Lightweight Superscalar Task Execution in Distributed Memory

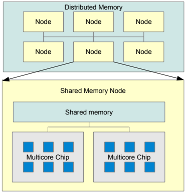
Asim YarKhan[1] and Jack Dongarra[1,2,3]

[1] Innovative Computing Lab, University of Tennessee, Knoxville, TN
[2] Oak Ridge National Lab, Oak Ridge, TN
[3] University of Manchester, Manchester, UK

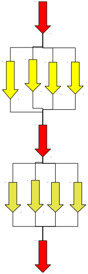
MTAGS 2014
7th Workshop on Many-Task Computing on Clouds, Grids, and Supercomputers
New Orleans, Lousiana

Nov 16 2014

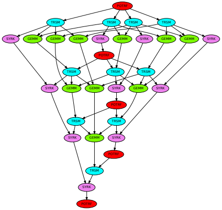
Architecture and Missed Opportunities



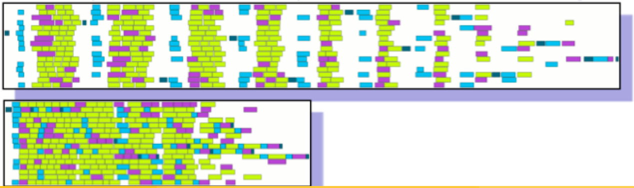
- Parallel Programming is difficult (still, again, yet).
    - Coding is via Pthreads, MPI, OpenMP, UPC, etc.
    - User handles complexities of coding, scheduling, execution, etc.
- Efficient and scalable programming is hard
    - Often get undesired synchronization points.
    - Fork-join wastes cores and reduces performance.
    - We need to access more of provided parallelism.
        - Larger multicore architectures
        - More inactive cores = more waste



Productivity, Efficiency, Scalability



- **Productivity** in Programming
  - Have a simple, serial API for programming.
  - Runtime environment handles all the details.
- **Efficiency** and **Scalability**
  - Tasks have data dependencies.
  - Tasks can execute as soon as data is ready (async).
  - This results in a task-DAG (directed acyclic graph).
  - Nodes are tasks; edges are data dependencies
  - Uses available cores in shared memory.
  - Transfers data as required in distributed memory

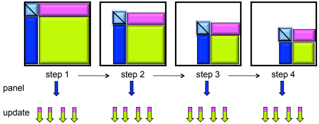


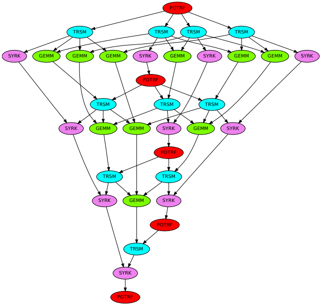
Related Projects

- PaRSEC [UTK] : Framework for distributed memory task execution. *Requires specialized parameterized compact task graph description*; parameterized task graphs are hard to express. Very high performance is achievable. Implements DPLASMA.
- SMPss [Barcelona] : Shared memory. Compiler-pragma based, runtime-system with data locality and task-stealing, *emphasis on data replication*. MPI available via explicit wrappers.
- StarPU [INRIA] : Shared and distributed memory. Library API based, *emphasis on heterogeneous scheduling (GPUs)*, smart data management, - similar to this work.
- Others: Charm++, Jade, Cilk, OpenMP, SuperMatrix, FLAME, ScaLAPACK, ...

Driving Applications: Tile Linear Algebra Algorithms

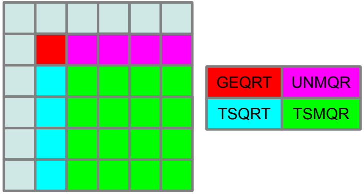
- Block algorithms
  - Standard linear algebra libraries (LAPACK, ScaLAPACK) gain parallelism from BLAS-3 interspersed with less parallel operations.
  - Execution is fork-join (or block synchronous parallel).
- Tile algorithms
  - Rewrite algorithms as tasks acting on data tiles.
  - Tasks using data $\Longrightarrow$ data dependencies $\Longrightarrow$ DAG
  - Want to execute DAGs asynchronously and in parallel $\Longrightarrow$ runtime.
  - QUeuing and Runtime for Kernels for Distributed Memory



