Scalable Shared Memory Programming with OpenMP

and Current Trends …

Workshop on Large-Scale Computer Simulation

March 9-11, 2001

Aachen / Jülich

Dieter an Mey, Christian Terboven

{anmey,terboven}@rz.rwth-aachen.de

Overview

- OpenMP in a Nutshell
- Scalable OpenMP Programming
- Hybrid Parallelization
- New Features in OpenMP 3.0 / 3.1
- Towards OpenMP 4.0
- Summary

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OpenMP – What is it about?

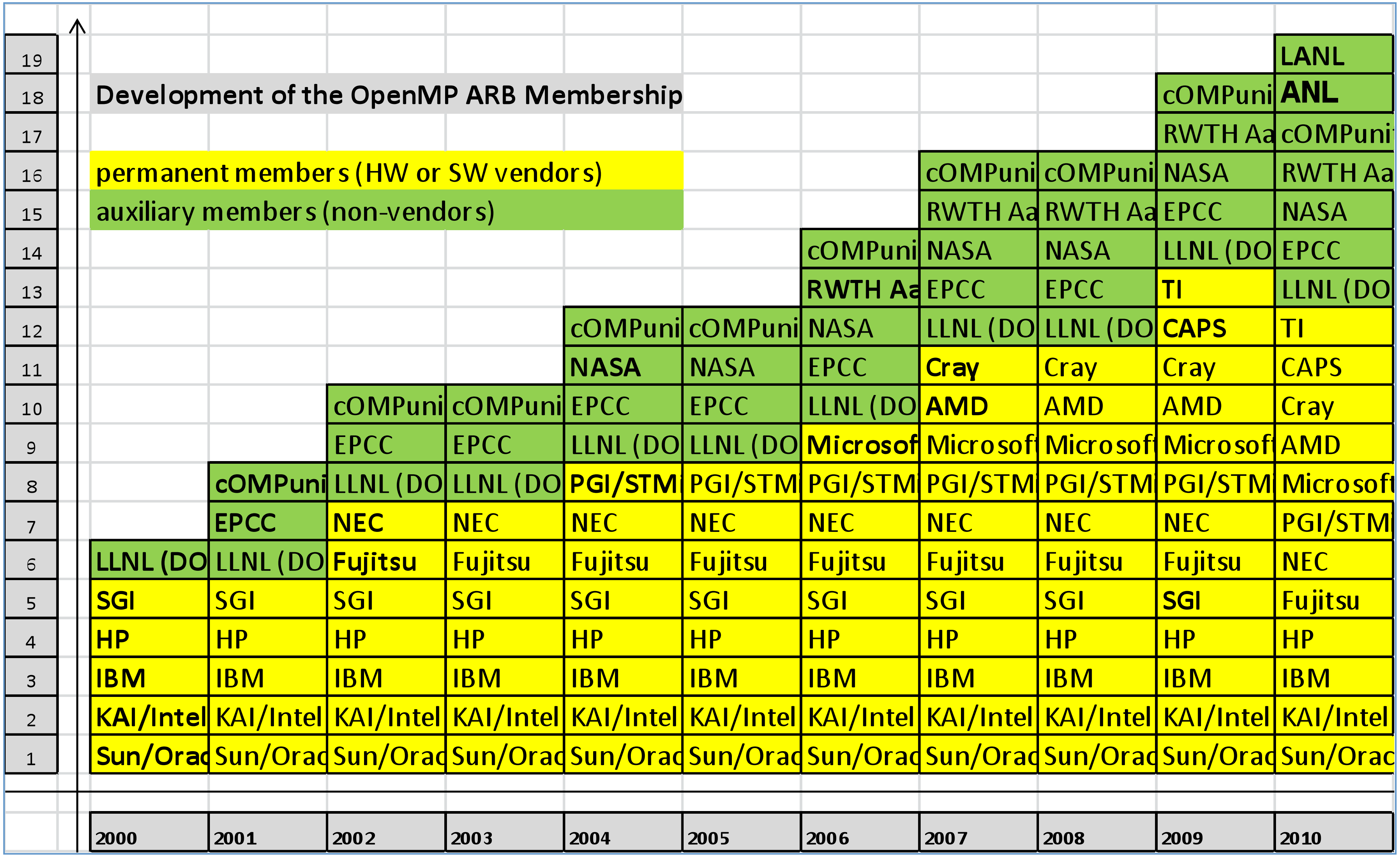
- OpenMP is an Application Progam Interface (API) for
  - **explicit**
  - **portable**
  - **shared-memory parallel programming**
  - in **C/C++** and **Fortran**.
- OpenMP consists of
  - **compiler directives**,
  - **runtime calls** and
  - **environment variables**.
- Today it is supported by all major compilers on Unix and Windows platforms
  - GNU, IBM, Oracle, Intel, PGI, Absoft, Lahey/Fujitsu, PathScale, HP, MS, Cray

http://openmp.org/wp/openmp-specifications/

OpenMP - Organisations

- OpenMP Architecure Review Board *www.openmp.org*
  - Non-profit corporation which owns the OpenMP brand and controls the specification
  - Directors: Josh Simons (Vmware), Sanjiv Shah (Intel), Koh Hotta (Fujitsu)
  - CEO: Larry Meadows (Intel)
- OpenMP Language Committee
  - works on the specification
- OpenMP User Community – cOMPunity *www.compunity.org*
  - cOMPunity has one vote in the ARB
  - Non-ARB-members are invited to contribute through cOMPunity
- Int‘l Workshop on OpenMP (IWOMP) *www.iwomp.org*
  - Annual OpenMP Workshop organized by cOMPunity and the ARB
  - IWOMP 2011, June 13-15 in Chicago, USA

OpenMP Architecture Review Board



Development of the OpenMP ARB Membership

permanent members (HW or SW vendors)

