SimTech Cluster of Excellence

University of Stuttgart
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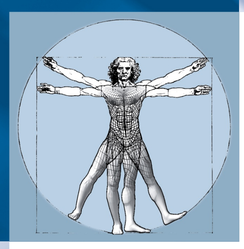

Simulation on Reconfigurable Heterogeneous Architectures

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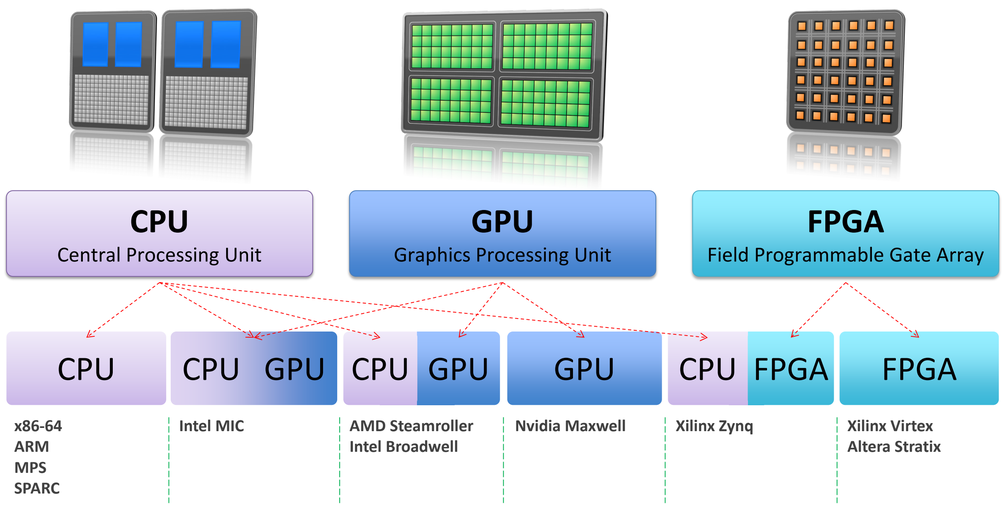
Motivation

- Heterogeneous computer architectures are integrated into single chips

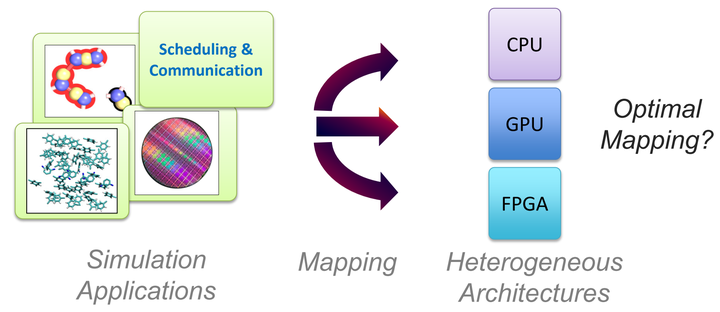


Overview of current heterogeneous architectures

- Upcoming: Reconfigurable Heterogenous Computer Architectures
- **Goal**
  - **Fast** and **reliable** execution of simulation applications on innovative **reconfigurable heterogeneous computer architectures**

Challenges

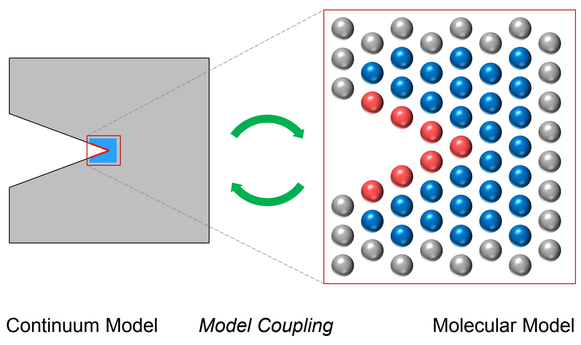
- Reliability
  - Simulation applications are often executed for days and months
  - CMOS devices, manufactured in 12nm technology and below:
    - vulnerable to transient effects, process variations and latent defects, as well as stress and aging mechanisms
  - Fault-tolerant execution, memories and communication are required
    - **Focus**: Fault-tolerant simulation algorithms
- Achieving optimal performance
  - Performance depends on the combination of implementation and utilized architecture



Current Work

Vulnerability of Multiscale and Multiphysics Simulation Algorithms

- **Goal:** Fault-tolerant techniques tailored to multiscale/multiphysics algorithms
- **Now:** Investigation of reliability issues



