Panel on

Insertion Paths for Algorithms and Software into Multiphysics Applications

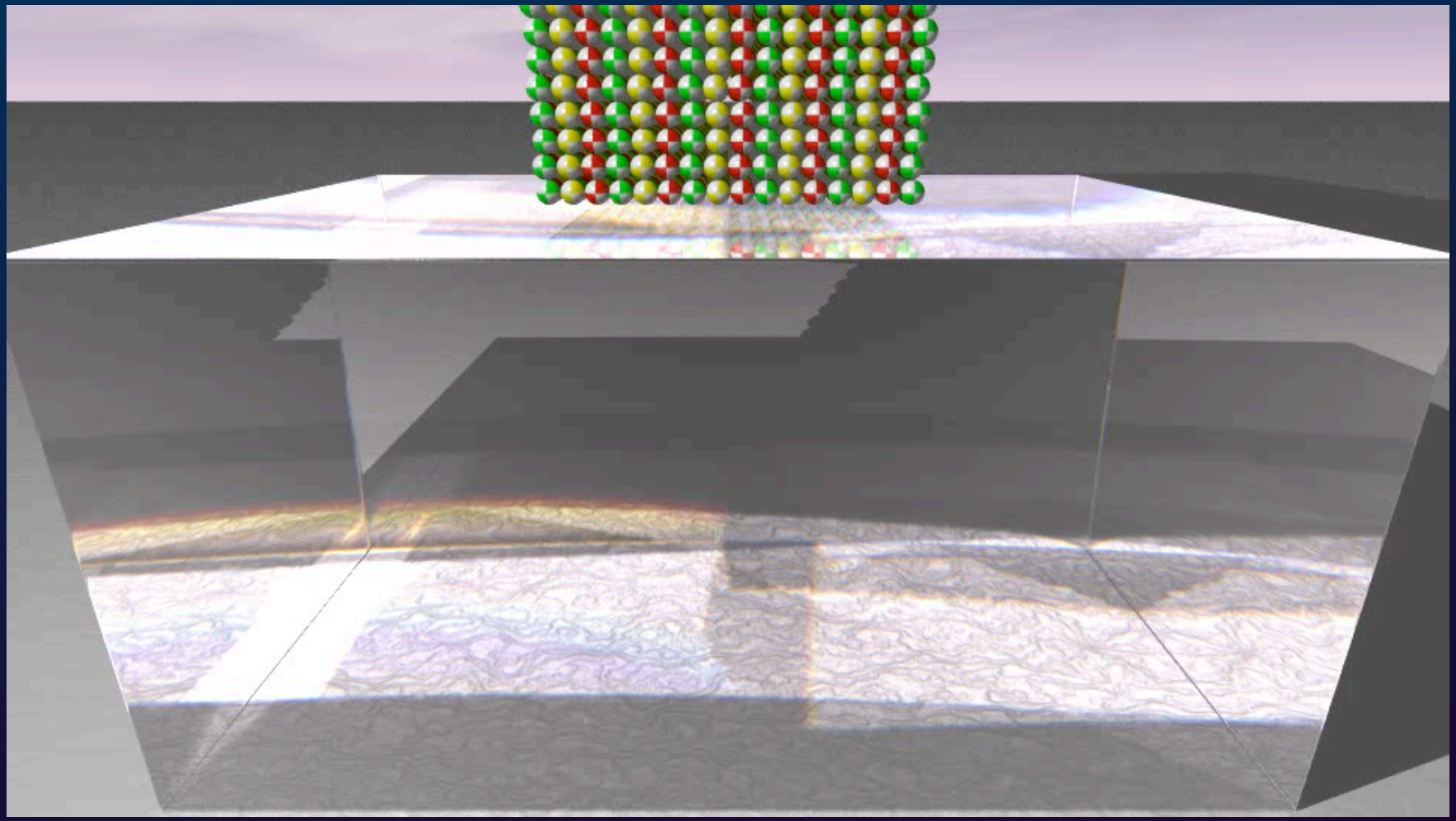
U. Rüde (LSS Erlangen, ruede@cs.fau.de)

