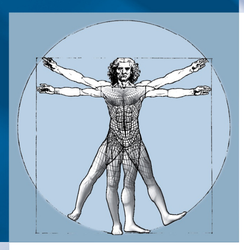
SimTech Cluster of Excellence

University of Stuttgart
Germany

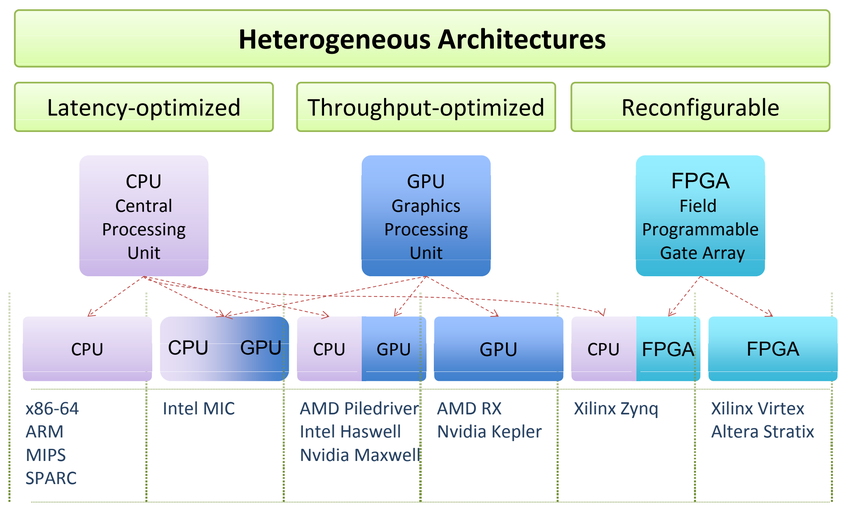


Simulation on Reconfigurable Heterogeneous Architectures

Dipl.-Inf. Alexander Schöll, Prof. Dr. Hans-Joachim Wunderlich
Institute of Computer Architecture and Computer Engineering, University of Stuttgart, Germany

Motivation

- Heterogeneous computer architectures are integrated into single chips

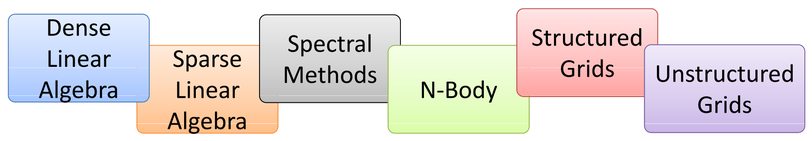


Overview of current heterogeneous architectures

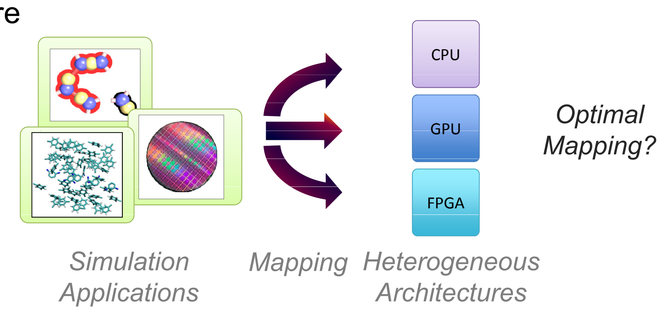
- **Upcoming**: Reconfigurable Heterogeneous Computer Architectures
- **Goal**
  - Development of new methods that enable the **direct mapping** of simulation applications to innovative **reconfigurable heterogeneous computer architectures**

Challenges

- Mapping of simulation applications
  - Simulation applications contain algorithms from distinct problem classes



  - Many different programming paradigms and languages
- Achieving optimal performance
  - Particular aspects of underlying hardware structures must be considered
  - Performance depends on the combination of implementation and utilized architecture



- Reliability
  - Simulation applications are executed for days and months
  - Fault-tolerant execution, memories and communication required

Current Collaborations

Expansion of the Pro-Apoptotic Receptor Clustering Model

Cooperation with M. Daub • G. Schneider

- Inclusion of the extracellular space
- Simulation of random impact of Ligands on the cell membrane
- Simulation on multiple time scales for optimal balance between biological process resolution and computation costs
- Mapping of particle simulation to heterogeneous architectures