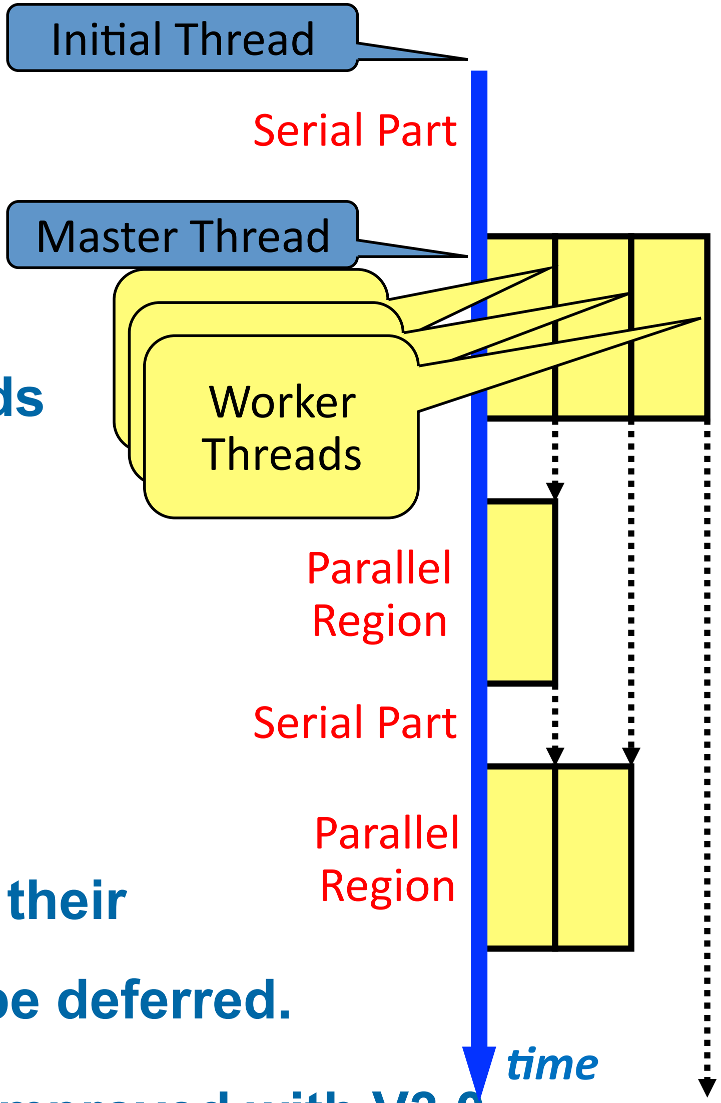
auxiliary members (non-vendors)

19											LANL
18										cOMPuni	ANL
17										RWTH Aa	cOMPuni
16								cOMPuni	cOMPuni	NASA	RWTH Aa
15								RWTH Aa	RWTH Aa	EPCC	NASA
14							cOMPuni	NASA	NASA	LLNL (DO	EPCC
13							RWTH Aa	EPCC	EPCC	TI	LLNL (DO
12					cOMPuni	cOMPuni	NASA	LLNL (DO	LLNL (DO	CAPS	TI
11					NASA	NASA	EPCC	Cray	Cray	Cray	CAPS
10			cOMPuni	cOMPuni	EPCC	EPCC	LLNL (DO	AMD	AMD	AMD	Cray
9			EPCC	EPCC	LLNL (DO	LLNL (DO	Microsof	Microsoft	Microsoft	Microsoft	AMD
8		cOMPuni	LLNL (DO	LLNL (DO	PGI/STM	PGI/STM	PGI/STM	PGI/STM	PGI/STM	PGI/STM	Microsoft
7		EPCC	NEC	NEC	NEC	NEC	NEC	NEC	NEC	NEC	PGI/STM
6	LLNL (DO	LLNL (DO	Fujitsu	Fujitsu	Fujitsu	Fujitsu	Fujitsu	Fujitsu	Fujitsu	Fujitsu	NEC
5	SGI	SGI	SGI	SGI	SGI	SGI	SGI	SGI	SGI	SGI	Fujitsu
4	HP	HP	HP	HP	HP	HP	HP	HP	HP	HP	HP
3	IBM	IBM	IBM	IBM	IBM	IBM	IBM	IBM	IBM	IBM	IBM
2	KAI/Intel	KAI/Intel	KAI/Intel	KAI/Intel	KAI/Intel	KAI/Intel	KAI/Intel	KAI/Intel	KAI/Intel	KAI/Intel	KAI/Intel
1	Sun/Orac	Sun/Orac	Sun/Orac	Sun/Orac	Sun/Orac	Sun/Orac	Sun/Orac	Sun/Orac	Sun/Orac	Sun/Orac	Sun/Orac
	2000	2001	2002	2003	2004	2005	2006	2007	2008	2009	2010

OpenMP - History

- **October 1997 OpenMP version 1.0 for Fortran.**
- **October 1998 OpenMP version 1.0 for C/C++.**
  - November 2000 OpenMP version 2.0 for **Fortran**.
  - March 2002 OpenMP version 2.0 for **C/C++**.
  - May 2005 OpenMP version 2.5 combined for **C/C++** and Fortran
- **May 2008 OpenMP Version 3.0 for C/C++ and Fortran**
- **February 2011 OpenMP Draft Version 3.1 for public comment**

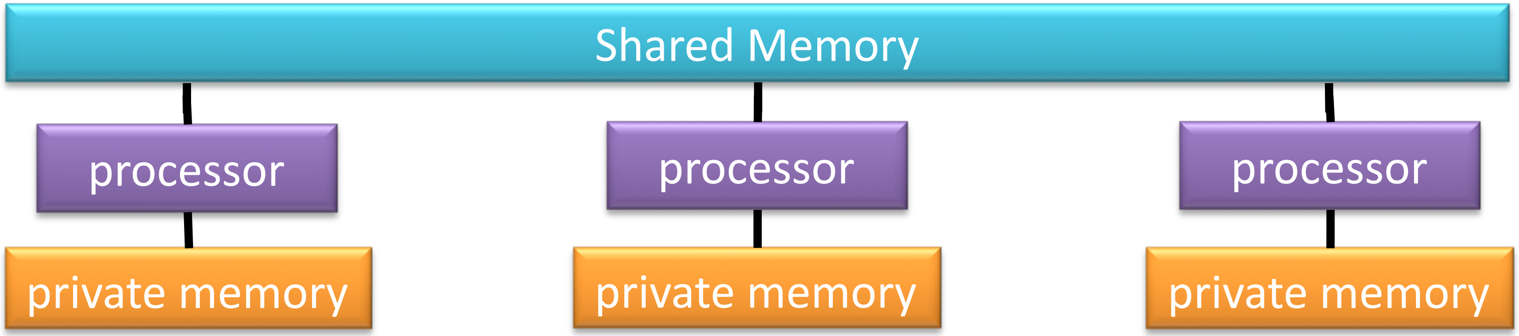
OpenMP in a Nutshell
Execution Model



- **Fork-join model of parallel execution**
- ***Parallel regions*** **are executed (redundantly) by a team of threads.**
- **Work can be distributed among the threads of a team by *worksharing constructs***
  - like the ***parallel loop construct***, which provides powerful **scheduling** mechanisms.
- **Since V3.0 (2008) *Tasks* (code plus data) can be enqueued by a *task construct* and their execution by any thread of the team can be deferred.**
- **Support for *Nested parallelism* has been improved with V3.0.**

OpenMP in a Nutshell
Memory Model

- **Shared-Memory model**
  - All threads share a common address space (shared memory)
  - Threads can have private data
- **Relaxed memory consistency**
  - Temporary View ("*Caching*"):
    Memory consistency is guaranteed only after synchronization points, namely implicit and explicit `flush`es
    - Each OpenMP `barrier` includes a `flush`
    - Exit from worksharing constructs include barriers by default (***but not entries!***)
    - Entry to and exit from `critical` regions include a `flush`
    - Entry to and exit from lock routines (OpenMP API) include a `flush`



