Windows-HPC @ RWTH Aachen University

Christian Terboven
terboven@rz.rwth-aachen.de

Center for Computing and Communication
RWTH Aachen University

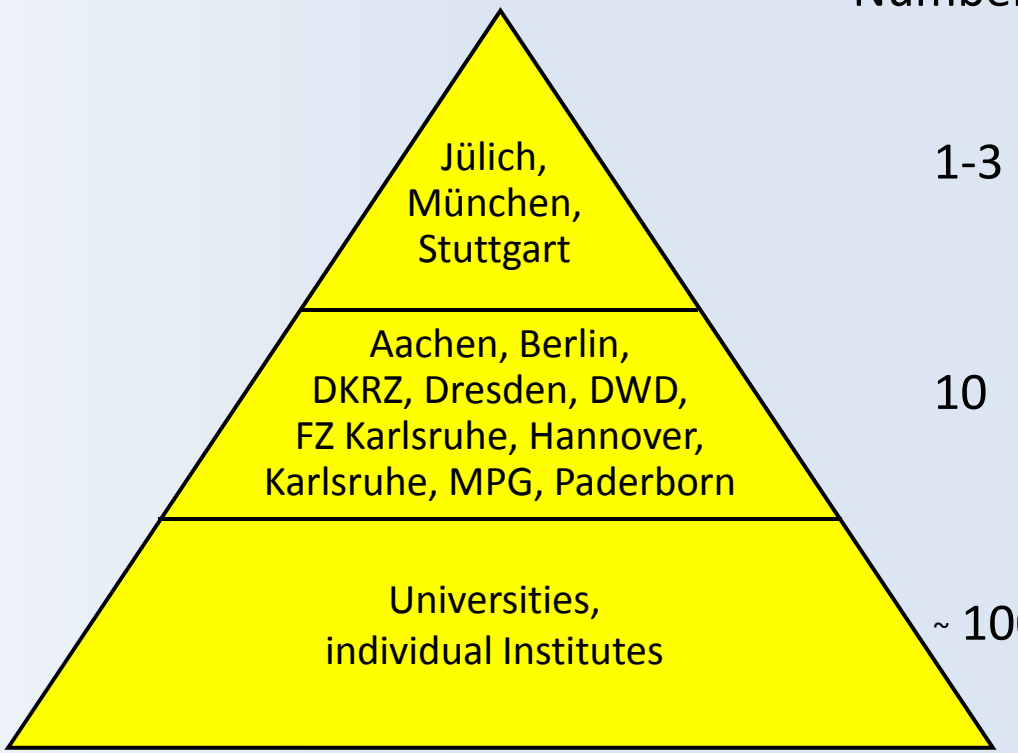
Windows-HPC User Group Meeting
17 November, Austin, TX, USA

Agenda

- HPC in Germany & Aachen
- HPC on Windows: Case Studies
- HPC on Windows: Outlook
- Summary

HPC-Pyramid

- Proposal of the *HPC @ DE* task force:



- 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.*

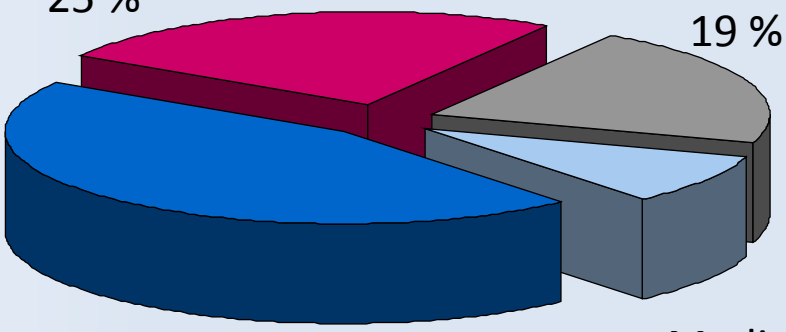
RWTH Aachen University (2007)