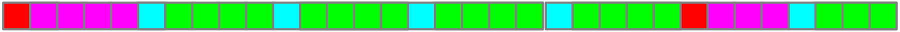


Tile QR Factorization Algorithm

```
for k = 0 ... TILES-1
  geqrt( $A^{rw}_{kk}$ , $T^{w}_{kk}$ )
  for n = k+1..TILES-1
    unmqr( $A^{r}_{kk-low}$ , $T^{r}_{kk}$ , $A^{rw}_{kn}$ )
  for m = k+1..TILES-1
    tsqrt( $A^{rw}_{kk-up}$ , $A^{rw}_{mk}$ , $T^{rw}_{mk}$ )
    for n = k+1..TILES-1
      tsmqr( $A^{r}_{mk}$ , $T^{r}_{mk}$ , $A^{rw}_{kn}$ , $A^{rw}_{mn}$ )
```

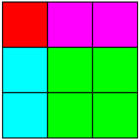


List of tasks as they are generated by the loops



Tile QR Factorization: Data Dependencies

F0 geqrt(A^{rw}_{00} , T^{w}_{00})
F1 **unmqr**(A^{r}_{00} , T^{r}_{00} , A^{rw}_{01})
F2 **unmqr**(A^{r}_{00} , T^{r}_{00} , A^{rw}_{02})
F3 **tsqrt**(A^{rw}_{00} , A^{rw}_{10} , T^{w}_{10})
F4 **tsmqr**(A^{rw}_{01} , A^{rw}_{11} , A^{r}_{10} , T^{r}_{10})
F5 **tsmqr**(A^{rw}_{02} , A^{rw}_{12} , A^{r}_{10} , T^{r}_{10})
F6 **tsqrt**(A^{rw}_{00} , A^{rw}_{20} , T^{w}_{20})
F7 **tsmqr**(A^{rw}_{01} , A^{rw}_{21} , A^{r}_{20} , T^{r}_{20})
F8 **tsmqr**(A^{rw}_{02} , A^{rw}_{22} , A^{r}_{20} , T^{r}_{20})
F9 geqrt(A^{rw}_{11} , T^{w}_{11})
F10 **unmqr**(A^{r}_{11} , T^{w}_{11} , A^{rw}_{12})
F11 **tsqrt**(A^{rw}_{11} , A^{rw}_{21} , T^{w}_{21})
F12 **tsmqr**(A^{rw}_{12} , A^{rw}_{22} , A^{r}_{21} , T^{r}_{21})
F13 geqrt(A^{rw}_{22} , T^{w}_{22})



Data dependencies from the first five tasks in the QR factorization

A_{00} : $F0^{rw} : F1^{r} : F2^{r} : F3^{rw}$
A_{01} : $F1^{rw} : F4^{rw}$
A_{02} : $F2^{rw} : F5^{rw}$
A_{10} : $F3^{rw} : F4^{r} : F5^{r}$
A_{11} : $F4^{rw}$
A_{12} : $F5^{rw}$
A_{20} :
A_{21} :
A_{22} :

Tile QR Factorization: Dependencies to Execution

First step in execution - Run task (function) $F0$.

F0 geqrt(A_{00}^{rw} , T_{00}^{w})
F1 unmqr(A_{00}^{r} , T_{00}^{r} , A_{01}^{rw})
F2 unmqr(A_{00}^{r} , T_{00}^{r} , A_{02}^{rw})
F3 tsqrt(A_{00}^{rw} , A_{10}^{rw} , T_{10}^{w})
F4 tsmqr(A_{01}^{rw} , A_{11}^{rw} , A_{10}^{r} T_{10}^{r})
F5 tsmqr(A_{02}^{rw} , A_{12}^{rw} , A_{10}^{r} T_{10}^{r})

A_{00} : $F0^{rw} : F1^{r} : F2^{r} : F3^{rw}$
A_{01} : $F1^{rw} : F4^{rw}$
A_{02} : $F2^{rw} : F5^{rw}$
A_{10} : $F3^{rw} : F4^{r} : F5^{r}$
A_{11} : $F4^{rw}$
A_{12} : $F5^{rw}$
T_{00} : $F0^{w} : F1^{r} : F2^{r}$
T_{10} : $F3^{w} : F4^{r} : F5^{r}$

Second step in execution - Remove $F0$; Now $F1$ and $F2$ are ready.

