The Emergence of Predictive Science
Computational Science and Engineering

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Outline

- What is this CSE about?
  - The Logic of Predictive Science
- The Scientific Tourist’s short guide through CSE (using examples from LSS)
  1. Solid phase - rigid body dynamics
  2. Fluid phase - lattice Boltzmann method
  3. Coupled Systems - Particulate Flows
  4. Electrostatics - particles in eletrostatics
  5. Gas phase - free surface tracking, volume of fluids
  6. Supercomputing: scalable algorithms and efficient software
  7. An example application
- Perspectives for the 21 century
The Two Principles of Science

Three

Theory
- mathematical models, differential equations, Newton

Experiments
- observation and prototypes, empirical sciences

Computational Science
- simulation, optimization, (quantitative) virtual reality

Computational methods open the path to Predictive Science
The Logic of Predictive Science: What is it?  
thanks to T. J. Oden, UT Texas, ICES

Predictive Science: the scientific discipline concerned with assessing the predictability of mathematical and computational models of reality. It embraces the processes of model selection, calibration, validation, verification, and their use in forecasting the relevant features of reality with quantified uncertainty.

- Mathematical constructions based on physical principles or empirical relations - generally derived from inductive theories that attempt to characterize abstractions of physical reality.
- The process of adjusting the parameters of a model to improve the predictions of the model to better agree with experimental measurements.
- The process of determining the accuracy with which a model can predict features of reality.
- The quantities of interest (QI): the goals of the simulation.
- UQ: quantitative analysis of the uncertainties in the predicted QI.

Predictability requires knowledge of the physical laws that are proposed to explain realities and requires recognizing and quantifying uncertainties.
The imperfect paths to knowledge
Building block I:
Granular Media Simulations
with the physics engine

with T. Preclik and K. Iglberger


Shaker scenario with sharp edged hard objects

Tobias Preclik
Sharp-edged Granular Matter in a High Amplitude Horizontal Shaker
31.3.2014

Computed with the PE software at LSS
Building Block II:

Scalable Flow Simulations with the Lattice Boltzmann Method

Flow simulations and animation with the waLBerla software framework at LSS
Computational Fluid Dynamics with waLBerla

with: F. Schornbaum, C. Godenschwager, E. Fattahi:
Simulation of phantom vocal fold geometry using the waLBerla framework at LSS
Direct Numerical Simulation for periodic and random dense sphere packings

joint work with Ehsan Fattahi, Christian Waluga, Barbara Wohlmuth
Construction of random spherical structure for porous media with the PE
Turbulent flow over a permeable wall

- $Re \approx 3000$, DNS
- 3 level of refinement used
- Volume rendering of velocity magnitude
- Periodic in X and Y direction
- Flow driven by periodic-pressure boundary condition
- Non-uniform pressure gradient
- 6 mega cells in the simulation
- 300 loops of flow over periodic channel
- Video from transition regime
- I10 cluster
- $7(\text{nodes}) \times 32(\text{cores}) \times 19(\text{h}) = 4256$ core hours
- 1,300,000 timesteps
- 8 times more timestep on the finest level
Building Block III:
Multi-Physics Simulations for Particulate Flows

Parallel Coupling with waLBerla and PE

with D. Bartuschat and K. Gustavsson (KTH Stockholm) coupled simulations with waLberla and PE at LSS
Fluid-Structure Interaction
direct simulation of Particle Laden Flows (4-way coupling)

Virtual Fluidized Bed

512 processors

Simulation Domain
Size: 180x198x360 cells of LBM

900 capsules and 1008 spheres = 1908 objects

Number time steps: 252,000

Run Time: 07h 12 min

coupled simulation of waLBerla and PE at LSS
Building Block IV (electrostatics)

Direct numerical simulation of charged particles in flow


6-way coupling

- electrostatic fields
  - FV-discretization - cell centered multigrid solver
  - lubrication correction
8.3 Weak Scaling

The runtimes of all parts of the algorithm are shown in Fig. 13 for different problem sizes, indicating their shares on the total runtime. This diagram is based on the BCs on the boundary. Whenever the relative proportion of the problem size scales with the diameter of the finite element MG solver in Gmeiner and Rüde (2014) according to required number of iterations, the growth in the condition number Shewchuk (1994). However, when doubling the problem size, CG iterations approximately double. The runtimes of all parts of the algorithm are shown for 240 time steps on increasing number of nodes. The problem size is successively doubled in all dimensions, as shown in Table 6 for V(3,3)-cycles and CG coarsest grid solver. The runtimes of charged particle algorithm sweeps for a Poisson problem with Dirichlet BCs. The runs were played. These include MG, setting the RHS of Poisson's equation (SetRHS), communication of the electric potential computation are distributed unevenly, making the sweeps on the parallel machine expensive. The ‘other’ sweeps scale perfectly—HydrF, LubrC, for a more precise evaluation, the exact figures are below 0.1% and each other sweep of 'Oth' is well below the overall performance. For the simulation for the animation, the load on the bottom wall are no longer evenly distributed, possibly causing load imbalances. However, they hardly affect the runs. For longer simulation times the particles attracted by the bottom wall are no longer evenly distributed, possibly causing load imbalances. However, they hardly affect the runs.