Lehrstuhl für Informatik 10 (Systemsimulation)
Universität Erlangen-Nürnberg

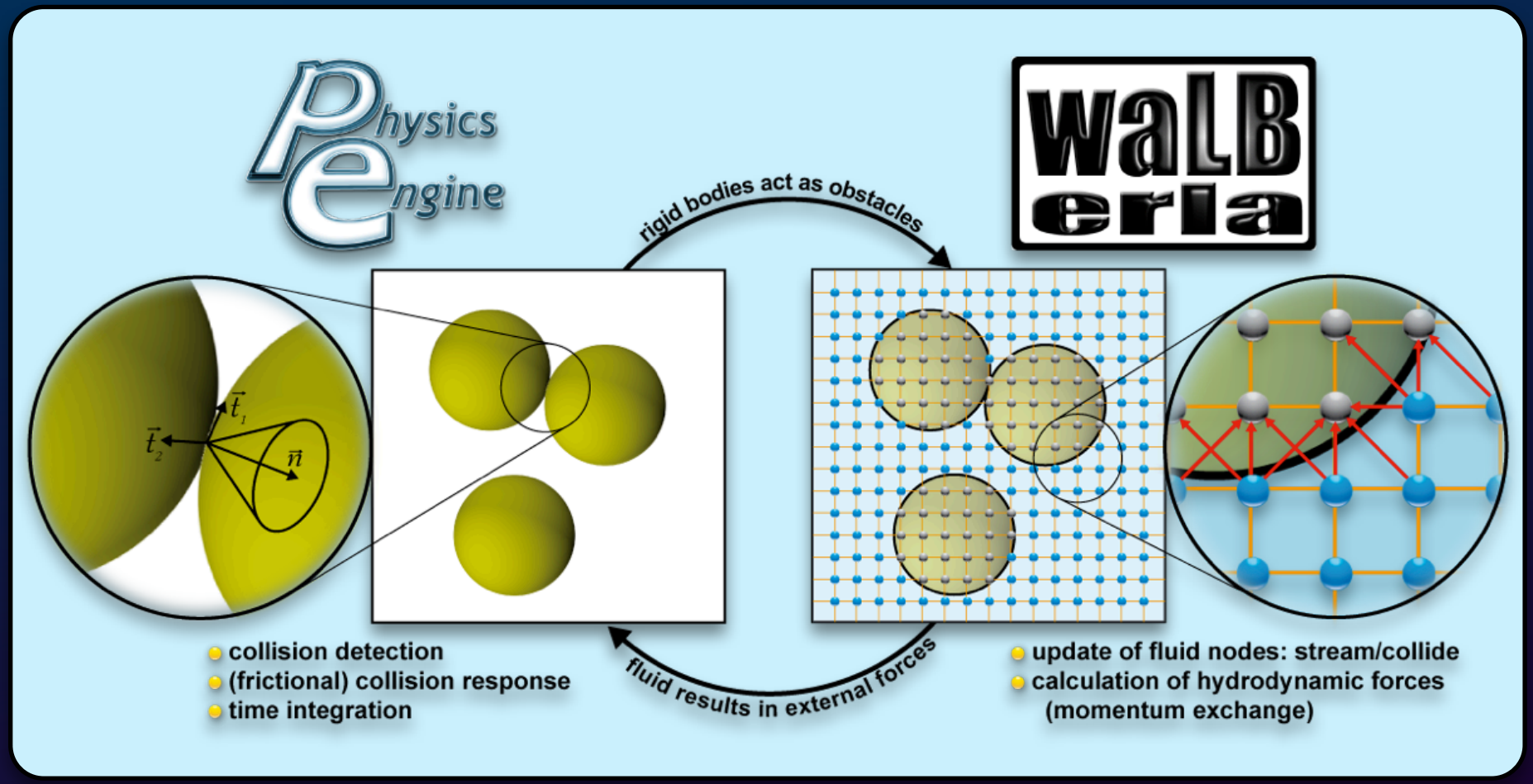
www10.informatik.uni-erlangen.de

ICiS Multiphysics Workshop
July 31 - August 6, 2011
Park City, Utah

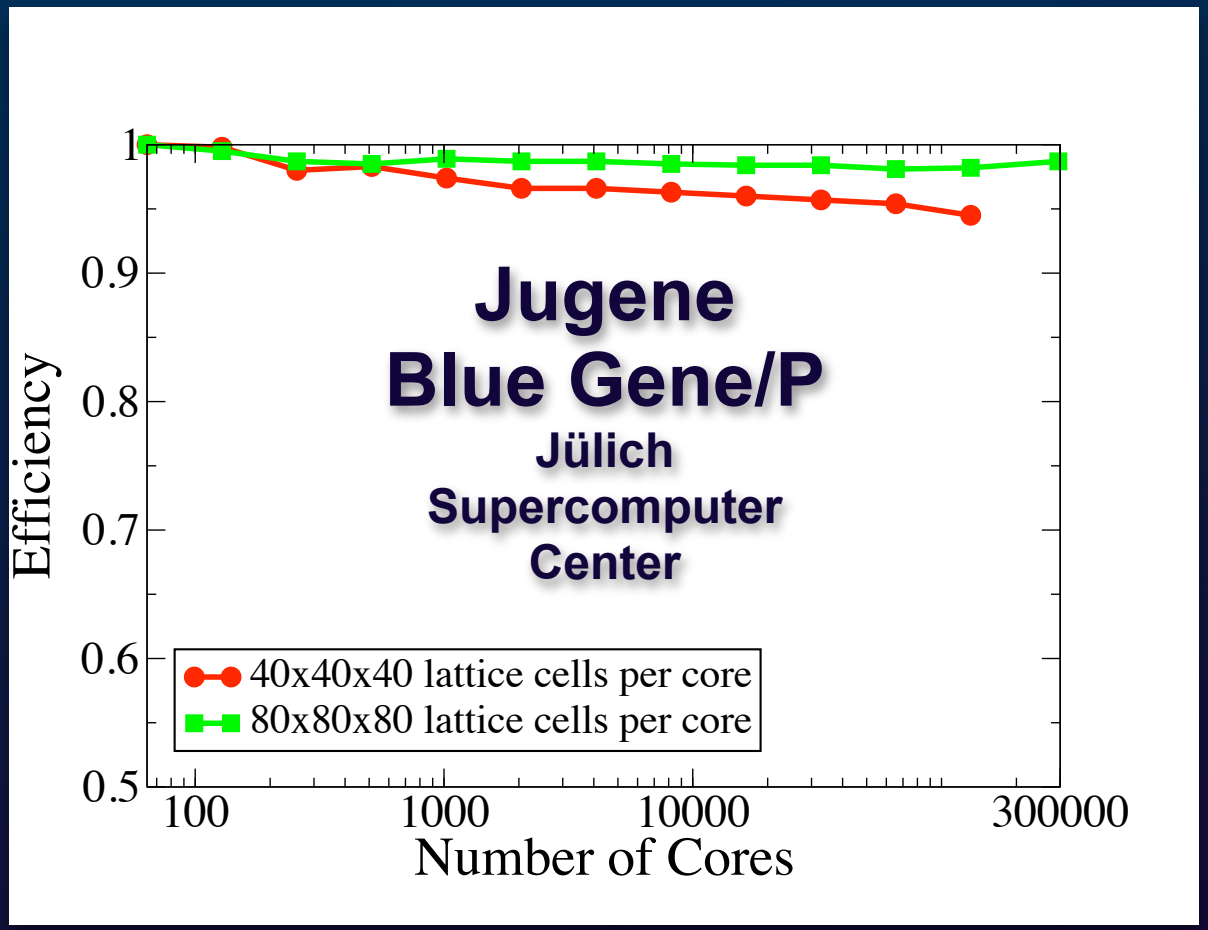
Fluid-Structure Interaction with Free Surface and Moving Objects



Fluid-Structure Interaction for particle ladden flows



Weak Scaling



- Scaling 64 to 294 912 cores
- Densely packed particles
- 150 994 944 000 lattice cells
- 264 331 905 rigid spherical objects

Questions / Challenges (0)

- For multiphysics we need extensible SW-architecture
  - PE: sandwich pattern
  - waLBerla:
    - patch-block data structure for waLBerla (coarse grain parallelism)
    - patches can have different „functionalities“: extensibility and heterogeneity
    - „sweep paradigm“ for expressing algorithms
    - identify performance critical kernels (fine grain parallelism)
  - flexibility and performance are often in conflict
- Legacy code: may range from „straightforward“ to „impossible“

Questions / Challenges (1)

- cross disciplinary collaboration for muliti-physics
  - software development is a long term project
  - difficult to find funding
  - and to sustain in the long term
- technical hurdles
  - complexity of HW & systems
  - complexity of models and math
  - emphasis of composition of building blocks rather than single-topic analysis
- sociological hurdles
  - must collaborate
    - individuals
    - teams
  - must be ready to admit ignorance

Questions / Challenges (2)

- structural hurdles
  - department structure
  - CS&E eco-system
  - community building
- scientific value system (where is the multi-physics journal?)

Is CS&E Research Adressing the „Real“ Problems?

