Parallelizing Dense Matrix Factorizations on Clusters of Multicore Processors using SMPSs

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Motivation

Solution of linear systems

- Systems of linear equations,

  $$Ax = b,$$

  are ubiquitous in scientific and engineering apps.

- “Large-scale” linear systems arise, e.g., in
  - Molecular dynamics simulations,
  - Fast acoustic scattering problems,
  - Dielectric polarization of nanostructures,
  - Magneto-hydrodynamics, etc.

  In these apps., A is dense and x can easily have $O(100,000)$ entries!

- The LINPACK benchmark (Top500) is a disguised linear system

Motivation

Matrix factorizations

- The most efficient method to solve

  $$Ax = b,$$

  when A is dense, is to “transform” (factorize) the matrix into a simpler form, and then solve the resulting linear systems

- Depending on the structure of the matrix:
  - Cholesky factorization for s.p.d. $A \rightarrow U^T U$
  - QR factorization for nonsquare $A \rightarrow QR$
  - LU factorization for general $A \rightarrow P^T LU$

- Computing the factorization requires a cubic number of flops, but solving the transformed linear systems is easy and cheap; e.g.,

  $$\begin{array}{llcll} 1. & A & \rightarrow & U^T U & \text{(Cholesky factorization)} \\ 2. & U^T y & = & b & \\ 3. & Ux & = & y & \end{array}$$

Motivation

Libraries for clusters

- Message-passing
  - ScaLAPACK: `http://www.netlib.org/scalapack/`
  - PLAPACK: `http://www.cs.utexas.edu/~plapack/`
- Clusters of multi-core processors?
  - One MPI process per node + multi-threaded BLAS
  - One MPI process per core

Both are suboptimal!

Motivation

Goal:

- Exploit task-level parallelism of dense matrix factorizations with little intrusion in existing legacy codes
- ScaLAPACK routine for the Cholesky factorization
- Other matrix factorizations/apps. parallelized as part of project text:

`http://www.project-text.eu/`

- Barcelona Supercomputer Center
- HLRS Stuttgart
- Jülich Supercomputer Center
- EPCC
- FORTH
- The University of Manchester
- Universitat Jaume I
- IBM Research Zurich
- Université de Pau

Outline

1. Introduction and motivation
2. Brief overview of Cholesky factorization
3. Message-passing Cholesky factorization in ScaLAPACK
4. MPI/SMPSs task-ification of ScaLAPACK/Cholesky
5. Performance evaluation
6. Conclusions

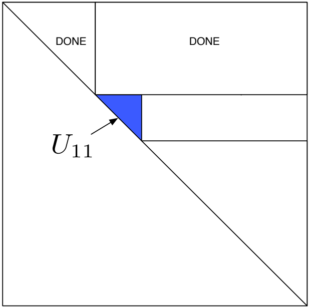
Right-Looking Blocked Cholesky Factorization

Definition

Factors A into the product $A = U^T U$, where A is s.p.d. and U upper triangular

Single R-L step

1. Factorize diagonal block
   $A_{11} \longrightarrow U_{11}^T U_{11}$



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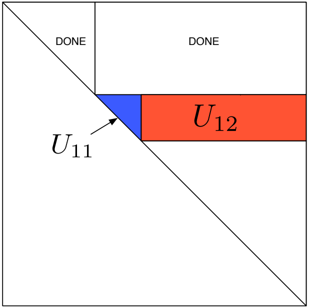
   $U_{12} \longleftarrow (U_{11}^T)^{-1} A_{12}$



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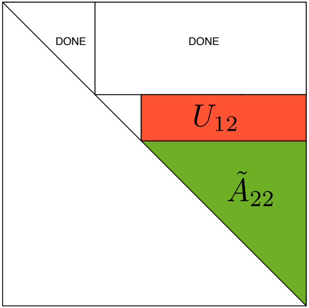
1. Factorize diagonal block
   $A_{11} \rightarrow U_{11}^T U_{11}$
2. Compute panel
   $U_{12} \leftarrow (U_{11}^T)^{-1} A_{12}$
3. Update trailing submatrix
   $\tilde{A}_{22} \leftarrow A_{22} - U_{12}^T U_{12}$



