



Methods for performance evaluation on modern HPC systems:

Performance analysis with Paraver

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Outline



The tools

Introduction

Paraver

Applied research: clustering and sampling

Analysis examples

Dimemas

Simulation examples

Some GPUs examples

GPUSs

HMPP

Extrae support

Our Tools

Since 1991

Based on traces

Core tools:

Paraver – offline trace analysis

Dimemas – message passing simulator

Exrae – instrumentation

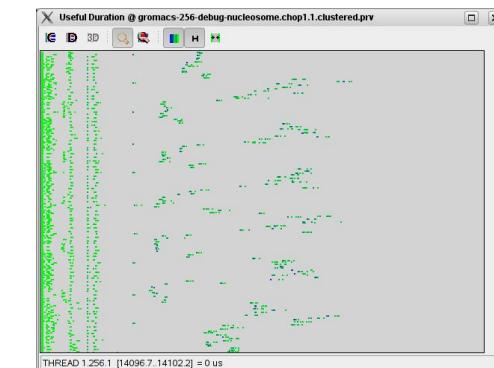
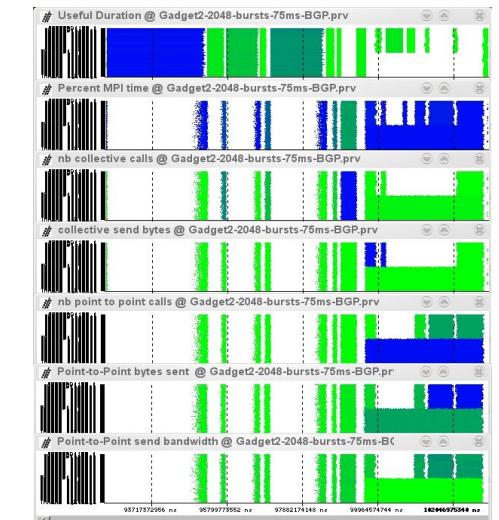
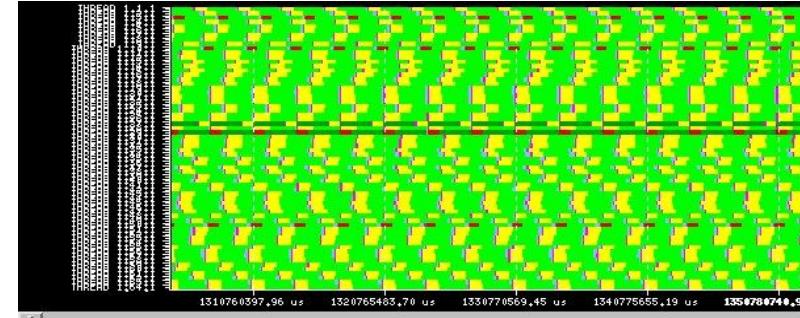
Detail and intelligence

analysis of applications at large scale

intelligent online data reduction

mixed instrumentation and sampling

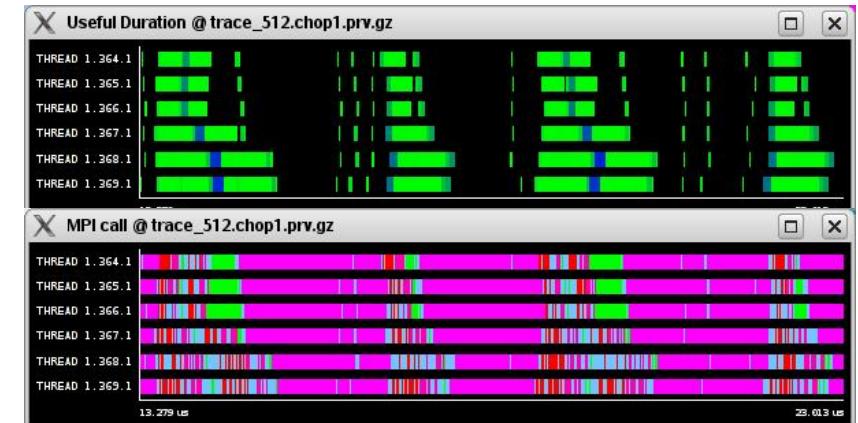
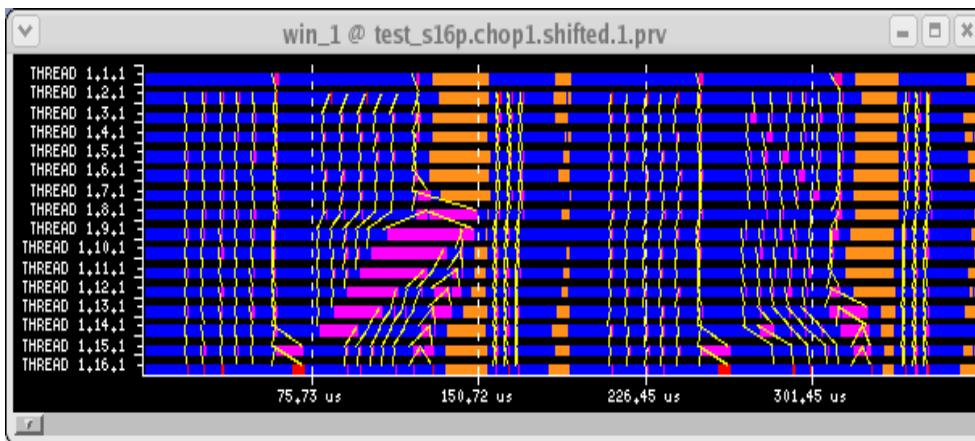
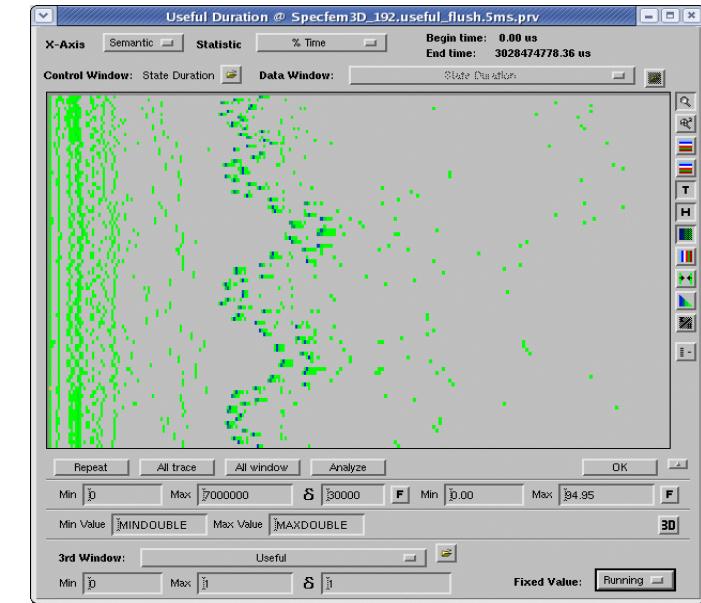
advanced modelling/prediction



Why traces?

Variability is important
along time, across processors

Highly non-linear systems
microscopic effects may have
macroscopic impact



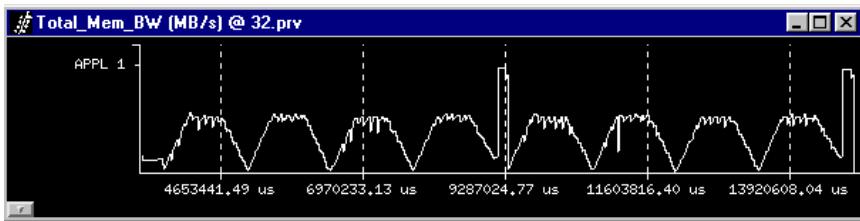
Paraver – Performance data browser



Goal = Flexibility

- No semantics
- Configurable

Timelines

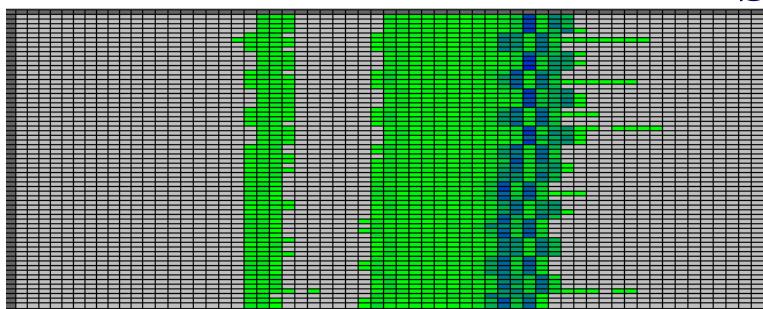


Identifier of function

Performance (IPC, Mflops...)

Routine duration

• • •



Statistics

Profiles

Average miss ratio per routine

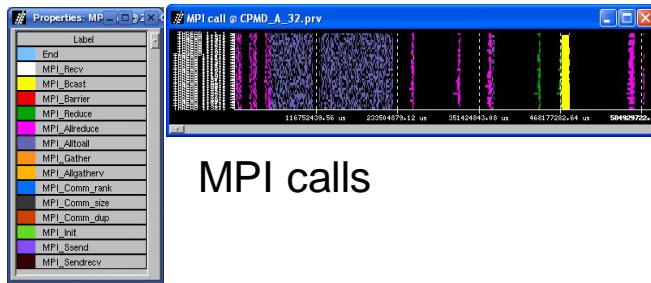
Histogram of routine duration

• • •

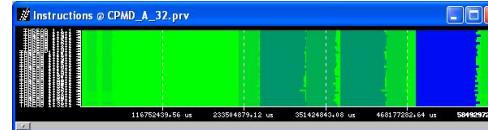
Views: Timelines

Raw events → Piece-wise constant functions of time → plots / colors

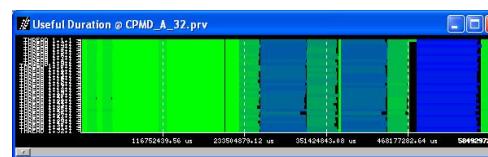
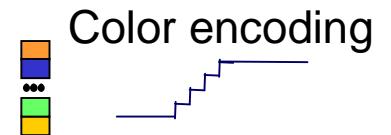
- Basic metrics



MPI calls



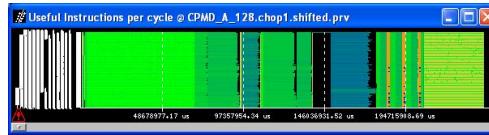
Instructions



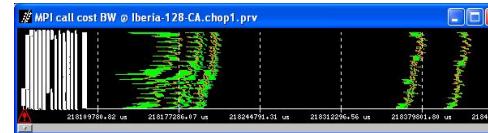
Useful duration

- Derived metrics

$$useful_{IPC} = \frac{instr}{cycles} \square useful$$



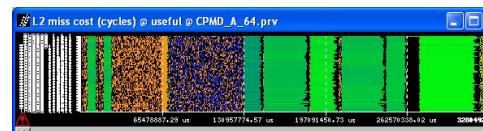
$$MPI_{call_cost} = \frac{MPI_{call_duration}}{bytes}$$



$$preempted_{time} = elapsed - \frac{cycles}{clock_{freq}}$$

- Models

$$L2_{miss}_{latency} = \frac{cycles - instr/idealIPC}{L2misses}$$

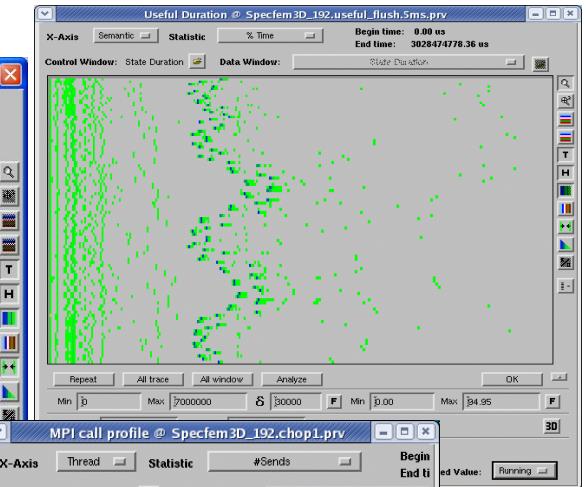
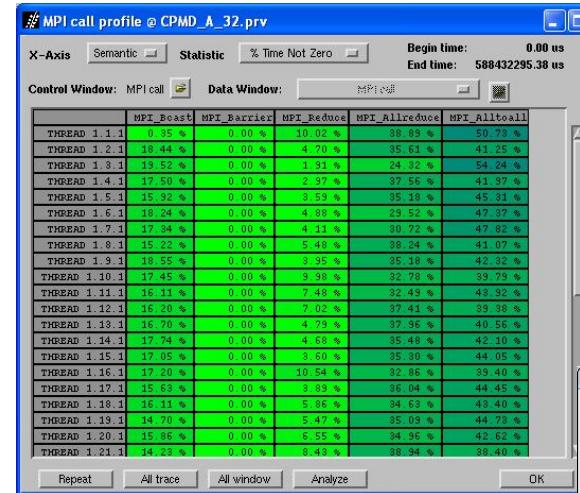


Views: Statistics

2D

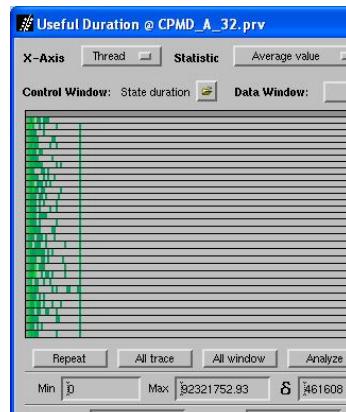
- Profiles
- Histograms
- Correlations
- Communication Patterns

MPI calls profile



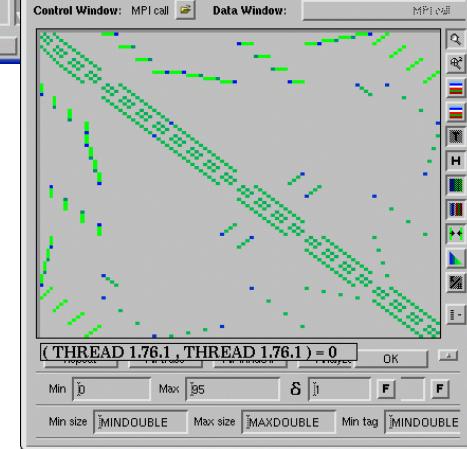
3D

Duration - IPC

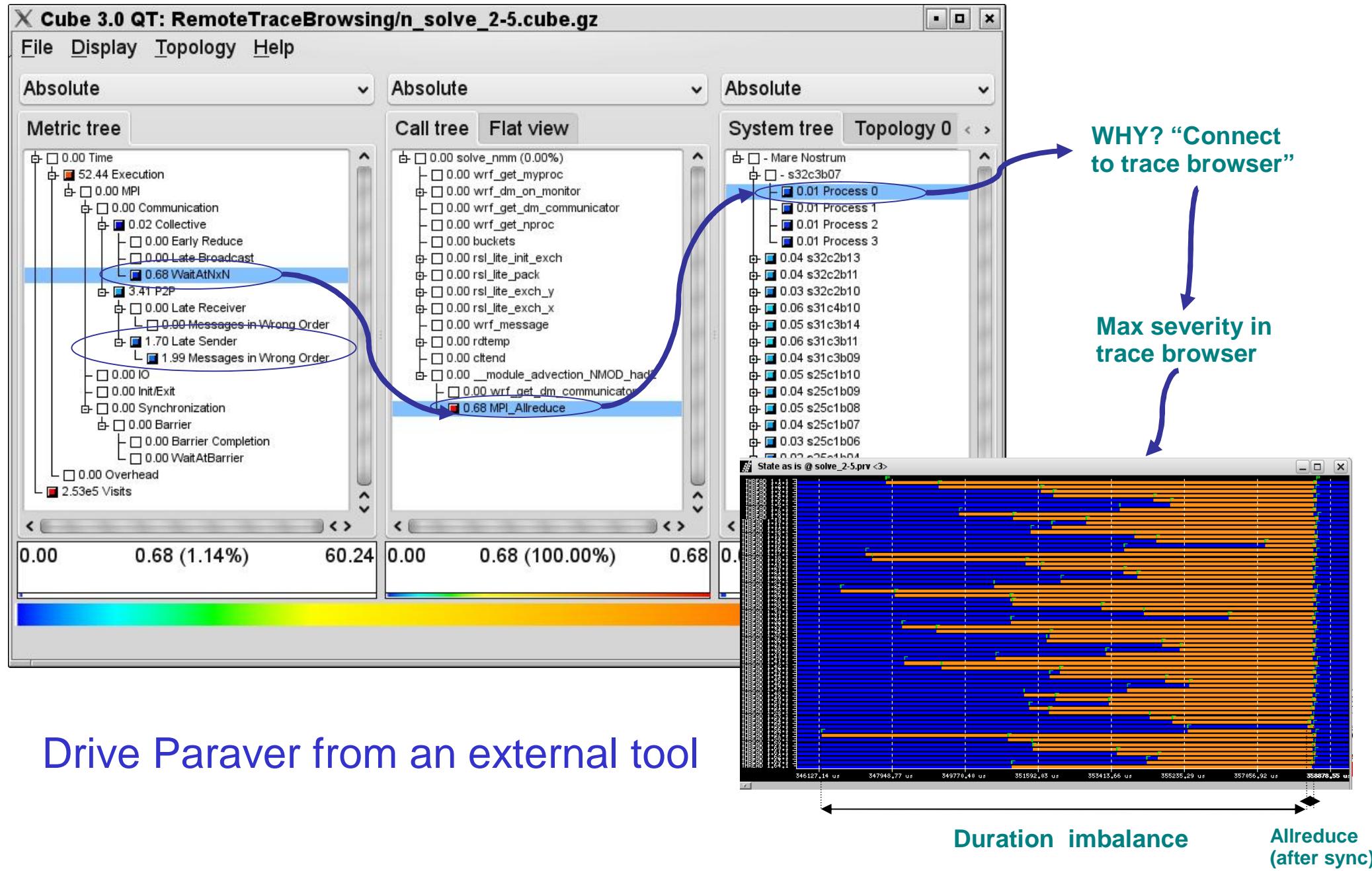


While computing

While communicating



Tools integration: CUBE + Paraver



Clustering module – detecting structure

Highlight structure

Clusters injected in trace

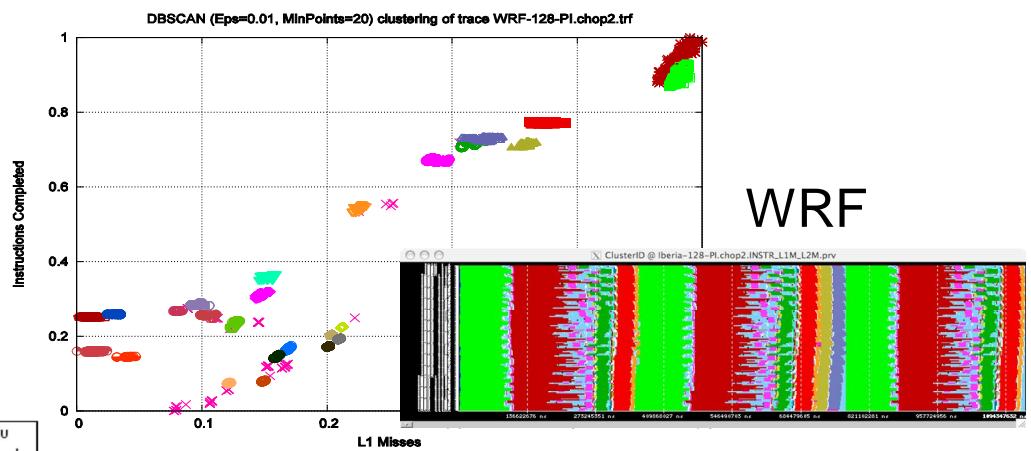
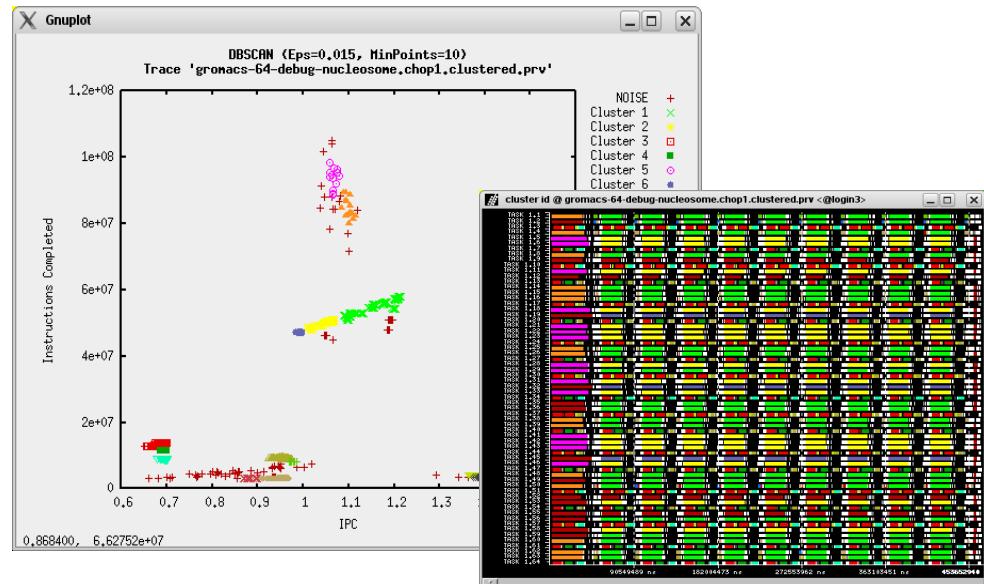
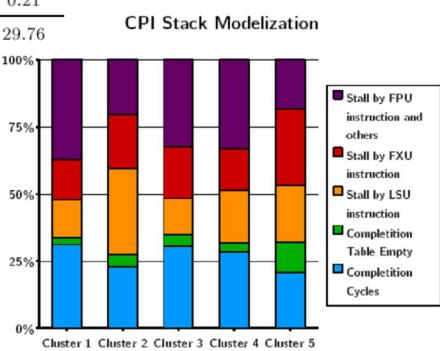
Phases vs. routines