OpenMP in a Nutshell
Parallel Region with a Single Simple Loop

- calculate Pi by numerical integration

$$\Pi = \int_0^1 \frac{4}{(1+x^2)} dx$$

```
double f(double x) {
   return (double)4.0 / ((double)1.0 + (x*x));
}


void computePi() {
        double h = (double)1.0 / (double)n;
        double sum = 0, x;
#pragma omp parallel for schedule(static) \
        private(x) shared(h,n) reduction(+:sum)
        for (int i = 1; i <= n; i++) {
                x = h * ((double)i - (double)0.5);
                sum += f(x);
        }

        myPi = h * sum;
}
```

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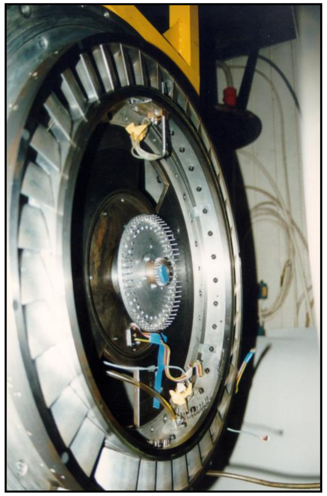
Increasing Scalability
Extend Parallel Region, Avoid Barriers

```
!$omp parallel private(n,m,l,i,j,k,lijk)
     do n = 1,7
       do m = 1,7
         !$omp do
         do l = LSS(itsub),LEE(itsub)
           i = IG(l)
           j = JG(l)
           k = KG(l)
           lijk = L2IJK(l)
           RHS(l,m)  = RHS(l,m)- &
             FJAC(lijk,lm00,m,n)*DQCO(i-1,j,k,n,NB)*FM00(l)  -  &
             FJAC(lijk,lp00,m,n)*DQCO(i+1,j,k,n,NB)*FP00(l)  -  &
             FJAC(lijk,l0m0,m,n)*DQCO(i,j-1,k,n,NB)*F0M0(l)  -  &
             FJAC(lijk,l0p0,m,n)*DQCO(i,j+1,k,n,NB)*F0P0(l)  -  &
             FJAC(lijk,l00m,m,n)*DQCO(i,j,k-1,n,NB)*F00M(l)  -  &
             FJAC(lijk,l00p,m,n)*DQCO(i,j,k+1,n,NB)*F00P(l)
         end do
         !$omp do nowait
       end do
     end do
!omp end parallel
```

partitioning the long loop

no barrier, zero overhead



Check for correctness !

(Intel Inspector, aka Thread Checker)

D. an Mey, S. Schmidt: From a Vector Computer to an SMP-Cluster - Hybrid Parallelization of the CFD Code PANTA, EWOMP 2000, Edinburgh

Increasing Scalability
Orphaning: 1 PR includes 69 Parallel Loops

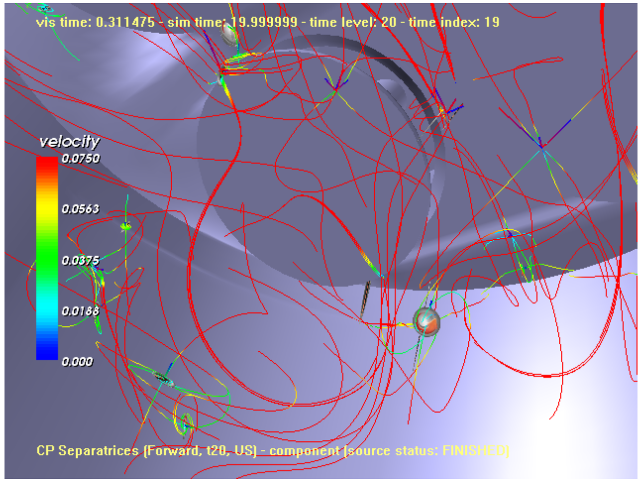
- **Simulation of the heat flow in a rocket combustion chamber**
- **Finite Element Method**
- **OpenMP Parallelization**
  - 30000 lines of Fortran
  - 200 OpenMP directives, 69 parallel loops,
  - 1 main parallel region
- **~40x Speed-up on 68 UltraSPARC III processors (Sun Fire 15K)**

- **OpenMP 3.1 Glossary: orphaned construct**
  - A *construct* that gives rise to a *region* whose *binding thread set* is the *current team*, but that is not nested within another *construct* giving rise to the *binding region*.

D. an Mey, T. Haarmann: Pushing Loop-Level Parallelization to the Limit *, EWOMP 2002, Rome*

Increasing Scalability
Load Imbalances, Nested Parallelism

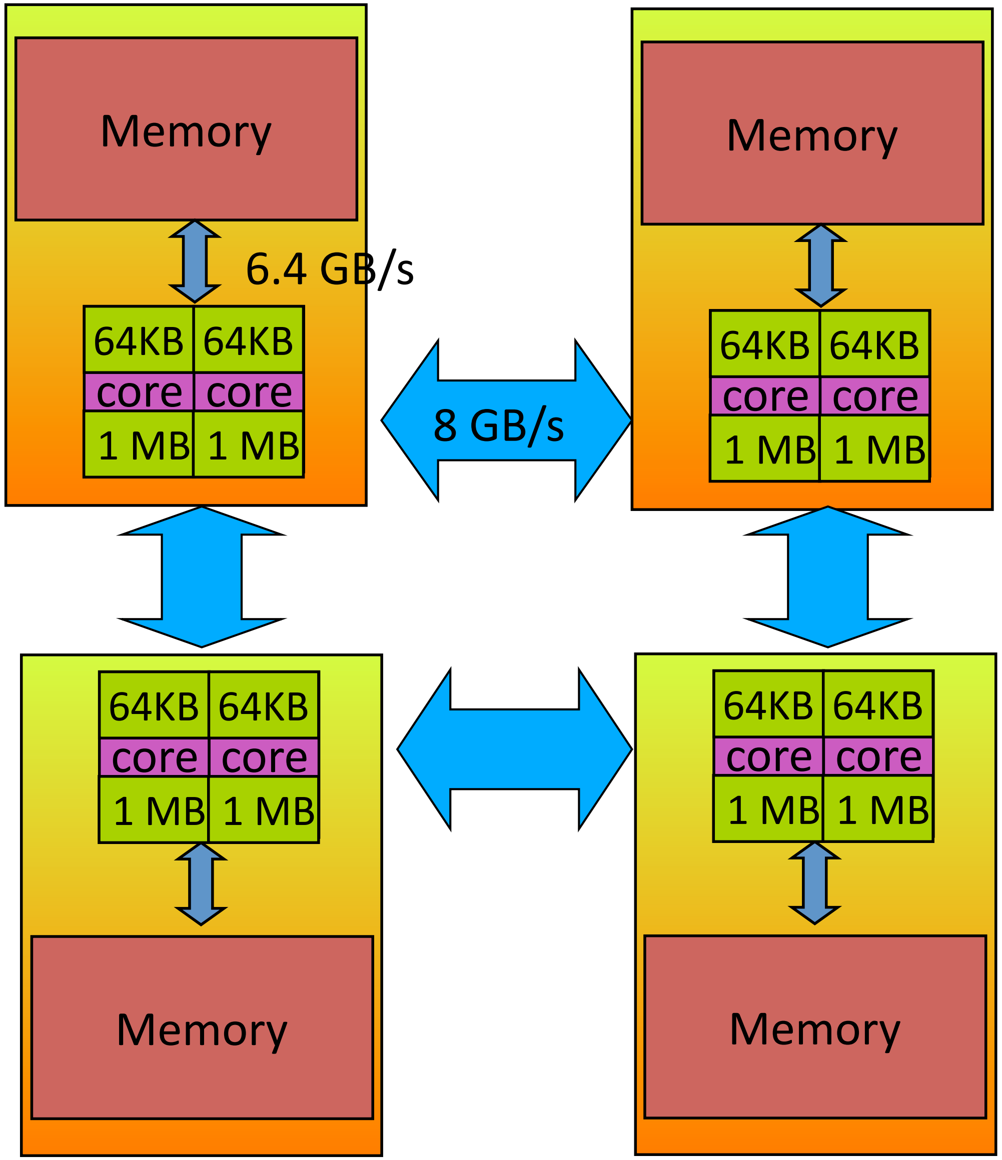
- **Analysis of complex and accurate fluid dynamics simulations**
- **Extraction of Critical Points for Virtual Reality (Location with velocity = 0)**
- **25-100% efficiency with 128 threads on 72 UltraSPARC IV dual core processors (Sun Fire E25K) depending on data set**


