Problem Solving Environments (PSEs): The Enabling Technologies for Simulation based Engineering Science

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Future Working Space



Outline of the Talk

- The Simulation Based Engineering Science (SBES) Discipline
- The CyberInfrastructure & CyberEngineering Landscape
- The Role of PSE in SBES
- Engineering Education for the 21st Century & the Role of PSEs
- Conclusion

Simulation-Based Engineering Science (SBES)

Definition

Simulation-Based Engineering Science (SBES) is the discipline that provides the scientific and mathematical basis for the simulation of engineered science systems.

SBES fuses the knowledge and techniques of the traditional engineering with the knowledge and techniques of fields like computer science, mathematics, and the physical and social sciences.

SBES empowers the engineers to predict and optimize systems affecting almost all aspects of our lives and work, including our environment, our security and safety, and the products we use and export.

Simulation - Based Engineering Science

Revolutionizing Engineering Science

through Simulation

May 2006

Report of the National Science Foundation Blue Ribbon Panel on Simulation-Based Engineering Science

SBES – Simulation based Engineering and Science Discipline

- SBES is a discipline central to advances of many new technologies and product development. There is ample evidence that developments in these new disciplines could significantly impact virtually every aspect of human experience.
- Formidable challenges stand in the way of progress in SBES research... one of those challenges is education of the next generation of engineers and scientists in the theory and practices of SBES.
- Realization of this vision requires changes in our educational system as well as changes in how basic research is funded.

Simulation - Based Engineering Science

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From physical models to simulation-based engineering sciences and decision making



The Main Infrastructure for Simulation based Engineering Science

o Computer Power
Not under our control
o Algorithmic Power
Our responsibility
o Programming Power
Mostly under our control

Computer Power: History/Future

• The amazing increase will persist for another decade or two

	1970	1995	2010
Speed	20Mflops	6 Gflops	10 Tflops
Memory	200 K words	50 M words	100 G words
Store	200 M words	500 G words	1 P words
Cents per 100 G add	20,000	70	0.02

Algorithmic Power

 Advances in models and algorithms have often to led to greater improvements in simulation capability than improvements in hardware



Example from magnetohydrodynamics: 2.5 orders of magnitude from hardware improvements; 3.5 orders of magnitude from modeling and algorithmic advances (From SCaLeS report, Vol 2 & SBES rpt)

Programming Power: History

- Slow productivity increase for programming in low level languages Cost of "raw" software will remain very high
- The number of well designed and tested library items has dramatically increased but software reuse is only moderate successful (<u>www.gams.org</u>)
- SBES domain specific application systems and PSEs have made very respectable progress reducing the cost of simulations
- Cost of programming is still the principal cost in simulations

Programming Challenges: New Computing Paradigms

- HPC Computing
- Global Computing
 - o Exploitation of the Web/Internet as a "distributed" heterogeneous computer (including HPC resources) and data storage infrastructure (**The Grid**) for running distributed parallel applications
- Service Oriented Computing
- SBES Finding

"Much of our current software in computational engineering science is inadequate for dealing with the multifaceted applications and challenges of SBES. New software tools, paradigms, and protocols will need to be developed so that software is more reusable. The multidisciplinary teams addressing SBES developments, we must incorporate experienced software developers who will work closely with engineering scientists to develop tomorrow's SBES software."

The Crisis of Knowledge Explosion

Prediction

A doubling of the world's knowledge: 1930 \rightarrow every 30 years 1970 \rightarrow every 7 years 2010 \rightarrow every 11 hours

Recommendation

- Meaningful advances in SBES will require dramatic changes in science and engineering education.
- Interdisciplinary education in computational science and computing technology must be encouraged and greatly improved.
- The traditional boundaries between disciplines in higher education must be made pervious to the exchange of information knowledge.

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- The Role of PSEs in Engineering Science Education and Training
- Conclusion

From physic prodels to simulation-based engineering screens and decision making



Distributed resources and knowledge

Resources can be of any information type (computing, storage, networking, /isualisation, etc)







Resources can be distributed worldwide





Virtual research and learning organisations

Grid: a key technology and service enabler



- An emerging middleware technology layer, capable of allocating resources and delivering access to them to users and applications
- Underlying high speed network is a key enabler!

