SimTech Cluster of Excellence

University of Stuttgart Germany

Simulation on Reconfigurable Heterogeneous Architectures

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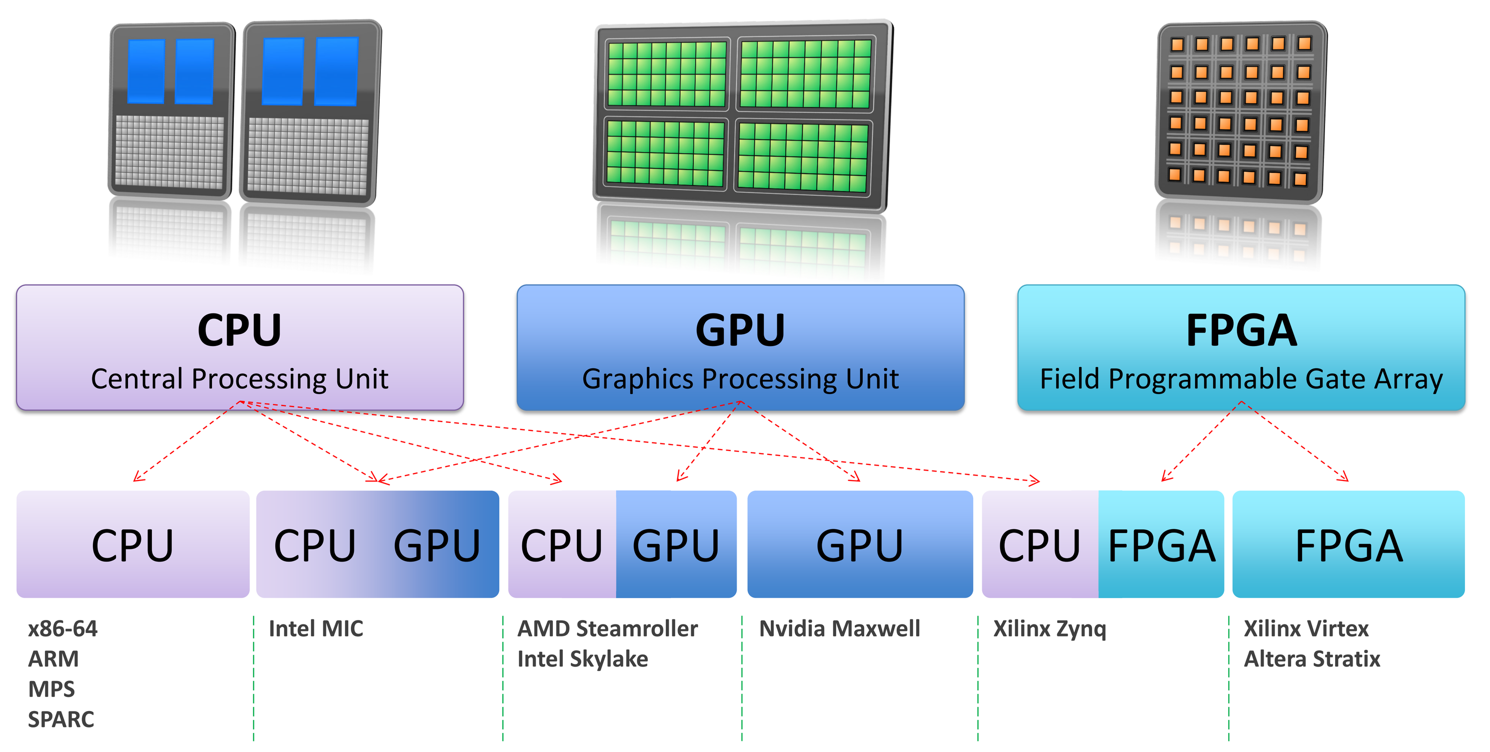
Motivation