F1 unmqr(A_{00}^{r} , T_{00}^{r} , A_{01}^{rw})
F2 unmqr(A_{00}^{r} , T_{00}^{r} , A_{02}^{rw})
F3 tsqrt(A_{00}^{rw} , A_{10}^{rw} , T_{10}^{w})
F4 tsmqr(A_{01}^{rw} , A_{11}^{rw} , A_{10}^{r} T_{10}^{r})
F5 tsmqr(A_{02}^{rw} , A_{12}^{rw} , A_{10}^{r} T_{10}^{r})

A_{00} : $F1^{r} : F2^{r} : F3^{rw}$
A_{01} : $F1^{rw} : F4^{rw}$
A_{02} : $F2^{rw} : F5^{rw}$
A_{10} : $F3^{rw} : F4^{r} : F5^{r}$
A_{11} : $F4^{rw}$
A_{12} : $F5^{rw}$
T_{00} : $F1^{r} : F2^{r}$
T_{10} : $F3^{w} : F4^{r} : F5^{r}$

QUARK-D API and Runtime

- QUARK-D
  - QUeuing and Runtime for Kernels in Distributed Memory
- Simple serial task insertion interface.

```
QUARKD_Insert_Task( quark , *function , *taskflags ,
  a_flags , size_a , *a, a_home_process , a_key ,
  b_flags , size_b , *b, b_home_process , b_key ,
  ... ,  0 );
```

- Manage the distributed details for the user.
  - Scheduling tasks (where should tasks run)
  - Data dependencies and movement (local and remote).
  - Transparent communication.
  - No global knowledge or coordination required.

Productivity: QUARK-D QR Implementation

The code matches the pseudo-code

```
for k = 0 ... TILES−1
  geqrt( $A_{kk}^{rw}$ , $T_{kk}^{w}$ )
  for n = k+1..TILES−1
    unmqr( $A_{kk-low}^{r}$ , $T_{kk}^{r}$ , $A_{kn}^{rw}$ )
  for m = k+1..TILES−1
    tsqrt( $A_{kk-up}^{rw}$ , $A_{mk}^{rw}$ , $T_{mk}^{rw}$ )
    for n = k+1..TILES−1
      tsmqr( $A_{mk}^{r}$ , $T_{mk}^{r}$ , $A_{kn}^{rw}$ , $A_{mn}^{rw}$ )
```

```
#define A(m,n) ADDR(A),HOME(m,n),KEY(A,m,n)
#define T(m,n) ADDR(T),HOME(m,n),KEY(T,m,n)

void plasma_pdgeqrf(A, T,.) {
 for (k = 0; k < M; k++) {
  TASK_dgeqrt(quark,.,A(k,k),T(k,k));
  for (n = k+1; n < N; n++)
   TASK_dormqr(quark,..,A(k,k),T(k,k),A(k,n));
  for (m = k+1; m < M; m++) {
   TASK_dtsqrt(quark,.,A(k,k),A(m,k),T(m,k));
   for (n = k+1; n < N; n++)
    TASK_dtsmqr(quark,.,A(k,n),A(m,n),
                            A(m,k),T(m,k));   }}}
```

Productivity: QUARK-D QR Implementation

The task is inserted into the runtime and held till data is ready.

```
void TASK_dgeqrt(
    Quark *quark,.., int m, int n,
    double *A, int A_home, key *A_key,
    double *T, int T_home, key *T_key )
{
 QUARKD_Insert_Task(quark,CORE_dgeqrt,...,
   VALUE, sizeof(int),&m,
   VALUE, sizeof(int),&n,
   INOUT|LOCALITY, sizeof(A),A,A_home,A_key,
   OUTPUT, sizeof(T),T,T_home,T_key,..,0);
}
```

When the task is eventually executed, the dependencies are unpacked, and the serial core routine is called.

```
void CORE_dgeqrt(Quark *quark)
{
 int m,n,ib,lda,ldt;
 double *A,*T,*TAU,*WORK;
 quark_unpack_args_9(quark,m,n,ib,A,
    lda,T,ldt,TAU,WORK);
 CORE_dgeqrt(m,n,ib,A,lda,T,ldt,TAU,WORK);
}
```