Counters projection

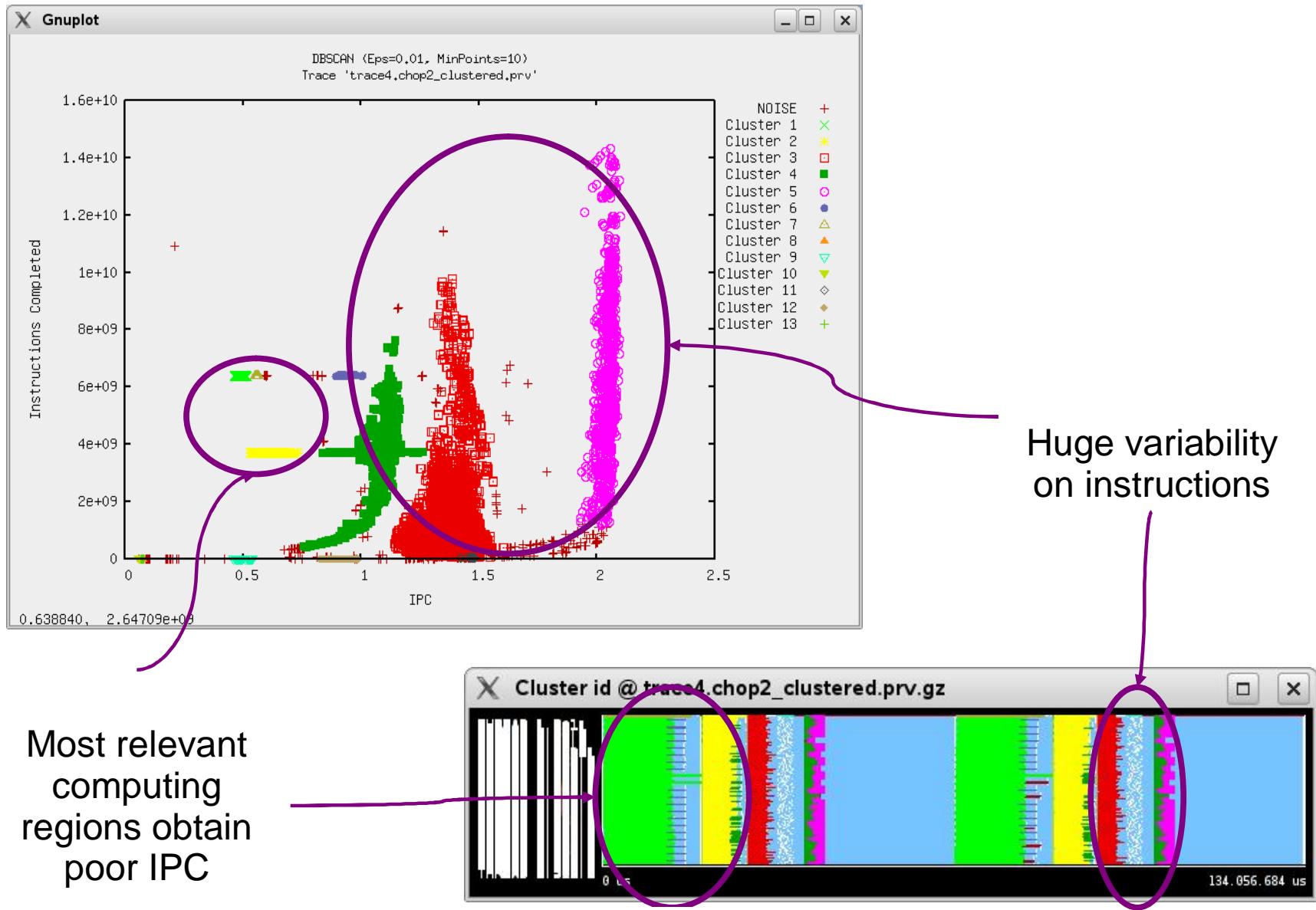
Statistics

Models (CPI stack)

CLUSTER	1	2	3	4	5
%TIME	54.88	17.96	16.90	6.44	1.42
AVG. BURST DUR. (ms)	1.02	0.78	13.14	2.50	1.11
IPC	1.02	0.65	0.89	0.91	0.53
MIPS	2231.8	1423.3	1966.5	2001.8	1163.0
MFLOPS	339.2	46.3	191.6	269.2	23.6
L1M/KINSTR	0.92	1.53	1.19	1.17	2.88
L2M/KINSTR	0.06	1.26	0.06	0.35	0.21
MEM.BW (MB/s)	16.79	218.47	13.87	85.77	29.76



Clustering module – detecting structure



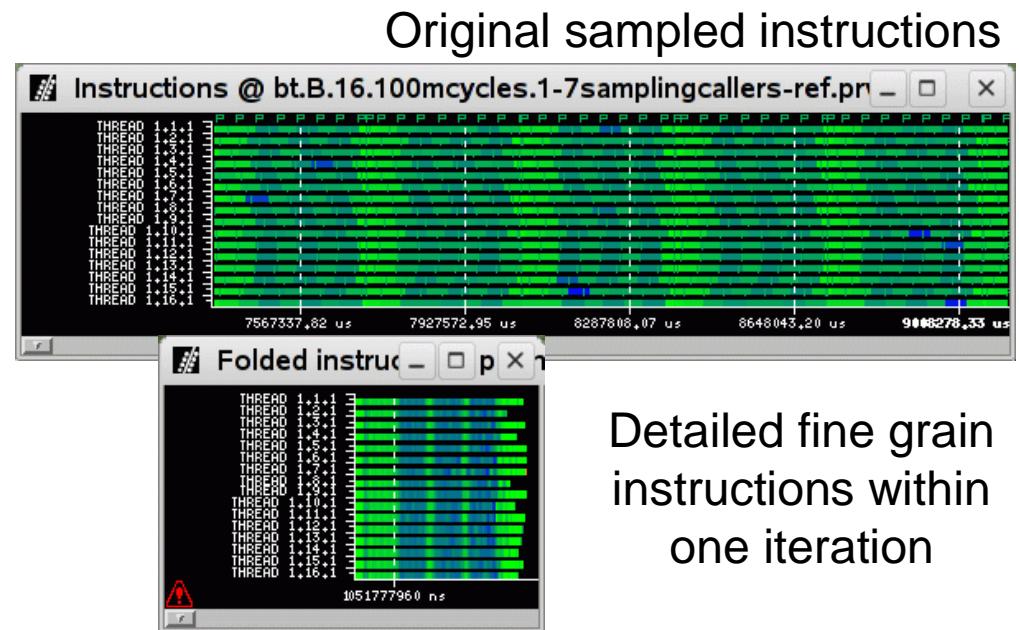
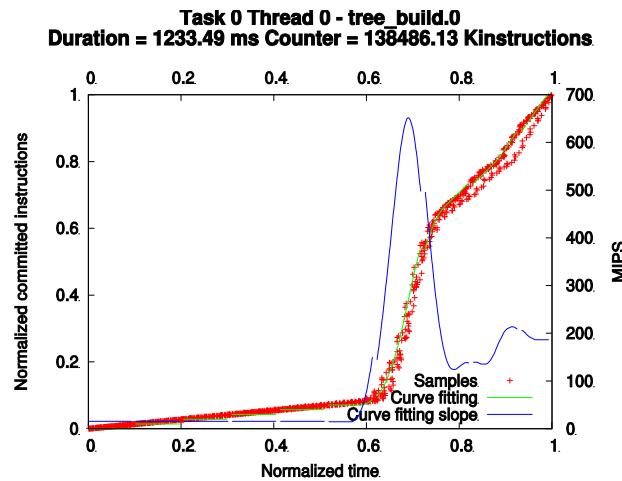
Folding samples – granularity / overhead

Application granularity vs. detailed granularity
Samples

hardware counters + callstack

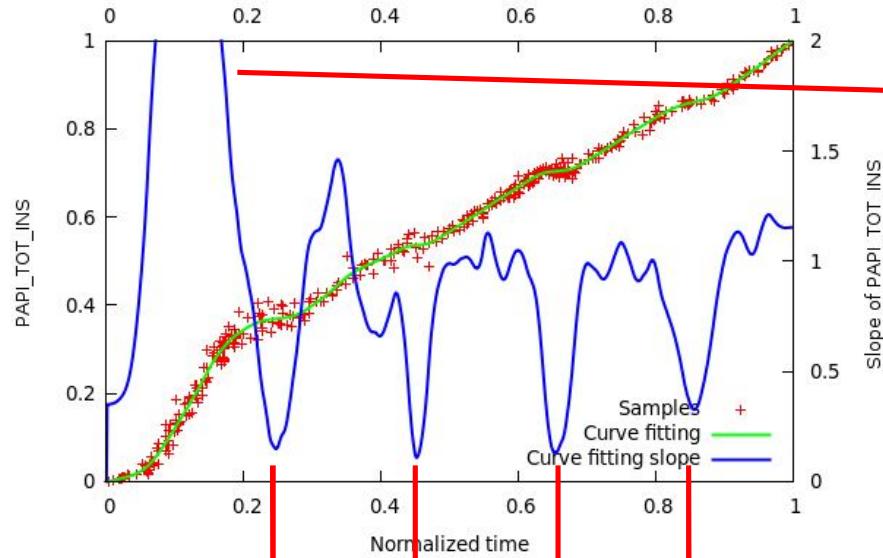
Folding

reduce sampling frequency / overhead
based on known structure: iterations,
routines, clusters

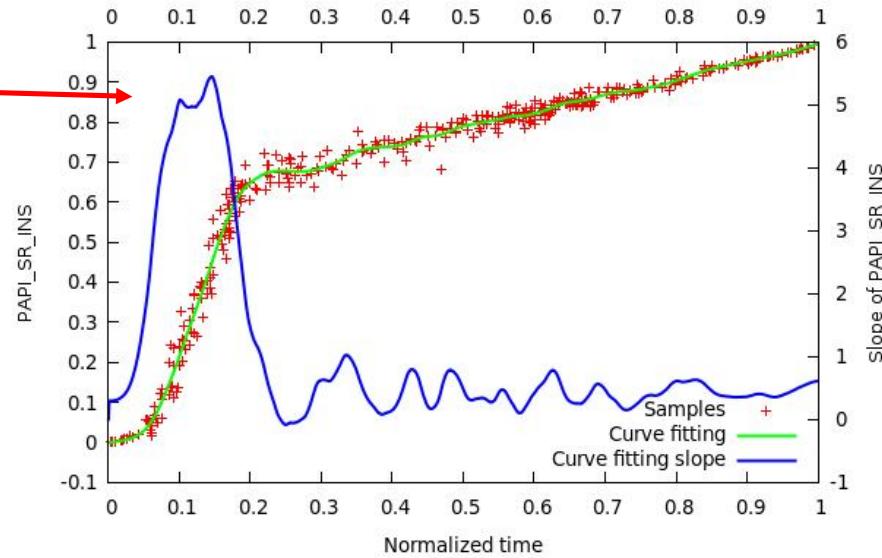


Folding samples – granularity / overhead

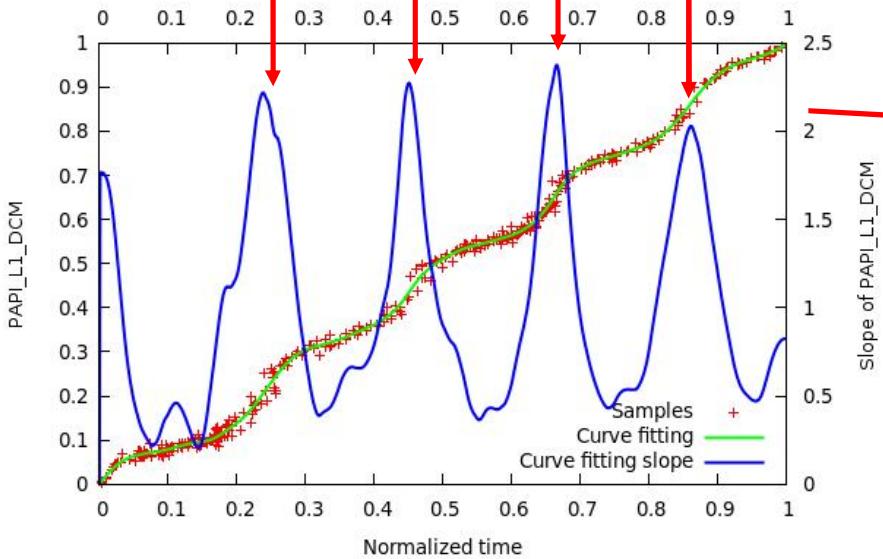
Task 4 Thread 0 -- COPY_FACES:[{copy_faces.f}:{4,7}-{320,9}]



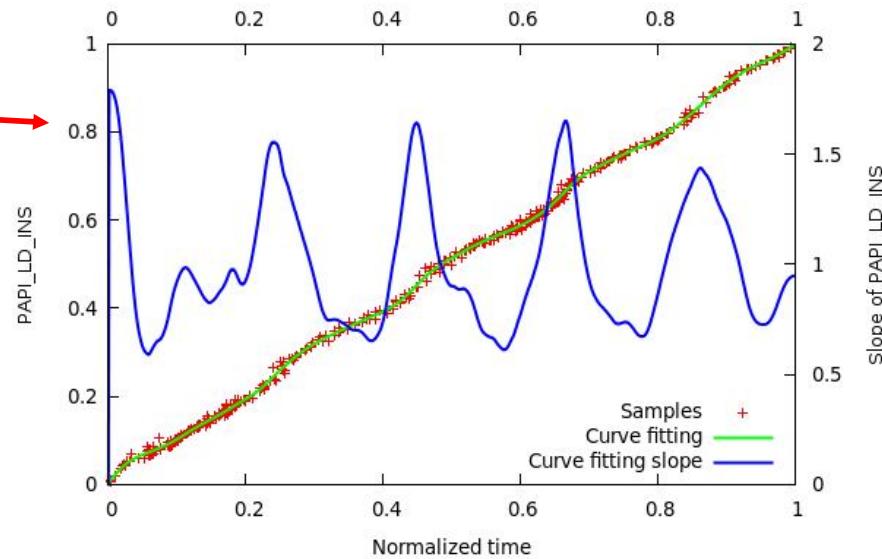
Task 4 Thread 0 -- COPY_FACES:[{copy_faces.f}:{4,7}-{320,9}]



Task 4 Thread 0 -- COPY_FACES:[{copy_faces.f}:{4,7}-{320,9}]

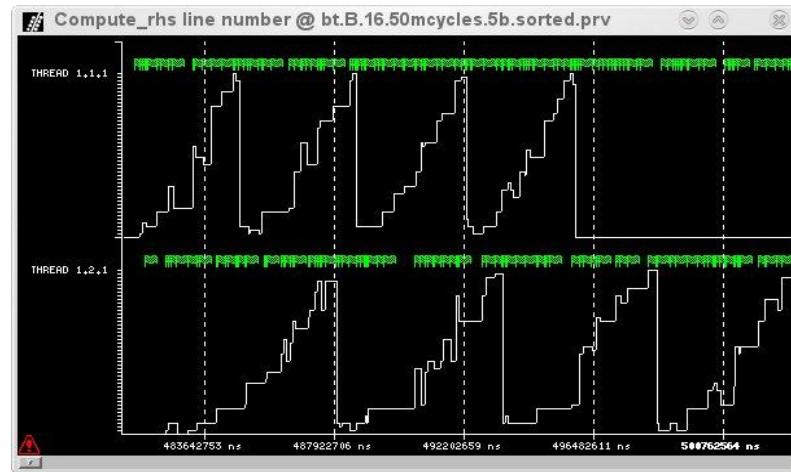


Task 4 Thread 0 -- COPY_FACES:[{copy_faces.f}:{4,7}-{320,9}]