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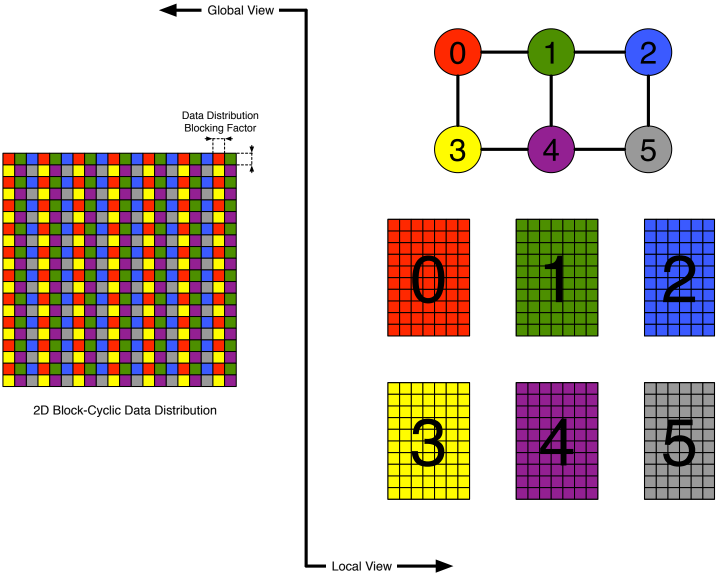
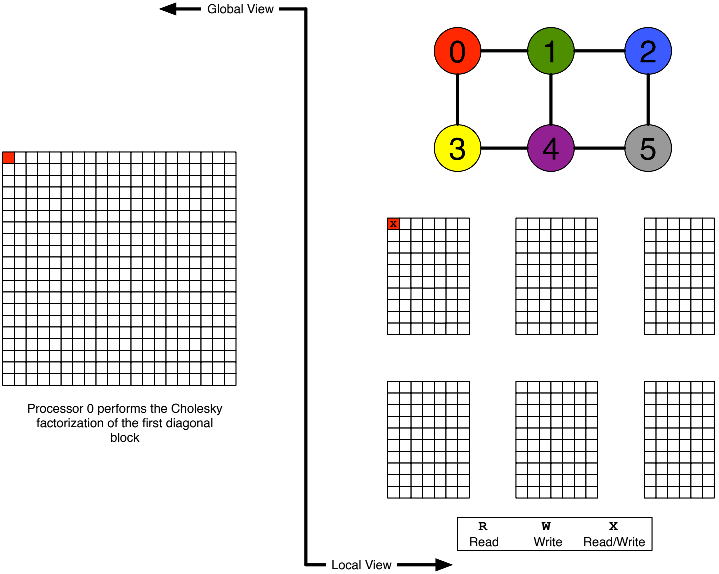
Routine `p_potrf` in ScaLAPACK



