the university** exposure to practical computational methods, and more generally to the idea of computers as problem-solving tools.
- Facilitate the adoption of computational tools and techniques for both research and education across campus, through education and faculty collaboration. A department facilitates the pursuit of these goals!

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# The department

- Administratively located in CNS
- Composed of 25-30 FTEs, including some current MSU faculty and a larger number of new hires (most from ACI).
- Most of these faculty will have joint appointments with other units on campus.
- Faculty will focus on data science and large-scale and high-performance computation
- Faculty will be incentivized to engage in cross-discipline and cross-college research collaborations
- Nurturing environment to attract these faculty and pursue large and interdisciplinary grants
- Close ties to ICER and MSU's HPCC

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# Benefits

- Recruitment of new faculty who are incentivized to collaborate across the university both in terms of research and education.
- Opportunities for existing MSU faculty to expand their computation-related capabilities, and to train students to use computational techniques.
- Broad and deep educational opportunities for both undergraduate and graduate students across the university.

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# New research opportunities

- Research challenges that require computation-oriented multidisciplinary and interdisciplinary approaches.
- Research problems that require "bleeding edge" (e.g., multi-petaflop/petabyte) computational approaches to interpret experimental data.
- Center-level funding opportunities (e.g., DoE SciDAC, NSF OCI $SI^2$).

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# Courses and degrees

- Undergraduate
  - Gateway "Introduction to Computational Science" course sequence - calculus-based (3 courses in sequence; requires Calc I)
  - Minor in CMSE
  - B.S. in Computational Modeling (with specializations in many disciplines)
  - B.S. in Data Science (with specializations in bioinformatics, statistics, data discovery, etc.)
- Graduate
  - Graduate Certificate in CMSE
  - M.S. in bioinformatics (joint w/MMG, Plant Bio, …)
  - M.S. in Computational Modeling and Scientific Computing
  - PhD in CMSE (also dual PhDs with other departments)

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# Steering Committee (2013-2014)

1) Titus Brown - Departments of Computer Science and Microbiology & Molecular Genetics

2) Robin Buell - Department of Plant Biology

3) Andrew Christlieb - Departments of Mathematics and Electrical and Computer Engineering

4) Ian Dworkin - Department of Zoology

5) Michael Feig - Department of Biochemistry

6) Kathy Hunt - Department of Chemistry

7) Mark Iwen - Departments of Mathematics and Electrical and Computer Engineering

8) Ben Levine - Department of Chemistry

9 Vince Melfi - Department of Statistics and Probability

10) Filomena Nunes - National Superconducting Cyclotron Laboratory / FRIB

11) Brain O'Shea - Lyman Briggs College and Department of Physics and Astronomy

12) Charles Ofria - Department of Computer Science

13) Bill Punch - Department of Computer Science

14) Shin-Han Shiu - Department of Plant Biology

15) Yang Wang - Departments of Mathematics

16) GuoWei Wei - Departments of Mathematics

17) John Verboncoeur - Department of Electrical and Computer Engineering

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# Timeline

| Faculty | Programs | Time to faclty governance | Projected Date of iImplementation |
|---|---|---|---|
| Exsiting FTE ~ 6 | Graduates certificate<br>Undergraduate Minor(x) | **Dec. 2014** | **Fall 2015** |
| | | | |
| 10 NEW FTEs<br>4 in progress start Fall 2015(*)<br>8 searches in Fall 2015(**) | Graduate programs<br>PhD<br>MS | **Aug. 2015** | **Fall 2016** |
| | | | |
| 6+ FTEs search in fall 2016 | Graduate programs<br>MS Bio informatics (Joint with Plant Bio) (***)<br>Dual PhD's Phy. Chem, Bio, EGR | **Dec. 2016** | **Dec. 2017** |
| | | | |
| 5+ FTEs search in fall 2017 | Undergraduate programs Jan. 2015<br>BS - CMSE Comp Phy<br>BS - CMSE Comp Chem<br>BS - CMSE Comp Bio | **Aug. 2017** | **Fall 2018** |