Vision: creating an e-infrastructure...







Mobile User Interface Environment





Web Evolution

- Any technological change that is a quantum leap in our ability to rapidly share solutions over the Web by providing modular reusable building blocks of functionality constitutes a version change.
- Web 1.0 Connected computers together using a set of standardized protocols invented by Internet pioneer <u>Vint Cerf</u>.
- Web 2.0 Marked by the appearance of <u>Web Services</u> which are modular solutions to complex problems, made available over the Web to external developers via an application program interface (API).
- Web 3.0 The marriage of artificial intelligence and The Human Computing Layer (HCL) and their subsequent integration into the Web, making powerful pattern recognition solving capabilities widely available to web surfers and developers alike.

The SBES Application Domain

- Multi-physics phenomena
- Multi-scale Phenomena
- Validation
- Crisis management real time and data driven simulations
- Virtual laboratories
- Collaborating simulations
- Dynamic simulations

Requirements SBES applications

- Visualization and steering
- Access and analysis of large remote datasets
- Access to remote data sources and special instruments (satellite data, particle accelerators)
- Distributed in wide-area networks
- Accessed through collaborative and multidisciplinary Computational Environments and via the Web

SBES Report: Example applications



Simulation-based planning for vascular bypass surgery. From left: MRI image data, preoperative geometric solid model, operative plan, computed blood flow velocity in aorta and proximal end of bypass, and postoperative image data used to validate predictions.

Simulation-based medicine (C. Taylor, Stanford)



Biomimetic Devices: functionalized carbon nanotube to mimic biological ion channels (N. Aluru, UIUC)



Multi-scale design of a composite component of an aircraft (SCOREC, RPI)

Gas Turbine Engine Application



Not every simulation looks like a FORTRAN program? Softlab Project



Crisis Management: Fire-Fighting



Building on fire (Has temperature sensors)

Clinical Applications of Biomechanical Simulation

PD Dr. F. Kruggel¹², Dr. M. Tittgemeyer², G. Wollny² 1 Dept. of Computer Science, University of Leipzig, Leipzig, Germany 2 MPI of Cognitive Neuroscience, Leipzig, Germany



F. Kruggel Advanced Environments and Tools for High Performance Computing



Analysis, Prediction & Design









Using HPC Computational Technology







n



F. Kruggel Advanced Environments and Tools for High Performance Computing

0,14 0,12 0,1 0,08 0,06 0,04

0.5

Elongation (mm)

15



Mid-Face Therapeutic Intervention





F. Kruggel Advanced Environments and Tools for High Performance Computing

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The Principal Challenges in SBES Realization

- How do we exploit the enormous power of algorithms and hardware to deliver "cheap" simulations to very complex applications?
- How can we capture this power to support problem solving and learning within specific domains of knowledge at various educational levels?

Mathematical Software History

- 1948's: First "mathematical" software
- 1960's: HLL, Manufacturer libraries
 - o 1963: Culler & Fried paper
 - o 1966: Rice & Rosen "Numerical Analysis PS systems"
- 1970's: Mathematical software community
 - o IMSL, NAG, EISPACK, FISHPAK, ACM library
 - o ELLPACK
 - o WG2.5 group
 - o TOMS ACM Journal

• 1980's: Maturation towards definition

- o Standardization: BLAS, LAPACK
- o Distribution: Netlib, ACM Algorithms

The GIPPS Project (1980s)

- Objective: Smart notebook supported by natural language, handwriting, computer based geometry, domain specific knowledge bases and compilers
- Outcome:
 - o Failure due to
 - Lack of computer power and technologies
 - Very ambitious objectives
 - Skepticisms
 - Technophobia
 - o Vision became the basis of less ambitious projects

What are PSEs?

"A PSE is a computer system that provides all the computational facilities necessary to solve a target class of problems"

These features include advanced solution methods, automatic and semiautomatic selection of solution methods, and ways to easily incorporate novel solution methods. Moreover, PSEs use the language of the target class of problems, so users can run them without specialized knowledge of the underlying computer hardware or software. By exploiting modern technologies such as interactive color graphics, powerful processors, and networks of specialized services, PSEs can track extended problem solving tasks and allow users to review them easily. Overall, they create a framework that is all things to all people: they solve simple or complex problems, support rapid prototyping or detailed analysis, and can be used in introductory education or at the frontiers of science."