30260 students

450 professorships

4000 academic staff

280 institutes



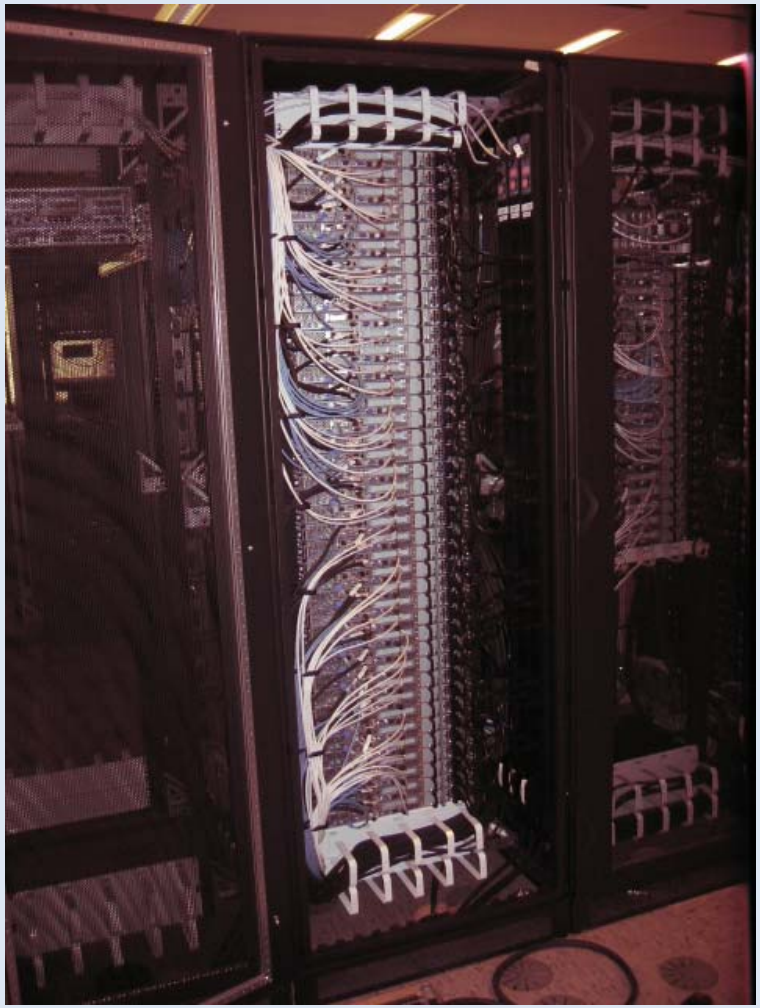
HPC on Windows @ RWTH Aachen

- 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

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 activites 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

FFT Computation in MATLAB (1/2)

- Example: FFT computation

```
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

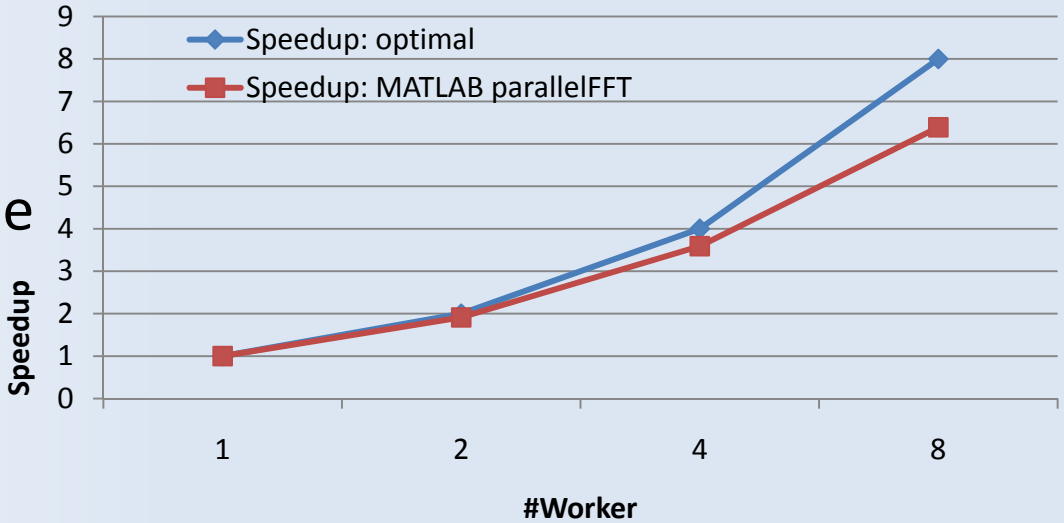
→ Simple approaches to exploit multi-core machines and clusters.

FFT Computation in MATLAB (2/2)

- Example: FFT computation, parallel

```
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:



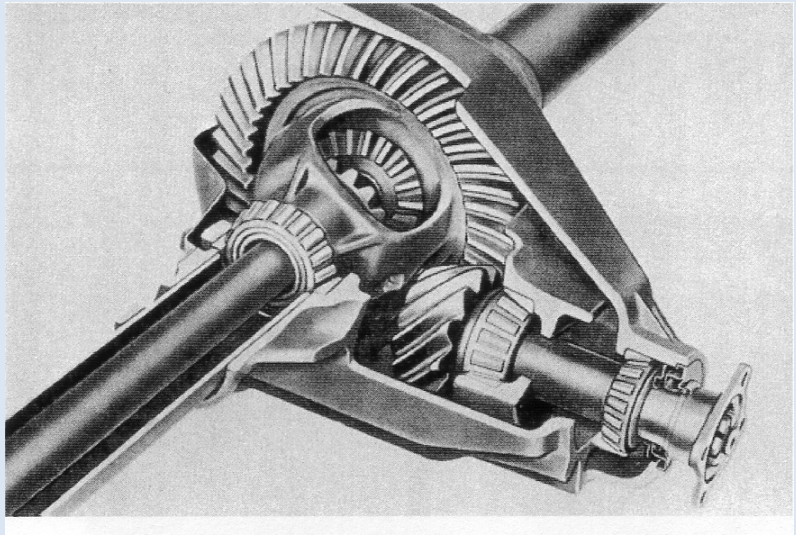
- Windows: Job Submission via „press this button“.
- Linux: Job Submission requires scripting + file copying + …
- Experiments have been done with Frank Gräber, The Mathworks Germany.

Case Study: KegelToleranzen (1/4)