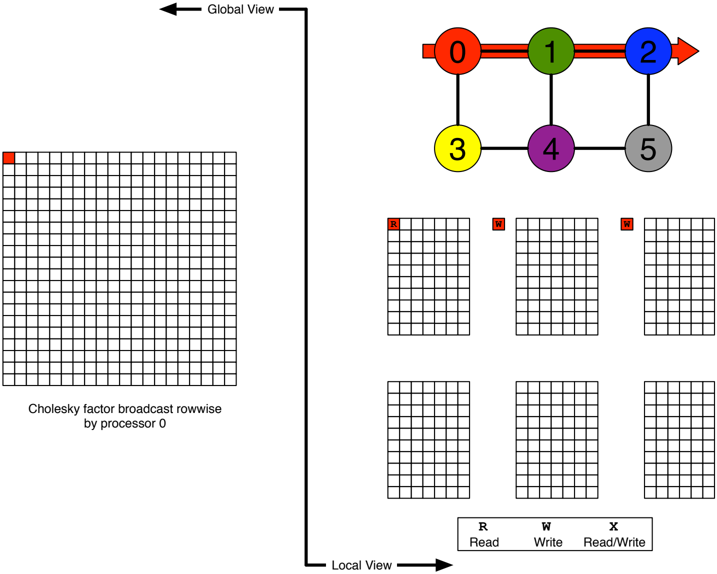
2D Block-Cyclic Data Distribution

Routine `p_potrf` in ScaLAPACK



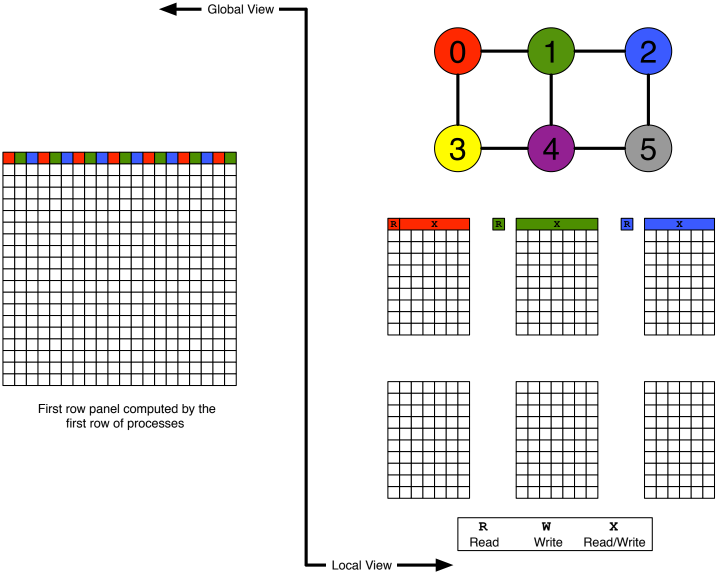
Processor 0 performs the Cholesky factorization of the first diagonal block

Routine `p_potrf` in ScaLAPACK



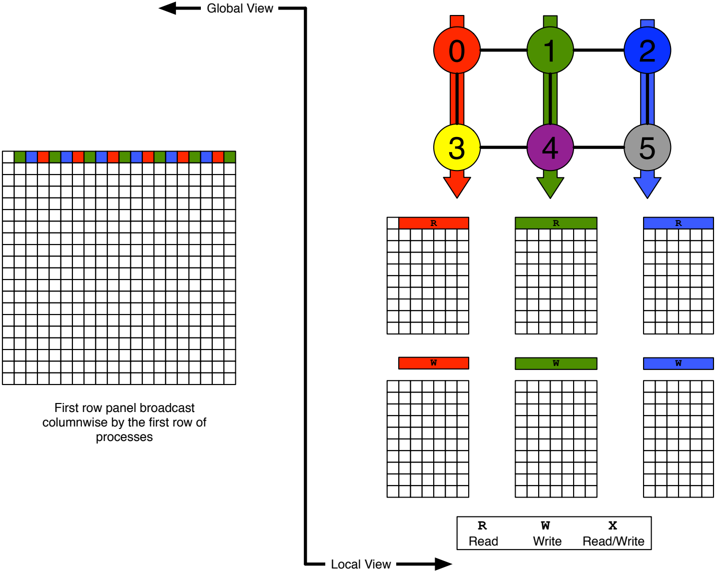
Cholesky factor broadcast rowwise
by processor 0

Routine `p_potrf` in ScaLAPACK



First row panel computed by the first row of processes

Routine `p_potrf` in ScaLAPACK



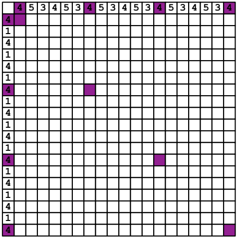
Global View

First row panel broadcast columnwise by the first row of processes

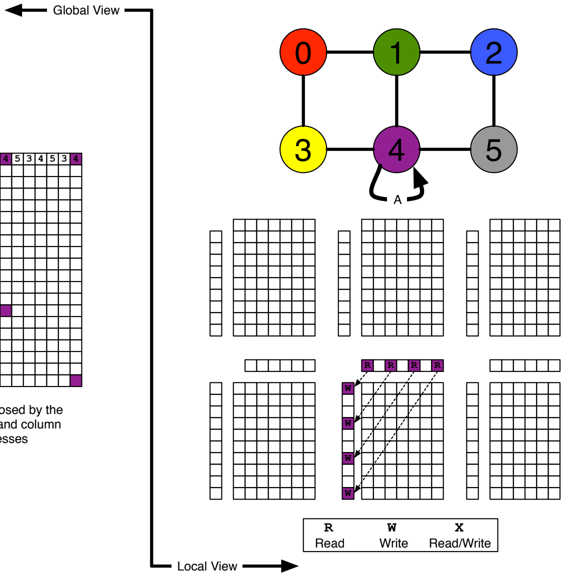
R	W	X
Read	Write	Read/Write

Local View

Routine `p_potrf` in ScaLAPACK



First row panel transposed by the second row (source) and column (target) of processes



