FRIEDRICH-ALEXANDER
UNIVERSITÄT
ERLANGEN-NÜRNBERG
FACULTY OF ENGINEERING

High End Simulation in Practice

12.04.2021

Prof. Dr. Harald Köstler

Lehrstuhl für Informatik 10 – Systemsimulation

FRIEDRICH-ALEXANDER
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Lecture 1

Logo

Organisation

Educational Goals, Lecture, Exercises, Exam, Contents, Literature

Logo

Educational Goals

- Know basics of CUDA, OpenCL and parallel programming
- Be able to do modular and efficient implementations of numerical algorithms on GPUs
- Learn basics of particle simulation / molecular dynamics
- Design software in a group

- What do you expect from the lecture?

Lecture

- Two parts
  - OpenCL, CUDA and parallelization part
  - Physical part molecular/rigid body dynamics
- First part is somehow continuation of lecture Advanced Programming Techniques (C++)
- Ask and give feedback
- Schedule
  - Online lecture Monday 10:15-11:45,
    https://fau.zoom.us/j/63354369071?pwd=Q2twRnBtNU5NK3RiN2lTcDFHZnJGQT09

Exercise

- Responsible: Rafael Ravedutti
- You will develop software in a group of 2-4 students
- Exercise sheets are found in Studon
- Schedule online (see Studon)

Exam

- Oral exam
- Based on the lecture and exercises

Contents

- Introduction to GPU architecture (Lect. 2)
- Introduction to OpenCL and CUDA (Lect. 3)
- Introduction to molecular dynamics (Lect. 4+5)
- Parallel Programming concepts and tools (Lect. 6+7)
- Introduction to rigid body dynamics (Lect. 8)
- Modern CUDA and C++ concepts for designing portable software (Lect. 9+10)

Basic literature

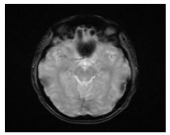
- Griebel, M., Knapek, S., Zumbusch, G., Numerical simulation in molecular dynamics. Springer, 2007 (available online)
- Pöschel, T.,Schwager, T., Computational granular dynamics: models and algorithms. Springer, 2005
- OpenCL/CUDA Programming Guide (Nvidia, AMD/ATI, or Intel)

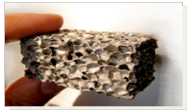
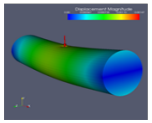
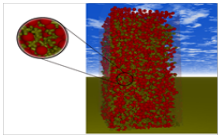
Introduction

Motivation

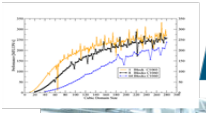
Logo

Computational Science and Engineering



Applications
- Tsunami
- fluid, rigid bodies
- medical engineering
- solidification

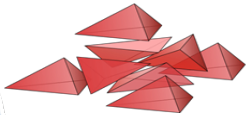
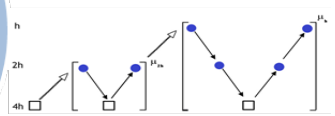
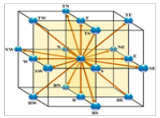



Computer Science
- HPC / architectures
- performance engineering
- **software design**
- **code generation**

```
USE_SweepSection(
getLBMsweepUID() ){
 USE_Sweep(){

swUseFunction(„LBMSweep::LBMSw
eep,FSUIDSet::all(),hsCPU,BSUIDS
et::all());
 }
 USE_After(){
  //Communication
 }
}
```


