Mapping Simulation Algorithms to Parallel Architectures

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

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

<table>
<thead>
<tr>
<th></th>
<th>Methane (CH₄)</th>
<th>Glycine (H₂NCH₂COOH)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Matrix dimensions</td>
<td>140x140</td>
<td>1100x1100</td>
</tr>
<tr>
<td>Disk space needed</td>
<td>80 MB</td>
<td>330 GB</td>
</tr>
<tr>
<td>Elapsed time on single cpu</td>
<td>&lt; 1 min</td>
<td>40 h</td>
</tr>
</tbody>
</table>

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

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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