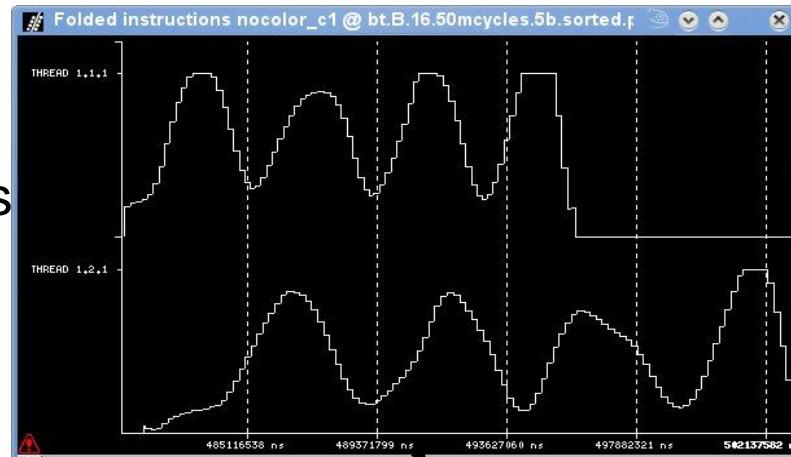


Folding samples – granularity / overhead

Source line

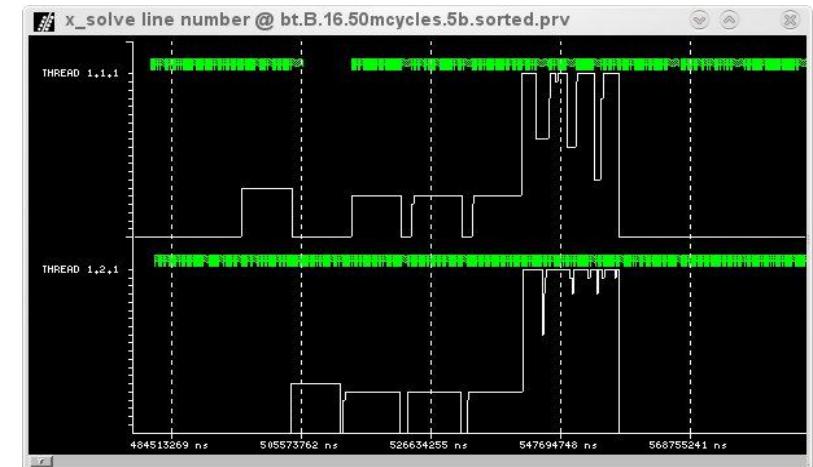


Instantaneous
MIPS



4 iterations outer loop

x_solve

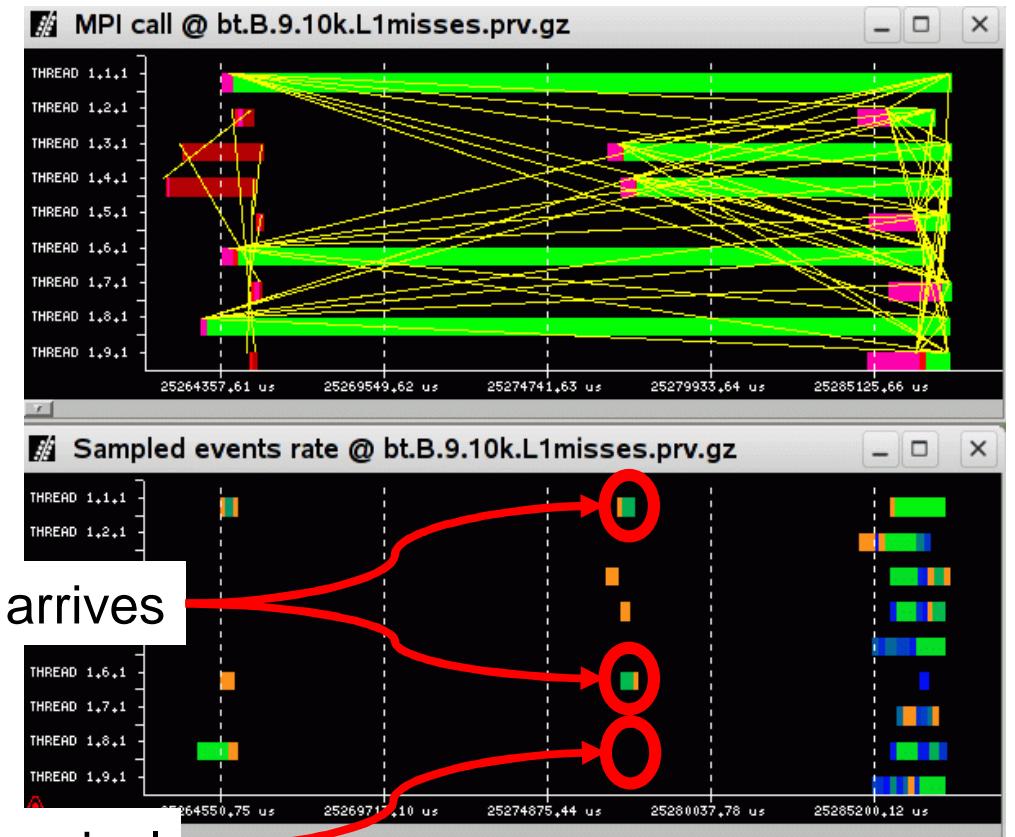
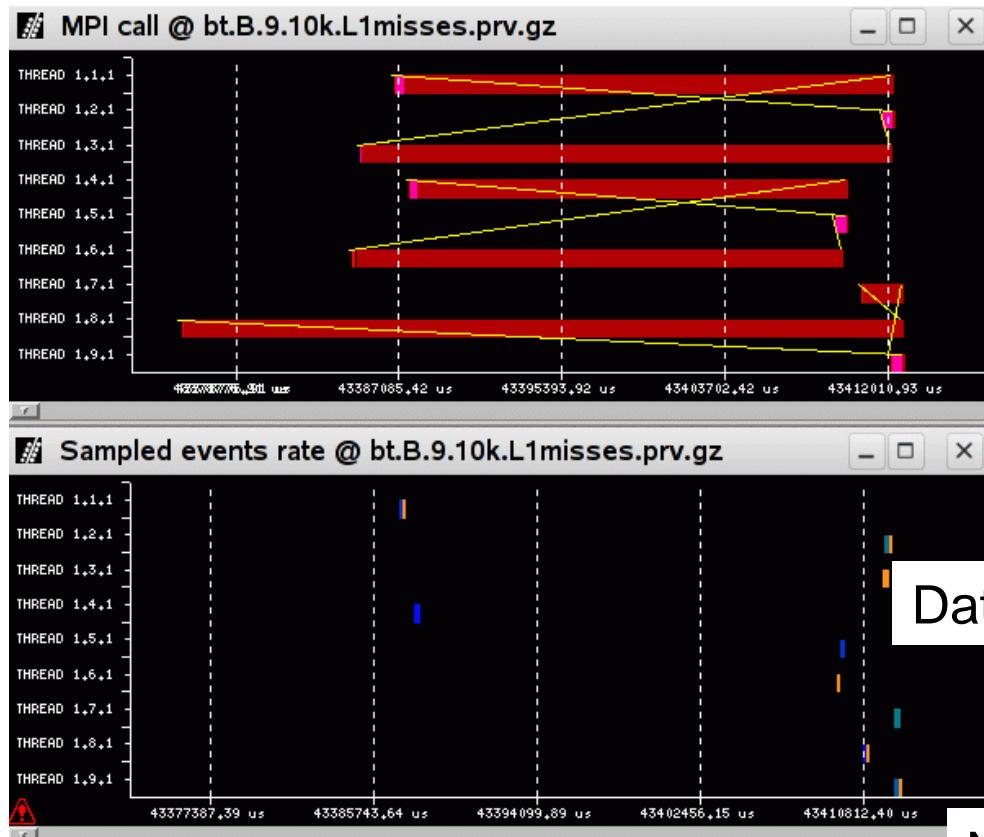


4 x_solve_cell4 backsubstitute

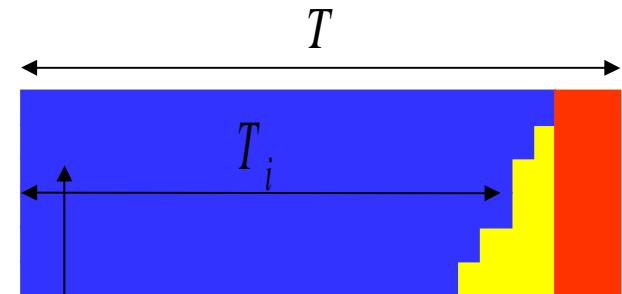
Sampling driven by other HWC



Density of L1 misses within MPI in a SMPs: when the data actually arrives



Scalability model



$$IPC \#instr$$

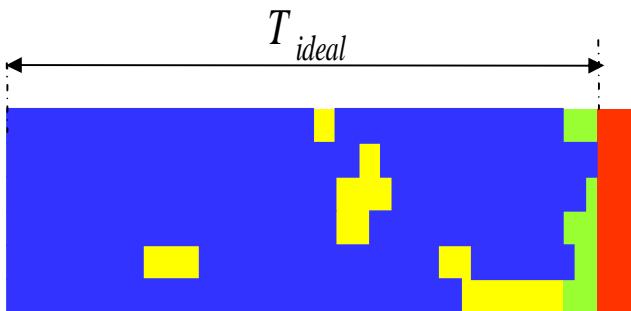
$$eff_i = \frac{T_i}{T}$$

$$LB = \frac{\sum_{i=1}^P eff_i}{P * \max eff_i}$$

$$Sup = \frac{P}{P_0} \cdot \frac{LB}{LB_0} \cdot \frac{CommEff}{CommEff_0} \cdot \frac{IPC}{IPC_0} \cdot \frac{instr_0}{instr}$$

Directly from real execution metrics

$$CommEff = \max eff_i$$



Migrating/local load
imbalance

Serialization

$$microLB = \frac{\max T_i}{T_{ideal}}$$

$$Sup = \frac{P}{P_0} \cdot \frac{macroLB}{macroLB_0} \cdot \frac{microLB}{microLB_0} \cdot \frac{CommEff}{CommEff_0} \cdot \frac{IPC}{IPC_0} \cdot \frac{instr_0}{instr}$$

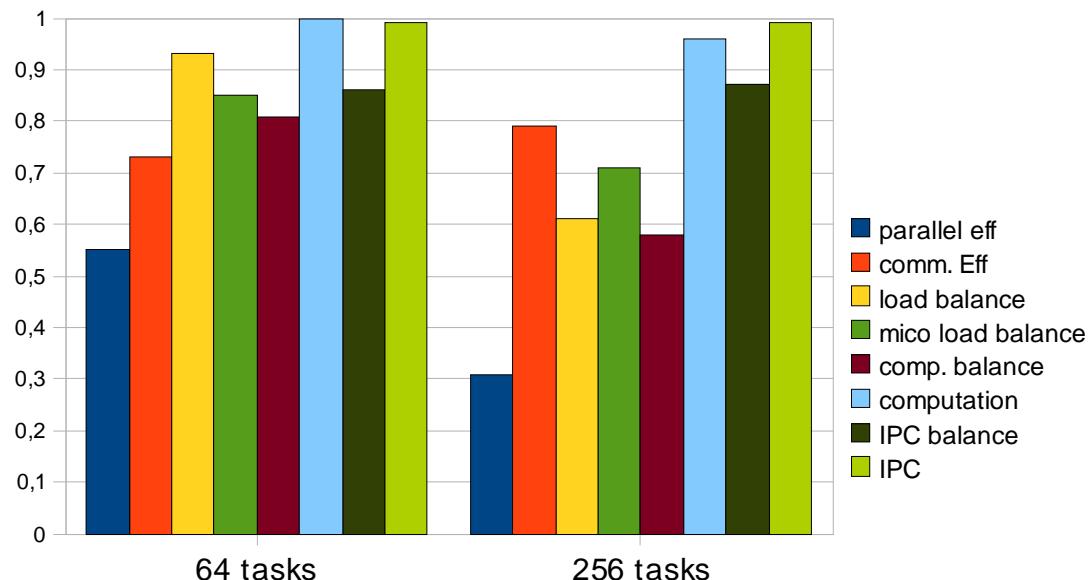
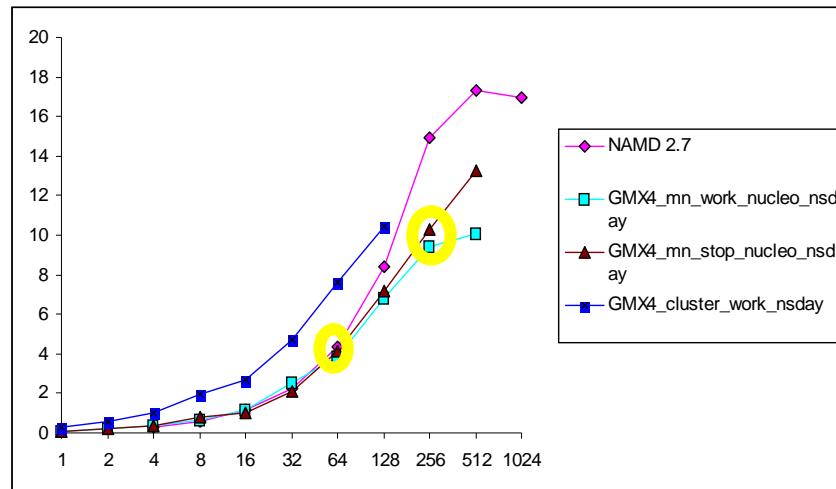
Requires Dimemas simulation

$$CommEff = \frac{T_{ideal}}{T}$$

Example: From quick analysis...



GROMACS analysis



Main scalability problems:
• Load balance
• Computation balance

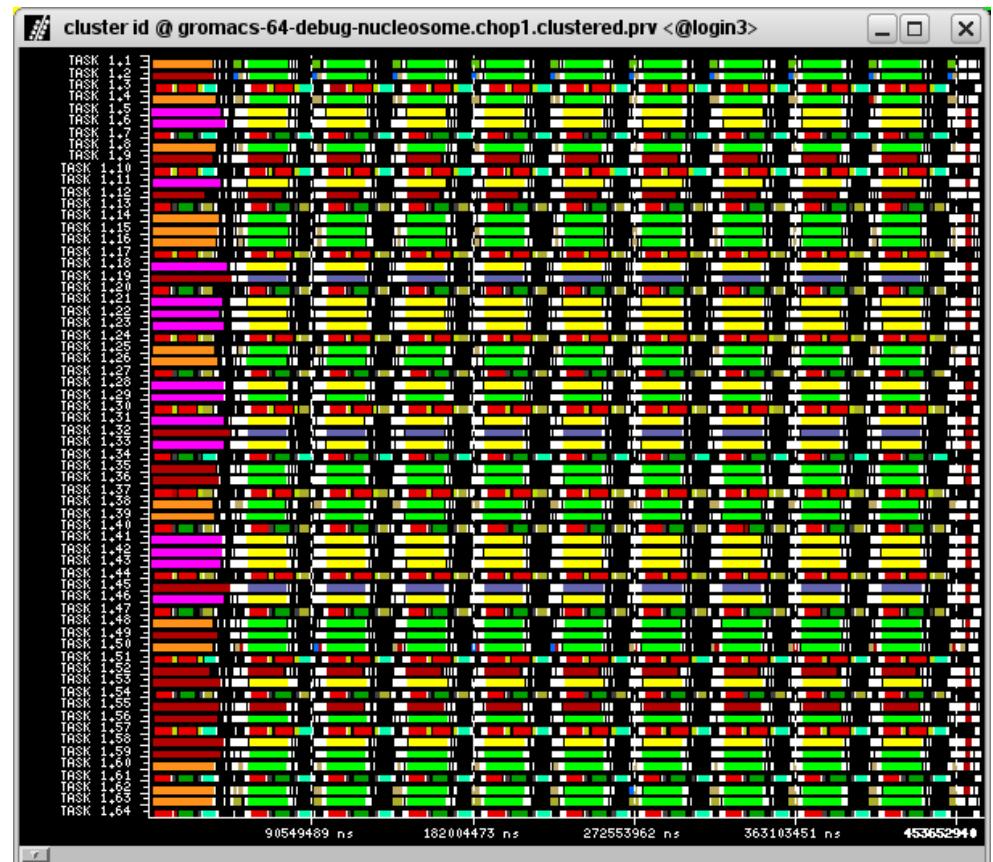
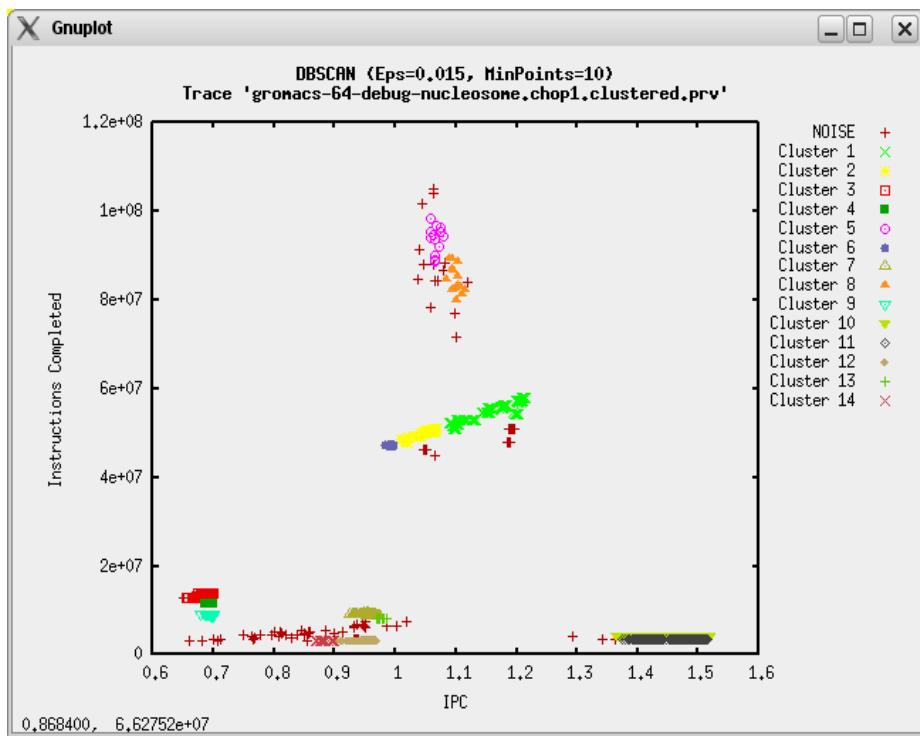
4% of code replication

64 tasks already poor efficiency!
• Communication problem

Example: ... to details



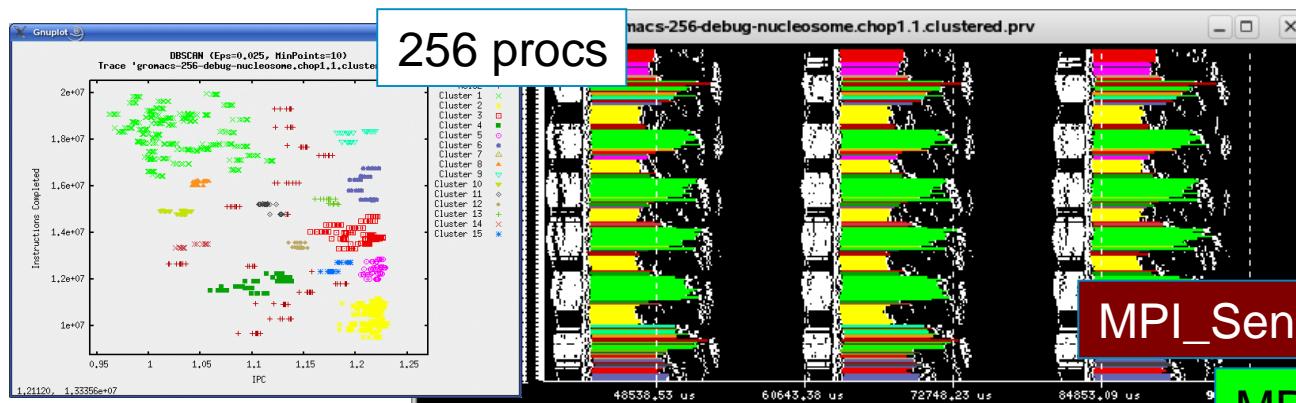
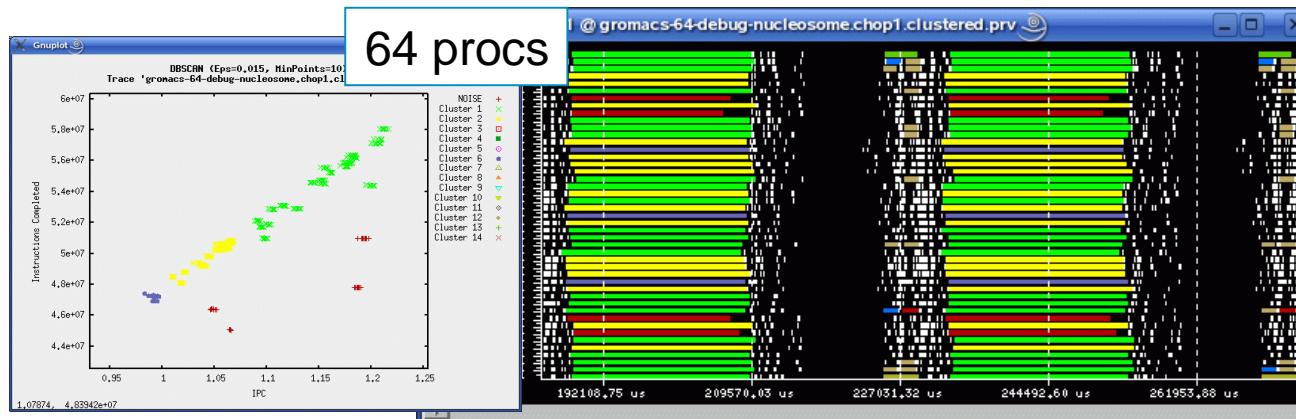
GROMACS structure, 64 tasks