From "Computer as Thinker/Doer: Problem-Solving Environments for Computational Science" by Stratis Gallopoulos, Elias Houstis and John Rice (IEEE Computational Science and Engineering, Summer 1994).

PSE publication trends till 2008

cumulative pubs



PSE functionality (A comparison of mathematical programs for data analysis by Stefan Steinhaus)

Tested PSEs	GAUSS	Maple	Mathematica	Matlab	O-Matrix	Ox Prof.	Scilab
	(8.0)	(V11)	(6.0)	(2008a)	(6.3)	(5.0)	(4.1.2)
Installation, learnability and usability (15%)	35%	88%	96%	77%	41%	34%	40%
Mathematical functionality (35%)	70%	55%	76%	69%	37%	54%	45%
Graphical functionality (10%)	61%	61%	85%	88%	47%	44%	51%
Functionality of the programming							
environment (11%)	63%	51%	65%	72%	42%	72%	62%
Data handling (5%)	62%	64%	76%	73%	50%	55%	54%
Available platforms (2%)	77%	69%	100%	77%	15%	92%	46%
Speed comparison (22%)	22%	11%	39%	55%	83%	42%	25%
Overall result	52%	51%	71%	70%	49%	50%	43%

Comparison of mathematical programs for data analysis by Stefan Steinhaous (Edition 5.03, April 2008)

Software Engineering Definition

PSE = Natural language + Problem Solving Libraries + Knowledge Base + Geometry Modelers + Visualization and Steering Tools+ Ambient Intelligent and Web Enable Interfaces + Software Bus or Middleware
Knowledge & Information Resources for Simulation Software and PSEs

- GAMS
- Mathematical Software and PSEs for Engineering and Science Education
 - o Mathematics WWW Virtual Library
 (http://www.math.fsu.edu/Virtual/)
 - o http://www.personal.kent.edu/~rmuhamma/Mathem atics/mathsoftware.html

Virtual Library of 210 Math Software and PSEs for Mathematics and Physics Education

- Libraries (113)
- Toolkits (36)
- Toolboxes (9)
- PSEs (51)
- Visualization tools (16)
- Data analysis tools (3)
- Add-ons (5)
- Tutors / workbenches (9)
- Simulators (4)
- Calculators (9)
- Applet libraries & environments (4)
- NA programming languages (3)
- Math software Recourses (75)
- Unclassified math software (11)

Medical Diagnosis and Imaging Problem Solving Environment

L.O. (Bob) Hertzberger Computer Architecture and Parallel Systems Group Department of Computer Science Universiteit van Amsterdam



Medical Diagnosis and Imaging Problem Solving Environment



Courtesy of L.O. (Bob) Hertzberger Computer Architecture and Parallel Systems Group Department of Computer Science Universiteit van Amsterdam



Application pull

Vision for PSEs: From PSEs to Webservices or Scientific Portals

- PSEs signal a new era in scientific computing, both in power and how resources are accessed, used, and programmed
- PSEs will become the main gateway for scientists to access terascale computing resources
- PSEs will allow users to access these resources from any web connection
- PSE's support for collaborative computational science & engineering will change the research culture, making it more open, accountable, and boundary independent

Service-Based PSEs

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- Problem specification tools
- Recommender systems

Applications and supporting tools (toolkits, Grid-enabled libraries, etc)

Application development and execution support services (CORBA, Globus, Jini, etc)

Generic web services (monitoring, security, brokering, fault management, etc)

Distributed resources (computers, storage, instruments, sensors, visualisation, etc)

PSEs: Problem Specification and Solution

- Most used
 - o Visual programming environment to link software components
 - o High-level language specification
- Less used
 - o Recommender systems to help user choose best way to solve problem and locate software (i.e. myPythia)
 - Intelligent compilation based on content than programming syntax (i.e. Andes physics workbench)
- Intelligence needed
 - o Collaborative and distributed computing adds new types of complexity to the software environment.
 - o PSEs need to be intelligent to minimize impact of this complexity on users.

