Oliver Röhrle
Ulrich Rüde
Barbara Wohlmuth

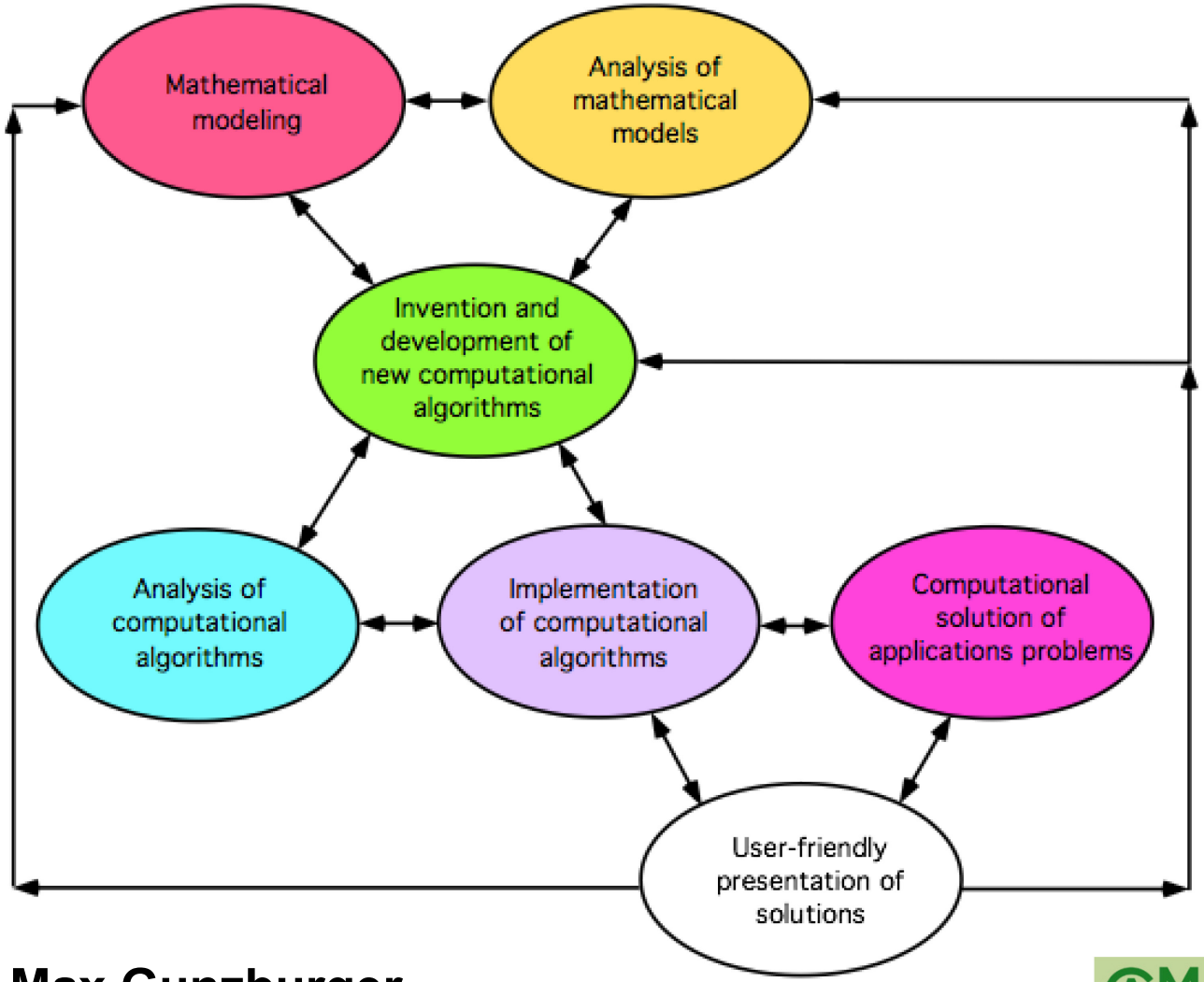
Garching, September 17/18, 2012

COMPUTATIONAL SCIENCE & ENGINEERING

"Leading-edge science and engineering depend on advanced computing for understanding, prediction, and control. In response to these needs, the field of computational science and engineering (CS&E) is evolving rapidly, to the point that it is now widely considered to be a new discipline by itself and a third pillar of the scientific enterprise, a peer alongside theory and physical experiment. CS&E is unique in that it enables progress in virtually all other disciplines by providing windows of discovery when traditional means of research reach their limits."