Example: ... to details



GROMACS PMEs balance / scalability



MPI_Allreduce: 286@pme_pp.c
MPI_Recv: 427@pme_pp.c

MPI_Senredv: 1533@domdec.c

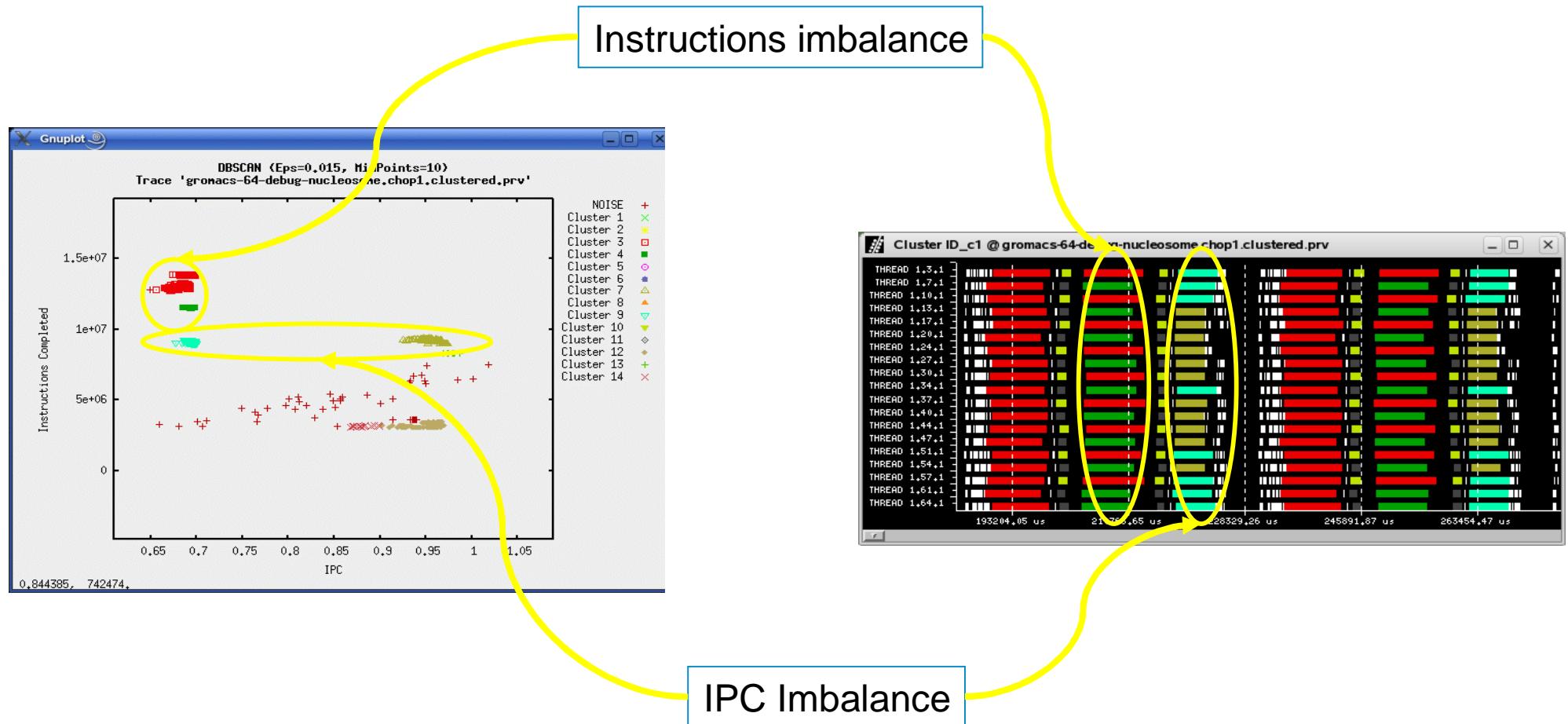
MPI_Waitall: 126@demdec_network.c

Color represents MPI caller line

Example: ... to details



GROMACS FFTs balance

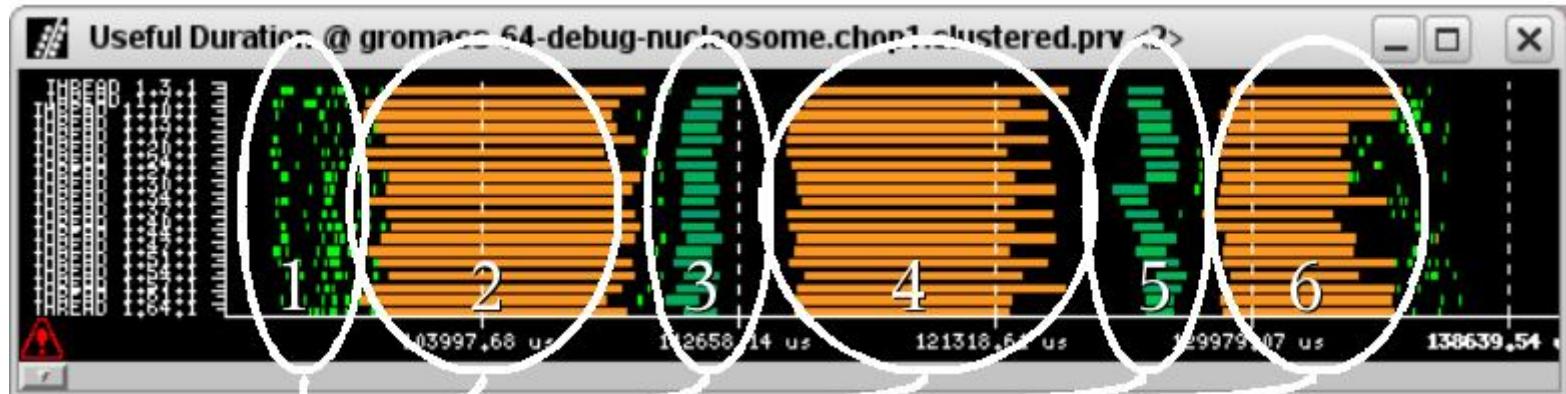


Example: ... to details

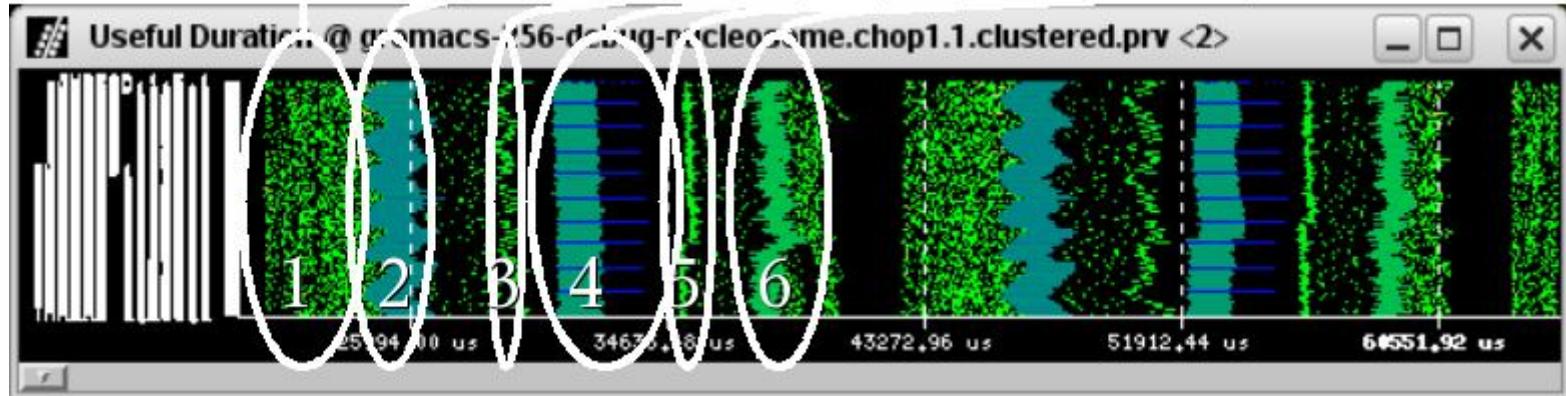


GROMACS: Comparing computation time for FFTs

64 tasks
(one iteration)



256 tasks
(2,2 iterations
in the same
time interval,
4 times more
resources)



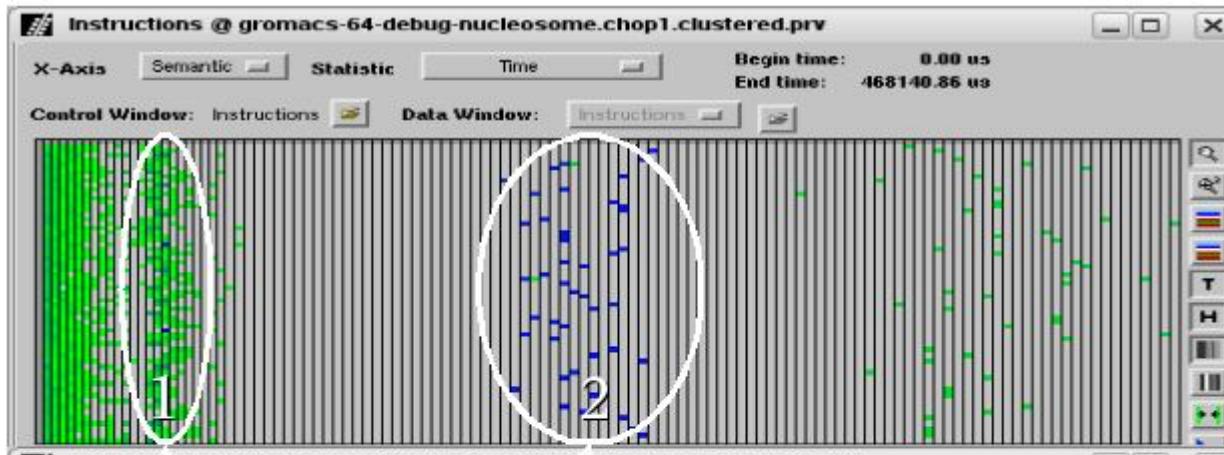
Zone 4 has a potentially structured imbalance with scalability problems (MPI_Alltoallv: 241@fftgrid.c)

Example: ... to details

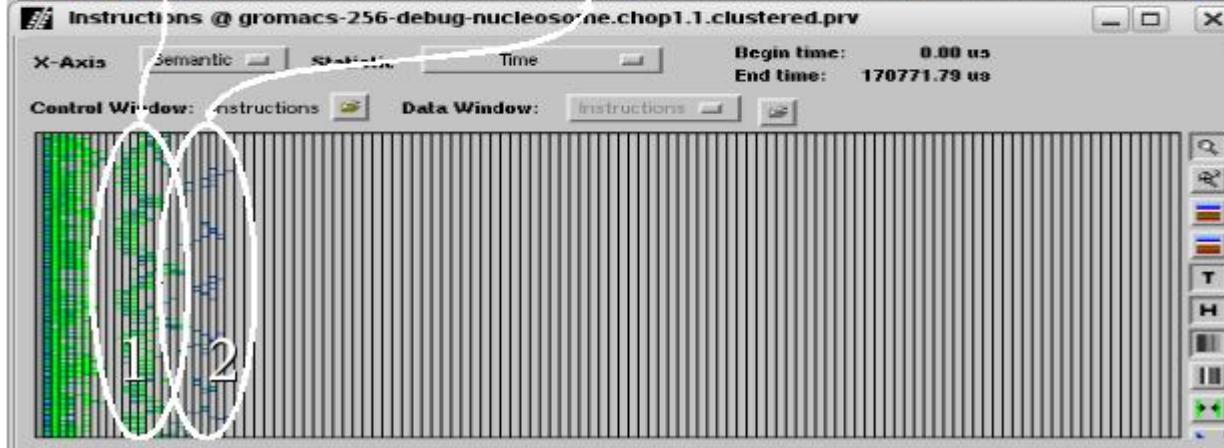


GROMACS Computational load balance

64 tasks



256 tasks



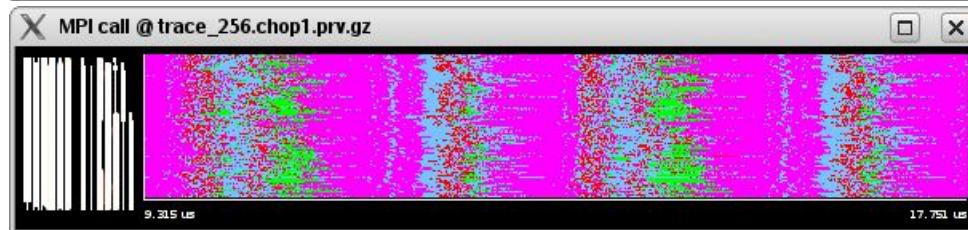
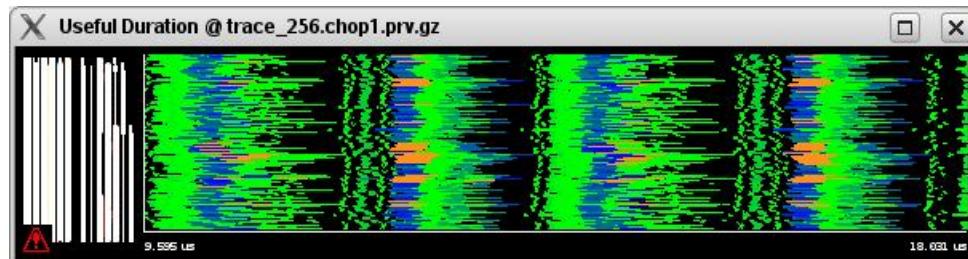
Zone 1 does not scale and increases imbalance!

Example: Code optimization



Short diagnosis: FrontFlowRed – 256 vs 512 tasks

- Unbalance and MPI time increases
- Sequence of MPI_Allreduce calls
- Poor IPC, high cache misses

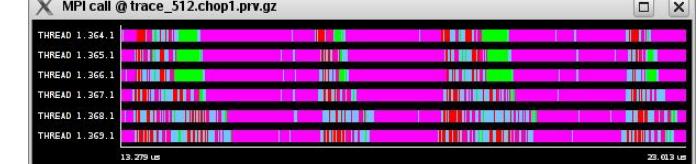
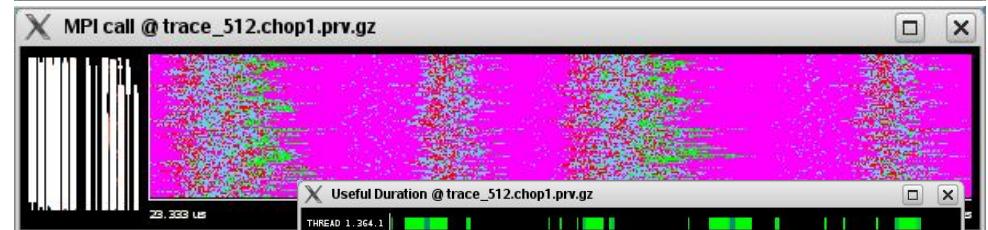
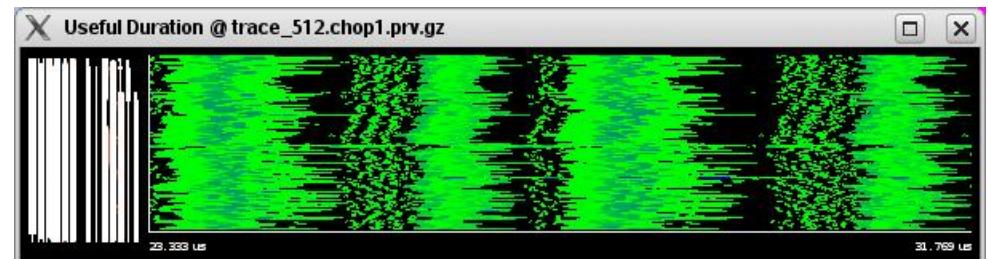


256 512

Parallel efficiency 27% 19%

Load balance 56% 48%

% MPI_Allreduce avg time 50% 62%



Example: Code optimization



Modifications in the source code

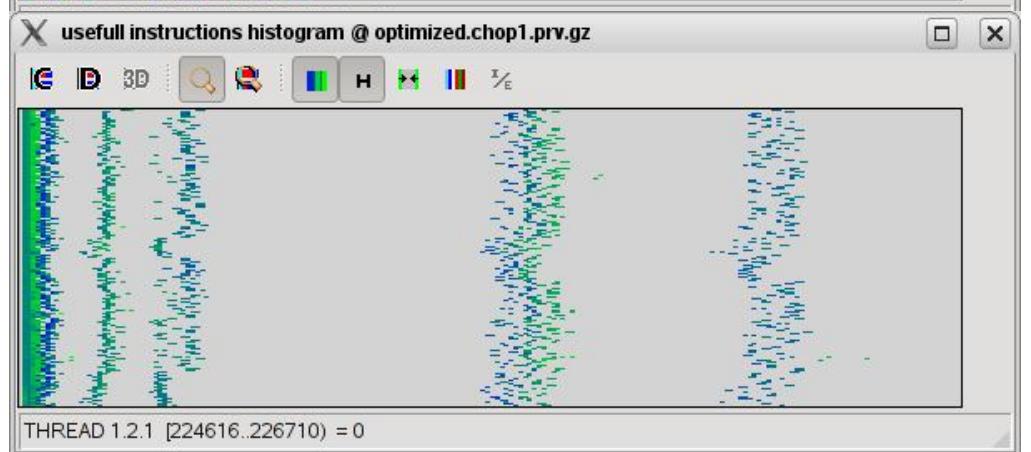
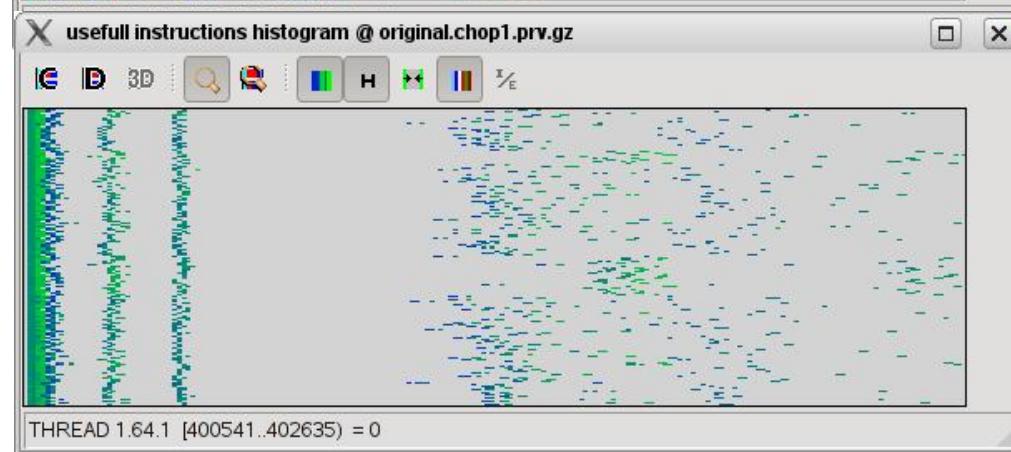
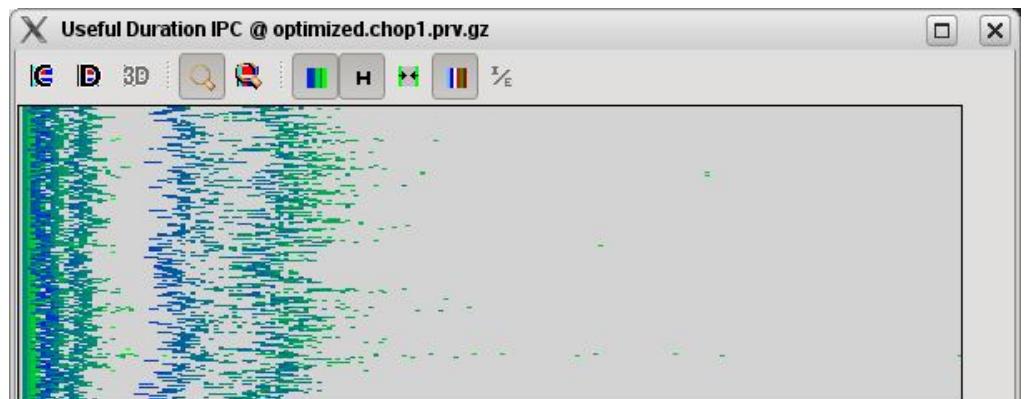
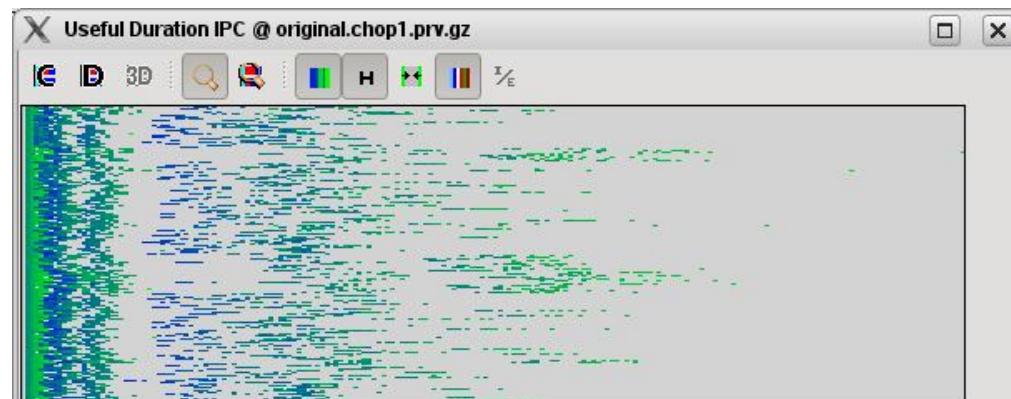
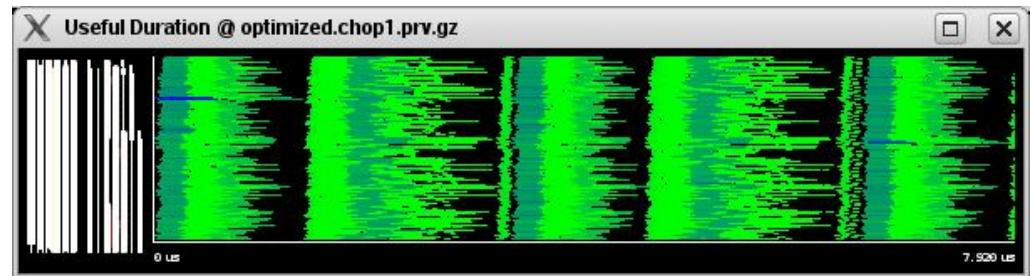
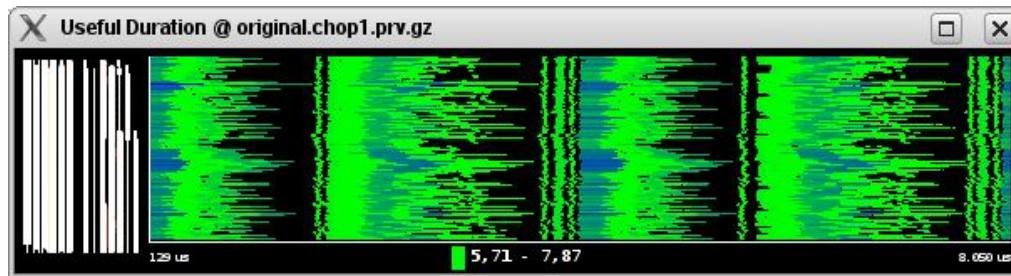
- Improved load balance – weight nodes based on their connectivity, balance total weight
- Reduction of all to all communications – half of MPI_Allreduce calls were eliminated
- Reduce cache misses – reordering node number