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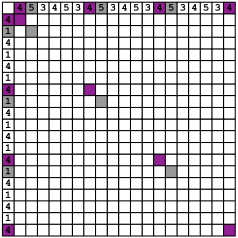

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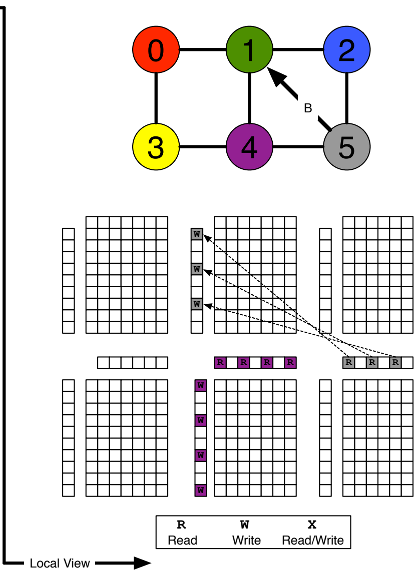
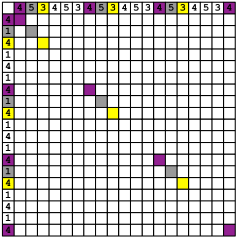


R	W	X
Read	Write	Read/Write

Routine `p_potrf` in ScaLAPACK

Global View



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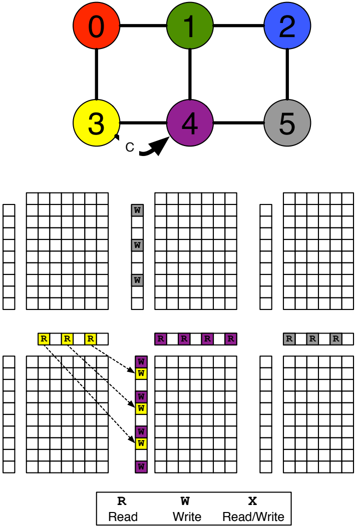
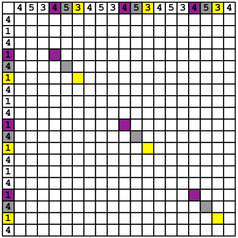


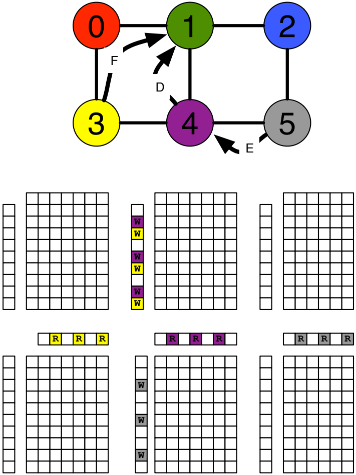
Local View

Routine `p_potrf` in ScaLAPACK

Global View



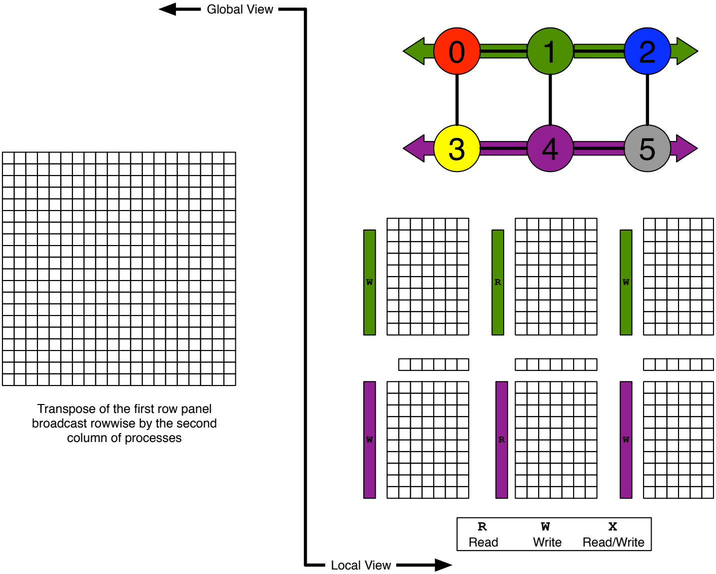
First row panel transposed by the second row (source) and column (target) of processes



