Agenda

- HPC in Germany & Aachen
- HPC on Windows: Case Studies
- HPC on Windows: Outlook
- Summary
Proposal of the HPC @ DE task force:

- **Tier 0**: Jülich, München, Stuttgart
  - Number of Institutions: 1-3

- **Tier 1**: Aachen, Berlin, DKRZ, Dresden, DWD, FZ Karlsruhe, Hannover, Karlsruhe, MPG, Paderborn
  - Number of Institutions: 10

- **Tier 2**: Universities, individual Institutes
  - Number of Institutions: ~100

Simulation Science: Main Pillar of Research

RWTH: *The simulation of complex models lies at the core of innovative products and basic research at RWTH Aachen.*
RWTH Aachen University (2007)

- 30,260 students
- 450 professorships
- 4,000 academic staff
- 280 institutes

- Natural Sciences: 25%
- Humanities, Social Sciences and Economics: 19%
- Engineering: 45%
- Medicine: 9%

HPC in Germany & Aachen
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HPC on Windows @ RWTH Aachen

- We do HPC on Unix for many years - why try Windows?
  - Third party cooperations sometimes depend on Windows
  - Some users look out for the Desktop-like HPC experience
  - Windows is a great development platform

- We started early:
  - 03/04: Intel ThreadingTools GUI only available on Windows
  - 2004: Visual Studio 2005 with OpenMP support (beta program)
  - 2005: Windows Compute Cluster Server (beta program)
  - 2007: Windows (HPC) Server 2008 (beta program)

- Cooperation with Microsoft since 2008:
  WinHP3C = Windows High Performance Cluster Competence Center
  - [http://www.rz.rwth-aachen.de/winhp3c](http://www.rz.rwth-aachen.de/winhp3c)
Top500 run (LINPACK) on Windows

- Cluster installed in Q1/2008:
  - Fujitsu-Siemens Primergy RS 200 S4 Server
    - 2x Intel Xeon 5450 (quad-core, 3.0 GHz)
    - 16 / 32 GB memory per node
    - 4x DDR InfiniBand:
      - MPI latency: ~5 us
      - MPI bandwidth: 1250 MB/s

- LINPACK-Tuning in Excel 😊

- Rank 100 in Top500 Liste in June 2008: 18,81 Tflop/s.
  - Windows HPC Server 2008 beta
WinHP3C activities in 2008

- Windows-HPC activities as part of the WinHP3C are open (free) for external participants:
  - 04/2008: Windows-HPC user group meeting in Germany
    • 1.5 days, over 110 participants from Industry and Academia
  - 04/2008: Windows HPC Deep Dive Training in Aachen
    • 3 days, 20 invited participants
  - 07/2008: Windows-HPC 2008 Workshop
    • 2 days, 55 participants
    • Opportunity to tune and parallelize your own codes!
  - 09/2008: Windows-HPC 2008 Workshop in english
  - 09/2008: Windows HPC Server 2008 Deployment Workshop

- Materials (Slides + Videos) are available online.
Agenda

- HPC in Germany & Aachen

- HPC on Windows: Case Studies
  - FFT Computation: MATLAB, Tasks
  - KegelToleranzen: Fortan90, OpenMP
  - DROPS: C++, Hybrid (MPI + OpenMP)

- HPC on Windows: Outlook

- Summary
Example: FFT computation

```matlab
fid = fopen("data.bin", "rb")
A = fread(fid, interval, "double")

F = fft(A)
```

MATLAB allows for simple approaches to parallel computing:

- `parfor`: Distribute loop iterations over a pool of works
- Distributed Arrays and Parallel Algorithms:
  - Store segments of data across participating workers
  - Over 150 parallel MATLAB functions available to work on distributed arrays

→ Simple approaches to exploit multi-core machines and clusters.
Example: FFT computation, parallel

```matlab
fid = fopen(„data.bin”, „rb”) 
A = fread(fid, interval, „double”) 
B = distributed(A, distributor()) 
F = fft(B)
```

- Speedup that can be achieved by this one-line change:
- Windows: Job Submission via „press this button“.
- Linux: Job Submission requires scripting + file copying + ...
- Experiments have been done with Frank Gräber, The Mathworks Germany.
Case Study: KegelToleranzen (1/4)

- Contact analysis simulation of Bevel Gears
  - Written in Fortran, using Intel Fortran 10.1 compiler
  - Very cache-friendly $\rightarrow$ runs at high Mflop/s rates

Laboratory for Machine Tools and Production Engineering, RWTH Aachen
Case Study: KegelToleranzen (2/4)

○ Comparing Linux and Windows Server 2003:

Performance of KegelToleranzen

- Linux 2.6: 4x Opteron dual-core, 2.2 GHz
- Windows 2003: 4x Opteron dual-core, 2.2 GHz

Comparing Linux and Windows Server 2003: 24% better
Comparing Linux and Windows Server 2008:

Performance gain for the user: Speedup of 5.6 on one node. Even better from starting point (desktop: 220 MFlop/s). MPI parallelization is work in progress.
Comparing Linux and Windows Server 2008:

Intel’s Fortran runtime library for Windows seems to have higher overhead than the version for Linux...

