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Integrating Computational Science in the Curriculum

Steven Gordon
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Preparing the Workforce

- Need for a workforce which understands both modeling and simulation principles and applications of models and data analysis at large scale
  - Requirements for high fidelity models of complex systems
  - Managing and understand large datasets – data science
  - Applications across a wide range of science, social science, and increasingly humanities

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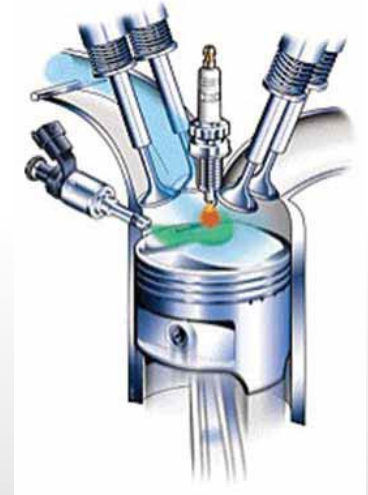
The Need For Computational Scientists

- A number of national studies document the need for computational scientists
    - …" computer modeling and simulation are the key elements for achieving progress in engineering and science." NSF Blue Ribbon Panel on Simulation-Based Engineering Science
    - "A persistent pattern of subcritical funding overall for SBE&S threatens U.S. leadership and continued needed advances…" International Assessment Of Research And Development In Simulation-Based Engineering And Science
    - Nearly 100% of the respondents indicated that HPC tools are indispensable, stating that they would not exist as a viable business without them or that they simply could not compete effectively. IDC Study for Council on Competitiveness of Chief Technology Officers of 33 Major Industrial Firms

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Crucial Tools for Manufacturing

- At Ford, HPC …allows us to build an environment that continuously improves the product development process, speeds up time-to-market and lowers costs.

- The ongoing use of modeling and simulation resulted in new packaging and product design that propelled the brand to a leading market position over a several-year period.
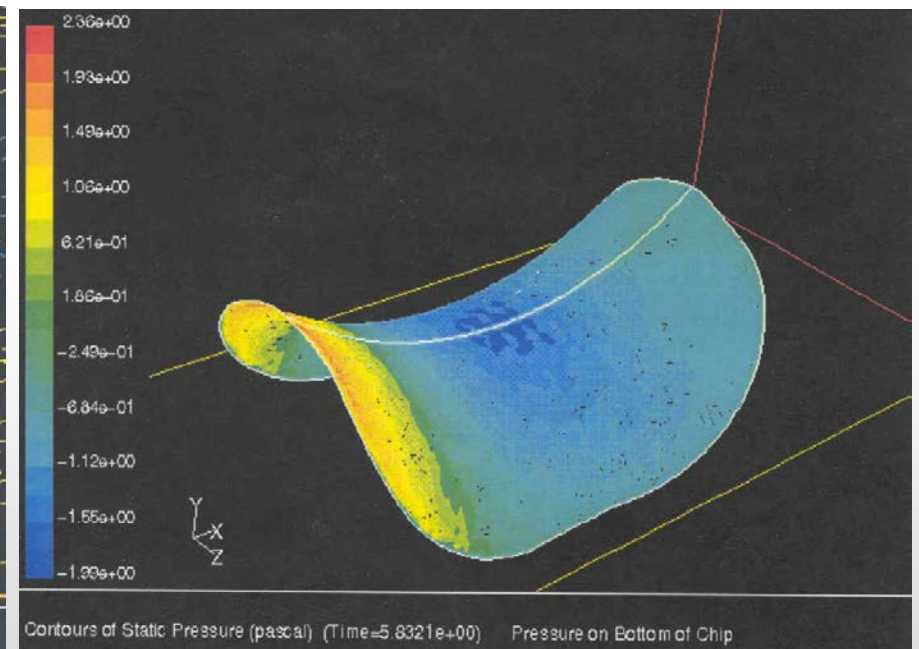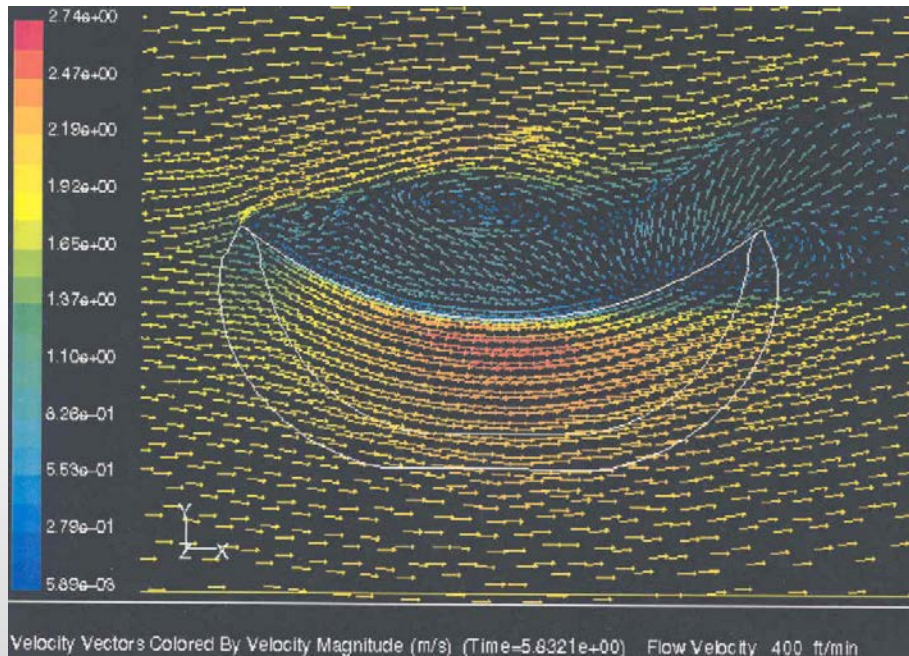
Ford EcoBoost Technology