Mapping of Domain Decomposition for the Nonlinear Wave Equation to Heterogeneous Architectures

Cooperation with M. Daub • G. Schneider

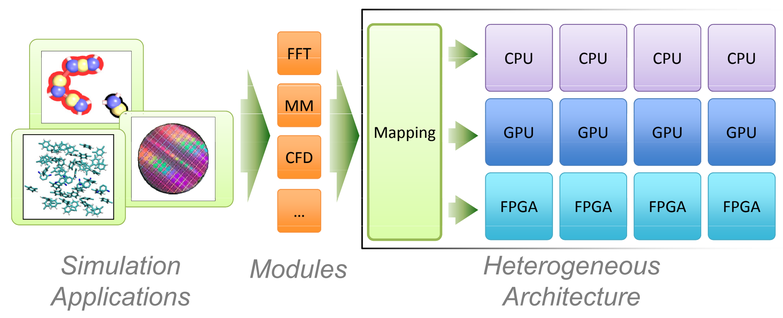
- Problem: Solve the nonlinear wave equation on large domains with a huge amount of nodes

$$u_{tt} = u_{xx} - d_c u + n_c u^3$$

- Mapping of equation solver to reconfigurable heterogeneous architectures

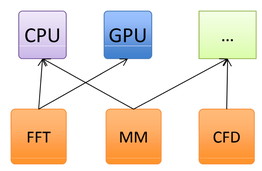
Current Work

- Implementation of specific compute modules for heterogeneous architectures
  - Modules perform basic tasks in targeted simulation applications
  - Implementation in distinctive realizations for different types of computing resources
  - Goal: Abstract and hide the actual execution of modules from the simulation application



- Development of resource management and load-balancing mechanisms
  - Investigation of efficient module organization and execution strategies

    Goal: Optimization of simulation performance and adaption to changing system conditions during runtime



- Development of fault-tolerance measures for modules
  - Repeated or redundant execution of modules and comparison of results
  - Algorithm-based fault-tolerance

SimTech Phase I: Simulation Applications and Collaborations

Parallel Simulation of Pro-Apoptotic Receptor Clustering on GPGPU Many-Core Architectures[1]

C. Braun • M. Daub • A. Schöll • G. Schneider • H.-J. Wunderlich

- Apoptosis: Structured decomposition of damaged or infected cells in multi-cellular organisms
- Initiated by signal competent clusters of tumor necrosis factor receptors (TNFR) and corresponding TNF Ligands on the cell membrane.
- Particle simulation has been mapped to GPGPU many-core architecture.
- **Reduction of simulation times from months to hours enables practical application of the model in research (Speedup: 300x)**

Acceleration of Markov-Chain Monte-Carlo Molecular Simulations on Hybrid Computer Architectures[2]

C. Braun • S. Holst • J. Castillo • J. Groß • H.-J. Wunderlich

- Markov-Chain Monte-Carlo (MCMC) simulations are the core of many tasks in thermodynamics
- Problem: Inherent serial dependencies make this method very hard to parallelize
- Typically coarse-grained parallelization and distribution of simulation instances on clusters or workstation grids is applied
- MCMC molecular simulation has been mapped to GPGPUs, exploiting parallel energy calculations and speculative evaluation of Monte-Carlo moves
- **Speedups of up to 400x**

[1] C. Braun, M. Daub, A. Schöll, G. Schneider, and H.-J. Wunderlich, "**Parallel Simulation of Apoptotic Receptor-Clustering on GPGPU Many-Core Architectures**", in Proc. IEEE International Conference on Bioinformatics and Biomedicine, BIBM 2012, Philadelphia, USA, 4.-7. October, 2012, pp. 155-160.

[2] C. Braun, S. Holst, J. Castillo, J. Groß, and H.-J. Wunderlich, "**Acceleration of Monte-Carlo Molecular Simulations on Hybrid Computing Architectures**", in Proc. 30th IEEE International Conference on Computer Design, ICCD'12, Montreal, Canada, 30.9.-3.10.2012, pp. 207-212.