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

Bevel Gear Pair

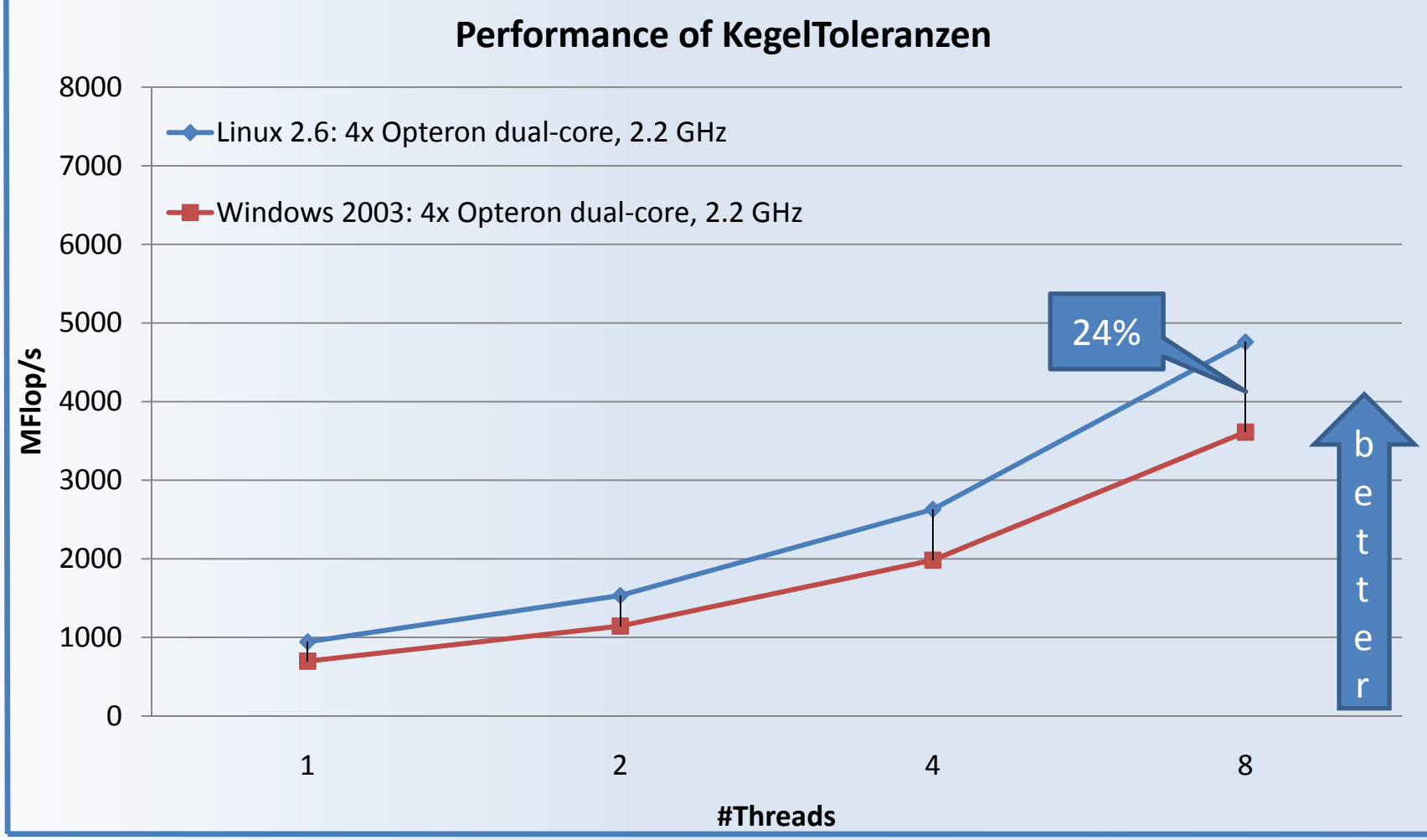
Differential Gear



Laboratory for Machine Tools and Production Engineering, RWTH Aachen

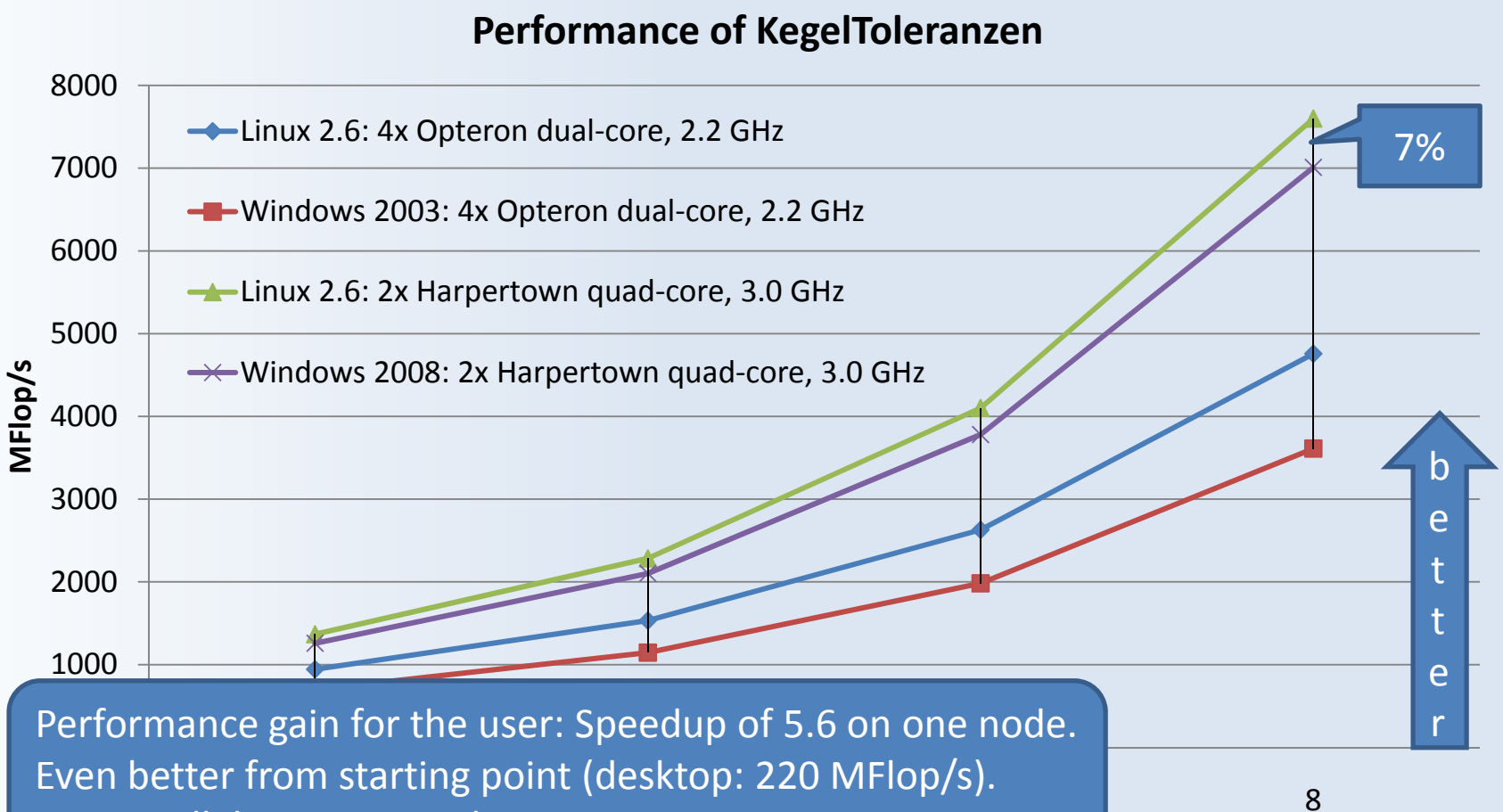
Case Study: KegelToleranzen (2/4)