Table 7 for one node and 2048 nodes. The total runtime (Whl) is less than the sum of the individual sweeps. Below, the cost of sweeps of the individual sweeps. The sweeps that scale perfectly—HydrF, LubrC, for a more precise evaluation, the exact figures are below 0.1% and each other sweep of 'Oth' is well below the overall performance. For the simulation for the animation, the load on the bottom wall are no longer evenly distributed, possibly causing load imbalances. However, they hardly affect the runs.

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Volume of Fluids Method for Free Surface Flows

joint work with Regina Ammer, Simon Bogner, Martin Bauer, Daniela Anderl, Nils Thürey, Stefan Donath, Thomas Pohl


Computational Fluid Dynamics
Lattice Boltzmann Method

- 1000 Bubbles
- $510 \times 510 \times 530 = 1.4 \times 10^8$ lattice cells
- 70,000 time steps
- 77 GB
- 64 processes
- 72 hours
- 4,608 core hours

Visualization
- 770 images
- Approx. 12,000 core hours for rendering

Bubbly flow using the massively parallel waLBerla framework at LSS
Example Application:

Additive Manufacturing
Fast Electron Beam Melting


Motivating Example: Simulation of Electron Beam Melting Process (Additive Manufacturing)

- EU-Project Fast-EBM
  - ARCAM (Sweden)
  - TWI (Cambridge)
  - WTM (FAU)
  - ZISC (FAU)
- Generation of powder bed
- Energy transfer by electron beam
  - modeling penetration depth
- Joint work with C. Körner, M. Markl, R. Ammer

- heat transfer
- Flow dynamics
- Melting/solidification
- phase transition
- surface tension
- fluid flow
- wetting, capillary forces
Simulation of Electron Beam Melting

Simulating powder bed generation using the PE framework

High speed camera shows melting step for manufacturing a hollow cylinder

WaLBerla Simulation
Building Block VI:

Current and Future High Performance Supercomputers

SuperMuc: 3 PFlops
How fast are computers today?

- $10^6 = 1$ MegaFlops: Intel 486 33MHz PC (~1989)
- $10^9 = 1$ GigaFlops: Intel Pentium III 1GHz (~2000)
  - If every person on earth computes one operation every 7 seconds, all humans together have ~1 GigaFlops performance (less than a current laptop)
- $10^{12} = 1$ TeraFlops: HLRB-I 1344 Proc., ~2000
- $10^{15} = 1$ PetaFlops
  - 122 400 Cores (Roadrunner, 2008)
  - 294 912 Cores (Jugene, Jülich, 1 PFlops, 1.44 $10^{14}$ Bytes Memory)
  - 155 000 Cores (SuperMuc, 3 PFlops, 3.33 $10^{14}$ Bytes Memory)
- If every person on earth runs a 486 PC, we all together have an aggregate Performance of 7 PetaFlops.
- ExaScale (~$10^{18}$ Flops) around 2020?
Summary of Performance Evaluation on Coronary Geometry

Weak scaling on JUQUEEN with 458,752 processes

- over a trillion ($10^{12}$) fluid lattice cells
  - Cell sizes of 1.27µm (diameter of red blood cells about 7µm)
  - 2.1 $10^{12}$ cell updates per second
  - 0.41 PFlops

Strong scaling at cell sizes of 0.1 mm

- In excess of 6000 time steps per second on 32,768 cores of SuperMUC
- 2.1 million fluid cells

Mega=$10^6$, Giga=$10^9$, Tera=$10^{12}$, Peta=$10^{15}$, Exa=$10^{18}$

- World has a population of $7 \times 10^9$ humans
- Earth is $4.6 \times 10^9$ years old
  - the oceans together have ca. $1.3 \times 10^9$ km$^3$
  - the mantle has $0.91 \times 10^{12}$ km$^3$
  - $10^{12}$ finite elements can resolve the volume of the mantle with ca. 1 km resolution
- Number of stars in the galaxy: $10^{11}$
- Avogadro’s constant: $6 \times 10^{23}$ mol$^{-1}$
- The recirculatory system contains $2.5 \times 10^{13}$ red blood cells
- The brain has ca. $10^{11}$ Neurons
- Processor chip has
  - $5 \times 10^9$ transistors
  - 3 GHz clock rate: $3 \times 10^9$
  - can perform $10^{11}$ (= 100 Giga) Flops
  - Supercomputer at 2020: $10^{18}$ Flops

An exa-scale computer system with $10^{18}$ Flops should suffice to resolve the meso-scale
Why are asymptotically optimal algorithms essential?