- Think in new modeling paradigms!
  - can we do process scale direct simulation fully resolving the level of
    - pores?
    - grains?
    - fibers?
    - molecules?
    - atoms?
- Performance? We do not have good metrics!
  - O(N) complexity versus time to solution
  - or O(h) convergence versus accuracy per MWh
- We will be drowned by the Tsunami of Parallelism
- Validation?
  - rigorous theory vs. experimental validation
- „Abstract“ numerical algorithms vs. high quality software
- Monolithic models vs. coupling a variety of „algorithmic building blocks“

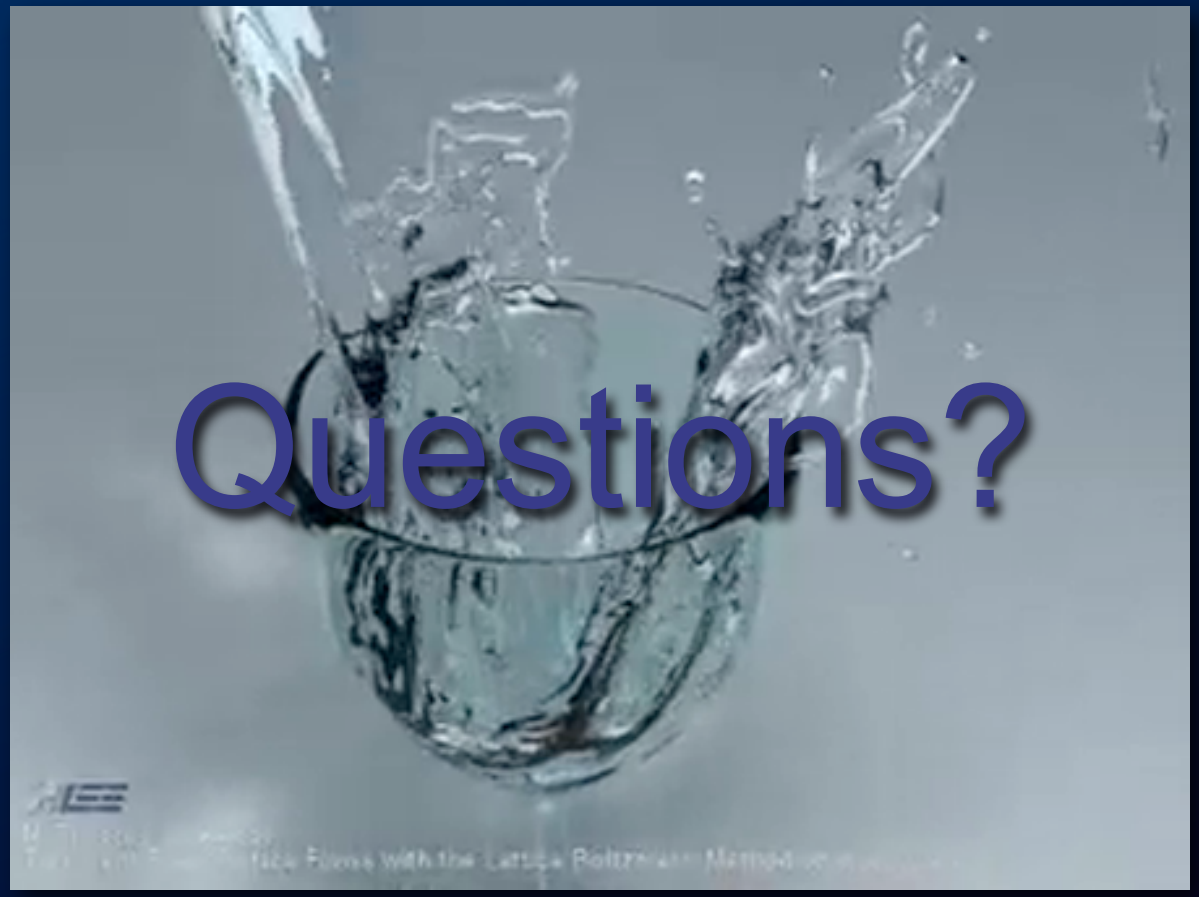
SIAM J. Scientific Computing

editor-in-chief: Hans Petter Langtangen, Oslo
(Uli Ruede until 12-2010)

SISC papers are classified into three categories:

- **Methods and Algorithms for Scientific Computing.** Papers in this category may include theoretical analysis, provided that the relevance to applications in science and engineering is demonstrated. They should contain meaningful computational results and theoretical results or strong heuristics supporting the performance of new algorithms. (section editor: Jan Hesthaven, Brown)
- **Computational Methods in Science and Engineering.** Papers ... will typically describe novel methodologies for solving a specific problem in computational science or engineering. They should contain enough information about the application to orient other computational scientists but should omit details of interest mainly to the applications specialist. (section editor: Irad Yavneh, Technion)
- **Software and High-Performance Computing.** Papers .... should concern the development of high-quality computational software, high-performance computing issues, novel architectures, data analysis, or visualization. The primary focus should be on computational methods that have potentially large impact for an important class of scientific or engineering problems. (section editor: Tamara Kolda, Sandia)

Thank you for your attention!



Slides, reports, thesis, animations available for download at:

www10.informatik.uni-erlangen.de