- Comparing Linux and Windows Server **2003**:



Case Study: KegelToleranzen (3/4)

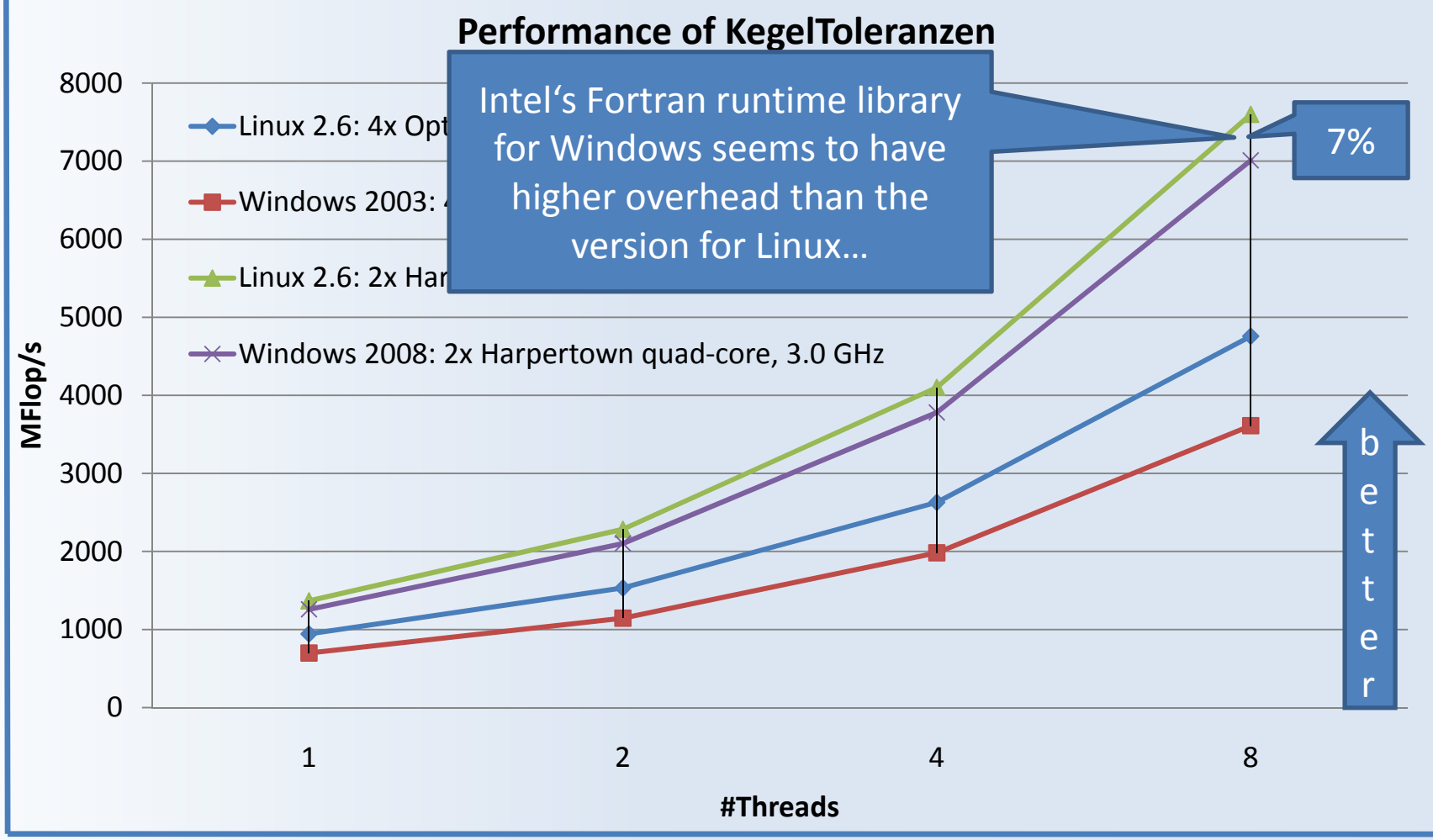
- Comparing Linux and Windows Server **2008**:



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.