Thought Experiment

- $10^9$ elements/nodes
- assume that every entity must contribute to any other (as is typical for an elliptic problem)
- equivalent to either
  - multiplication with inverse matrix
  - $n \times n$ Coulomb interaction
- Results in $10^{18}$ data movements
  - each 1 NanoJoule (optimistic)
- Together: $10^9$ Joule = 277 kWh

Thought Experiment

10 elements/nodes assume that every entity must contribute to any other (as is typical for an elliptic problem) equivalent to either multiplication with inverse matrix $n \times n$ Coulomb interaction.

Results in $10^{24}$ data movements each 1 NanoJoule (optimistic).

Together: $10^{15}$ Joule

Figure 5: With new scaling rules and massive growth in parallelism, data locality is increasingly important. This diagram shows the cost of a double-precision multiply-add at different levels of the memory hierarchy (from the cost of performing the flop to the movement of data operands from registers, different distances on-chip, and distances off-chip). The model or FPU and register access is based on the Tensilica LX2 core energy model, the energy consumed for cross-chip wires uses the Orion2 power model which is based on Balfour’s model [6], memory access is based on the JEDEC DDRx memory roadmap, and cross-system is based on projections for VCSEL-based optical transceivers.

2.4 New Communication and Synchronization Mechanisms

Increased use of non-conventional (non-cache-coherent) methods for interprocessor communication on chip (e.g. GPU Warps and Intel SCC inter-processor hardware message queues) suggests new approaches are needed for expressing data locality so that runtime systems can manage data movement instead of increasing the burden on the application programmer.

Configurable Caches: Increased use of configurable caches (automatic vs. user-managed) to explicitly manage vertical data movement. Motivates new APIs for making effective use of these new hardware locality management features in a cross-platform manner.

Coordinated Power Management: Local power management decisions (such as Intel/Sandybridge thermal-throttling of FPU clock rates) will result in system-wide performance inhomogeneity. This motivates systemwide coordinated power management.

Energy Aware Data Movement/Load-Balancing: New sources of transient load-imbalance are increasing (such as software-based fault resilience mechanisms, and localized power management), but rebalancing the load may be more costly than tolerating it. Balancing the cost of fixing a load-imbalance vs. tolerating its continuation requires an API for expressing the energy-costs of data movement to the application and runtime.

ASCR Exascale Programming Challenges Workshop

277 GWh or 240 Kilotons TNT

the picture shows the Badger-Explosion of 1953 with 23 Kilotons TNT

The future:

Bringing Things Together in Computational Science and Engineering

Max Gunzburger's (FSU) diagram on CSE
The Simulation Pipeline

Basis of CSE

thanks to H.J. Bungartz, TU Munich

Predictive Computational Science - Ulrich Rüde
The Simulation Pipeline
Basis of CSE

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Mathematical model
\[ \frac{\partial u}{\partial t} + (u \cdot \nabla) u + \frac{1}{\rho} \nabla p - \nu \Delta u = 0 \]

Discretization & solver
\[ A \dot{u}_h + D u_h + C(u_h) u_h - M^T p_h / \rho = 0 \]

Parallel implementation, HPC

Insight, Design

Exploration

Validation

Software

Predictive Computational Science - Ulrich Rüde
All this is just about to take off...

slide thanks to H.J. Bungartz, TU Munich
Conclusions and Perspectives

- Supercomputer power
- Versatile tools
  - lattice Boltzmann
  - multi-body dynamics
- Limitations to pore scale resolution
  - ensemble size
  - time steps
- Gain insight
  - multi-scale
  - multi-physics
- Challenges
  - multi-core (parallel computing)
  - validation
  - software
Reviewing IEWA @ Kanpur

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Impressions (I)
Impressions (II)
Impressions (III)
Impressions V
Thank you for your attention!

Videos, preprints, slides at https://www10.informatik.uni-erlangen.de
Thank You!