Durable coffee package for P&G

Will Pringles Fly?

Velocity Vectors Colored By Velocity Magnitude (m/s) (Time=5.8321e+00)   Flow Velocity 400 ft/min

Contours of Static Pressure (pascal) (Time=5.8321e+00)   Pressure on Bottom of Chip

High Speed Conveying
Create Vortices
Shedding…
…'Rocking Chips'
NOT GOOD!

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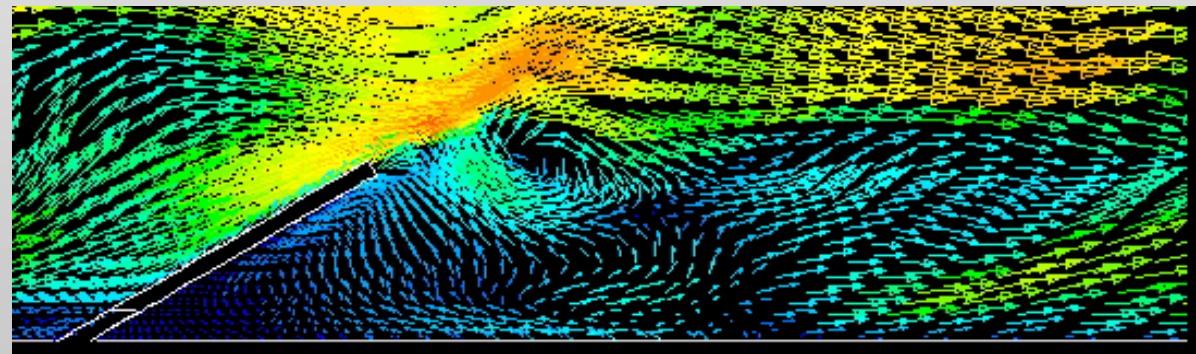
Approaches to Curriculum Change