Half an hour meeting for the analysis, few days of work to modify code → 25% of improvement

Example: Code optimization



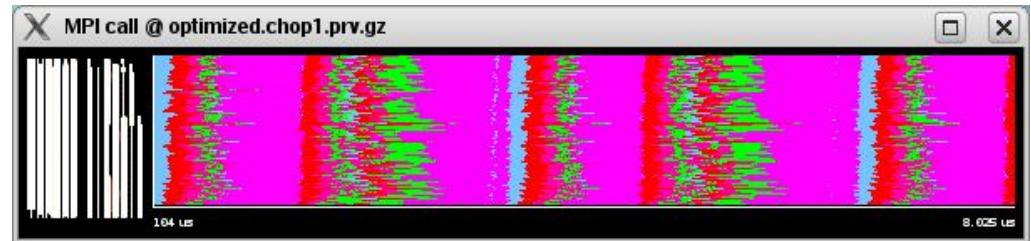
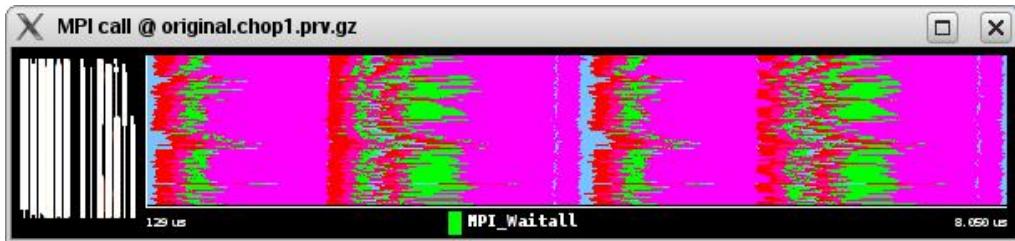
256 tasks – Load balance



Example: Code optimization



256 tasks – MPI time



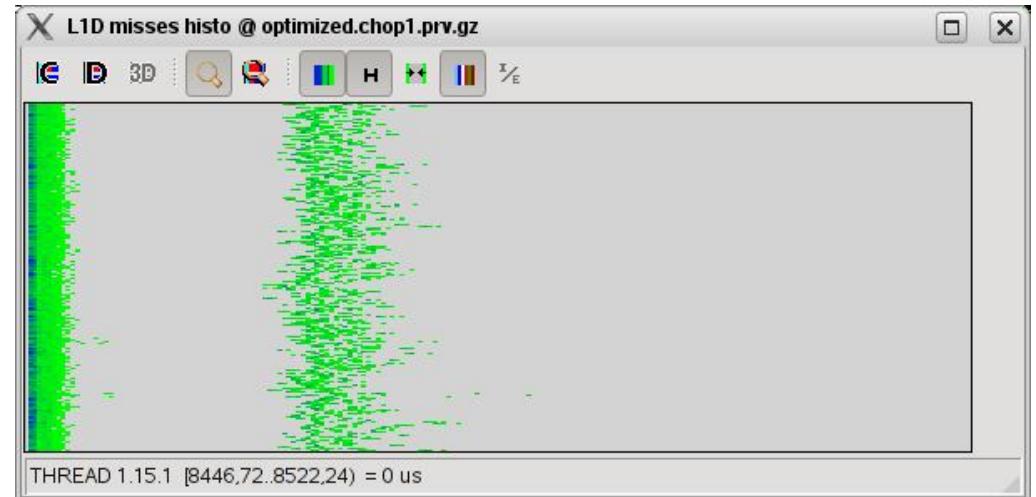
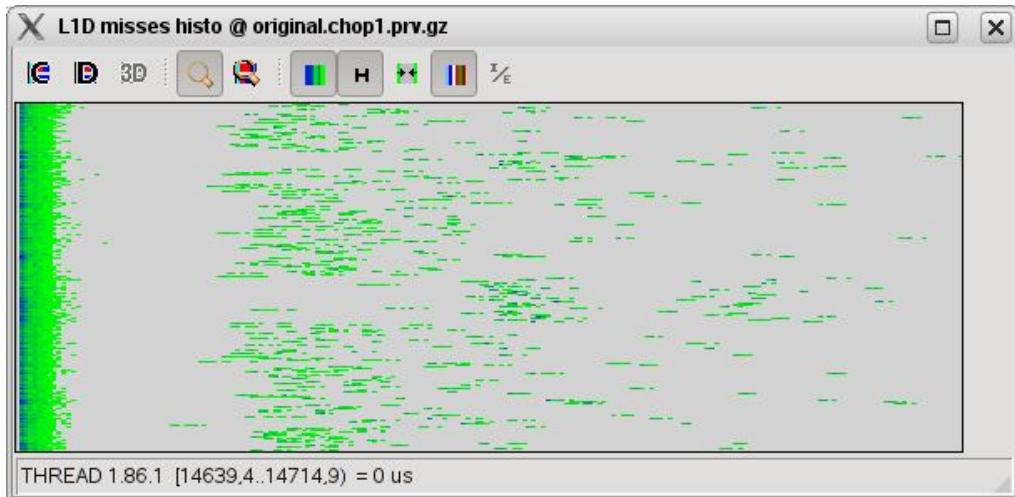
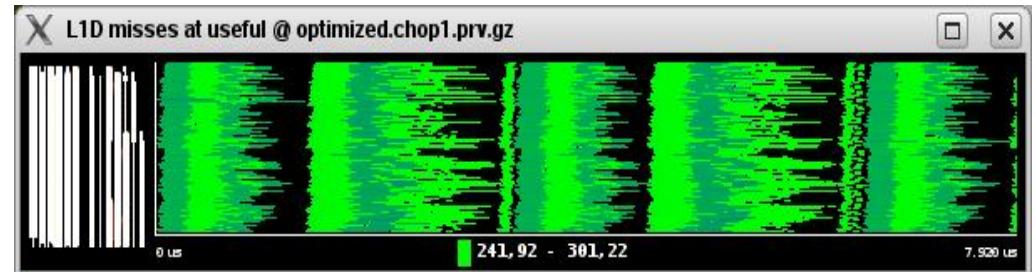
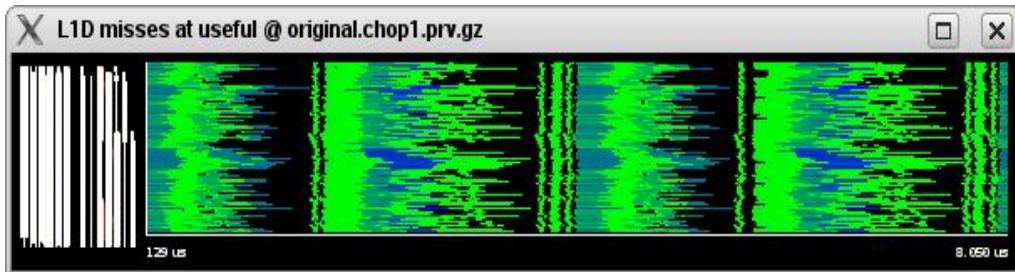
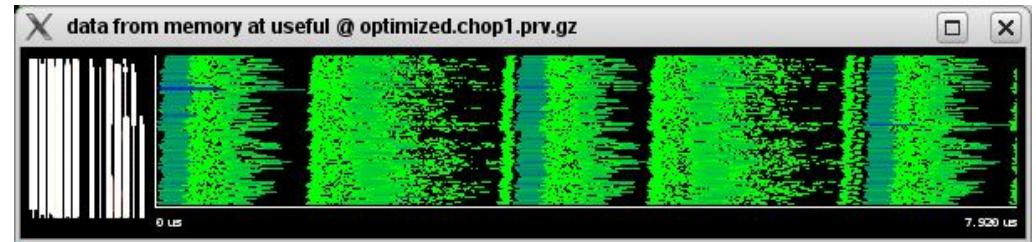
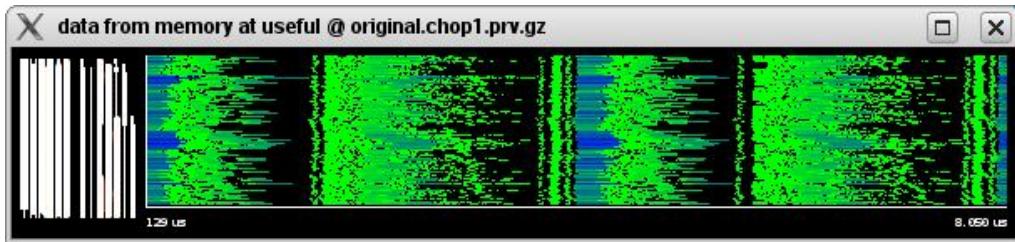
	End	MPI_Isend	MPI_Irecv	MPI_Waitall	MPI_Allreduce
Total	7.617,81 %	2.432,05 %	1.772,21 %	2.245,19 %	11.532,74 %
Average	29,76 %	9,50 %	6,92 %	8,77 %	45,05 %
Maximum	51,85 %	18,11 %	13,00 %	28,59 %	67,69 %
Minimum	17,59 %	1,65 %	1,37 %	1,46 %	14,88 %
StDev	8,04 %	3,33 %	2,39 %	6,05 %	11,03 %
Avg/Max	0,57	0,52	0,53	0,31	0,67

	End	MPI_Isend	MPI_Irecv	MPI_Waitall	MPI_Allreduce
Total	9.089,05 %	3.100,13 %	2.107,96 %	1.511,02 %	9.791,83 %
Average	35,50 %	12,11 %	8,23 %	5,90 %	38,25 %
Maximum	51,05 %	20,77 %	14,59 %	21,31 %	64,34 %
Minimum	22,99 %	3,47 %	3,21 %	1,72 %	10,90 %
StDev	5,92 %	3,62 %	2,61 %	3,89 %	10,13 %
Avg/Max	0,70	0,58	0,56	0,28	0,59

Example: Code optimization



256 tasks – Memory access



Outline



The tools

Introduction

Paraver

Applied research: clustering and sampling

Analysis examples

Dimemas

Simulation examples

Some GPUs examples

GPUSs

HMPP

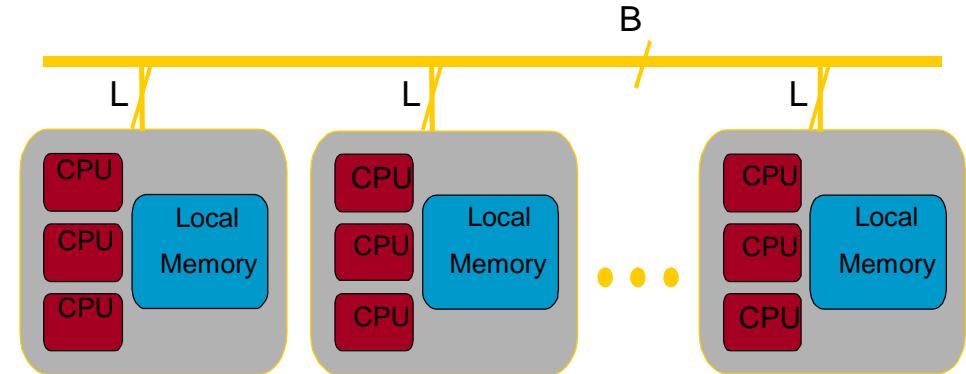
Extrae support

Key factors influencing performance

Abstract architecture

Basic MPI protocols

No attempt to model details



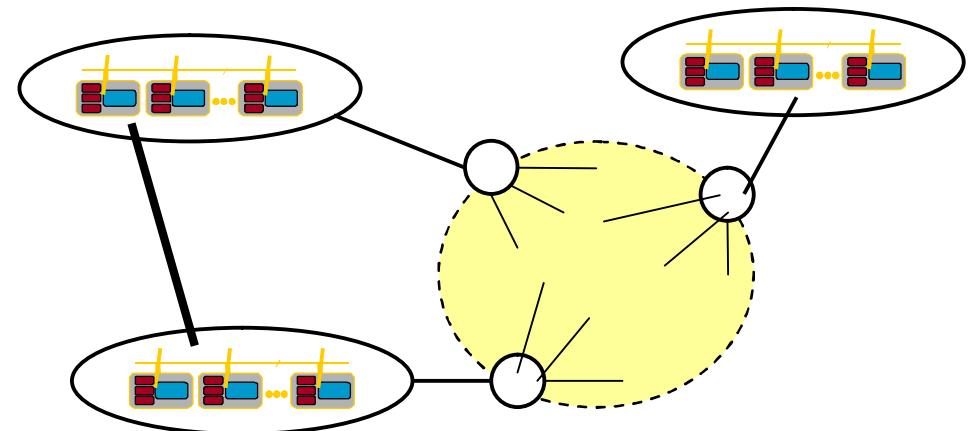
$$T = \frac{\text{MessageSize}}{\text{BW}} + L$$

Objectives

Simple / general

Fast simulations

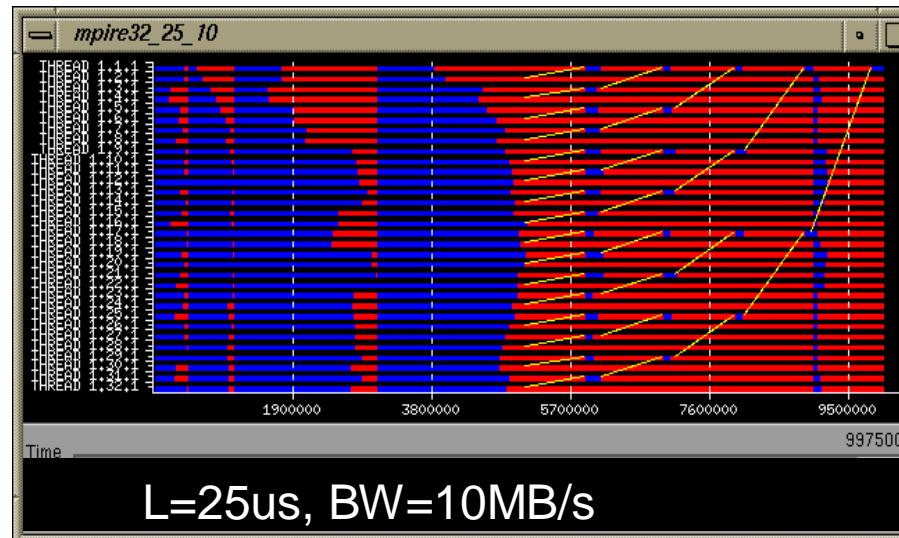
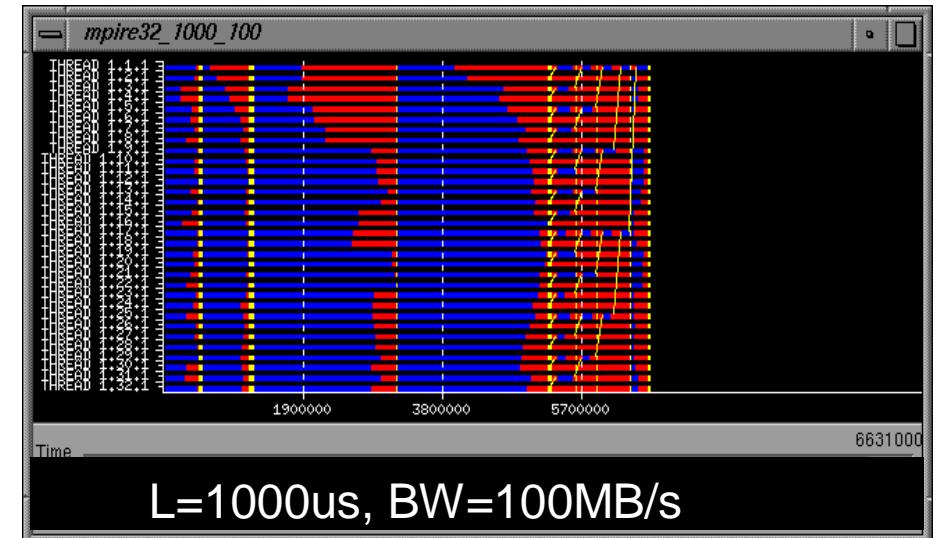
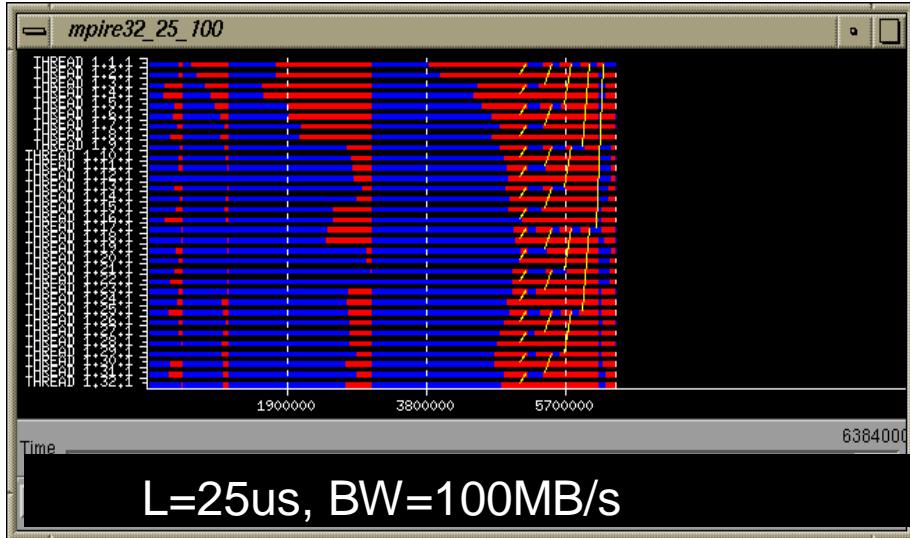
Network of SMPs / GRID



Understanding applications



MPIRE 32 tasks, no network contention

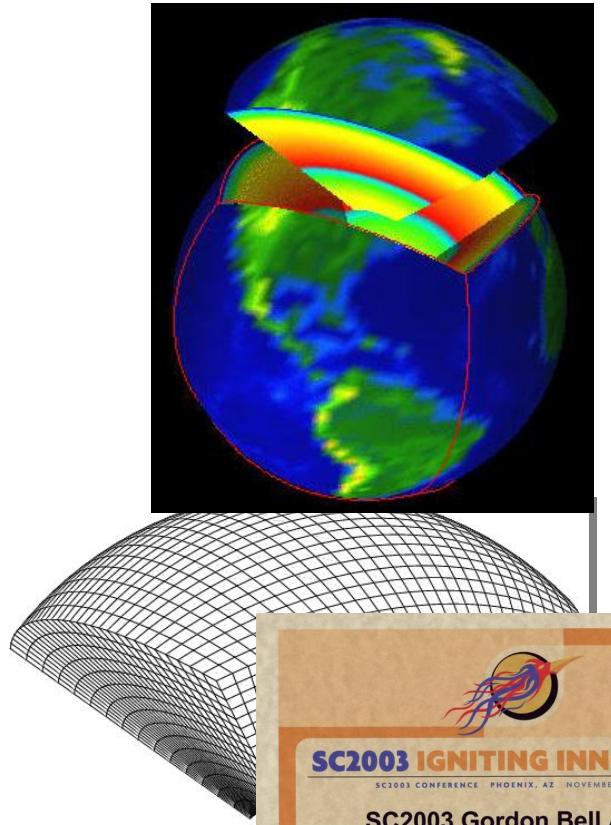


All windows same scale

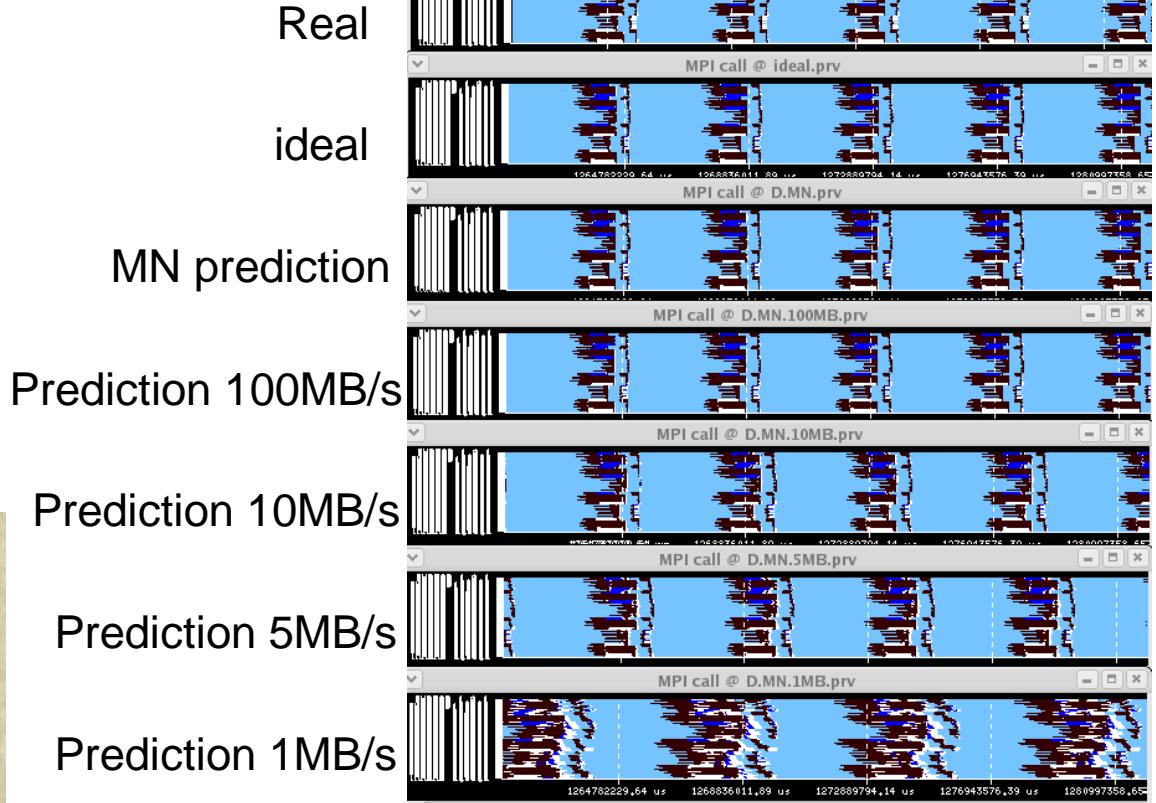
Predicting performance



SPECFEM3D – asynchronous communication?



