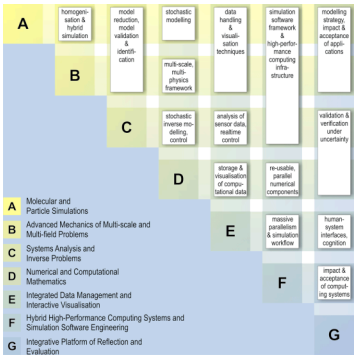
Mapping Simulation Algorithms to Parallel Architectures

SimTech Cluster of Excellence

ITI Institut für Technische Informatik, Universität Stuttgart

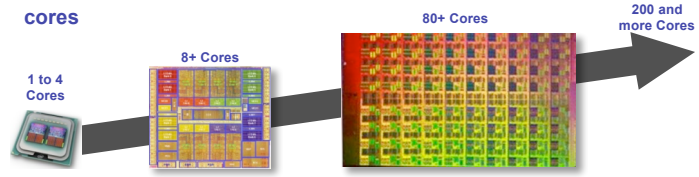
The Challenge

- Modern simulation algorithms demand enormous amounts of computing power
- SimTech Research Areas A – F: E.g. Molecular and Particle Simulation, etc.
- Problem: Very long turn around times limit the usage of simulation



The Technology

- The steady increase of clock frequency has reached its limits
- Nonetheless: Much more computing power is still needed
- Architectures move from classic Single-Core to Multi-Core
- The future will bring Many-Core architectures with thousands of cores



e.g. IBM POWER4 since 2001 — e.g. SUN UltraSparc T1 since 2005 — e.g. Intel TeraScale prototype since 2007

A First Case Study: Simulation of Quantum Mechanics in Parallel

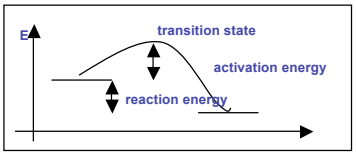
Cooperation with Prof. Dr. H.-J. Werner, Institute for Theoretical Chemistry

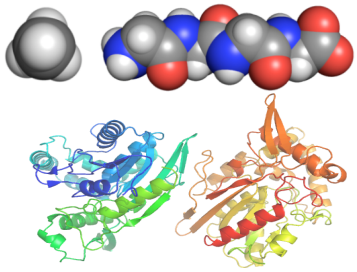
Calculating total energies ab initio

Important for:
- Reaction energies
- Determining transition states
- Chemical analysis, material research

Today: Calculations of molecules up to 100 atoms

Future:
- Investigation of complex biological systems
- Calculations of molecules up to thousands of atoms



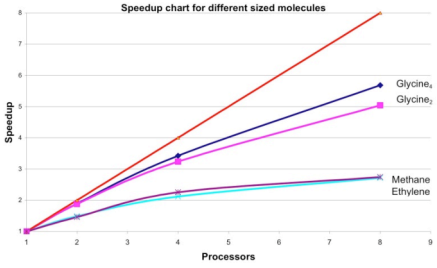


- Interdisciplinary work with student participation
- MOLPRO: (Commercial) program for molecular electronic structure calculations
- Calculations of integrals and large matrices
- Coarse-grain parallelization on a 8 core system

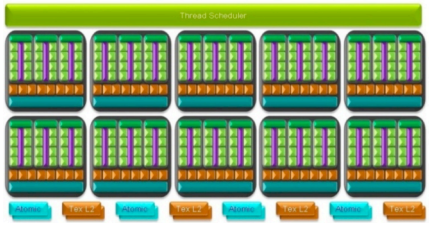
	Methane (CH_4)	Glycine$_4$
Matrix dimensions	140x140	1100x1100
Disk space needed	80 MB	330 GB
Elapsed time on single cpu	< 1min	40 h

The Next Steps & Future Work

- On a system with 8 cores a speedup of nearly 6 could be reached
- Next Step: Parallelization for Many-Core architectures with thousands of cores



Graphics Processing Units (GPU):
- GPUs offer 240+ cores and can be linked to Multi-GPU systems
- GPGPU: Research on general-purpose calculations on GPUs



NVIDIA GeForce GTX 280 Parallel Computing Architecture

Outlook:
- Effective mapping of simulation problems to thousands of cores
  - Coarse and fine grain parallelization
  - Research on other par. architectures
- How can reconfigurable HW be used to support and simplify the mapping?
- Thousands of cores: How can fault tolerance (HW & SW) be guaranteed to ensure maximum performance and maximum availability?

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