- Introducing computational science into existing courses
  - Provide model examples to illustrate scientific principles
  - Engage students with inquiry-based assignments
- Creating formal programs
  - Minor or certificate programs focusing on a handful of elective courses
  - New emerging majors and graduate programs for example
    - Bioinformatics
    - Data science
- Inter-institutional collaboration for specialized course instruction
  - Example – [Applications of Parallel Computers](#)

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Example Programs

- Several in Ohio created as part of previous NSF grants
- Based on competencies created to guide program development and content
  - [Competencies in computational science and data science](#)
  - Augmented and updated by the XSEDE project

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	Topic	Course	Credit Hours	Terms offered	Required/Elective
Prerequisites	Calculus	MATH 1151.xx	5	Au, Sp	
		MATH 1152.xx or Math 1172	5	Au, Sp	
Core Courses	Simulation and Modeling (Choose one of these courses)	MATH 1157	3	Sp	Required
		CSE 2021	3	Sp	
		ISE 5100	3	Au, Sp	
		ME 5372	3	Au	
		MATSCEN 4321	3	Au	
	Programming and Algorithms (Choose one of these courses)	CSE 1222	3	Au, Sp	Required
		CSE 2221	4	Au, Sp, Su	
	Numerical Methods (Choose one of these courses)	AERO 3581	3	Au	Required
		CSE 5361	3	Au, Sp	
		ECE 5510	3	Au	
		MATH 3607	3	Sp	
		MATH 5401	3	Sp	
		MECHENG 2850	3	Au, Sp	

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		CIVILEN 4000.01	2	Au, Sp	
Discipline Specific Courses	**Capstone Research/Internship Experience (minimum 3 credits)**	MATH 4998; CHEM 4998 or other approved individualized research credits **	3-5	Au, Sp, May, Su, May + Su/ Au, Sp/Au, Sp	**R e q u i r e d**
	Discipline-specific Computationally oriented Course	CSE 3521	3	Au, Sp	R e q u i r e d
		CSE 3341	3	Au, Sp	
		MICRBIO 5161H	3	N/A	
		BMI 5730	3	Sp	
		CHEM 5440	3	Au	
		MATH 5651	3	Sp	
		PHYS 6810	4	Sp	
		LING 5801	3	Au	
		LING 5802	3	Sp	
		ECON 4050	3	Au, Sp	
		ECON 5001	3	Au, Sp	
		GEOG 5221	3	Au	
		PSYCH 5608	3	Sp	
Elective: Choose at least one course from the following (3 credits total required)	Differential Equation and Discrete Dynamical Course	MATH 2255	3	Su, Au, Wi, Sp	E l e c t i v e
		MATH 2415	3	Su, Au, Wi, Sp	E l e c t i v e
		MATH 2568	3	Su, Au, Wi, Sp	
	Parallel Programming	CSE 5441	3	Au	E l e c t i v e
	Scientific Visualization	CSE 5544	1-5	Su, Au, Wi, Sp	E l e c t i v e
		CEG (CIVILEN) 4760	3	Sp	

Data Analytics Minor - University of Mary Washington		
Total credits: 23		
Required Courses	MATH 220	Introduction to Statistics
	MATH 200	Linear algebra
	CPSC220 Computer Science 1	Programming and Algorithms
	CPSC419	Data mining
	CPSC420	Modeling and Simulation
One of these electives	CPSC230 Computer Science II	Data structures
	BUAD 400	Analytics Application Development
One of these electives	BUAD 403	Foundations and Applications of Data Analytics
	CPSC 425	Parallel Processing

Other Resources

- [HPCUniversity index of computational science education resources](#)
- Online training materials
  - [XSEDE](#)
  - [Argonne National Labs](#)
- Workshops
  - OSC workshops
  - [XSEDE faculty professional development workshops](#)

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Possible Roles for OSC

- Provide computing and data services for classroom use
- Create mechanisms to build a statewide community of interested faculty
- Facilitate the sharing of instructional materials
- Facilitate inter-institutional course sharing
- In-depth discussion of these and other topic after lunch

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Questions

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