Case Study: KegelToleranzen (4/4)

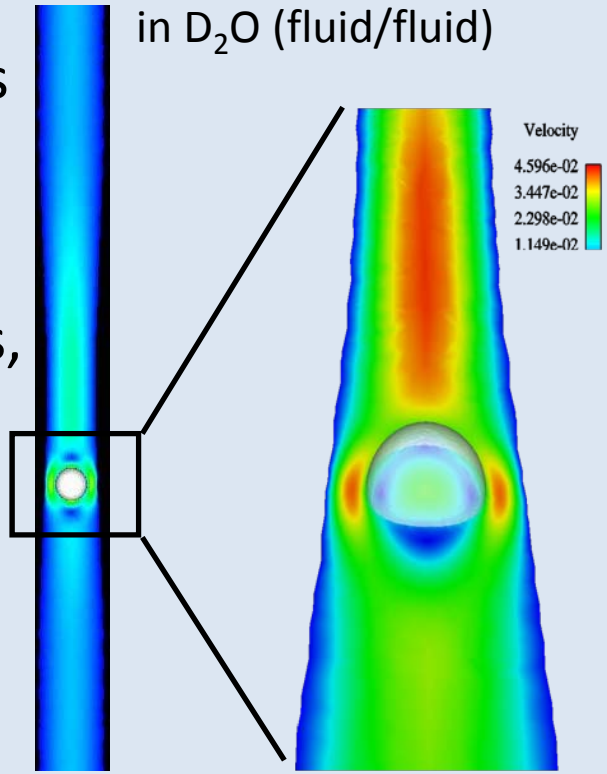
- Comparing Linux and Windows Server **2008**:



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_2O (fluid/fluid)



DROPS: A Navier-Stokes Solver in C++ (2/4)

```
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!

DROPS: A Navier-Stokes Solver in C++ (3/4)

```
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
    […]
    q = A * p;
    double alp
    x += alpha
    r -= alpha
    […]
```

```
y_Ax_par(&q.raw()[0],
   A.num_rows(), A.raw_val(),
   A.raw_row(), A.raw_col(),
   Addr( p.raw()));
```

```
a omp for reduction
                (+:alpha_sum)
ong j=0; j<n; j++)
ha_sum += p[j]*q[j];

a omp single {
ha = rho/alpha_sum;
```

C++: Transformation can be done invisible to the user via suitable template expression facility → introduce parallelism by using existing abstractions (work in progress).