R	W	X
Read	Write	Read/Write

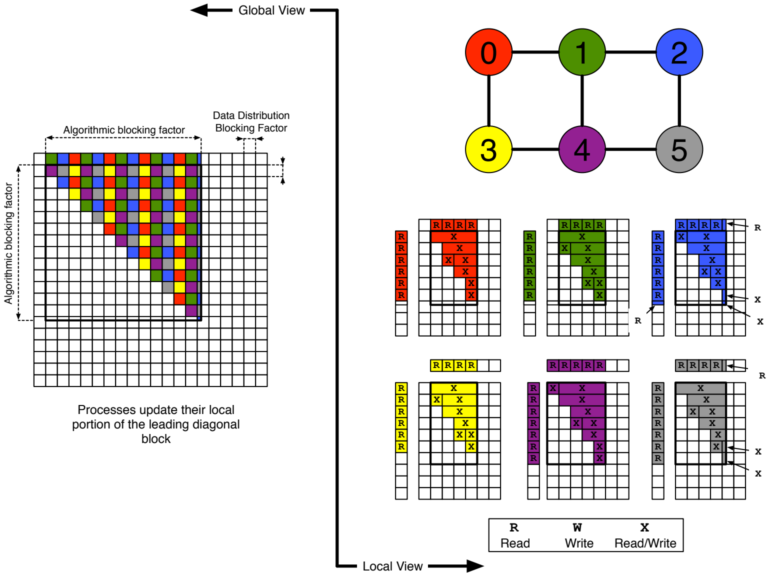
Local View

Routine `p_potrf` in ScaLAPACK



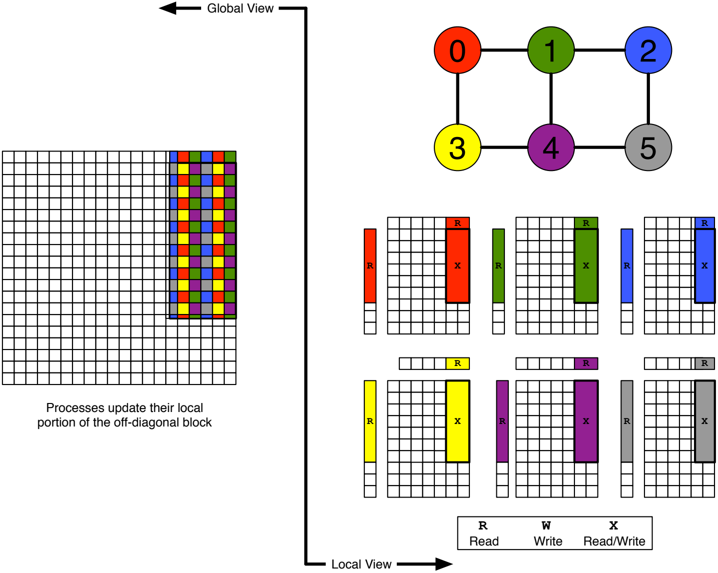
Transpose of the first row panel broadcast rowwise by the second column of processes

Routine `p_potrf` in ScaLAPACK



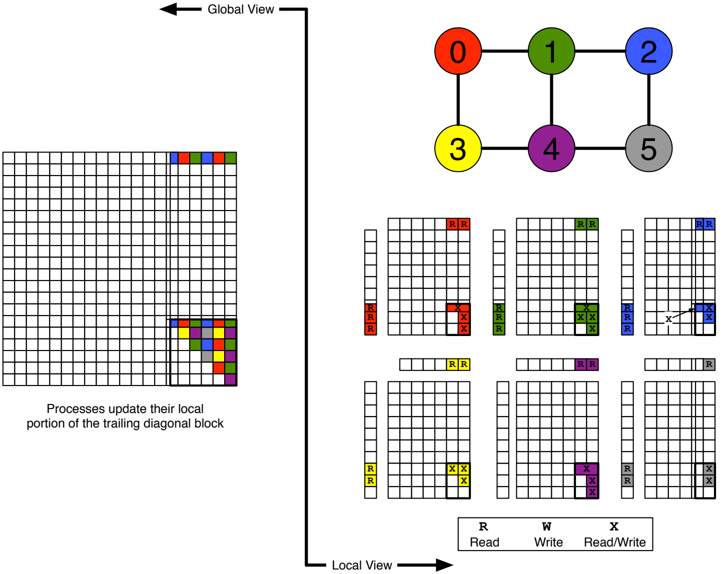
Processes update their local portion of the leading diagonal block