Distributed Memory Algorithm

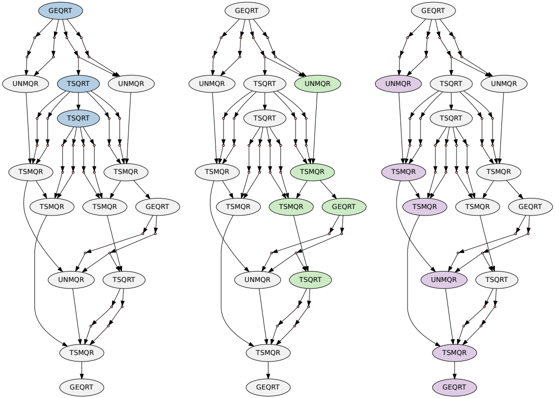
This pseudocode manages the distributed details for the user.

```
// running at each distributed node
for each task $T$ as it is inserted
    // determine $P_{exe}$ based on dependency to be kept local
    $P_{exe}$ = process that will run task $T$
    for each dependency $A_i$ in $T$
        if (I am $P_{exe}$ ) && ( $A_i$ is invalid here )
            insert receive tasks ($A_i^{rw}$)
        else if ( $P_{exe}$ has invalid $A_i$ ) && ( I own $A_i$ )
            insert send tasks ($A_i^r$)
        // track who is current owner, who has valid copies
        update dependency tracking
    if ( I am $P_{exe}$ )
        insert task $T$ into shared memory runtime
```

QUARK-D Running the Distributed Memory Algorithm

A00	A01	A02
A10	A11	A12
A20	A21	A22

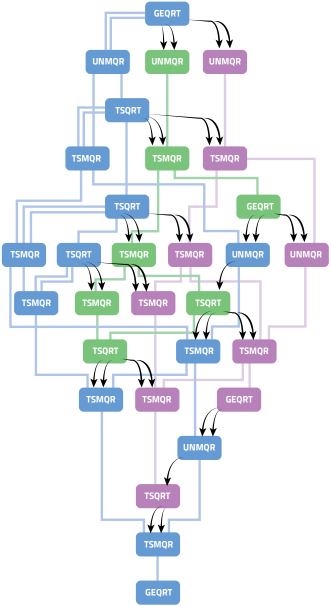
F0 **geqrt**(A^{rw}_{00} , T^{w}_{00})
F1 **unmqr**(A^{r}_{00} , T^{r}_{00} , A^{rw}_{01})
F2 **unmqr**(A^{r}_{00} , T^{r}_{00} , A^{rw}_{02})
F3 **tsqrt**(A^{rw}_{00} , A^{rw}_{10} , T^{w}_{10})
F4 **tsmqr**(A^{rw}_{01} , A^{rw}_{11} , A^{r}_{10} , T^{r}_{10})
F5 **tsmqr**(A^{rw}_{02} , A^{rw}_{12} , A^{r}_{10} , T^{r}_{10})
F6 **tsqrt**(A^{rw}_{00} , A^{rw}_{20} , T^{w}_{20})
F7 **tsmqr**(A^{rw}_{01} , A^{rw}_{21} , A^{r}_{20} , T^{r}_{20})
F8 **tsmqr**(A^{rw}_{02} , A^{rw}_{22} , A^{r}_{20} , T^{r}_{20})
F9 **geqrt**(A^{rw}_{11} , T^{w}_{11})
F10 **unmqr**(A^{r}_{11} , T^{w}_{11} , A^{rw}_{12})
F11 **tsqrt**(A^{rw}_{11} , A^{rw}_{21} , T^{w}_{21})
F12 **tsmqr**(A^{rw}_{12} , A^{rw}_{22} , A^{r}_{21} , T^{r}_{21})
F13 **geqrt**(A^{rw}_{22} , T^{w}_{22})



(a) P0 (b) P1 (c) P2

Execution of a small QR factorization (DGEQRF). Three processes (P0, P1, P2) are running the factorization on 3x3 tile matrix using a 1 × 3 process grid. Note that TSQRT and TSMQR have locality on second RW parameter.

QUARK-D: QR DAG



QUARK-D's principles of operation. Scheduling the DAG of the distributed memory QR factorization. Three distributed memory processes are running the factorization algorithm on a 3x3 tile matrix. One multi-threaded process runs all the blue tasks, another multi-threaded process runs the green tasks, and a third runs the purple tasks. Colored links show local task dependencies. Black arrows show inter-process communications.

QUARK-D: Key Developments

- Distributed scheduling
    - A function tells us which process is going to run a task; usually based on data distribution (2D block cyclic) but any function that will evaluate the same on all processes.
    - Execution within a multi-threaded process is completely dynamic.
- Decentralized data coherency protocol
    - Processes coordinate the data movement without any control messages.
    - Coordination is enabled by a data coherency protocol, where each process knows who is the current owner of a piece of data, and which processes have valid copies of that data.
- Asynchronous data transfer
    - Data movement is initiated by tasks, then the message passing continues asynchronously without blocking other tasks.
    - The data movement protocol is an eager protocol initiated by a send-data task. The receive-data task is activated by the message passing engine, and can get the data asynchronously (from temporary storage if necessary).