```
#pragma omp for
for (long j=0; j<n; j++){
   x[j] += alpha * p[j];
   r[j] -= alpha * q[j];
}
```

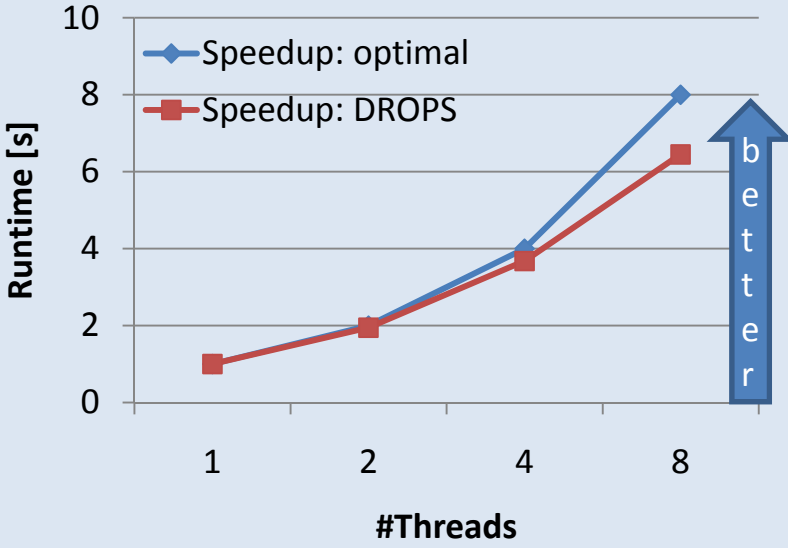
- This programming style asks for a solid integration of compiler and debugger!

DROPS: 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
  - DROPS: Winner of Microsoft Student Program for HPC

    Porting of ParMETIS: Graph partitioning for load balancing

    Porting of DDD: Library for high-level network communication

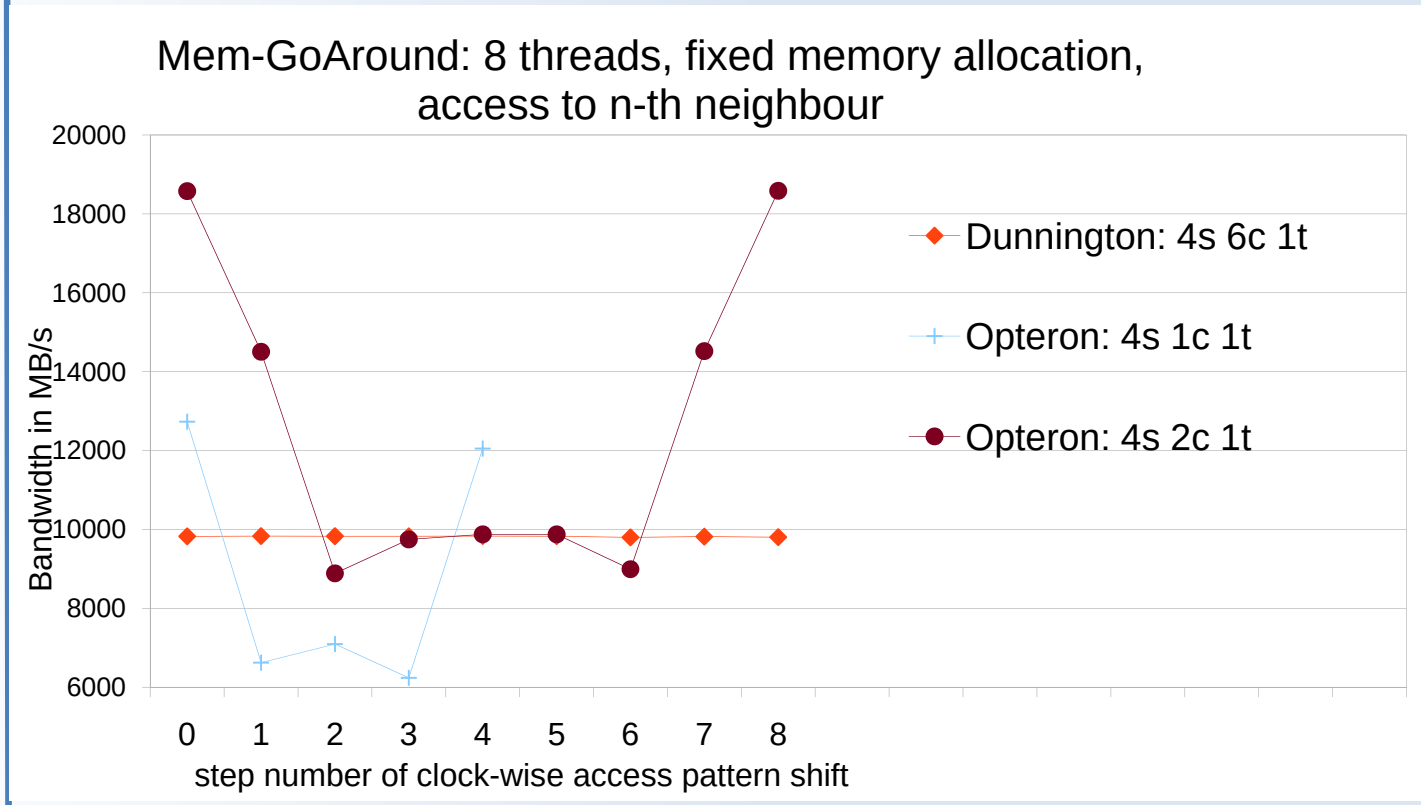


- MPI parallelization is still in development:
  Adaptive solver with load balancing is available already.

Agenda

- HPC in Germany & Aachen
- HPC on Windows: Case Studies
- HPC on Windows: Outlook
- Summary

Shared-Memory systems go cc-NUMA!



- 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.

Agenda

- HPC in Germany & Aachen
- HPC on Windows: Case Studies
- HPC on Windows: Outlook
- Summary

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