Courtesy Dimitri Komatitsch



Parametric studies – network sensitivity

WRF, Iberia 4Km, 4 procs/node

None sensitive to latency

NMM

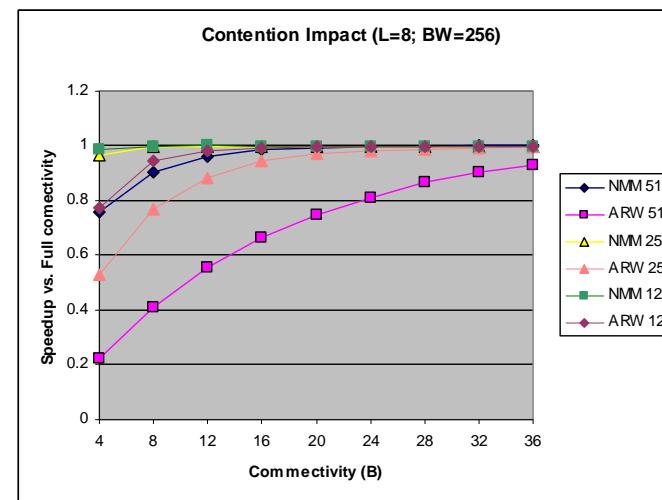
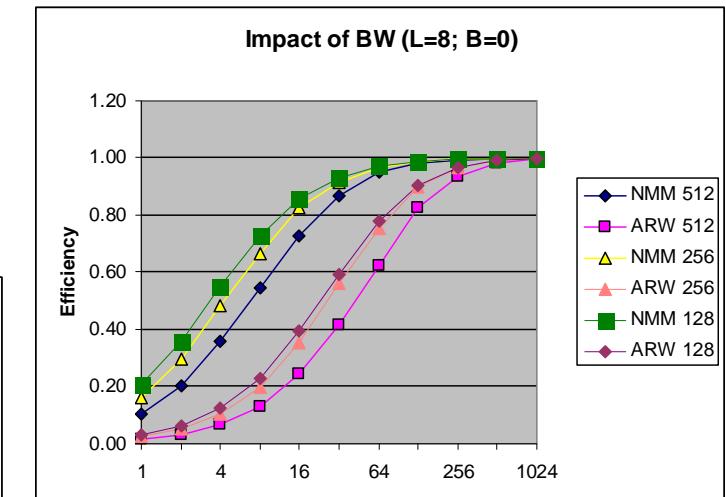
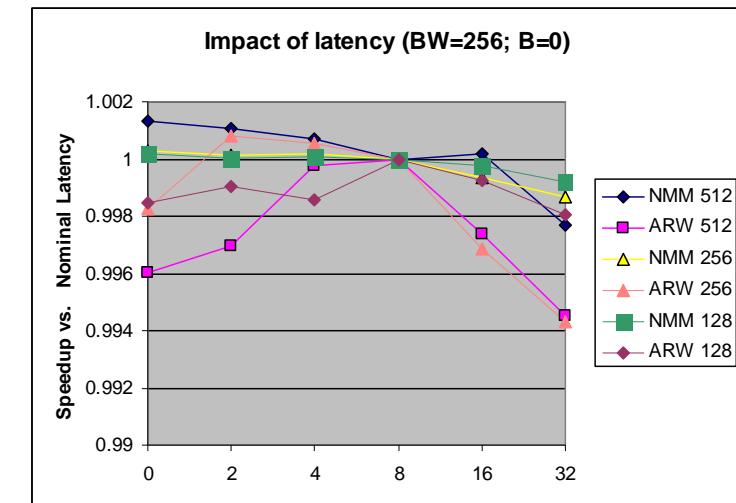
Bw – 256MB/s

512 – sensitive to contention

ARW

Bw - 1GB/s

Sensitive to contention



Multiscale simulation: L2 size vs network bw

Left: clusters IPC with different cache sizes

- 64KB - 512MB

Right: execution time with different network bw and cache size

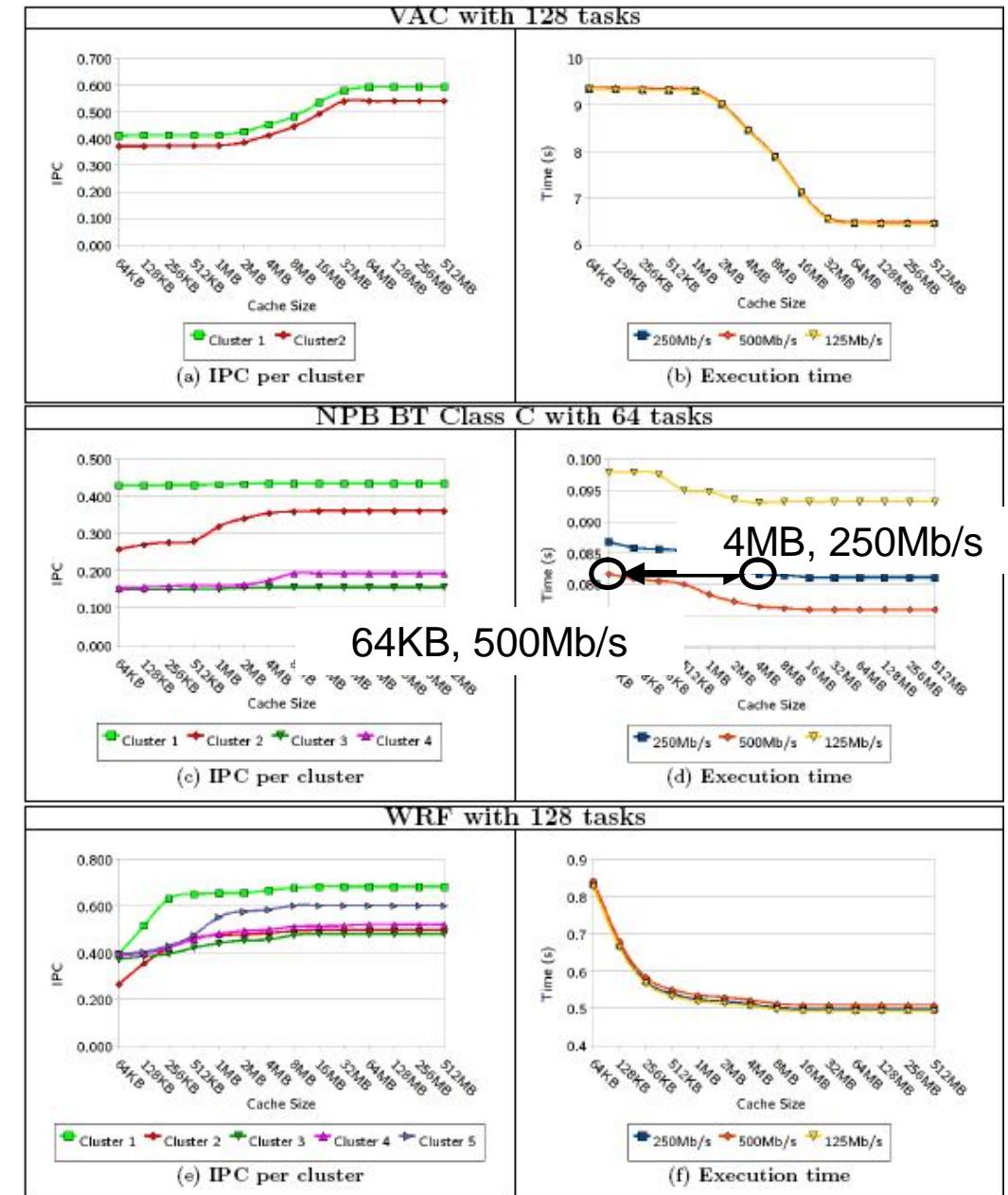
- 125Mb/s - 500Mb/s

NAS BT

- Can compensate cache reduction with more network bw

VAC, WRF

- Dominated by comp.

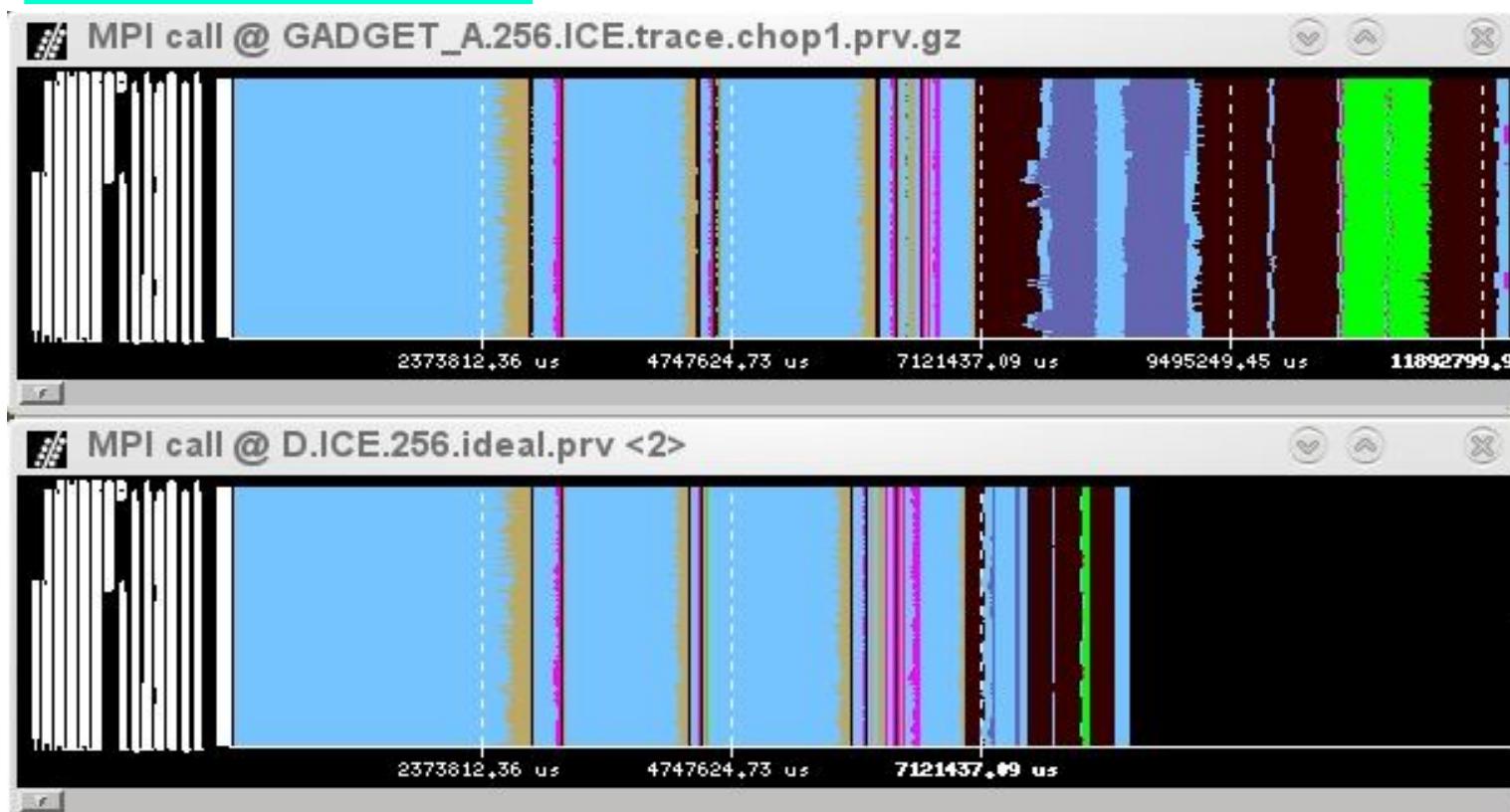


Fighting Amdahl's law



GADGET behavior: load balance / dependences?

Real run



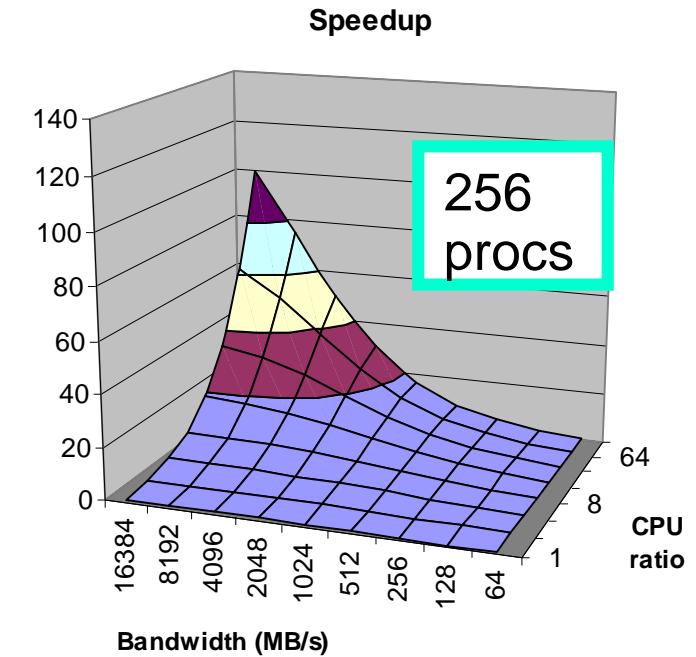
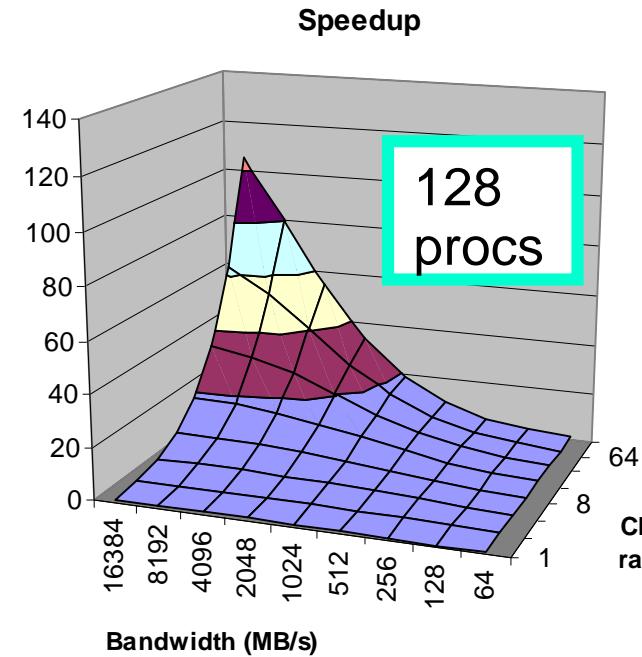
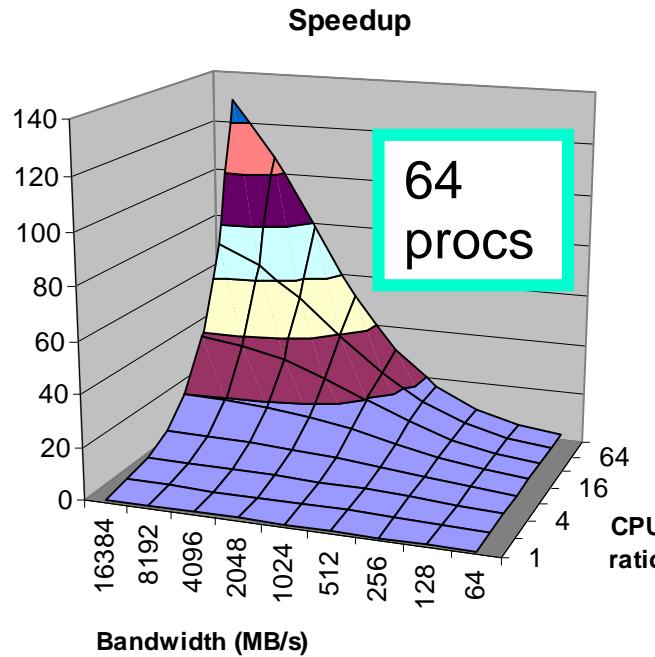
Ideal network: infinite bandwidth, no latency