Routine `p_potrf` in ScaLAPACK



Processes update their local portion of the off-diagonal block

Routine `p_potrf` in ScaLAPACK

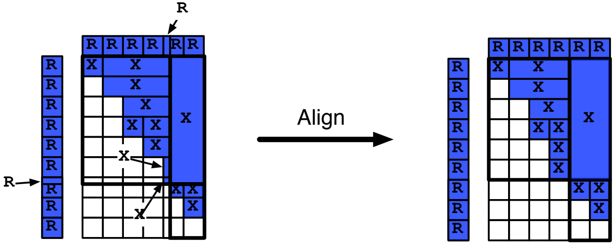


Processes update their local portion of the trailing diagonal block

Outline

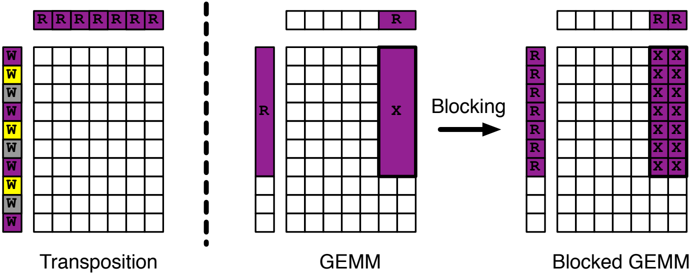
Taskification of computational kernels

- The parallel/distributed symmetric rank-k update uses a larger algorithmic blocking factor to increase level-3 BLAS granularity
- Algorithmic and data distribution partitionings don't need to be aligned
  → Blocking factors chosen independently (library vs. user)
- If level-3 BLAS kernels are naively encapsulated into SMPSs tasks ...
  → Accessed data can partially overlap the accesses of others tasks
  → Base-address dependency test cannot handle this scenario as is
- Solution: align algorithmic/data distribution partitionings



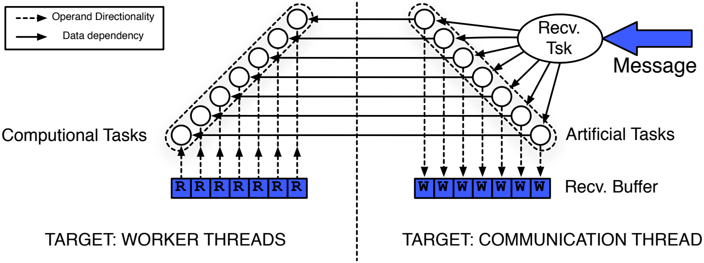
Taskification of computational kernels

- Coarse-grain level-3 BLAS update off-diagonal blocks, load unbalance → Need for finer-grain parallelism via blocking techniques
- Desirable that granularity of tasks could be determined independently of the distribution blocking factor, but . . .
- . . . transposition operations of a row panel (i.e., pack, unpack) are blocked conformally/aligned with data distribution partitioning
- Solution: granularity determined by the distribution blocking factor



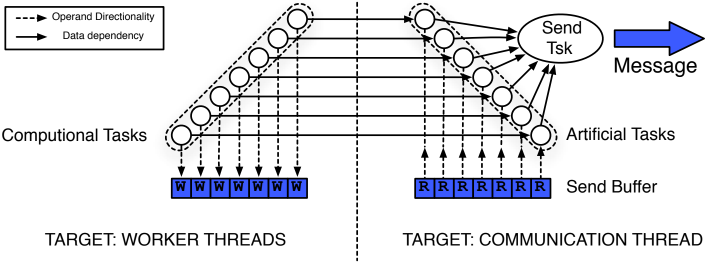
Taskification of communication kernels

- Recv. calls must be blocked conformally with computational kernels
- Avoid decomposing a Recv. call into a set of receives
  → Preserve latency/bandwidth requirements of the original application
- We instead decompose a Recv. call into:
  - Recv. Task: actually receives the message
  - Set of artificial/void/ghost? tasks: do nothing, used to create the data dependency path among communication and computation kernels



Taskification of communication kernels

- Send calls must be blocked conformally with computational kernels
- Avoid decomposing a Send call into a set of sends
  → Preserve latency/bandwidth requirements of the original application
- We instead decompose a Send call into:
  - Send Task: actually sends the message
  - Set of artificial/void/ghost? tasks: do nothing, used to create the data dependency path among communication and computation kernels



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5. **Performance evaluation**
6. Conclusions