## Notes

(x) The proposed undergraduate minor can be talk with existing faculty

(*) Open Rank Searchs 2015

| | Data Science | Joint With |
|---|---|---|
| | 1) One in Applied Harmonic Analysis | 75% CMSE - 25% Math |
| | 2) One in Toplogy of Big Data | 75% CMSE - 25% Math |
| | 3) One in Bayesian Analysis | 75% CMSE - 25% Stat |
| | **Computational Modeling** | |
| | 1) Two in computational fluid dynamics | One 75% CMSE - 25% Mech Egr |
| | | One 25% CMSE - 75% Mech Egr |
| | 2) One in Computational Bio Chemistry | One 25% CMSE - 75% Bio Chem |
| | 3) One in Computational Chemistry | One TBD%-CMSE - TBD% Chem |

(**) 2 of the 8 Searches in 2016 Need to focous on Bio Infromatics
1 or 2 of the remaining 8 in Data Science and 4 or 5 on Computational Modeling

(***) The two in Bio Informatics are to help support the joint MS

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# Resources for Recruiting

- Leadership Endowments (2)
- Endowed Chairs (6)
- Endowed Visiting Chairs (2)
- Endowed Post Docs (20)
- Endowed Fellowships (20)

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# Example Scientist We Would Want to Recruit: Mathematical Foundations of Data Science

- Mauro Maggioni, Professor at Duke in Mathematics, ECE, and Computer Science Departments.
- Interests are in harmonic analysis, wavelets, multiscale analysis in general, and in particular with applications to the analysis of graphs and data sets viewed as discrete or sampled continuous geometric structures embedded in high-dimensional spaces. …

1. Diffusion Wavelets:
2. Diffusion Geometries:
3. Analysis of Molecular Dynamics Data:
4. Multiscale Analysis of Markov Decision Processes
5. Visualization of large data sets.
6. Harmonic Analysis and Wavelets:
7. HyperSpectral Imaging and Pathology:

Reduced order time accurate models based on finding low dimensional manifolds where solutions live and automated development of low order ODE models for time accurate dynamics on manifolds

http://www.math.duke.edu/~mauro/

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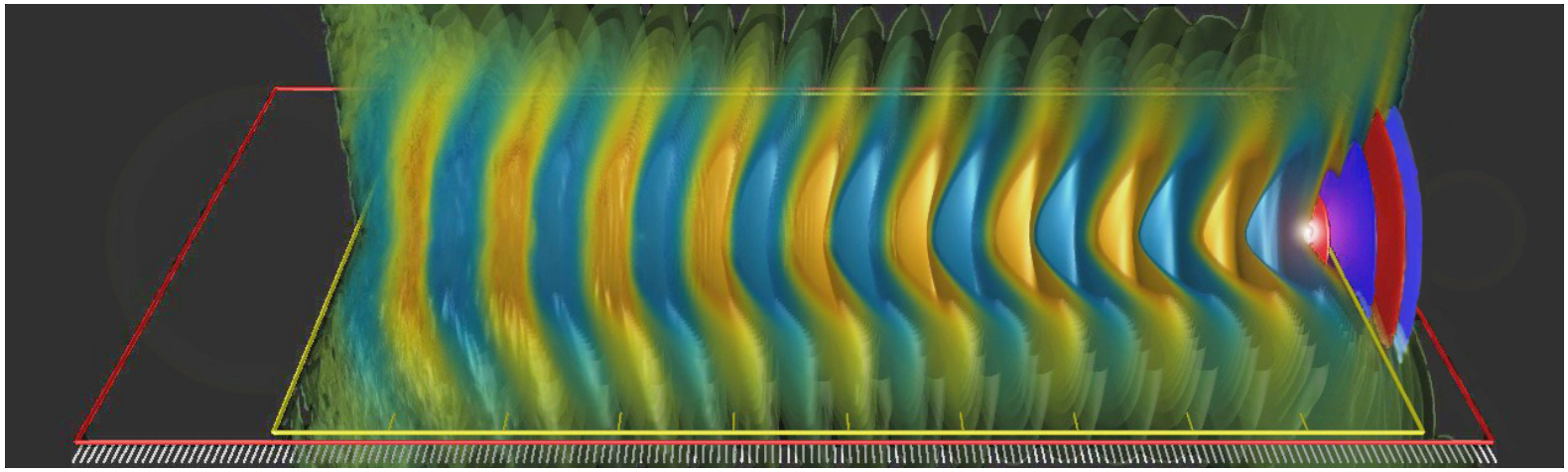
# Example Scientist We Would Want to Recruit: Modeling of Accelerator Technology