Fighting Amdahl's law



Speeding up **all** computation burst by CPU ratio

The more processes, less speed up – higher impact of bw limitations

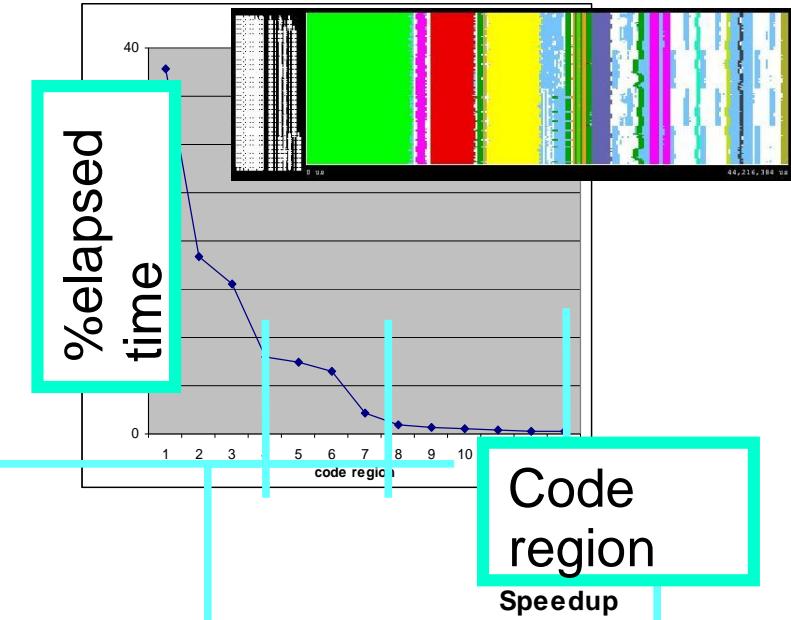


Fighting Amdahl's law



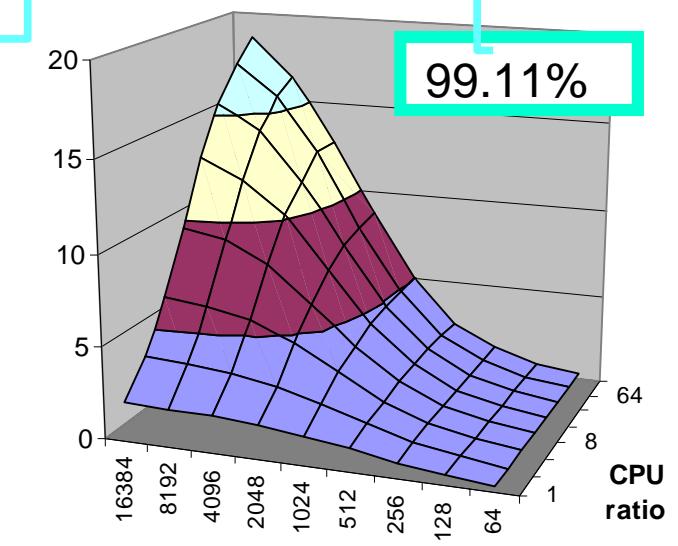
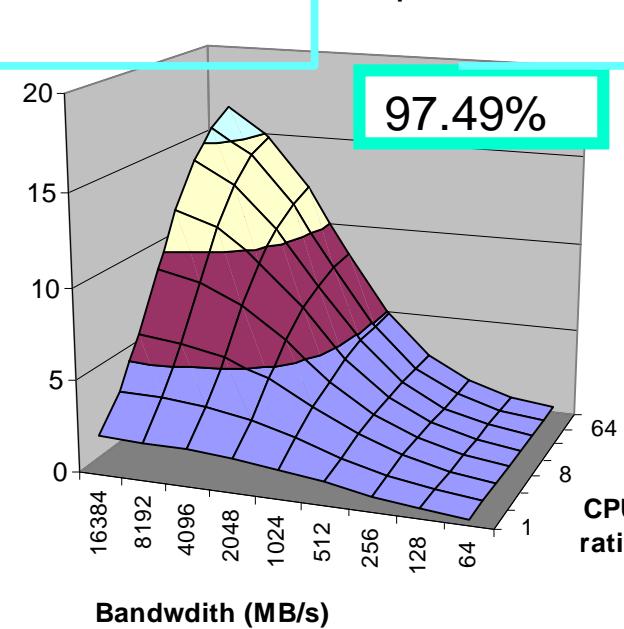
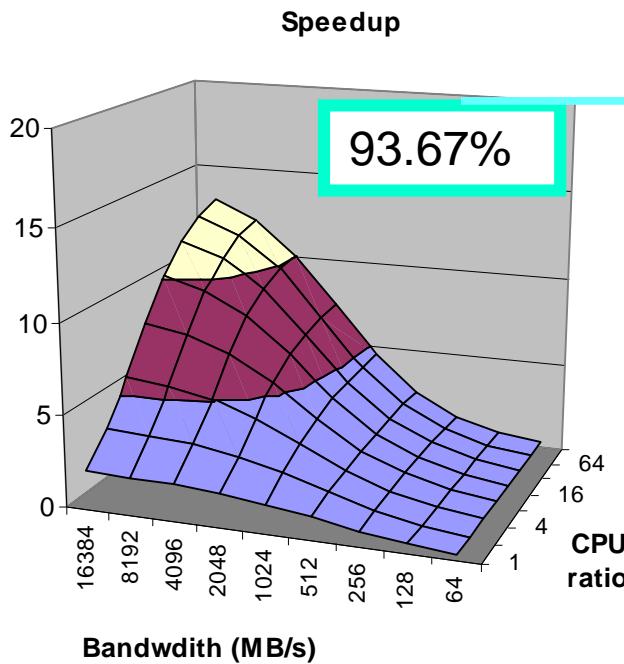
Hybrid parallelization (128 procs)

Speed up only selected regions
by CPU ratio



Code region

Speedup



Outline



The tools

Introduction

Paraver

Applied research: clustering and sampling

Analysis examples

Dimemas

Simulation examples

Some GPUs examples

GPUSs

HMPP

Extrae support

StarSs: a sequential program...



Understandable to a numerical analyst

```
void Cholesky( float *A ) {
    int i, j, k;
    for (k=0; k<NT; k++) {
        spotrf (A[k*NT+k]) ;
        for (i=k+1; i<NT; i++)
            strsm (A[k*NT+k], A[k*NT+i]);
        // update trailing submatrix
        for (i=k+1; i<NT; i++) {
            for (j=k+1; j<i; j++)
                sgemm( A[k*NT+i], A[k*NT+j], A[j*NT+i]);
            ssyrk (A[k*NT+i], A[i*NT+i]);
        }
    }
}
```

```
void spotrf (float *A);

void ssyrk (float *A, float *C);

void sgemm (float *A, float *B, float *C);

void strsm (float *T, float *B);
```



Compiler translate source to runtime calls

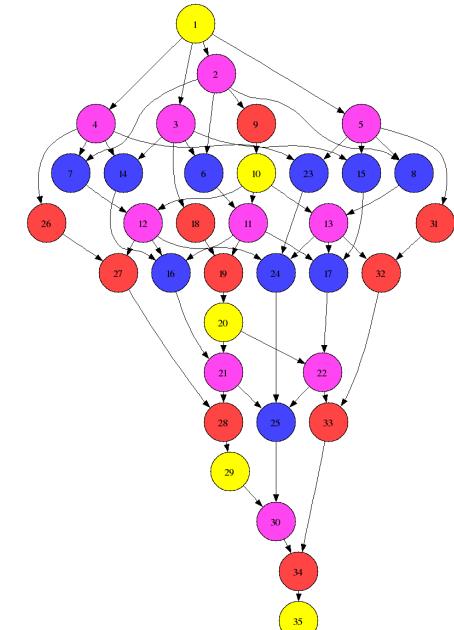
```
void Cholesky( float *A ) {
    int i, j, k;
    for (k=0; k<NT; k++) {
        spotrf (A[k*NT+k]) ;
        for (i=k+1; i<NT; i++)
            strsm (A[k*NT+k], A[k*NT+i]);
        // update trailing submatrix
        for (i=k+1; i<NT; i++) {
            for (j=k+1; j<i; j++)
                sgemm( A[k*NT+i], A[k*NT+j], A[j*NT+i]);
            ssyrk (A[k*NT+i], A[i*NT+i]);
        }
    }
}

#pragma omp task inout ([TS][TS]A)
void spotrf (float *A);
#pragma omp task input ([TS][TS]A) inout ([TS][TS]C)
void ssyrk (float *A, float *C);
#pragma omp task input ([TS][TS]A,[TS][TS]B) inout ([TS][TS]C)
void sgemm (float *A, float *B, float *C);
#pragma omp task input ([TS][TS]T) inout ([TS][TS]B)
void strsm (float *T, float *B);
```

StarSs: ... and dynamically executed

Data flow model – graph generated at run time

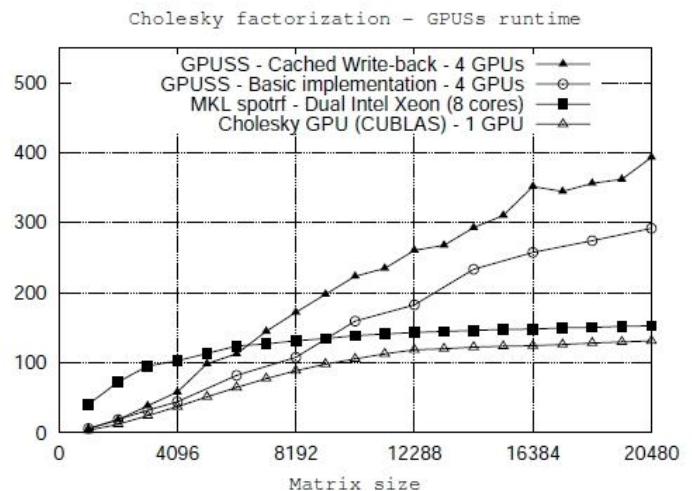
```
void Cholesky( float *A ) {  
    int i, j, k;  
    for (k=0; k<NT; k++) {  
        spotrf (A[k*NT+k]) ;  
        for (i=k+1; i<NT; i++)  
            strsm (A[k*NT+k], A[k*NT+i]);  
        // update trailing submatrix  
        for (i=k+1; i<NT; i++) {  
            for (j=k+1; j<i; j++)  
                sgemm( A[k*NT+i], A[k*NT+j], A[j*NT+i]);  
            ssyrk (A[k*NT+i], A[i*NT+i]);  
        }  
    }  
  
    #pragma omp task inout ([TS][TS]A)  
    void spotrf (float *A);  
    #pragma omp task input ([TS][TS]A) inout ([TS][TS]C)  
    void ssyrk (float *A, float *C);  
    #pragma omp task input ([TS][TS]A,[TS][TS]B) inout ([TS][TS]C)  
    void sgemm (float *A, float *B, float *C);  
    #pragma omp task input ([TS][TS]T) inout ([TS][TS]B)  
    void strsm (float *T, float *B);
```





GPUSs

Cholesky @ 1-4 GPUs



Same source any target

Possibly optimised tasks
Different implementations

Transparent data transfer

Prefetch, double buffer
Locality aware scheduler

```
#pragma css task inout (A[TS][TS])
void chol_spotrf (float *A);
```

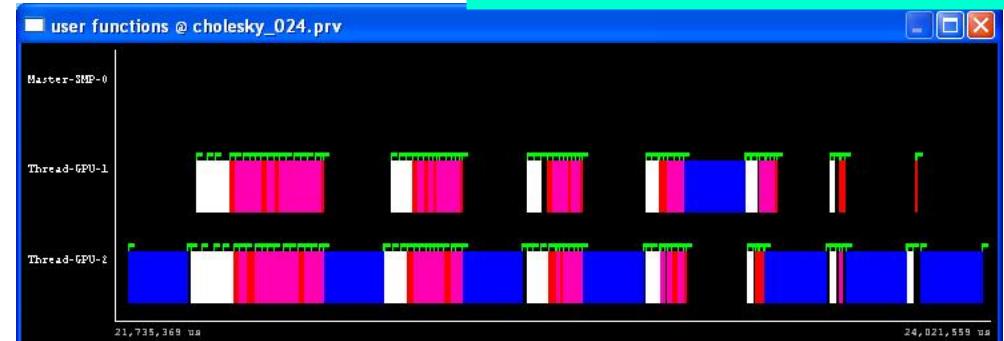
```
#pragma css target device (cell, cuda) copy_deps
#pragma css task input (A[TS][TS], B[TS][TS}) inout (C[TS][TS])
void chol_sgemm (float *A, float *B, float *C);
```

Block matrix storage at CPU



n = 8192; bs = 1024

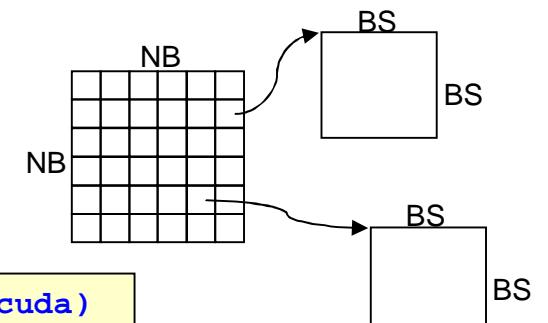
Source code independent of #devices



```
void blocked_cholesky( int NT, float *A ) {  
    int i, j, k;  
    for (k=0; k<NT; k++) {  
        spotrf (A[k*NT+k]) ;  
        for (i=k+1; i<NT; i++)  
            strsm (A[k*NT+k], A[k*NT+i]);  
        // update trailing submatrix  
        for (i=k+1; i<NT; i++) {  
            for (j=k+1; j<i; j++)  
                sgemm( A[k*NT+i], A[k*NT+j], A[j*NT+i]);  
                ssyrk (A[k*NT+i], A[i*NT+i]);  
        }  
    }  
}
```

Spotrf: Slow task @ GPU - In critical path (scheduling problem)

```
#pragma css task input([NB*NB]A, [NB*NB]B) inout([NB*NB]C) target device (cuda)  
void sgemm(float *A, float *B, float *C, unsigned long NB)  
{  
    unsigned char TR='T', NT='N';  
    float DONE=1.0, DMONE=-1.0;  
    cublasSgemm( NT, TR, NB, NB, NB, DMONE, A, NB, B, NB, DONE,C, NB );  
}
```

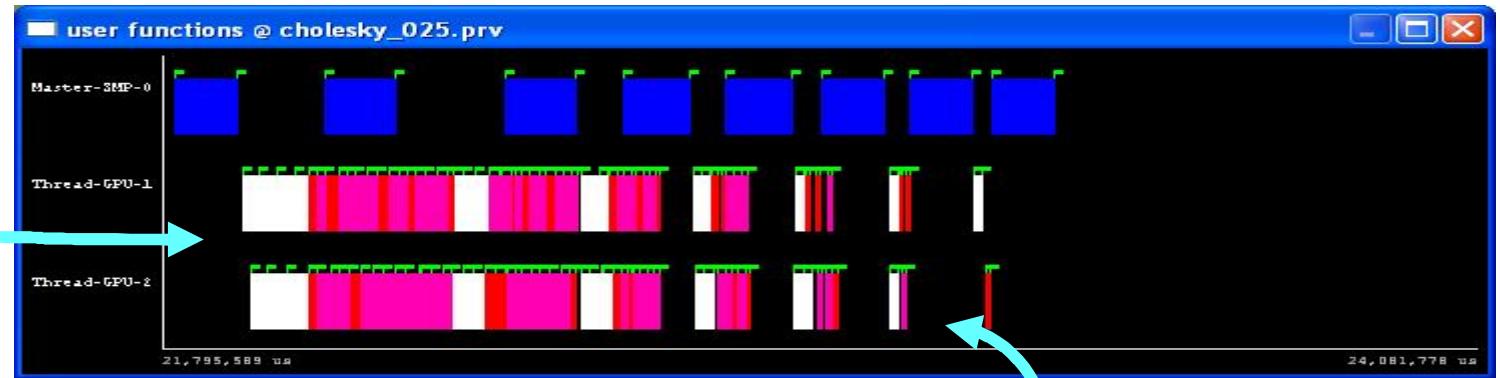


Heterogeneous execution



Spotrf more efficient at CPU
Overlap between CPU and GPU

n = 8192; bs = 1024



```
#pragma omp task inout([NB*NB]A) target device (smp)
void spotrf_tile(float *A, int NB)
{
    long INFO;
    char L = 'L';

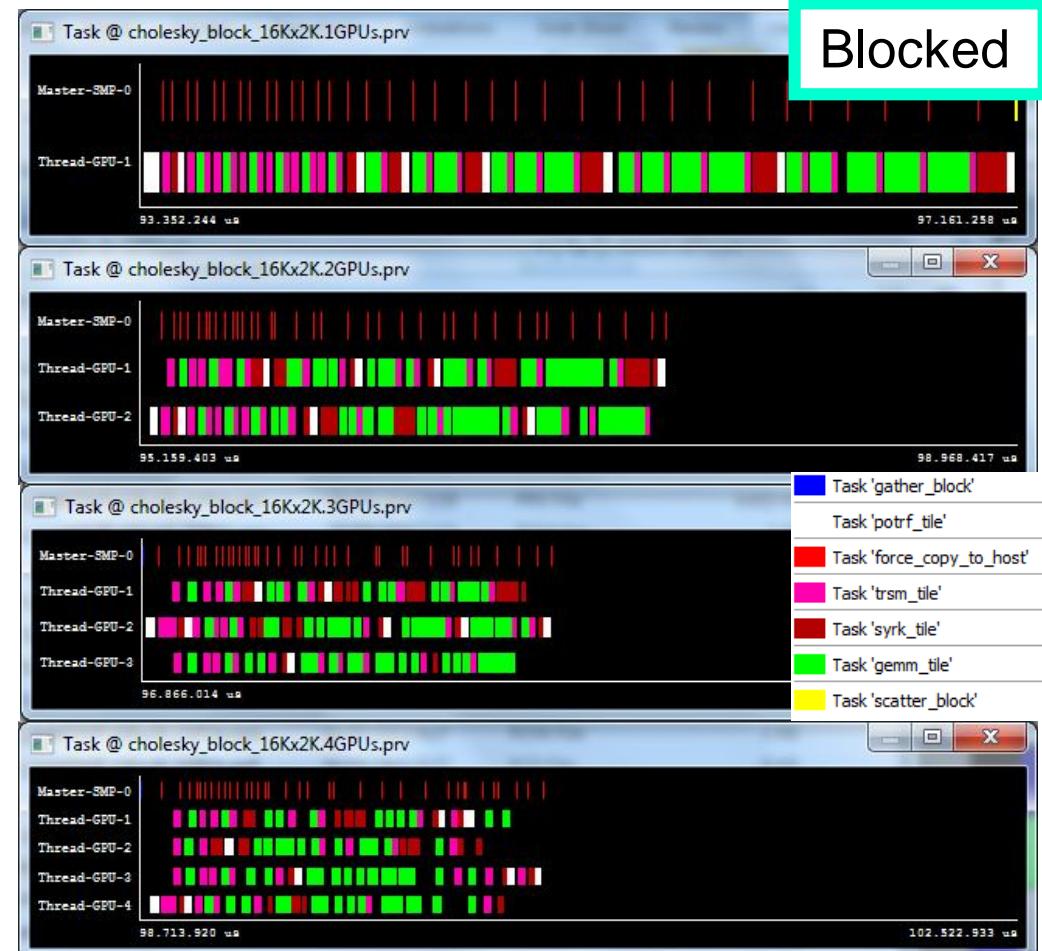
    spotrf_( &L, &NB, A, &NB, &INFO );
}
```

Cholesky performance



Matrix size: 16K x 16K

- Block size: 2K x 2K
- Storage: Blocked / contiguous
- Tasks:
 - `spotrf`: Magma
 - `trsm`, `syrk`, `gemm`: CUBLAS



Two Intel Xeon E5440, 4 cores
4 Tesla S2050 GPUs

Comparing 2GPUs and 4GPUs

% running time significantly decreases

	Master-SMP-0	Thread-GPU-1	Thread-GPU-2
SHUTDOWN	-	-	-
ERROR	-	-	-
IDLE	66,18 %	4,72 %	4,31 %
RUNTIME	29,45 %	9,72 %	8,83 %
RUNNING	1,13 %	70,48 %	71,55 %
SYNCHRONIZATION	3,17 %	0,02 %	0,01 %
SCHEDULING	0,04 %	0,01 %	0,01 %
CREATION	0,02 %	-	-
DATA TRANSFER TO DEVICE	-	15,04 %	15,27 %
DATA TRANSFER TO HOST	0,01 %	0,00 %	0,00 %
LOCAL DATA TRANSFER IN DEVICE	-	-	-