vis time: 0.311475 - sim time: 19.999999 - time level: 20 - time index: 19
velocity
0.0750
0.0563
0.0375
0.0188
0.000
CP Separatrices [Forward, t20, US] - component [source status: FINISHED]

```
//  Loop over time levels
#pragma omp parallel for num_threads(nTimeThreads) schedule(dynamic,1)
for (curT=1; curT<=maxT; ++curT) {
//  Loop over Blocks
#pragma omp parallel for num_threads(nBlockThreads) schedule(dynamic,1)
for (curB=1; curB<=maxB; ++curB) {
//  Loop over Cells
#pragma omp parallel for num_threads(nCellThreads) schedule(guided)
for (curC=1; curC<=maxC; ++curC) {
FindCriticalPoints (curT, curB, curC); //  highly adaptive algorithm (bisectioning)
} } }                                  //  huge load imbalances
```

A. Gerndt, S. Sarholz, et.al.: 3-D Critical Points Computed by Nested OpenMP *, SC 2006, Tampa*

Non Uniform Memory Architectures (NUMA)



Sun Fire V40z
one of the early popular NUMA systems
with 4 dual core x86-64 processors

AMD Opteron 875, dual core, 2.2 GHz

Cache-coherent
HyperTransport
Connections

Memory Allocation Policy

- **If data is setup in serial region, but the computation in parallel regions, the data to thread affinity may hurt performance very badly !**
  - Either take care of thread binding explicitly + first-touch parallel initialization

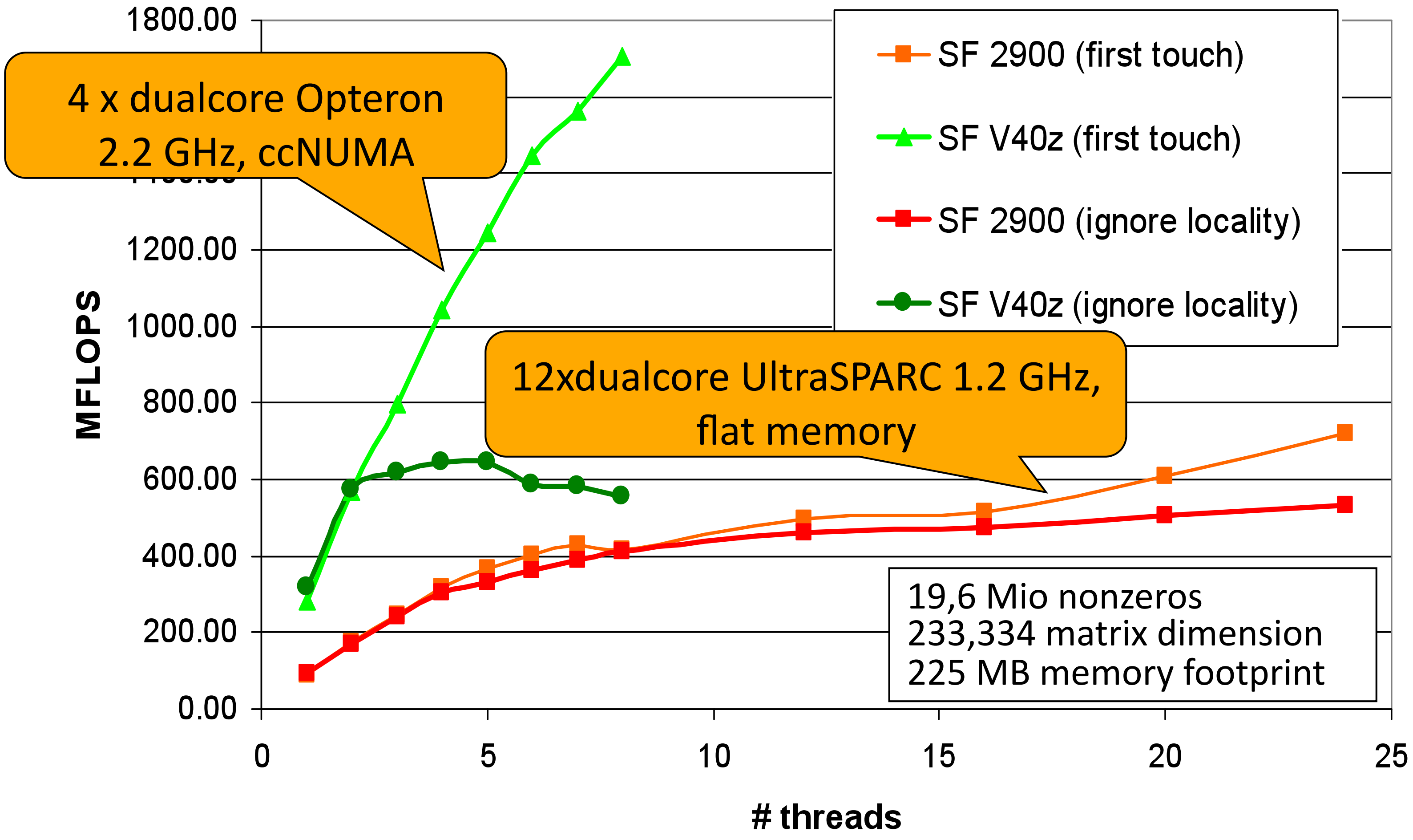
    or apply random / round robin data placement

```
//  allocation of arrays
double *a, *b, *c;
a, b, c = (double*) malloc(N*sizeof(double));

//  parallel initialization of data where used later on
# pragma omp parallel for schedule(static)
for (i=0;i<N;i++) a[i]=…=0.0;

//  calculation with optimal memory placement and identical schedule
#pragma omp parallel for schedule(static)
for(i=0;i<N;i++) a[i]=b[i]+scalar*c[i];
```