Applied Math
- LBM, multigrid
- FEM / DG
- Neural nets
- Genetic programming

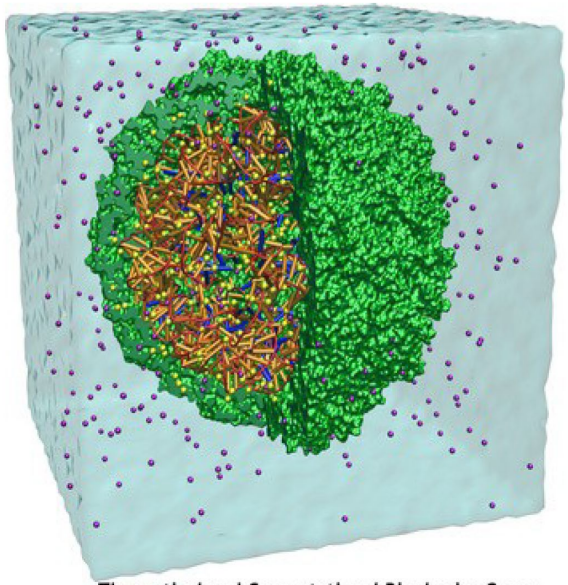




High Performance Computing: Applications

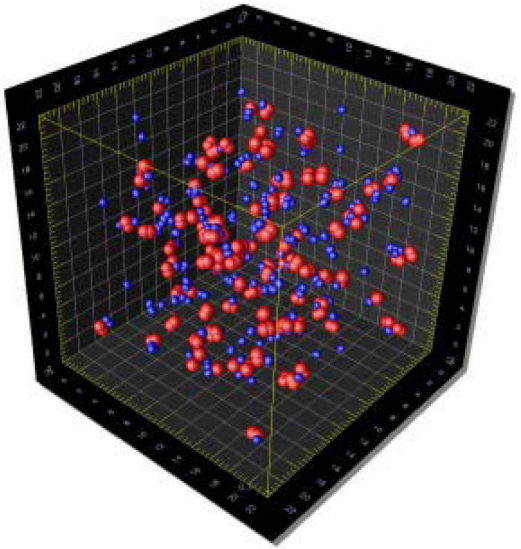
real-time
simulation
e.g. medicine

Large-scale
simulation
e.g. multi-physics

Molecular dynamics



Theoretical and Computational Biophysics Group
Beckman Institute
University of Illinois at Urbana-Champaign



Snapshot from
BGCE project **MolDyn**

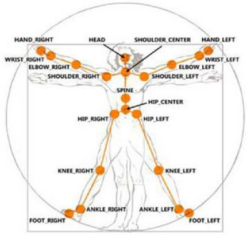
Computational Steering: Granular Convection

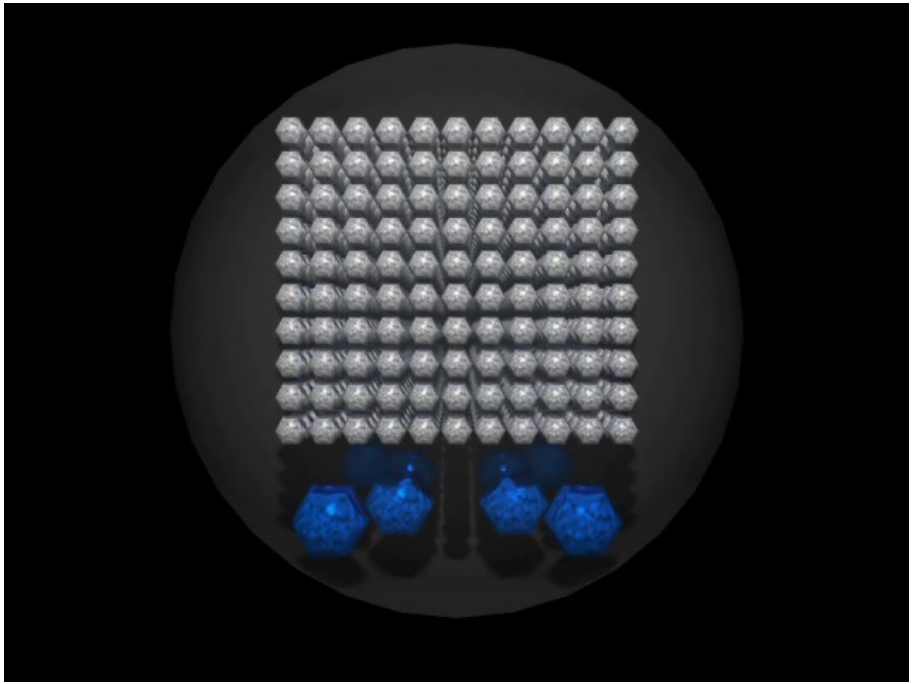
- Newton's second law of motion

$$F = m \cdot a$$

$$M = J \cdot \alpha$$

- Discrete Element Method
- OpenCL + DirectX
- Microsoft Kinect sensor





Next time…

- Current super computers
- Current GPU architectures
- Basic GPU programming