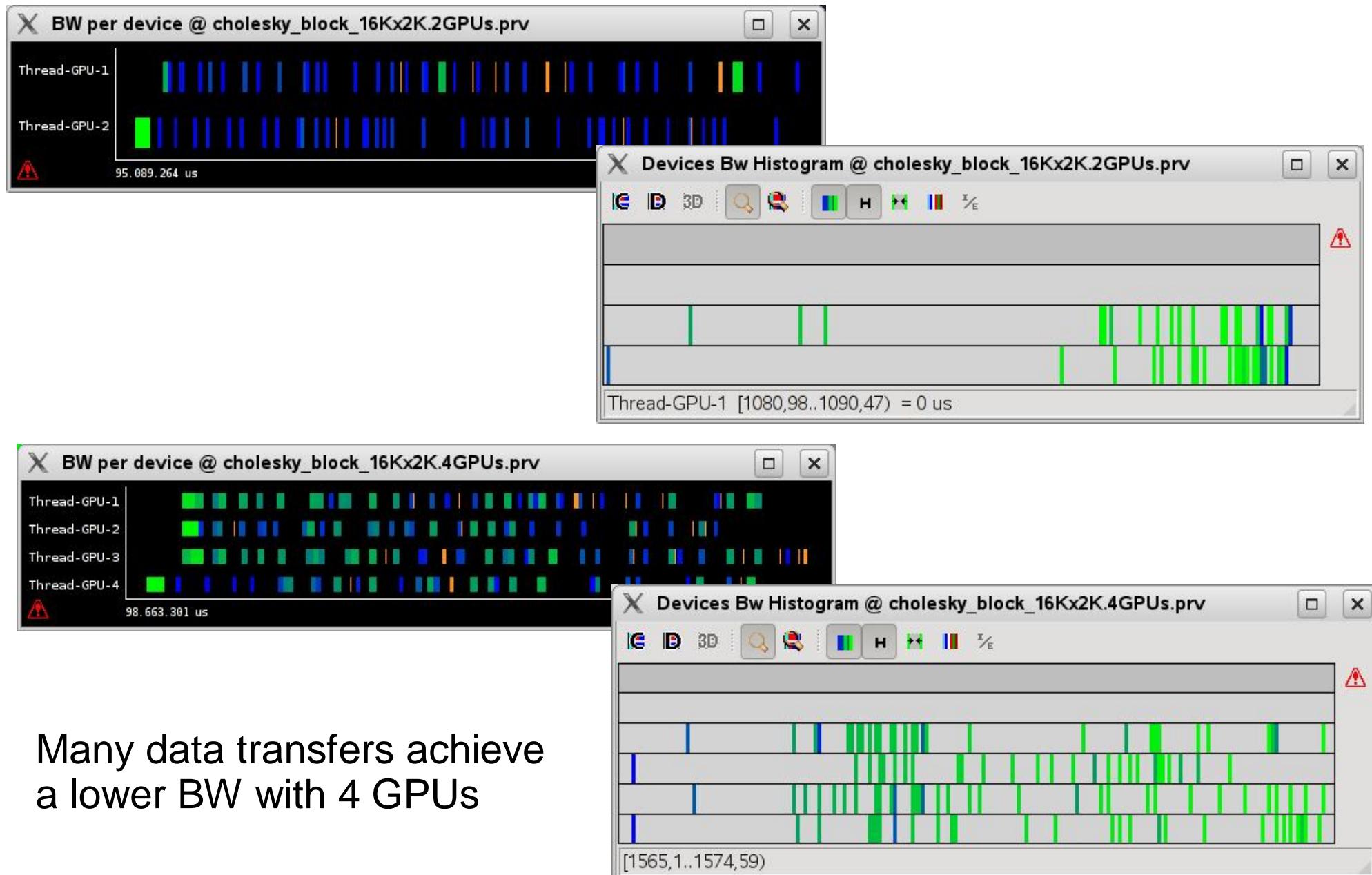
	Master-SMP-0	Thread-GPU-1	Thread-GPU-2	Thread-GPU-3	Thread-GPU-4
SHUTDOWN	-	-	-	-	-
ERROR	-	-	-	-	-
IDLE	50,77 %	12,25 %	20,66 %	7,05 %	14,63 %
RUNTIME	45,07 %	13,62 %	11,71 %	14,18 %	11,61 %
RUNNING	0,05 %	46,11 %	45,29 %	50,99 %	51,40 %
SYNCHRONIZATION	4,05 %	0,02 %	0,01 %	0,02 %	0,01 %
SCHEDULING	0,02 %	0,01 %	0,00 %	0,01 %	0,01 %
CREATION	0,03 %	-	-	-	-
DATA TRANSFER TO DEVICE	-	27,97 %	22,31 %	27,73 %	22,32 %
DATA TRANSFER TO HOST	0,01 %	0,00 %	0,00 %	0,00 %	0,00 %
LOCAL DATA TRANSFER IN DEVICE	-	-	-	-	-

while average data transfer increases

	Master-SMP-0	Thread-GPU-1	Thread-GPU-2
SHUTDOWN	-	-	-
ERROR	-	-	-
IDLE	20.619.067,57 ns	581.564,06 ns	574.129,30 ns
RUNTIME	1.593.852,11 ns	186.670,27 ns	177.580,28 ns
RUNNING	128.155,07 ns	26.207.403,23 ns	28.442.120,69 ns
SYNCHRONIZATION	1.462.820 ns	6.967,74 ns	5.758,62 ns
SCHEDULING	7.714,29 ns	8.259,26 ns	6.805,56 ns
CREATION	3.886,79 ns	-	-
DATA TRANSFER TO DEVICE	-	9.371.324,32 ns	9.029.515,62 ns
DATA TRANSFER TO HOST	5.972,22 ns	4.000 ns	4.000 ns
LOCAL DATA TRANSFER IN DEVICE	-	-	-

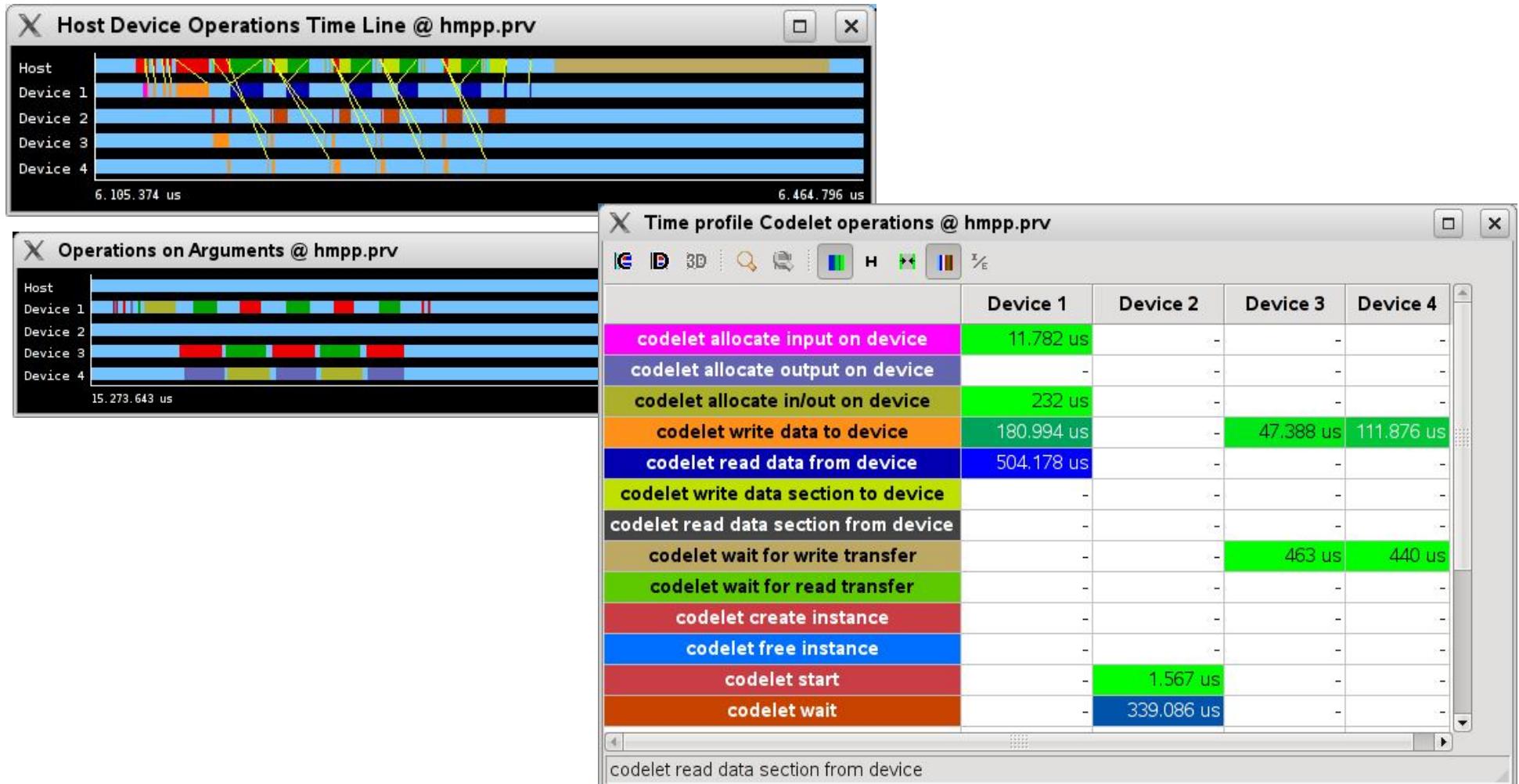
	Master-SMP-0	Thread-GPU-1	Thread-GPU-2	Thread-GPU-3	Thread-GPU-4
SHUTDOWN	-	-	-	-	-
ERROR	-	-	-	-	-
IDLE	12.752.000 ns	2.333.265,43 ns	4.068.342,66 ns	1.342.990,70 ns	2.756.242,79 ns
RUNTIME	2.018.561,59 ns	376.358,85 ns	343.966,10 ns	388.232,23 ns	318.495,25 ns
RUNNING	5.930,96 ns	26.636.066,67 ns	27.066.344,83 ns	29.455.166,67 ns	28.734.258,06 ns
SYNCHRONIZATION	1.798.128,21 ns	9.133,33 ns	6.586,21 ns	10.166,67 ns	7.225,81 ns
SCHEDULING	11.250 ns	9.217,39 ns	5.400 ns	5.409,09 ns	6.833,33 ns
CREATION	7.421,88 ns	-	-	-	-
DATA TRANSFER TO DEVICE	-	13.466.916,67 ns	12.470.903,23 ns	13.350.527,78 ns	12.477.187,66 ns
DATA TRANSFER TO HOST	7.441,18 ns	5.500 ns	5.400 ns	5.000 ns	5.000 ns
LOCAL DATA TRANSFER IN DEVICE	-	-	-	-	-

Comparing 2GPUs and 4GPUs





Same analysis tool, different programming model,
different concepts

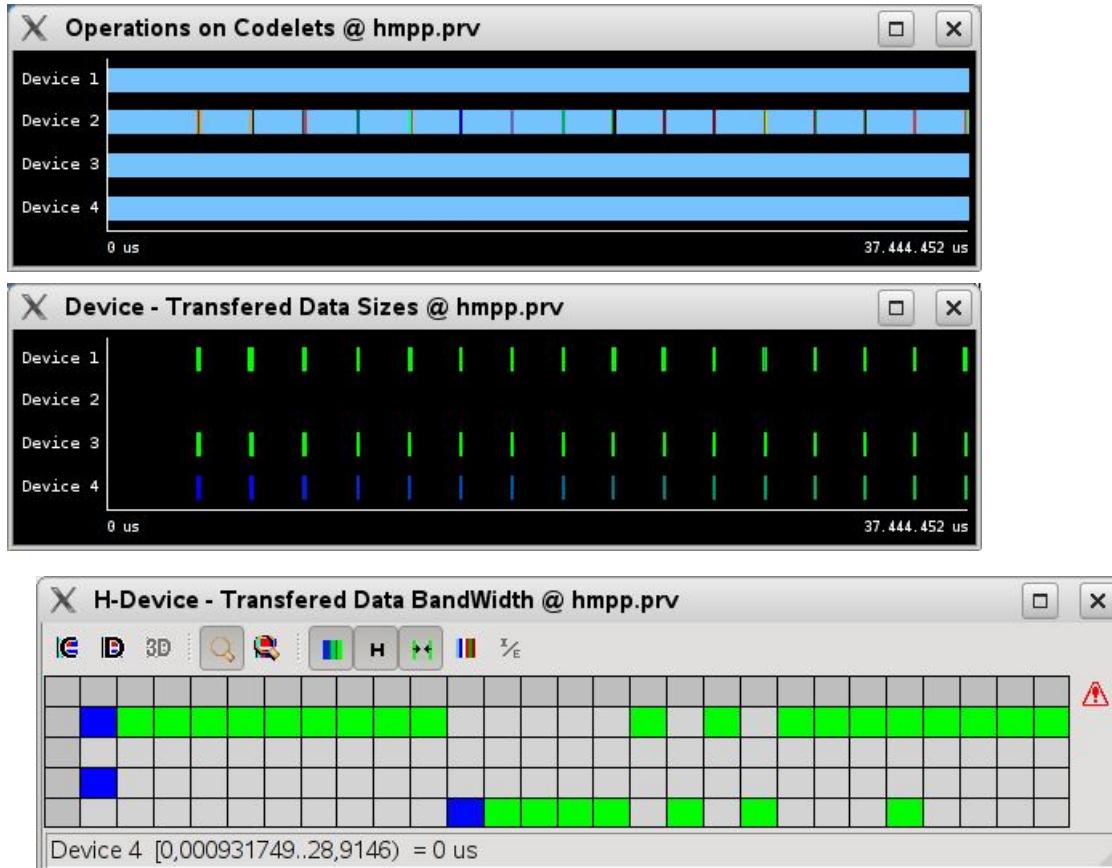


HMPP methodology



Analysis methodology predefined

- CAPS distribute it with a complete set of views
 - If sequenced, can be used as an exploratory tree

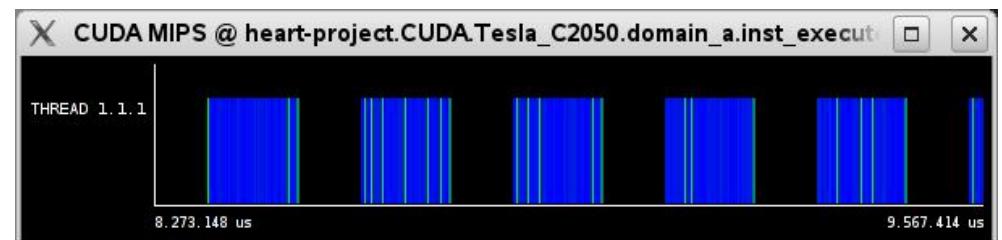
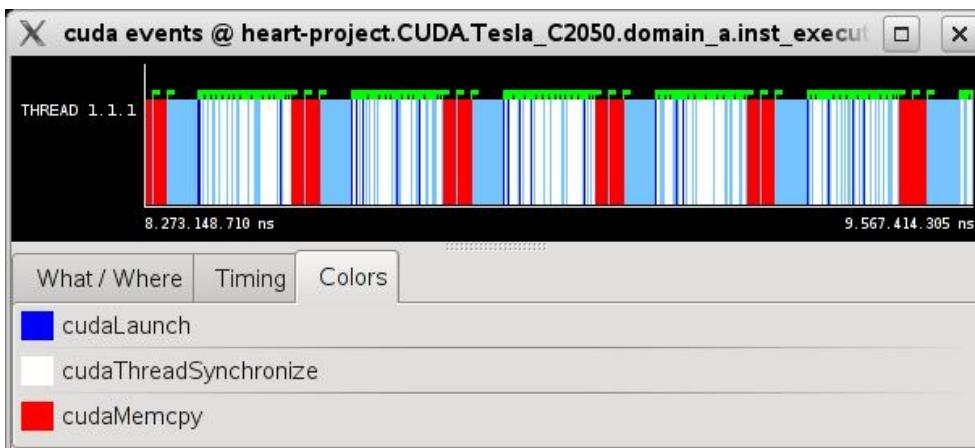


H-Codelet Operation Durations @ hmpp.prv	
TASK 2.1	
[59800..1,84447e+07)	1.158 us
[1,84447e+07..3,68296e+07)	34.221 us
[3,68296e+07..5,52146e+07)	28.898 us
[5,52146e+07..7,35995e+07)	59.878 us
[7,35995e+07..9,19844e+07)	49.857 us
[9,19844e+07..1,10369e+08)	112.297 us
[1,10369e+08..1,28754e+08)	52.466 us
[1,28754e+08..1,47139e+08)	21.243 us
[1,47139e+08..1,65524e+08)	4.079 us
[1,65524e+08..1,83909e+08)	17.514 us
[1,83909e+08..2,02294e+08)	3.278 us
[2,02294e+08..2,20679e+08)	-
[2,20679e+08..2,39064e+08)	5.066 us
[2,39064e+08..2,57449e+08)	-
[2,57449e+08..2,75834e+08)	-
[2,75834e+08..2,94219e+08)	-
[2,94219e+08..3,12604e+08)	-
[3,12604e+08..3,30988e+08)	-
[3,30988e+08..3,49373e+08)	7.296 us
[3,49373e+08..3,67758e+08]	4.625 us
Total	401.876 us
Average	28.705,43 us
Maximum	112.297 us
Minimum	1.158 us
StDev	30.227,18 us

Extrاء support to CUDA



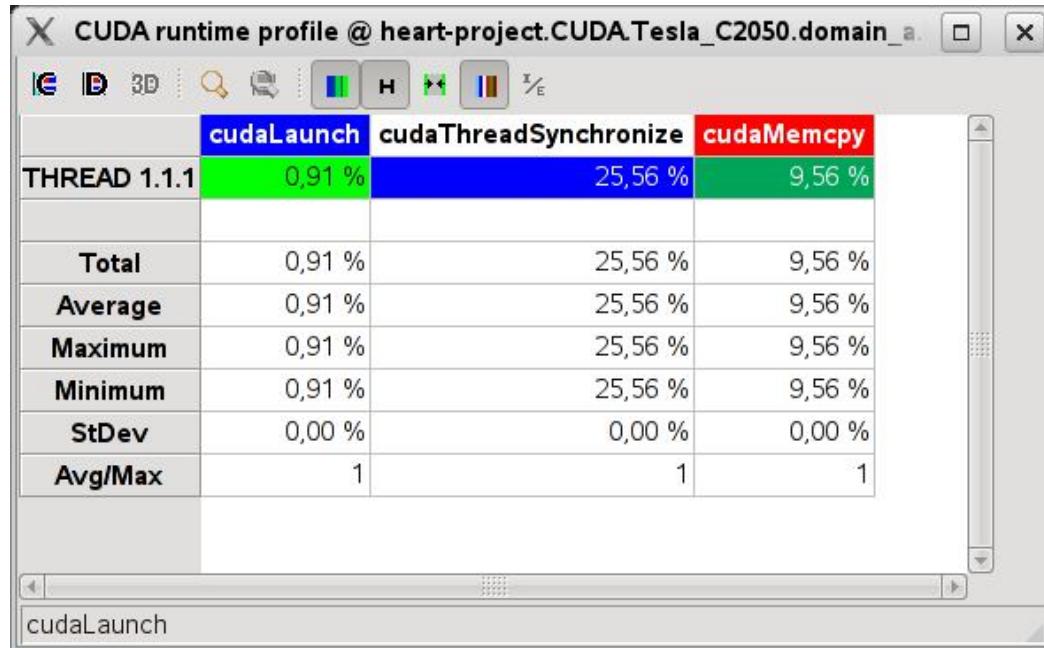
- Just starting
- Support to BSC/CASE department
 - Propagation of an electrical shock wave across the cardiac tissue
- Captured information
 - From CPU perspective
 - CUDA runtime calls
 - PAPI CUDA counters



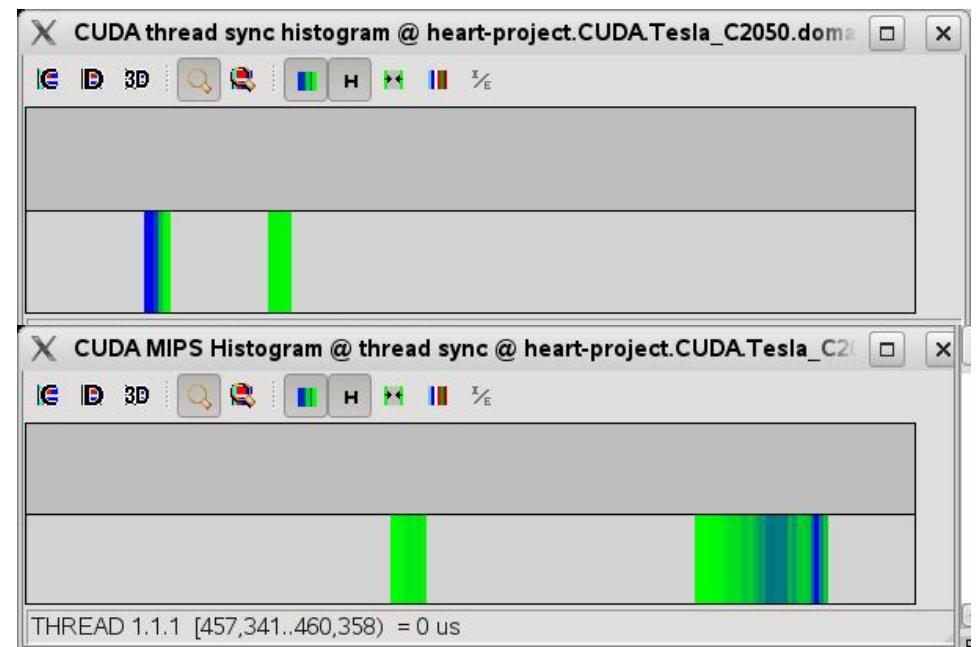
Example of CUDA analysis



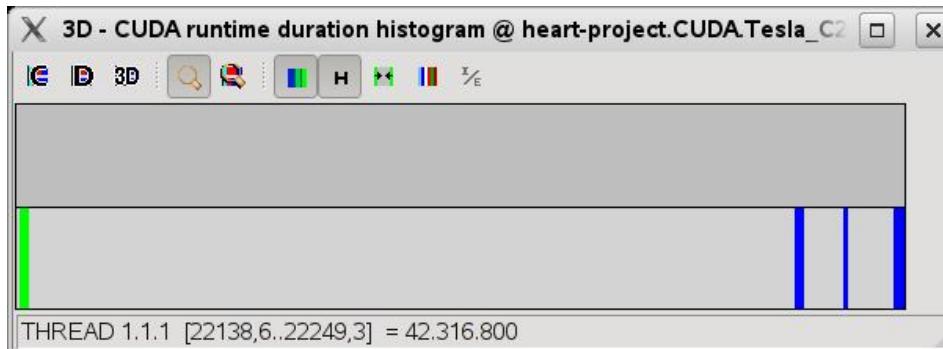
CUDA runtime profile



CUDA ThreadSync histogram



CUDA Memcpy histogram vs size



Conclusions



- The complexity of heterogeneous systems pushes the need for tools
- Same tools and similar methodology maybe used for very different scenarios
- Do not speculate about your code performance behaviour, look at it

www.bsc.es/paraver