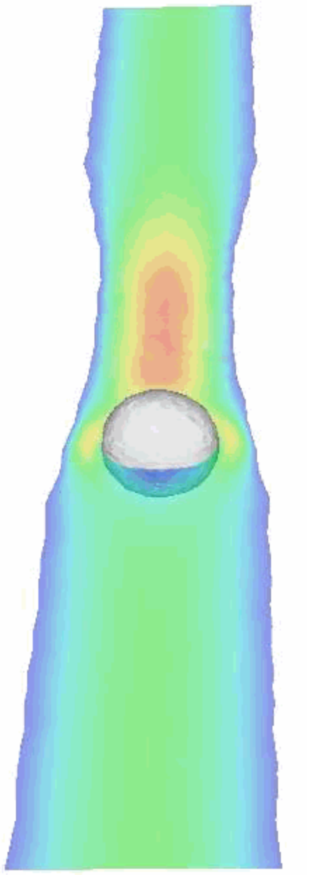
Sparse Matrix-Vector Multiplication on NUMA



4 x dualcore Opteron
2.2 GHz, ccNUMA

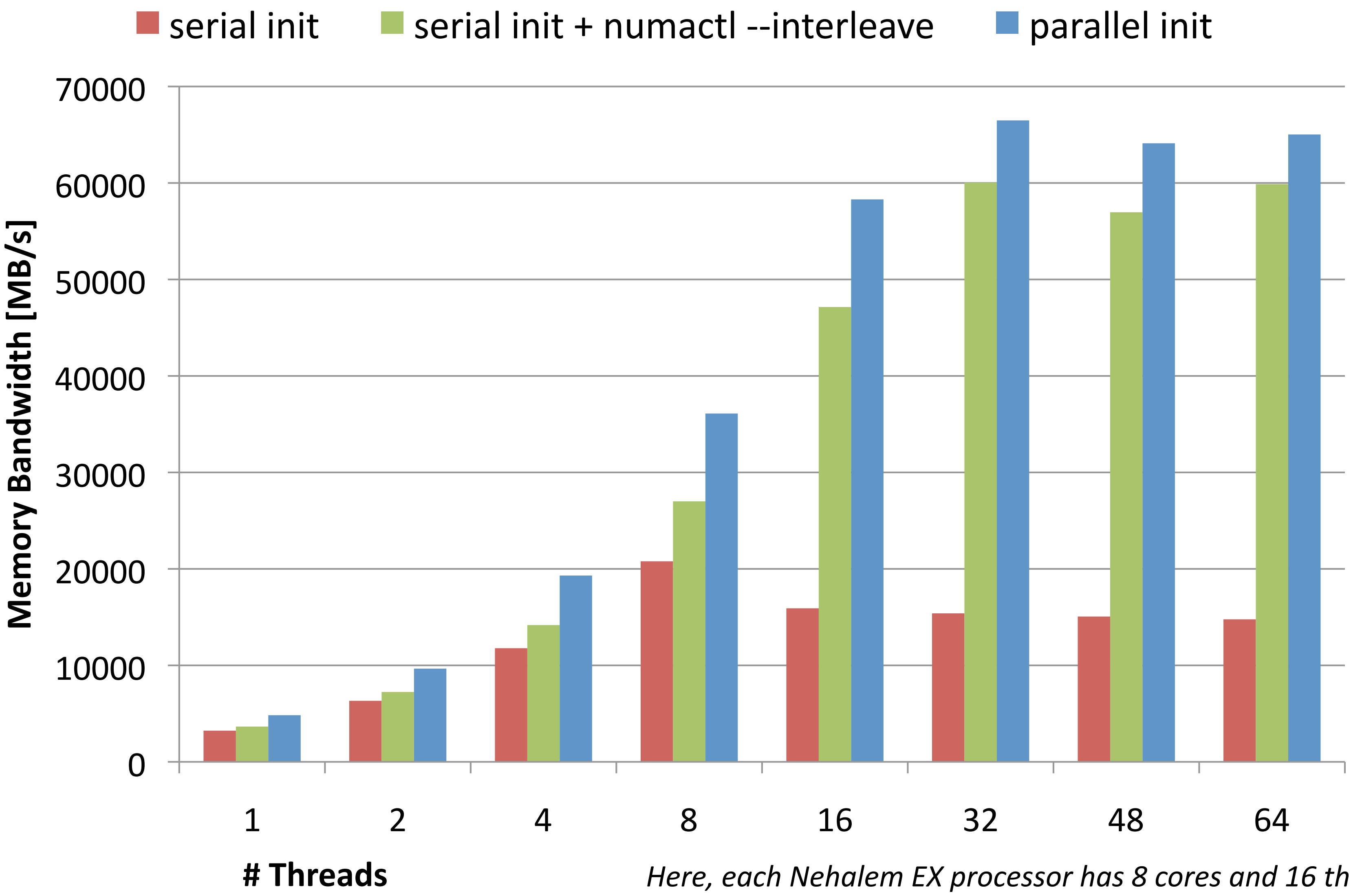
12xdualcore UltraSPARC 1.2 GHz,
flat memory

19,6 Mio nonzeros
233,334 matrix dimension
225 MB memory footprint



C. Terboven, et.al.: Parallelization of the C++ Navier-Stokes Solver DROPS with OpenMP , *ParCo 2005, Malaga*

Memory Bandwidth on a 4-way Nehalem EX System (Stream Triad)