**Performance of KegelToleranzen**

- **Linux 2.6**: 4x Opteron dual-core, 2.2 GHz
- **Windows 2003**: 4x Opteron dual-core, 2.2 GHz
- **Linux 2.6**: 2x Harpertown quad-core, 3.0 GHz
- **Windows 2008**: 2x Harpertown quad-core, 3.0 GHz
DROPS: A Navier-Stokes Solver in C++ (1/4)

- Numerical Simulation of two-phase flow
- Modeled by instationary and non-linear Navier-Stokes equation
- Level Set function is used to describe the interface between the two phases
- Written in C++: is object-oriented, uses nested templates, uses STL types, uses compile-time polymorphism,
- (Adaptive) Tetrahedral Grid Hierarchy
- Finite Element Method (FEM)

Example: Silicon oil drop in D$_2$O (fluid/fluid)
This programming style asks for a solid integration of compiler and debugger!

```cpp
PCG(const MatrixCL& A, VectorCL& x, const VectorCL& b,
    const PreCon& M, int& max_iter,
    double& tol)
{
    VectorCL p(n), z(n), q(n), r(n);
    [...]
    for (int i=1; i<=max_iter; ++i) {
        [...]
        q = A * p;
        double alpha = rho / (p*q);
        x += alpha * p;
        r -= alpha * q;
    }
    y_Ax_par(&q.raw()[0],
             A.num_rows(), A.raw_val(),
             A.raw_row(), A.raw_col(),
             Addr( p.raw()));
    #pragma omp for reduction (+:alpha_sum)
    for (long j=0; j<n; j++)
        alpha_sum += p[j]*q[j];
    #pragma omp single {
        alpha = rho/alpha_sum;
    }
    #pragma omp for for (long j=0; j<n; j++){
        x[j] += alpha * p[j];
        r[j] -= alpha * q[j];
    }
```
This programming style asks for a solid integration of compiler and debugger!

C++: Transformation can be done invisible to the user via suitable template expression facility → introduce parallelism by using existing abstractions (work in progress).
DROS: A Navier-Stokes Solver in C++ (4/4)

- **Strength of Windows Development Platform:**
  - Visual Studio is a powerful C++ development environment
  - Exceptional support for parallel Shared-Memory debugging
  - DROS: Winner of Microsoft Student Program for HPC

  *Porting of ParMETIS:* Graph partitioning for load balancing
  *Porting of DDD:* Library for high-level network communication

- **MPI parallelization is still in development:**
  Adaptive solver with load balancing is available already.
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○ Summary
○ Programmers (and Operating Systems) have to deal with that.
  – Windows HPC Server 2008 is cc-NUMA aware to some extent,
  – but is still missing memory page migration functionality.
The Crystal Ball is showing many, many cores

- SUN Microsystems just recently won our HPC procurement:
  - 2008: Dunnington-based systems with
    - 4s 6c 1t → 24 threads per node
  - 2009/2010: Nehalem-based systems with
    - 8s 8c 2t → 128 threads per node

- .NET is nice, but MSFT should not forget about native code:
  - We hope for soon-to-be-found OpenMP 3.0 support!

- Today’s severest issue of Windows-HPC in mixed env.: I/O
  - How far does CIFS scale (i.e. delivered by NetApp)?
  - We need clients for parallel filesystems, such as Lustre!
    Lustre: Intended cooperation between SUN and RWTH Aachen.
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Summary

- RWTH: *The simulation of complex models lies at the core of innovative products and basic research at RWTH Aachen.*
  - Simulation Science (HPC) is main pillar of Research.

- Windows HPC Server 2008 has proven to be a solid solution for HPC on Windows:
  - We experience a growing interest in Industry and Academia.

- Some issues still remain open:
  - Support for native parallel programming with OpenMP 3.0 (de-facto standard) + better cc-NUMA support.
  - Client availability for parallel file systems.
The End

Thank you for your attention!

WinHP3C:
http://www.rz.rwth-aachen.de/winhp3c

2nd German Windows-HPC User Group Meeting:
http://www.rz.rwth-aachen.de/go/id/siu

March 30./31. 2009, Dresden, Germany