- Emerging: **Heterogeneous computer architectures**

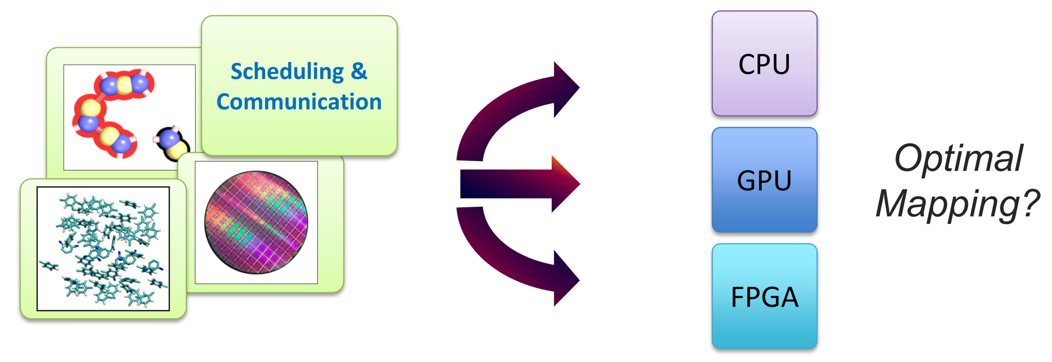


Overview of current heterogeneous architectures

- **Goal**
  - **Fast** and **fault-tolerant** execution of simulation applications on **runtime reconfigurable heterogeneous computer architectures**

Challenges

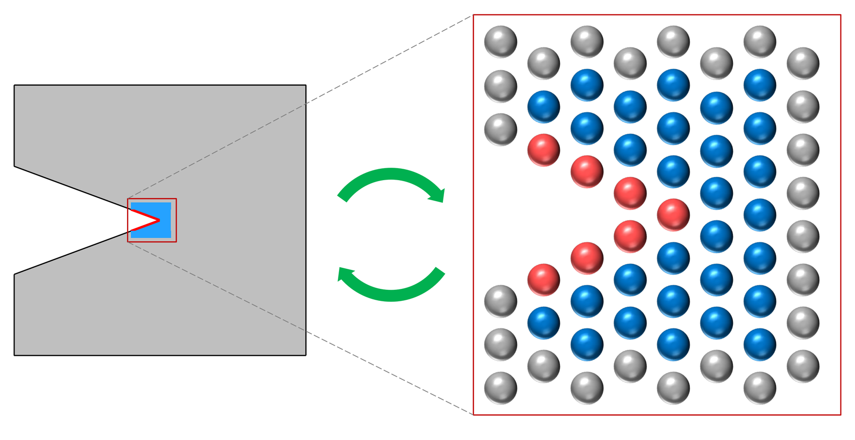
- **Reliability**
  - Simulation applications are often executed for days and months
  - CMOS devices, manufactured in 14nm technology and below:
    - vulnerable to transient effects, process variations and latent defects, as well as stress and aging mechanisms
  - Fault-tolerant execution, memories 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)[1,2]

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

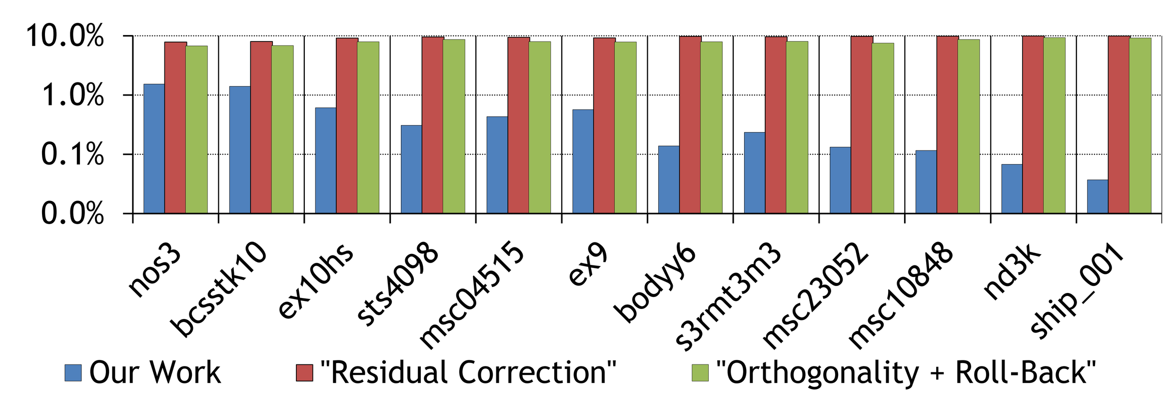
- Exploitation of global orthogonality and residual relationships to derive an **efficient error detection method**