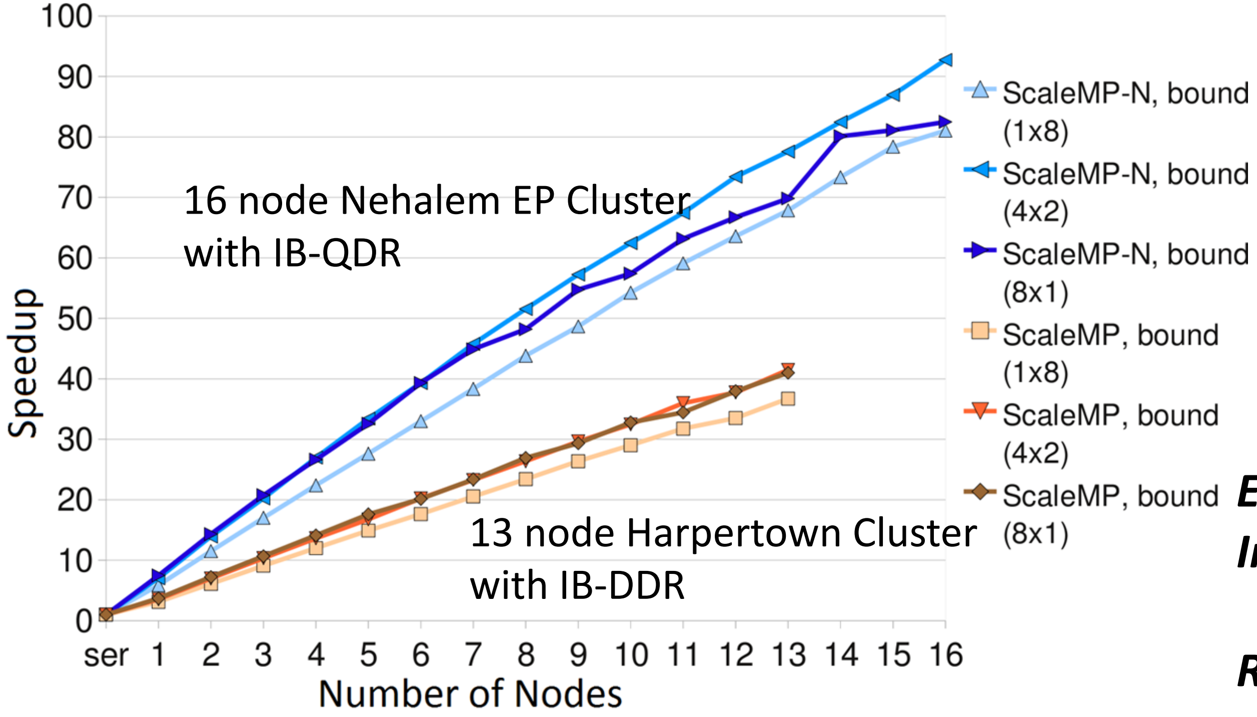


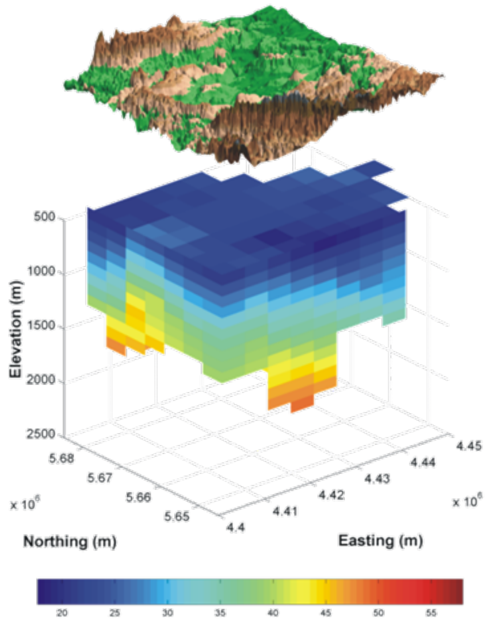
Here, each Nehalem EX processor has 8 cores and 16 threads which adds up to 32 cores and 64 threads (Intel HyperThreading)

Virtual Shared Memory Processing on an Infiniband-Cluster with ScaleMP

SHEMAT-Suite

- Geothermal Simulation of CO_2 Storage
- Simulating Groundwater flow, heat transfer and transport of reactive solutes
- ~10x speed-up with 2nd level of OpenMP





E.ON Energy Research Center Inst. of Appl. Geophysics and Geothermal Energy, RWTH Aachen University

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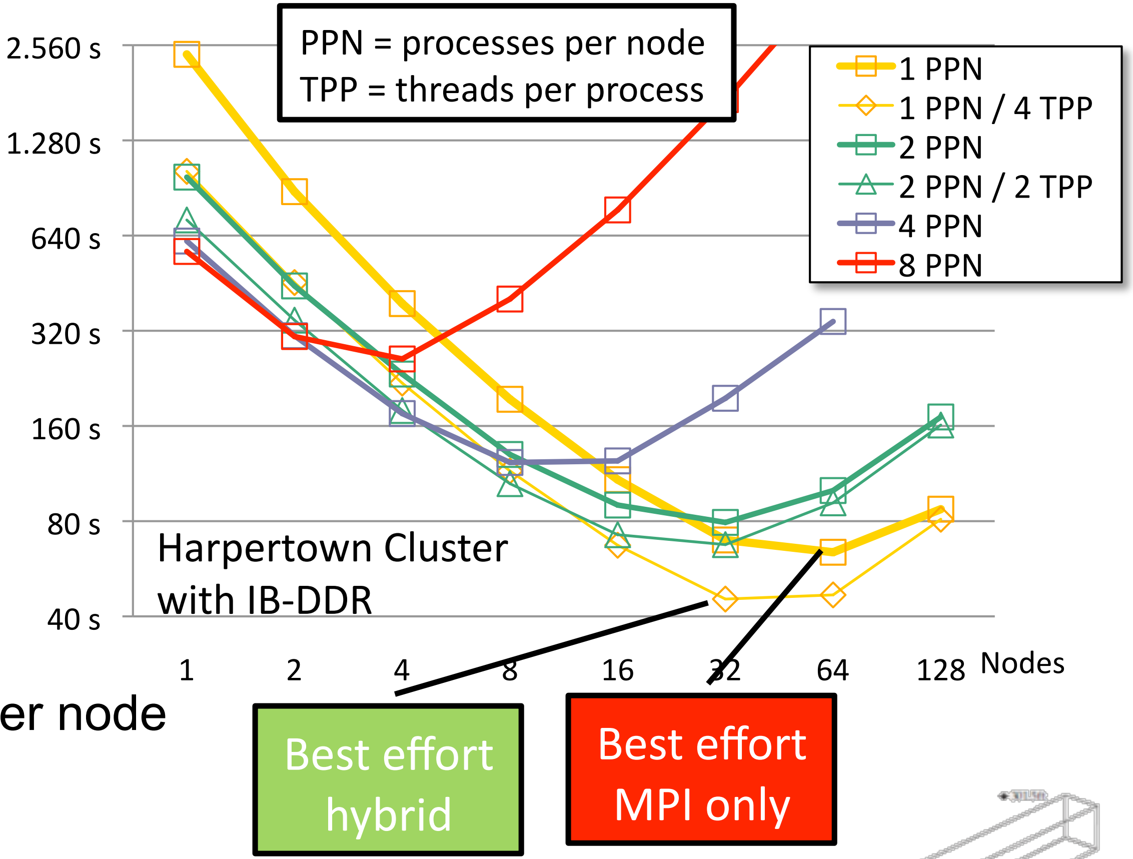
Adding OpenMP to MPI may be beneficial