- Editorial, SISC Special Issue on CS&E (2007)

CS&E IN MATHEMATICS



View: Max Gunzburger

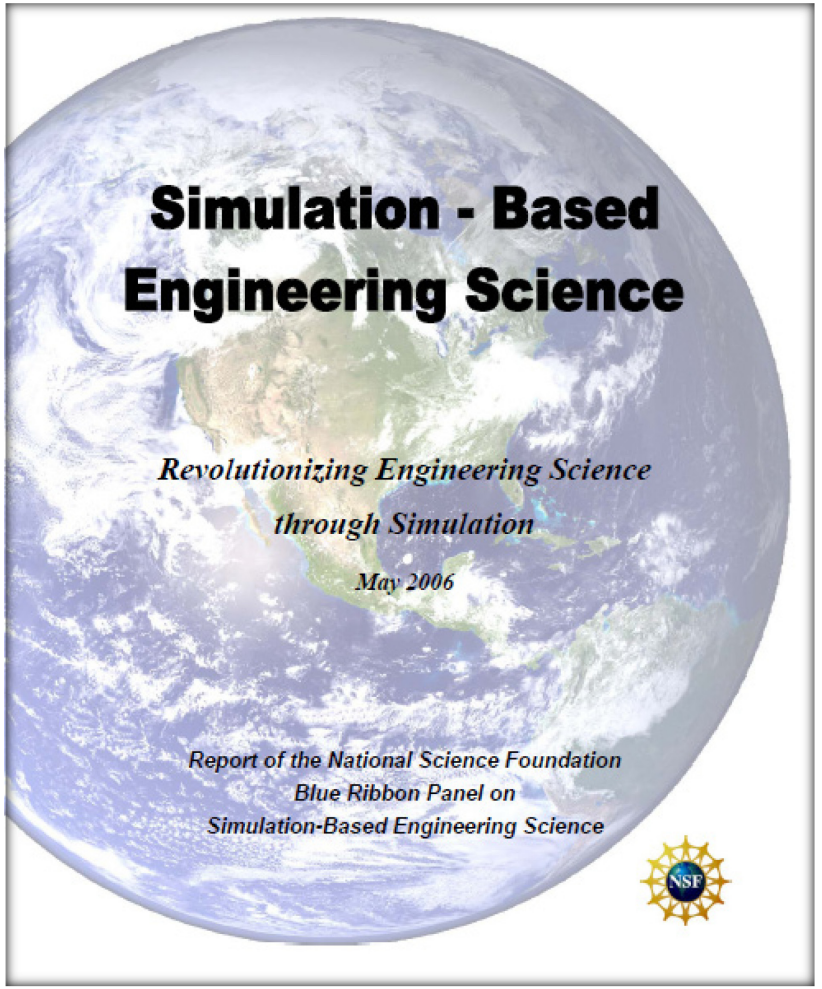
CS&E Pipeline in Informatics

- Data analysis
  - Pattern recognition, statistics, signal processing, parameter identification
- Simulation
  - Modeling approaches
    - *Physics, dynamical systems, continuums mechanics, fluid mechanics, ...*
    - *Differential equations, integral equations, statistics, geometry, ...*
    - *Model reduction, uncertainty quantification*
  - Discretisation techniques
    - *Approximation theory, functional analysis*
    - *Numerical analysis of PDEs and ODEs*
    - *Meshing, error estimators, adaptivity*
  - Algebraic solutions (*Linear algebra, iterative methods, multigrid)*
  - Optimization, steering, inverse problems
  - Implementations
    - *Hardware architecture*
    - *Parallel numerical algorithm*
    - *Software engineering for simulation tasks, efficient programming*
- Post-processing
  - Visualization, computer graphics
  - Computational steering

View: Uli Rüde

CS&E IN ENGINEERING

"Seldom have so many independent studies been in such agreement: simulation is a key element for achieving progress in engineering and science."