Method: Error Correction

- **Adaptive error correction** scheme
  - The **detected corruption** is evaluated and the most promising error correction technique is selected:
    - **Online** Correction
    - **Complete** or **corrective** rollback

Experimental Results

- **Experiments:** Evaluation of **runtime overhead** for error detection compared to unprotected execution of PCG

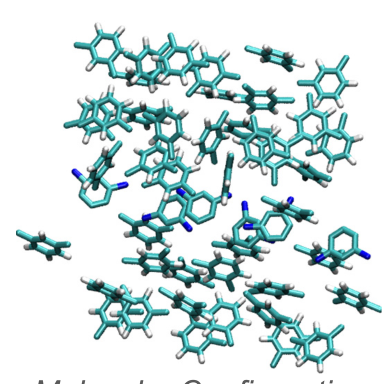


Current Collaborations

Acceleration of Markov-Chain Monte-Carlo Molecular Simulations[3]

Cooperation with J. Castillo • J. Groß

- **Marcov-Chain Monte-Carlo (MCMC) simulations** are the core of many tasks in thermodynamics
- **Problem:** Inherent serial dependencies make this method **very hard to parallelize**
- MCMC molecular simulation has been mapped to GPUs, exploiting **parallel energy calculations** and speculative evaluation of Monte-Carlo moves
- **Speedups of up to 400x**



Molecular Configuration

Adaptive Parallel Simulation of a Two-Timescale Model for Apoptotic Receptor-Clustering on GPUs[4]

Cooperation with M. Daub • G. Schneider

Motivation

- Deeper understanding necessary for the activation of *apoptosis* (I.e. Decomposition of cells in multi-cellular organisms)
- **Simulation:** Dominated by extensive computing times
  - **Large numbers** of simulations required to draw reliable conclusions

Goals

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

Computational Performance Results

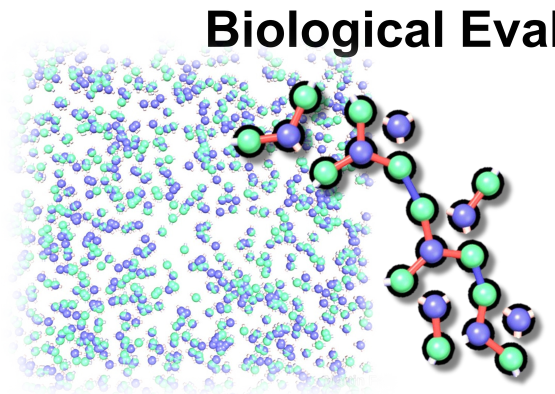
- **Reduction** of simulation time from **hours to seconds**

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



Evolution of ligand-receptor clusters in less than 0.5s

[1] A. Schöll, C. Braun, M. A. Kochte, and H.-J. Wunderlich, **"Efficient On-Line Fault-Tolerance for the Preconditioned Conjugate Gradient Method"**, in Proceedings of the IEEE International On-Line Testing Symposium (IOLTS'15), Elia, Halkidiki, Greece, 6.-8. July 2015, pp. 95-100.

[2] A. Schöll, C. Braun, M. A. Kochte, and H.-J. Wunderlich, **"Low-Overhead Fault-Tolerance for the Preconditioned Conjugate Gradient Solver"**, in Proceedings of the IEEE International Symposium on Defect and Fault Tolerance in VLSI and Nanotechnology Systems (DFT'15), Amherst, MA, USA, 12.-14. October 2015, pp. 60-66.

[3] C. Braun, S. Holst, J. Castillo, J. Groß, and H.-J. Wunderlich, **"Acceleration of Monte-Carlo Molecular Simulations on Hybrid Computing Architectures"**, in Proceedings of the 30th IEEE International Conference on Computer Design, ICCD'12, Montreal, Canada, 30. September-3. October 2012, pp. 207-212.

[4] 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.