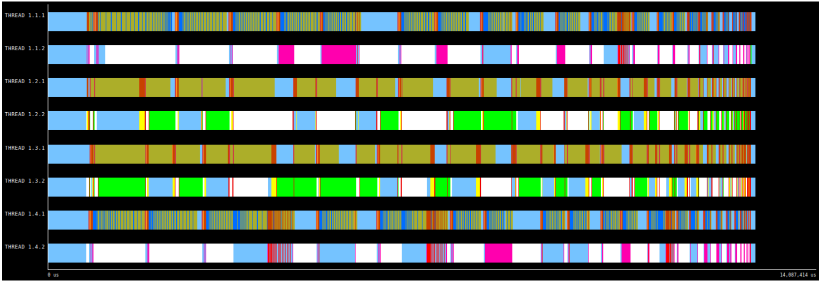
Experimental framework (small scale)

- Target platform:
    - `peco.act.uji.es`, small cluster at Universitat Jaume I
    - 8 nodes, 2 Intel QuadCore E5520 per node (64 cores total)
    - Infiniband interconnect
- Compilers and libraries:
    - Intel C and Fortran77 compilers v11.1
    - MPI/SMPSs rev13/svn/TRAC-TEXT
    - ScaLAPACK v1.8.0 + BLACS v1.1 (OpenMPI v1.4)
    - MKL 10.3 (single and multi-threaded BLAS)

Profile guided optimization

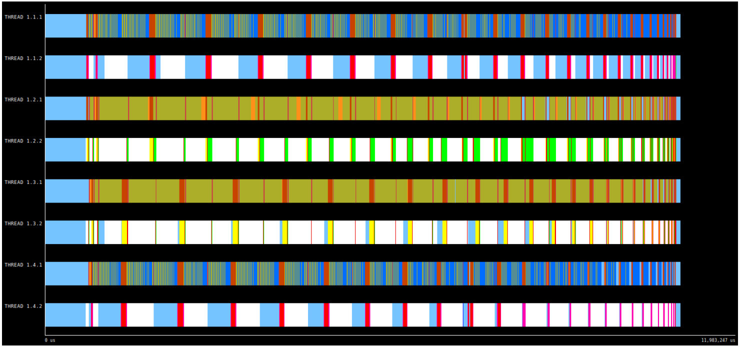
- We used `Extrae` and `Paraver` to extract execution traces
- Analysis of critical path and idle times allowed us to detect performance bottlenecks
- BSC used trace information to add scheduling options to SMPSs runtime