- **XNS (M. Behr, CATS, RWTH)**
  - Simulation of Hydro-Dynamic forces of the Ohio Dam
- **OpenMP Parallelization:**
  - 9 parallel regions
  - **Human effort: ~ 6 weeks**
- **Best MPI performance:**
  - 48 nodes, one MPI process per node
- **Best Hybrid performance:**
  - 32 nodes, one MPI process per node, 4 threads per process
  - **1,5x improvement to MPI-only**

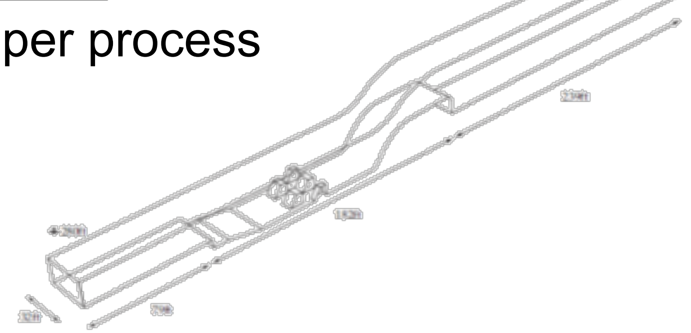


PPN = processes per node
TPP = threads per process

Harpertown Cluster with IB-DDR

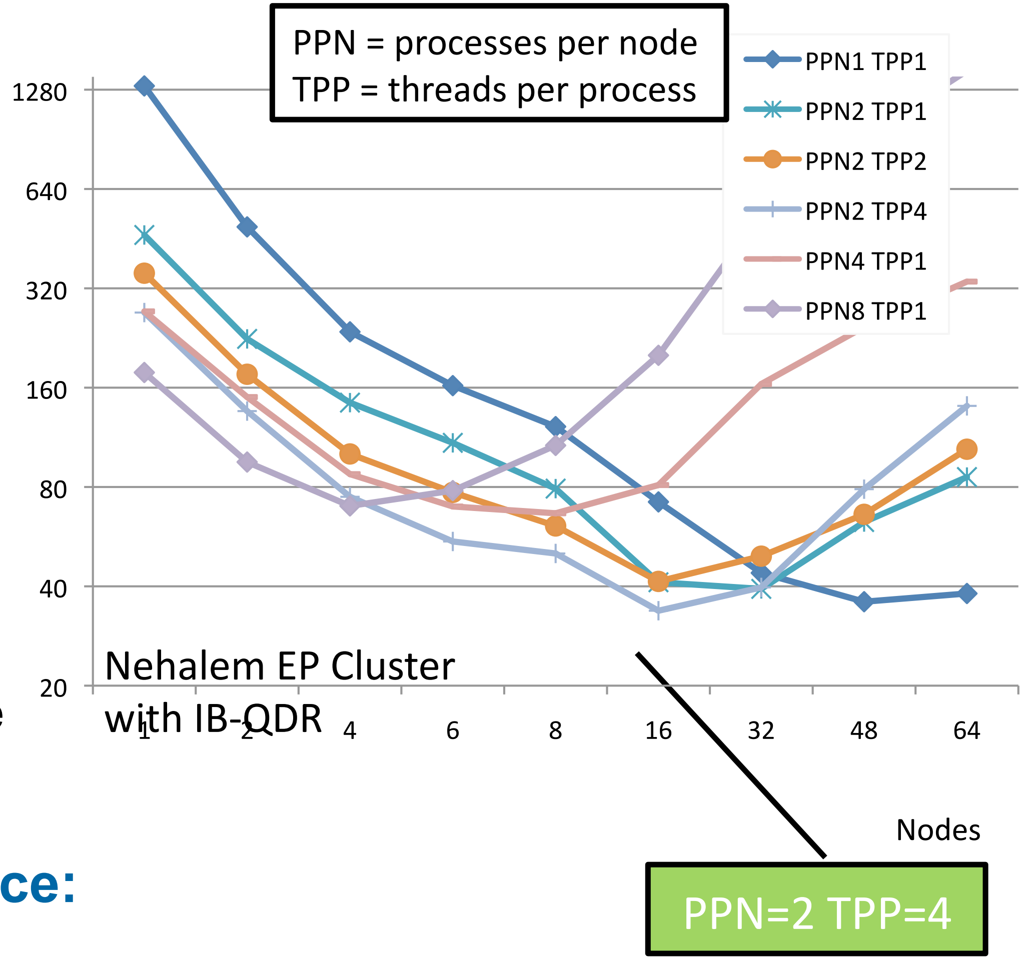
Best effort hybrid

Best effort MPI only



Adding OpenMP to MPI may be beneficial

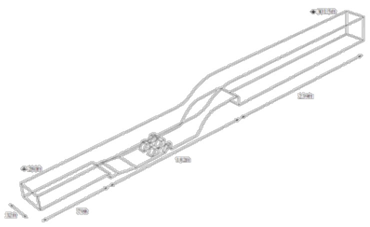
- **XNS (M. Behr, CATS, RWTH)**
  - Simulation of Hydro-Dynamic forces of the Ohio Dam
- **OpenMP Parallelization:**
  - 9 parallel regions
  - **Human effort: ~ 6 weeks**
- **Best absolute MPI performance:**
  - 48 nodes, 1 MPI process per node 35,9 sec
- **Best absolute Hybrid performance:**
  - 16 nodes, one MPI process per socket, 4 threads per process 33,7 sec



PPN = processes per node
TPP = threads per process

Nehalem EP Cluster
with IB-QDR

PPN=2 TPP=4



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New in OpenMP 3.0
Tasks

- **Tasks allow to parallelize irregular problems, e.g.**
  - unbounded loops
  - recursive algorithms
  - Producer / Consumer patterns
  - and more …

- ***Task*****: A unit of work which can be executed later**
  - Can also be executed immediately

- **Tasks are composed of**
  - Code to execute
  - Data environment
  - Internal control variables (ICV)

New in OpenMP 3.0
Tasking Example

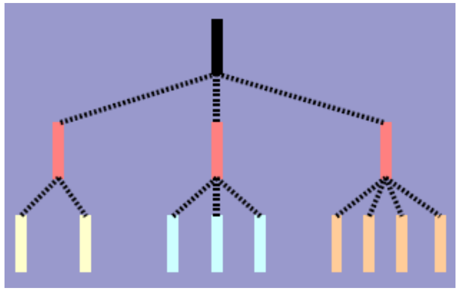
- **Parallelization of an unbounded while loop**
  - All loop iterations are independent from each other!
  - Number of iterations unknown up front
  - would have been unconvenient beforehand (inspector/executor method)

```
typedef list<double> dList;  dList myList;
#pragma omp parallel
{
#pragma omp single
    {
          dList::iterator it = myList.begin();
          while (it != myList.end())
          {
#pragma omp task firstprivate(it)
          { *it = processListItem(*it); }
          it++;
          }
    } // end single
} // end parallel region
```