Authors:
J. Oden, T. Belytschko, J. Fisch,
T. Hughes, C. Johnson, D. Keyes,
A. Laub, L. Petzold, D. Srlovitz, S. Yip

EDUCATION IN CS&E

- A CS&E-student should be an expert in developing (and using) computational methods – and not necessarily an expert regarding a specific application.
- Methods shall be applicable to several applications → application-spanning methodological competence. This is the main difference between a CS&E student and a specialist (e.g. engineer)
- The focus shall be therefore on the modeling and simulation techniques (and natural science). This is the difference between CS&E students and students in mathematics or computer science.
- Math and computer science need to be linked together in an interdisciplinary sense.

CS&E Activities Exist…

- International Association of Computational Mechanics (IACM) and its German section (GACM),
- Arbeitsgemeinschaft Simulation (ASIM), which is an activity group of the Gesellschaft Informatik (GI),
- As part of the excellence initiative: Cluster of Excellence for Simulation Technology (SimTech) and graduate schools at Aachen and Darmstadt,
- DFG Schwerpunktprogramm (priority program) on ExaScale Software, and
- SIAM Activity Group CSE.

CS&E

- CS&E is in-between mathematics,
  computer science and the respective application.
- Despite the existing national and international momentum, there exists no coordinated activity group that scientifically represents the full spectrum of CS&E in Germany.
- GAMM has traditionally strong links to mathematics and many CS&E relevant application fields.
- The GAMM has also strong links to the computer sciences, in particular with high performance computing, parallel algorithms, visualization and data analysis.

CS&E AS PART OF THE GAMM

- Submitted an application to the board of the GAMM to establish an activity group “Computational Science and Engineering”
- This application was approved at the last board meeting of the GAMM in Darmstadt in March 2012.
- Kick-off meeting

AIMS OF THE GAMM FA CS&E

- The activity group on CS&E shall represent the subject itself and provide a forum to discuss the interests of research and education concerning CS&E.
- To adequately represent the interdisciplinary nature of CS&E towards universities and research institutions and to promote the necessary link between mathematics, mechanics, physics, computer science, natural and engineering sciences.

AIMS OF THE KICK-OFF MEETING

- Discuss and define CS&E from different point of views (engineering, mathematics, computer science, high performance computing, industry, ...).
- Discuss research and funding environment
- CS&E in education
- Establish networking links
- Provide an international perspective on CS&E
- Constitute the GAMM activity group on CS&E
- Discuss further activities of the GAMM FA CS&E

AGENDA

Monday, September 17, 2012:

13:00	**Opening and Welcome (Coffee)**
13:30	GAMM Fachausschuss CSE (Barbara Wohlmuth, Oliver Röhrle, Ulrich Rüde)
14:00	Wolfgang Ehlers (Stuttgart & Simtech)
14:30	Hans-Joachim Bungartz (München & SPP EXA)
15:00	Petros Koumoutsakos (Zürich, ASME Fellow)
15:30	**Coffee break**
16:00	Karsten Urban (Ulm, WiR)
16:30	Panel Discussion on "Research & Money @CSE" (Marcus Wilms, Hans-Joachim Bungartz, Dirk Hartmann, and more)
17:30	Constitution of the FA CSE and election of the speaker
18:30	**Joint dinner** (more detailed information on the back)

AGENDA

Tuesday, September 18, 2012:

09:00	David Keyes (KAUST & Columbia)
09:45	Tod Laursen (President of Khalifa University)
10:15	Dirk Hartmann (Siemens)
10:45	**Coffee break**
11:15	Kirk Jordan (IBM & SIAM AG CSE)
11:45	Michael Hanke (Stockholm, COSSE Erasmus Mundus)
12:15	Discussion of further CSE activities of the GAMM FA CSE