GUI and Data Flow Interfaces



Data flow user interface



Designing in the New Millennium: Advanced Engineering Environments (AEE) Phase I & II http://www.nap.edu/

Definition: AEEs are specific computational and communications systems that create integrated virtual and/or distributed environments linking researchers, technologists, designers, manufacturers, supplies, customers, and other users involved in mission-oriented, leading-edge engineering teams in industry, government, and academia.

- o Enable complex new systems, products, and missions.
- o Greatly reduce product development cycle time and costs.
- o Lower technical, cultural, and educational barriers.
- o Apply AEEs broadly across government, industry, and academia.

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Culture of New Generation of Pupils: The "Sesame Street" and "Computer Games" calture





Immense amount of ICT infrastructure

- "Information and Communication Technologies (ICT) are driving at accelerating pace the production of any human enterprise, from manufacturing to entertainment, telecommunications, transportation and education"
- The supercomputing infrastructure of the near past already exists in many desks today
- "Very soon" all the schools will be connected to the Internet
- "Very soon" we will be able to solve any problem that has a known solution
- "There is such an immense amount of technology that can do such an immense amount of good around the world" Craig Barrett Intel chairman

New Dimensions of Engineering Problem Solving

(Hartikainen and Yrjanheikki, Learning Engineering Proplem Solving in Different Learning Environments)



Engineering Education in the 21st Century: Attributes of the engineer of 2020

- Strong analytical skills
- Practical ingenuity, creativity; innovator
- Good communication skills
- Business, management skills
- High ethical standards, professionalism
- Dynamic/agile/resilient/flexi ble
- Lifelong learner
- Able to put problems in their socio-technical and operational context
- Adaptive leader



National Academy of Engineering

Educational Pedagogy must Change

FROM

- Teacher Centric
- Single Medium
- Individual Work
- Passive Learning
- Artificial Context
- Didactic Approach
- Problem Solving
- Monological Thinking
- Mortal and Bricks
- Static learning
- Rigid Schedule
- Terminal Degree
- Books as Primary Medium
- Delivery in Classroom
- Technology as an Expense

TO

- Student Centric
- Multimedia
- Collaborative Work
- Active Learning
- Real Problems
- Dialogical Approach
- Problem Formulation
- Critical Thinking
- Bits and Bytes (E-learning)
- Real time learning
- Courses on Demand
- Lifelong Learning
- Information on Demand
- Delivery Anywhere
- Technology to Improve Efficiency and Productivity

A Proposal for Engineering Education

- An (optional) first-semester curriculum that involves students in cross-disciplinary studies as a way of learning fundamentals
- Integrates physics, math, and humanities into unified grouplearning experience
- Explores tutorial approach around projects rather than static classrooms
- Students learn from each other through inquiry (exponential impact)
- Addresses directly development of critical thinking through teaching by asking rather than by telling
- Utilization of Problem Solving Environments to Enable Engineering Problem Solving (EPS)

Engineering Problem Solving Dependence in "Professional" Mathematics

- Mathematical modeling and simulation is part of every engineering and scientific development today
- Examples
 - o optimal resource allocation in production,
 - o transportation, banking /trading,
 - o waste management,
 - o designing of drugs and engineering artifacts from bottles to planes and buildings,
 - o entertainment (computer games, movies),
 - o predicting the weather,
 - o cutting expensive materials such as leather, textile or wood
 - o Biomedical applications
- Mathematics education for all professional life of an engineer
- "Professional" vs. "Recreational" Mathematics

Difficulties in Teaching Engineering Students "Professional" Mathematics

- Mathematically *gifted* people syndrome
- Negative "image"
- Short term "learning"
- Learning by recognizing patterns
- The "Fun" and "Useful" phenomenon
- Huge amount of "professional math knowledge" must be acquired
- Performance of CE&C UTH students in the NA course: 2000 -2004
 - o 40% of students passed the course in the year taught
 - o 24% of students passed the course within 5 years
 - o 6% of students passed the course after 5 years
 - o 30% of students have not passed the course yet!!!
- Pole of Innovation of Thessaly
 - o Involves more than 100 scientists and engineers
 - o Involves 45 companies
 - o Spreadsheet mathematics
 - o Very few graduate students and professors involved knew the serious usage of this PSE!
- What is the solution
 - o New teaching and learning paradigms
 - o New curricula structures
 - o Utilization of PSEs
 - o Utilization of ICT technologies at all educational levels