New in OpenMP 3.0
Improved Support for Nested Parallelism

New runtime functions:

```
int omp_get_level()
    // Which current nested level?
int omp_get_active_level()
    //How many nested active parallel regions (>1 thread)?
int omp_get_ancestor_thread_num(int level)
    // thread-id of  ancestor thread at a given level?
int omp_get_team_size(int level)
    // Size of ancestor‘s team at a given level?
```



New environment variables (plus corresponding runtime functions)

- **OMP_MAX_NESTED_LEVEL** # maximum number of active parallel regions
- **OMP_THREAD_LIMIT** # maximum total number of OpenMP threads

News in OpenMP 3.0
Miscellaneous

Static schedule

```
#pragma omp for schedule(static) nowait
   for(i = 1; i < N; i++) a[i] = …
#pragma omp for schedule(static)
   for (i = 1; i < N; i++)c[i] = a[i]
```

Allowed in OpenMP 3.0 if and only if:
- Number of iterations is the same
- Chunksize is the same (or not specified)

Loop collapsing

```
#pragma omp for collapse(2)
   for(i = 1; i < N; i++)
      for(j = 1; j < M; j++)
          foo(i, j);
```

Iteration space from i-loop and j-loop is collapsed into a single one, if loops are perfectly nested and form a rectangular iteration space.

New variable types allowed in for-*Worksharing*

```
#pragma omp for
for (unsigned int i = 0; i < N; i++)  foo(i);

vector v; vector::iterator it;
#pragma omp for
for (it = v.begin(); it < v.end(); it++)
   foo(it);
```

Legal in OpenMP 3.0:
- Usigned integer types
- Pointer types
- Random access iterators (C++)

New in OpenMP 3.1 (1/2)

- **Many small corrections and clarifications throughout the whole spec**
- **A tiny step towards improved NUMA support:**
  - **`export OMP_PROC_BIND=true`**

    # please, don‘t move OpenMP threads between processes
  - **`export OMP_NUM_THREADS=4,3,2`**

    # control thread number for nested parallelism up front
- **Refinements to the OpenMP Tasking Model:**
  - The `taskyield` directive denotes a user-defined task scheduling point at which the current task may be suspended (and resumed later).
  - The `mergeable` clause indicates that the task may have the same data region as the generating task region.
  - The `final` clause denotes all descendent tasks to be executed sequentially in the same region (immediate execution).

New in OpenMP 3.1 (2/2)

More miscellaneous extensions:

- The `atomic` construct now accepts the clauses `read`, `write`, `update` and `capture` to ensure atomicity of the corresponding operations.
- The `firstprivate` clause accepts `const`-qualified types in C/C++ and `intent(in)` declared types in Fortran.
- For C/C++ the `reduction` clause now also accepts `min` and `max` reductions for built-in datatypes, still excluding aggregate types, pointer types, and reference types.
- The new `omp_in_final()` API routine allows to determine whether the calling task is final.

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Towards OpenMP 4.0
Overall Goals

- Error Model
- Interoperability and Composability
- NUMA Support („Affinity“)
- Accelerators
- Tasking Extensions

Towards OpenMP 4.0
OpenMP Error Model

- **C, C++ and Fortran suggest different approaches: Error Codes, Error Variables, Call Backs, Exceptions, …**

- **First step: Being able to react to an error.**

- **Current plan: Introduction of a directive to end the execution of OpenMP constructs and definition of *Cancellation* points**

- **#pragma omp done [scope]**
  - To end the current Parallel Region
  - To end the current Worksharing construct
  - To end the current Task

- **Pre-defined as well as user-defined Cancellation points at which the execution is guaranteed to end**

Towards OpenMP 4.0
NUMA Support

Issue / Ticket	Example	Version
Controlling the Number of Threads on Multiple … Levels	**export OMP_NUM_THREADS=4,3,2**	3.1
Controlling Thread Binding	**export OMP_PROC_BIND=TRUE**	3.1
Restricting the Processor Set for Program Execution	**setenv OMP_PROCSET 0,2,4,6, 8,10, 12,14**	4.x
Controlling the Placement of Threads within the Processor Set	**export OMP_AFFINITY=scatter,,compact** **!$omp parallel affinity(scatter)**	**4.x**
Controlling the Initial Placement of Shared Data	**export OMP_MEMORY_PLACEMENT=spread**	4.x
Adapting the Placement of Shared Data at Runtime	**!$omp migrate[(variable list)] strategy(…)**	4.x ?
Distance Matrix	?	4.x ?

Towards OpenMP 4.0
Accelerators

- **Accelerator Subcommittee led by James Beyer (Cray) is very active.**

- **Extensions to the Execution and Memory Model**
  - *Accelerator Tasks* can be created to execute an *Accelerator Region*
  - Data can reside on the *Host*, the *Accelerator Device*, or both.

    Directives control data transfer

    Details are left to the runtime

- **Accelerator Execution Region**
  - Marks the code to be executed on an accelerator

- **Accelerator Data Region**
  - define the data scope to be reused across multiple accelerator regions

Towards OpenMP 4.0
Tasking Extensions

- **Feedback from the user community:**
  - Tasks need *Reductions*
  - Tasks need *Dependencies*
- **There is currently no way to identify tasks (and it is not intended to create one), but we need a facility to denote tasks belonging together**
- **Current approach: *Taskgroup***
  - Defined as a structured block, an OpenMP Region
  - Reductions may be performed inside a Taskgroup
- **Current approach regarding dependencies: Expression via addresses, thus Array Shaping Expressions are necessary.**

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- **OpenMP scales**
  - within the node (there is a lot of resource sharing, though)
  - if you do it right (extend parallel regions, try to avoid barriers …)
  - Consider data-thread-affinity on NUMA, use OS tools for control
  - Beware of data races – there are verification tools (like Intel Inspector)
- **OpenMP may even scale across nodes (ScaleMP)**
- **OpenMP works well together with MPI**
  - Frequent sweet spot: one MPI process per socket, one thread per core
  - Again: Consider data-thread-affinity on NUMA
    (Depends on MPI implementation and resource management system)
- **OpenMP progresses slowly**
  - OpenMP is closely tight to into the base languages which makes it tough
  - Stay tuned for OpenMP on accelerators

PPCES, March 21-25, 2010, Aachen

www.rz.rwth-aachen.de/ppces

- Monday, March 21, afternoon

  Announcement of the upcoming RWTH Compute Cluster

  with renowned Speakers from Bull, Intel, GRS, and Oracle

- Tuesday, March 22 – Thursday, March 24,

  Tutorials in Serial, OpenMP and MPI Programming

- Friday, March 25

  GPGPU Programming with Michael Wolfe (PGI)