Default scheduling options

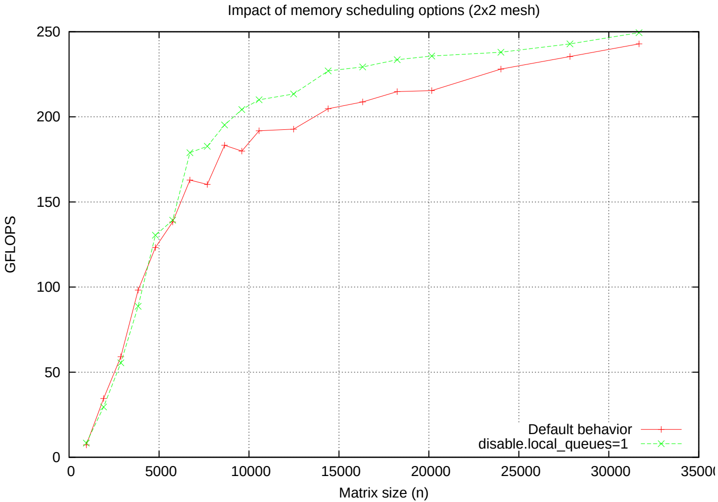


Excessive idle time

Local thread queues disabled



Performance Effect



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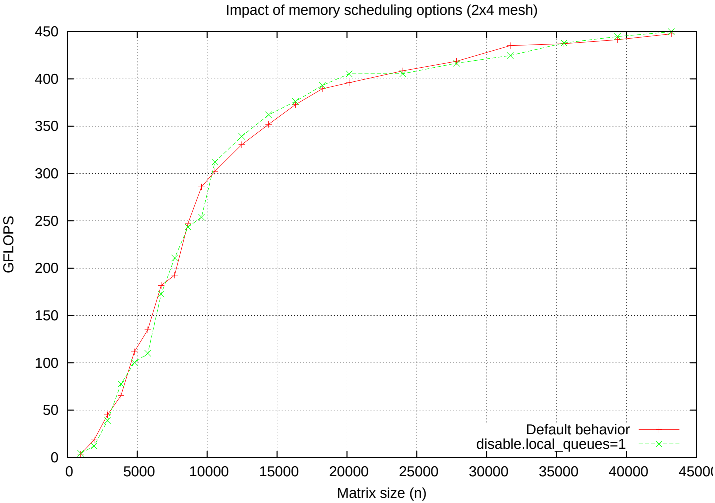
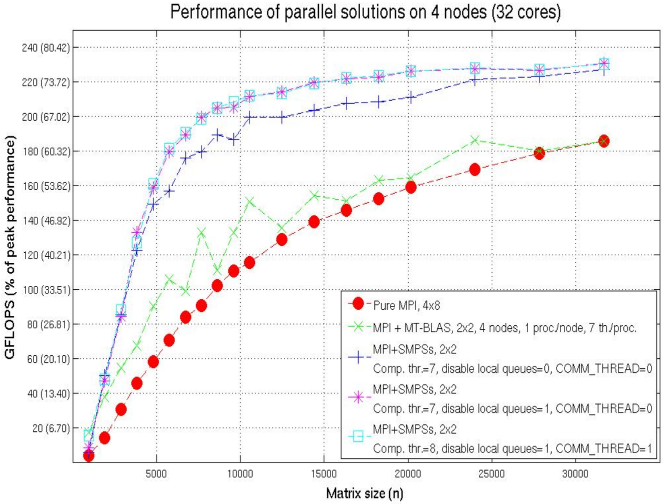
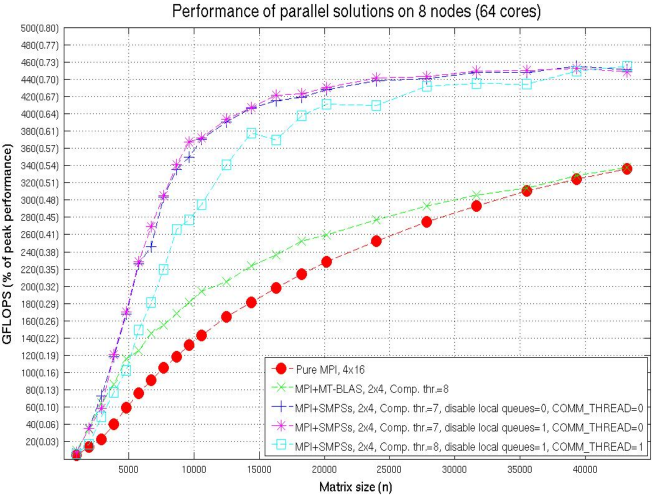


Performance evaluation on 32 cores



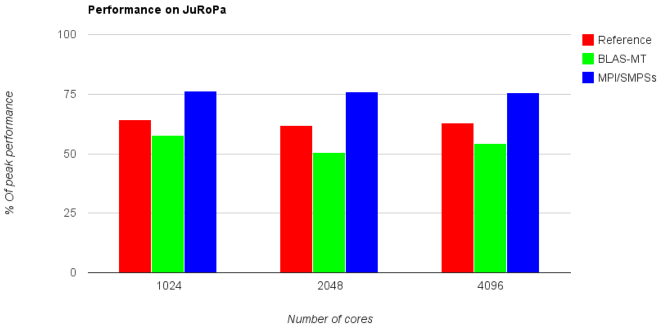
Performance evaluation on 64 cores



Experimental framework (large scale)

- Target platform:
  - `JuRoPa` at Juelich Supercomputing Center
  - 2,028 nodes, 2 Intel Xeon X5570 per node
  - Infiniband interconnect
- Compilers and libraries:
  - Intel C and Fortran77 compilers v11.1
  - MPI/SMPSs Minor changes from svn/TRAC-TEXT version
  - ScaLAPACK v1.8.0 + BLACS v1.1
  - MKL 10.3 (single and multi-threaded BLAS)

Preliminary large scale report



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Conclusions

- Current status:
  - ROutine for the Cholesky factorization in ScaLAPACK adapted to levarate current MPI/SMPSs for clusters
    → Match algorithmic and distribution blocking factors
  - Superior performance compared with conventional parallel solutions for clusters of multi-core processors
- Ongoing tasks:
  - Fine tuning, optimization guided by detailed performance analysis
  - Clusters of hardware accelerators
  - Other matrix kernels

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