The Role of Simulation Software in an Engineering Learning Environments^{*}

- Most of the Engineering Subjects are Taught Today through some form of Engineering Simulation Software
- Generally, more resources create a superior learning environment; the type of resource, however, is important
- There is superior software in the form of Libraries and PSEs waiting to be fully utilized in education

* D. Reamon and S. Sheppard, Center for Design Research, Stanford University

PSE based approach in learning mathematics

- Provide a greater proportion of students with the opportunity to apply sophisticated mathematical methods in problem-solving (*popularize mathematics*)
- Enable students to acquire knowledge for life since some of these PSEs are used as kernels to develop special toolkits for advanced engineering subjects and are updated regularly with the latest algorithmic and programming technologies
- Increase visualization, thus, the attractiveness of mathematics through graphics capabilities and special tools of analyzing the results of mathematical studies and experiments
- Produce logs and information-rich *documentation* of a particular effort in various publishing standards
- *Collaboration* with other students and teachers

PSE based approach in teaching mathematics (continue)

- Solving and prototyping real engineering problems in student's time frame (*support brain storming*)
- Provide *interaction and self validation* during the learning process and *increase independence of students*
- Allow the possibility to deal with larger and more *realistic problems*
- Be applied as a *supplement to traditional methods*
- Be used to stress the *numerical methods* in the mathematics curriculum
- Be used for *data analysis* and to simulate technical processes
- Used to develop active electronic books
- Increase the level of fun!

Do PSEs make parts of the standard mathematics curriculum redundant?

- PSEs are not expert systems yet! Garbage in Garbage Out
- PSEs assume that the user has an understanding of the basic concept
- PSEs reduce the time to train pupils in extremely specialized techniques and devote more time to mathematical culture (tools, concepts, history)
- PSEs can enhance the attractiveness, usefulness, intellectual excitement of mathematics
- PSEs can support users in all professional life
- PSEs can become an updated repositories of knowledge

Mathematics lecture at Berlin University of Technology using eChalk system



Whiteboard and Simulation Environment





ON/OFF

ischicker.

"There is such an immense amount of technology that can do such an immense amount of good around the world" Craig Barrett Intel chairman



"Education, training and research are the key to economic renewal ... we need an integrated strategy for education and research based on networking and mobility giving priority to the technologies of the future"



Gas Turbine Engine Application



The Collaborating Mathematical Modeling of a Multidisciplinary Applications



GasturbnLab MPSE Project

- Study Grid based Distributed Heterogeneous Collaborative and Parallel Computing from Algorithmic and Software Engineering Point of View
- Software Architecture of MPSEs
- Reuse of large scale legacy software
- Collaborating computing methodologies
- Measure performance

Problem Solving Environments (PSEs) and MPSEs: The Computer Science View

What is PSE?

"A PSE is a computer system that provides all the computational facilities needed to solve a target class of problems ...

PSE = Interface + Library + Tools + Knowledge Base + Software Bus (Middleware)

What is an MPSE?

"An MPSE is a framework and software kernel for combining PSEs from different disciplines towards the analysis and synthesis of a whole physical system ..."

"Computer as Thinker/Doer: Problem-Solving Environments for Computational Science" by Stratis Gallopoulos, Elias Houstis and John Rice (IEEE Computational Science and Engineering, Summer 1994).

Enabling Technologies for Computational Science: Frameworks, Middleware and Environments (E.N. Houstis, J.R. Rice, E. Gallopoulos and R. Bramley editors), Kluwer Academic Publishers, Boston, March 2000.

Aspects of PSEs

- Distributed
- Collaborative because interesting problems are often complex and draw on many types of expertise.
- Heterogeneity pervades network environments
- Transparency is usually desirable
- Intelligence is needed to deal with various types of complexity – especially complexity arising from the collaborative and distributed use of PSEs in heterogeneous dynamic environments.