QUARK-D: QR Trace

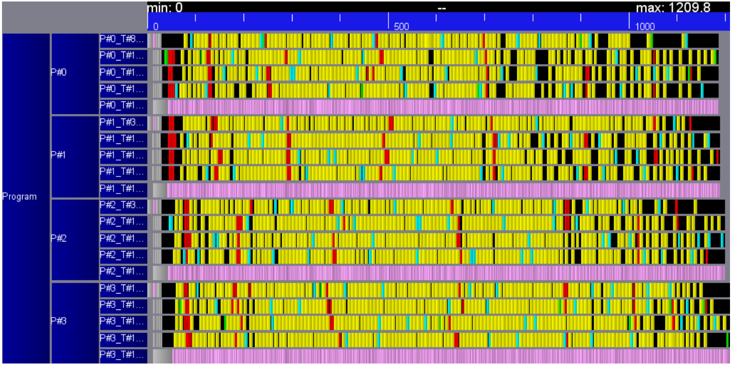


Figure: Trace of a QR factorization of a matrix consisting of 16x16 tiles on 4 (2x2) distributed memory nodes using 4 computational threads per node. An independent MPI communication thread is also maintained. Color coding: MPI (pink); GEQRT (green); TSMQR (yellow); TSQRT (cyan); UNMQR (red).

QUARK-D: QR Weak Scaling: Small Cluster

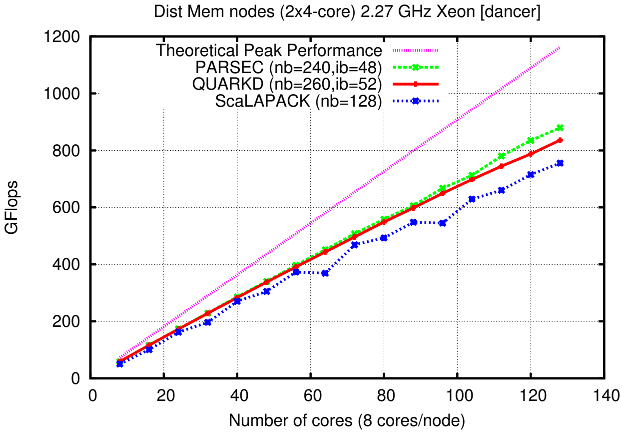


Figure: Weak scaling performance of QR factorization on a small cluster. Factorizing a matrix (5000x5000/per core) on up to 16 distributed memory nodes with 8 cores per node. Comparing QUARK-D, PaRSEC and ScaLAPACK (MKL).

QUARK-D: QR Weak Scaling: Large Cluster

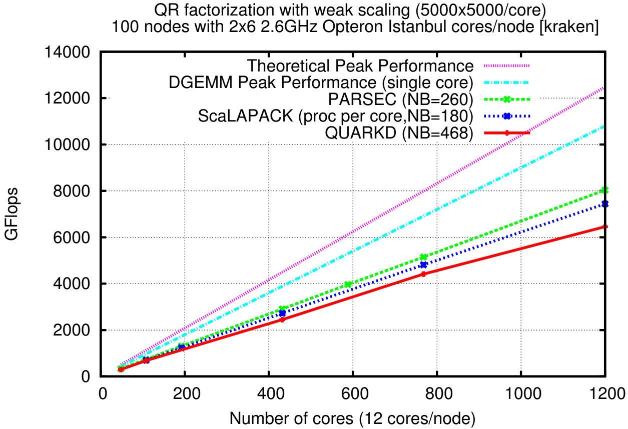


Figure: Weak scaling performance for QR factorization (DGEQRF) of a matrix (5000x5000/per core) on 1200 cores (100 distributed memory nodes with 12 cores per node). Comparing QUARK-D, PaRSEC and ScaLAPACK (libSCI).