- Jean-Luc Vay of the Accelerator and Fusion Research wins Prize for Achievement in Accelerator Science and Technology



- Vay's citation reads, in part, "For original contributions to the development of novel methods for simulating particle beams, particularly the Lorentz boosted frame techniques."
- Used knowledge of physics to reduce simulations on DoE super computers that would take years down to hours

http://today.lbl.gov/2013/04/17/afrds-jean-luc-vay-wins-prestigious-accelerator-prize/

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# Data Science

**Summary of Universities Polled**
**Data Science**

| | | | |
|---|---|---|---|
| Total | 88 | | MSU |
| | | | |
| Department | 27 | 31% | N |
| Program | 50 | 57% | Y |
| Center | 40 | 45% | Y |
| Minor | 18 | 20% | N |
| Undergrad | 22 | 25% | N |
| Masters | 48 | 55% | N |
| Doctoral | 37 | 42% | N |

Summary of Universities With
Departments that Focus on Both the Theory and Application of Data Scientific

| National | University | Department? | Department |
|---|---|---|---|
| 28 | University of Michgian | y | http://www.lsa.umich.edu/informatics/ |
| 36 | Georgia Institute of Technology-Main Campus | y | http://www.cse.gatech.edu |
| 41 | University of Wisconsin – Madison | y | http://www.biostat.wisc.edu/ |
| 52 | University of Wasington | y | https://ischool.uw.edu |
| 62 | University of Pittsburgh | y | http://www.ischool.pitt.edu/ist/ |
| 75 | Indiana University | y | http://www.soic.indiana.edu/ |

Key: Red - Data Science Department
Green - Similar to new department

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# Computational Science

**Summary of Universities Polled**
**Scientific Computing**

| | | | |
|---|---|---|---|
| Total | 95 | | MSU |
| Department | 11 | 12% | n |
| Program | 35 | 37% | y |
| Center | 51 | 54% | n |
| Minor | 23 | 24% | y |
| Undergrad | 22 | 23% | n |
| Masters | 29 | 31% | n |
| Doctoral | 25 | 26% | n |

Summary of Universities With
Departments that Focus on Scientific Computing

| National | University | Department? | Department |
|---|---|---|---|
| 1 | **Princeton University** | y | http://www.pacm.princeton.edu/ |
| 14 | Brown University | y | http://www.brown.edu/academics/applied-mathematics/ |
| 18 | Rice University | y | http://www.caam.rice.edu/index.html |
| 32 | New York University-Courant | y | http://www.cims.nyu.edu |
| 36 | **Georgia Institute of Technolog** | y | http://www.cse.gatech.edu |
| 49 | Northeastern University | y | http://www.esam.northwestern.edu |
| 52 | University of Washington-Seattle | y | http://depts.washington.edu/amath/ |
| 82 | Stony Brook University | y | http://www.ams.sunysb.edu/index.shtml |
| 86 | University of Colorado Boulder | y | http://amath.colorado.edu |
| 91 | **Florida State University** | y | https://www.sc.fsu.edu |
| 121 | **University of Utah** | y | http://www.cs.utah.edu |

Key: Blue- Applied Math with Heavy Scientific Computing

Red - Applied Math moving towards new department

Green - Similar to new department

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