Who is Involved in PSEs?

- Application end users (scientists, engineers, etc.)
 - o Solve a particular problem which is domain specific
 - o Undertake "what if" investigations
- Developers (programmers)
 - o Create components and place them in Component Repository
 - o Make new algorithms and techniques available to the end users.
- Software infrastructure builders
 - o Create services and interfaces
 - o Provide abstractions
 - o Develop standards

AEE System Components and Characteristics (Vision 1)

• Computation, Modeling, and Software

- o multidisciplinary analysis and optimization interoperability of tools, data, and models
- o system analysis and synthesis
- o collaborative distributed systems
- o software structures that can be easily reconfigured
- o deterministic and nondeterministic simulation methods
AEE System Components and Characteristics (Vision 2)

- Human-Centered Computing
 - o adaptive human-machine interfaces
 - o networked virtual environments
 - o immersive systems
 - o telepresence
 - o intelligence augmentation (enhance human performance through some form of AI)

AEE System Components and Characteristics (Vision 3)

- Hardware and Networks
 - o ultrafast computing systems
 - o large high-speed storage devices
 - o high-speed and intelligent networks

Rise of IT Technologies and

Orbital View of IT



Curriculum Innovation

Proposed Tools/Mechanisms

Design Oriented Education Real World Examples Connectivity in Curriculum Multidisciplinary Applications Internet Ready Instruction Modules (IRIM) Industrial Design Project Modules Faculty Research Modules

Concept Learning Through Experiments Virtual Lab Modules (VLAB)

Exposure to IT-Based Engineering Practice Subject Specific Software Software Applications Library Web-mediated Concurrent Engineering Startup Company Model

Outcome Based Assessment Knowledge-Based and Perception Based Assessment Mechanisms

Findings

- The development of effective multiscale modeling techniques will require major breakthroughs in computational mathematics and new thinking on how to model natural events occurring at multiple scales.
- While verification and validation and uncertainty quantification have been subjects of concern for many years, their further development will have a profound impact on the reliability and utility of simulation methods in the future. New theory and methods are needed for handling stochastic models and for developing meaningful and efficient approaches to the quantification of uncertainties. As they stand now, verification, validation, and uncertainty quantification are challenging and necessary research areas that must be actively Pursued.
- Research is needed to effectively use and integrate data-intensive computing systems, ubiquitous sensors and high-resolution detectors, imaging devices, and other data-gathering storage and distribution devices, and to develop methodologies and theoretical frameworks for their integration into simulation systems.
- Concomitant investments are also required in sensory-data computing, the collection and use of experimental data, and the facilitation of interactions between computational models and methods, all of which are necessary to achieve dynamic adaptive control of the computational process.

The Collaborating Mathematical Modeling of a Multidisciplinary Applications – GasTurbLab Project



Examples of Research Issues for PSEs

- Develop PSE architecture that supports the plug-and-play paradigm
- Exploit multi-level abstractions and complex properties of science
- *Reuse of legacy scientific software*
- Create test beds for components and combinations
- Create certain important difficult components
- Create knowledge bases for solvers and problems

Maxillo-Facial Biomechanics



Displacements are in the range of millimeters.



F. Kruggel Advanced Environments and Tools for High Performance Computing

Towards an "Ambient Intelligence"

ICT today

PC based... "Keyboard and screen"... "Writing and reading"... Mobile telephony (voice)...

Steep usage learning curve... "Word" based information search...

5% of global population on-line...

"Ambient Intelligence" tomorrow

... interface is "our surrounding" ... technology (almost) invisible ... use all senses, intuitive ... high-bandwidth mobile multimedia ... laid-back mode of interaction ... context-based knowledge handling ... >70% of population on-line

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Elias N. Houstis

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Algorithmic Power: History/Future I

- Fast Algorithms are as important as faster machines
- Resources to solve a particular 3D elliptic PDE on a fixed one 1 Gflops computer

	1945	1955	1960	1970	1980	1990
Time	3*10^6 years	200 years	6 hours	1 day	30 min	2 sec
Memory	10^9	5*10^6	3*10^7	2*10^5	10^5	10^5