Case Study: Multi-Scale Simulation of Materials

Efficient Fault-Tolerance for the Preconditioned Conjugate Gradient Method (PCG)

Motivation

- PCG is one of the most popular sparse linear system solvers *(Ax = b)*
  - Widely used in structural mechanics, computational fluid dynamics, electronic design automation
- PCG is still **vulnerable** to **transient errors**
  - Single errors may significantly increase computation times and **corrupt** the computed solution **without indication** to the user

Method: Error Detection

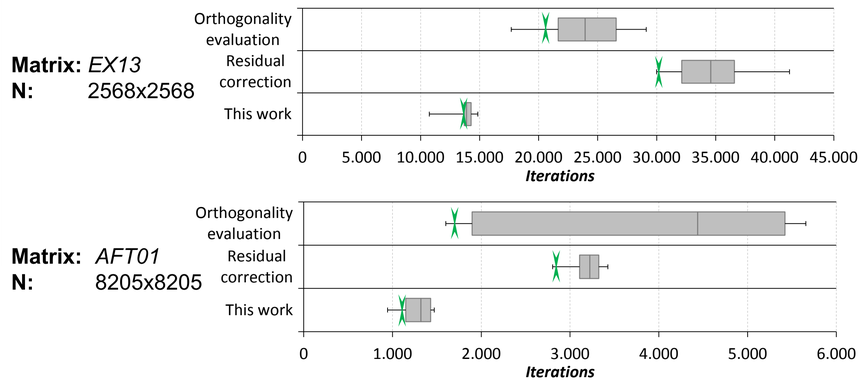
- Exploitation of global orthogonality and residual relationships to derive an **efficient error detection method**

Method: Error Correction

- **Adaptive error correction** scheme
  - Dependent on the **detected corruption** an **online correction**
  - … or a **rollback recovery** is performed

Experimental Results

- **Experiments:** Random injection of bit flips and comparison against error-free execution (✓)



Current Collaborations

Adaptive Parallel Simulation of a Two-Timescale Model for Apoptotic Receptor-Clustering on GPUs[1]

Cooperation with M. Daub • G. Schneider

Motivation

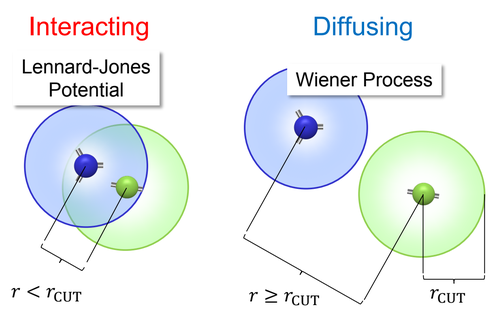
- Apoptosis: Structured decomposition of damaged or infected cells in multi-cellular organisms
- Deeper understanding of the activation necessary
- **Simulation:** Dominated by extensive computing times
  - Significant **computational requirements**
  - **Large numbers** of simulations required to draw reliable conclusions

Goals

- **Reduction** of **computation time**
- … to **obtain extensive** and **detailed conclusions** about the clustering behavior

Methods

- Simulation on multiple time scales for optimal balance between biological process resolution and computation costs
- Separation of particle dynamics
  - Adaptive refinement of time steps on each timescale in case of violations



- Mapping of particle simulation to heterogeneous architectures

Computational Performance Results

- Reduction of simulation time from hours to seconds

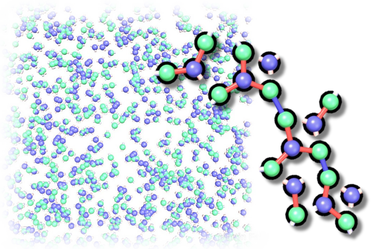
Computation times with different numbers of parallel instances on multiple GPUs

Parallel Simulation Instances	4	8	16	24	32
Previous work (s)	2082	3045	5203	7591	9778
This work (s)	**12**	**17**	**30**	**43**	**57**

Setup with 2496 monomer, 2496 dimer and 1344 ligand particles.

Biological Evaluation

- Temporal evolution of ligand-receptor clusters in less than 0.5s



[1] A. Schöll, C. Braun, M. Daub, G. Schneider, and H.-J. Wunderlich, **"Adaptive Parallel Simulation of a Two-Timescale Model for Apoptotic Receptor-Clustering on GPUs",** in Proceedings of the IEEE International Conference on Bioinformatics and Biomedicine, BIBM 2014, Belfast, UK, 2.-5. November, 2014, pp. 424-431.