Computational Science and Engineering Introduction

Yanet Manzano
Florida State University
manzano@cs.fsu.edu

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Research Today

Research Today (1)

- Computation: equal partner with theory and experimentation
- Computer models and simulations:
  - supplement in some cases replace experimentation
- Numerical simulation:
  - enables the study of complex systems and natural phenomena too expensive, dangerous, or even impossible, to study by direct experimentation

Research Today (2)

- Going from application area to computational results requires:
  - domain expertise
  - mathematical modeling
  - numerical analysis
  - algorithm development
  - software implementation
  - program execution
  - analysis
  - validation and visualization of results

Research Today (3)

- Quest higher levels of detail and realism in simulations:
  - requires enormous computational capacity
  - has provided the impetus for dramatic breakthroughs in computer algorithms and architectures

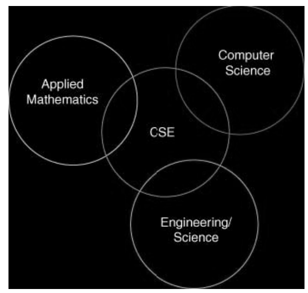
- Due to these advances, computational scientists and engineers can now solve large-scale problems that were once thought intractable

What is CSE ?

What is CSE?

- A rapidly growing multidisciplinary area with connections to the sciences, engineering, mathematics and computer science.

- Focuses on the development of problem-solving methodologies and robust tools for the solution of scientific and engineering problems



CSE an Emerging Discipline

CSE and Emerging Discipline

- Historically:
  - Simulation used as a qualitative guide for design and control
  - Not often expected to provide accurate results for realistic physical systems

- Increasingly:
  - Simulation used in a more quantitative way as an integral part of the manufacturing, design and decision-making processes, and as a fundamental tool for scientific research.

Examples

Examples of problems where CSE has played and is expected to continue to play a pivotal role

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Weather and Climate Prediction

Weather and Climate Prediction

- Climate modeling at the global, regional and local levels can:
  - reduce uncertainties regarding long term climate change
  - abate the impact of violent storms
- Computing power:
  - allows to incorporate knowledge about the interactions between the oceans, the atmosphere and living ecosystems into the models used to predict long-term change

Weather and Climate Prediction (Example)

- Weather modeling group at IBM Thomas J. Watson Research Center: utilize the latest developments in meteorology and information technology to enable reliable, affordable numerical predictions for customer applications.

- Also, posting local forecasts for the New York City area

Aircraft Design

- Computational simulation has been used in the performance analysis and design of aircraft components, such as:
  - the analysis of lift and drag of airfoil designs

- Computing Power:
  - increasing important as capabilities improve for such things as numerical modeling of combustion for engine design

Aircraft Design (Example)

Aircraft Design Example

- The Boeing 777
  - first jetliner to be 100% digitally designed, using 3D solid modeling
  - Throughout the design process, the airplane was preassembled on the computer, eliminating the need for a costly full-scale mark-up

Examples

Example of scientific areas where CSE tools are critical for experiments and in analyzing data and developing models

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Chemistry

Chemistry

- CC allows the prediction of chemical phenomena based on models
  - In real problem solving situations, these models are often combined to form and study "hybrid models“

- Simulations and quantum chemical calculations:
  - extremely compute-intensive
  - high accuracy required, which sets restrictions with regard to the method used to solve the partial differential equations involved.

Biology

Biology

- Simulation plays a major role in the conceptual development of medical devices used in:
  - diagnostic procedures (electromagnetic, ultrasonic, etc.)
  - in design of artificial organs (hearts, kidneys, etc.)

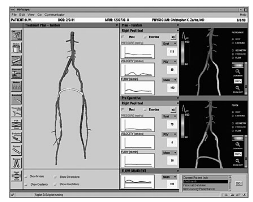
- Computational modeling key in emerging efforts to combine mathematics and biology in the genomic sciences (genome sequencing, gene expression profiling, genotyping, etc.).
  - Large scale simulations with complex computational

Example

Example

- Researchers funded by the joint NASA-Stanford University Center for Turbulence Research are using MRI data to create computer simulations of blood flow through vessels of patients with heart disease.

- The researchers are working with surgeons to predict the outcome of cardiovascular surgery.



My work so far: Modeling behavior of time-varying surfaces created from parametric equations

Variation on The Klein Bottle

Parametric Form:

• x = (A+cos(u/2)*sin(v)-sin(u*v/2)*sin(2*v))*cos(u);

• y = (A+cos(u/2)*sin(v)-sin(u*v/2)*sin(2*v))*sin(u);

• z = sin(u/2)*sin(v)+cos(u*v/2)*sin(2*v);

With u={ 0,2*pi},v={0,2*pi}

•A = cos(SimulationTime * frequency *2 *M_PI);

Conic Spiral or Seashell Surface

Parametric form :

• x = a*(1-v/(2*pi))*cos(n*v)*(1+cos(u))+c*cos(n*v)

• y = a*(1-v/(2*pi))*sin(n*v)*(1+cos(u))+c*sin(n*v)

• z = b*v/(2*pi)+a*(1-v/(2*pi))*sin(u)

Example: a=0.2,b=1,c=0.1,n=2,u={ 0,2*pi},v={0,2*pi}

• b = cos (SimulationTime) | n = 1/ sin(SimulationTime)

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