QUARK-D: Cholesky Weak Scaling: Small Cluster

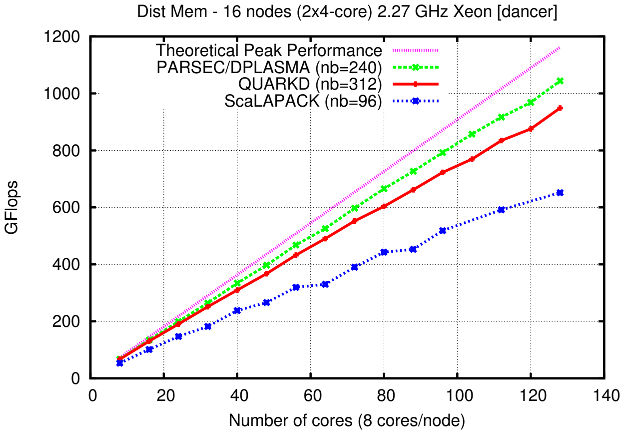


Figure: Weak scaling performance of Cholesky factorization (DPOTRF) of a matrix (5000x5000/per core) on 16 distributed memory nodes with 8 cores per node. Comparing QUARK-D, PaRSEC and ScaLAPACK (MKL).

QUARK-D: Cholesky Weak Scaling: Large Cluster

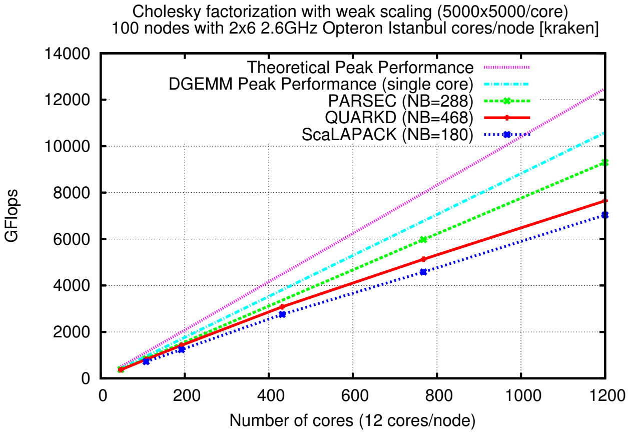
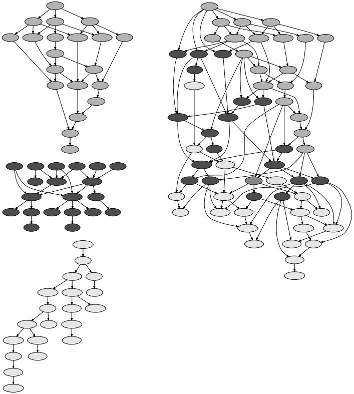
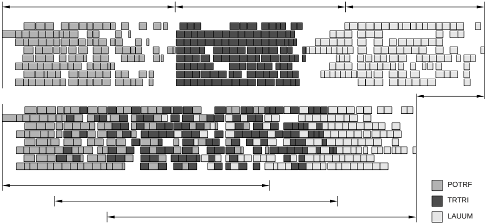


Figure: Weak scaling performance for Cholesky factorization (DPOTRF) of a matrix (7000x7000/per core) on 1200 cores (100 distributed memory nodes with 12 cores per node). Comparing QUARK-D, PaRSEC and ScaLAPACK (libSCI).

DAG Composition: Cholesky Inversion

- Cholesky Inversion
- POTRF, TRTRI, LAUUM
- DAG composition can compress DAGs substantially





QUARK-D: Composing Cholesky Inversion

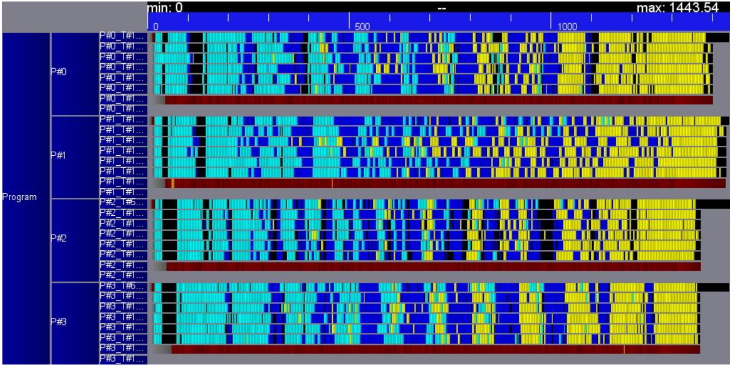


Figure: Trace of the distributed memory Cholesky inversion of a matrix with three DAGs that are composed (POTRF, TRTRI, LAUUM)

QUARK-D Summary

- Designed and implemented a runtime system for task based applications on distributed memory architectures.
- Uses serial task insertion interface with automatic data dependency inference.
- No global coordination for task scheduling.
- Distributed data coherency protocol manages copies of data.
- Fast communication engine transfers data asynchronously.
- Focus on *productivity*, *scalability* and *performance*.

The End