

# Comparative Study of One-Sided Factorizations with Multiple Software Packages on Multi-Core Hardware

Emmanuel AGULLO

Jack DONGARRA

Bilel HADRI

Jakub KURZAK

Hatem LTAIEF

Piotr LUSCZEK

Scheduling for Large-Scale Systems, Knoxville, TN, May 13-15, 2009



# Outline

## 1. Tile Algorithms

- Cholesky Factorization
- QR (&LU) Factorizations

## 2. Experimental environment

- Libraries
- Hardware
- Metrics

## 3. Tuning

- PLASMA

## 4. Comparison against other libraries

- Experiments on few cores
- Experiments on a large number of cores
- PLASMA scalability

## 5. Conclusion and current work

# Outline

## 1. Tile Algorithms

- Cholesky Factorization
- QR (&LU) Factorizations

## 2. Experimental environment

- Libraries
- Hardware
- Metrics

## 3. Tuning

- PLASMA

## 4. Comparison against other libraries

- Experiments on few cores
- Experiments on a large number of cores
- PLASMA scalability

## 5. Conclusion and current work

# Outline

## 1. Tile Algorithms

- Cholesky Factorization
- QR (&LU) Factorizations

## 2. Experimental environment

- Libraries
- Hardware
- Metrics

## 3. Tuning

- PLASMA

## 4. Comparison against other libraries

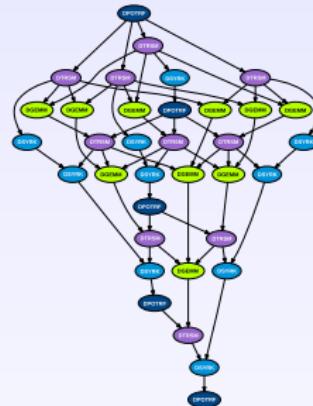
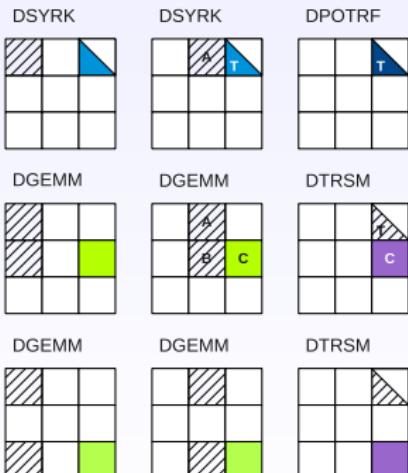
- Experiments on few cores
- Experiments on a large number of cores
- PLASMA scalability

## 5. Conclusion and current work

# Tile Cholesky Factorization

```

FOR k = 0..TILES-1
  FOR n = 0..k-1
    A[k][k] ← DSYRK(A[k][n], A[k][k])
    A[k][k] ← DPOTRF(A[k][k])
  FOR m = k+1..TILES-1
    FOR n = 0..k-1
      A[m][k] ← DGEMM(A[k][n], A[m][n], A[m][k])
      A[m][k] ← DTRSM(A[k][k], A[m][k])
    
```



- ★ Basically identical to the block algorithm (LAPACK).
- ★ Input matrix stored and processed by square tiles.
- ★ Complex DAG.

# Tile Cholesky Factorization - Static pipeline

```

void dsyrk(double *A, double *T);
void dpotrf(double *T);
void dgemm(double *A, double *B, double *C);
void dtrsm(double *T, double *C);

k = 0; m = my_core_id;
while (m >= TILES) {
    k++; m = m-TILES+k;
} n = 0;

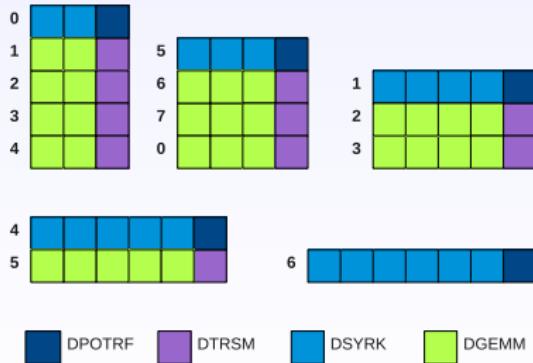
while (k < TILES && m < TILES) {
    next_n = n; next_m = m; next_k = k;

    next_n++;
    if (next_n > next_k) {
        next_m += cores_num;
        while (next_m >= TILES && next_k < TILES) {
            next_k++; next_m = next_m-TILES+next_k;
        } next_n = 0;
    }

    if (m == k) {
        if (n == k) {
            dpotrf(A[k][k]);
            core_progress[k][k] = 1;
        }
        else {
            while(core_progress[k][n] != 1);
            dsyrk(A[k][n], A[k][k]);
        }
    }
    else {
        if (n == k) {
            while(core_progress[k][k] != 1);
            dtrsm(A[k][k], A[m][kk]);
            core_progress[m][k] = 1;
        }
        else {
            while(core_progress[k][n] != 1);
            while(core_progress[m][n] != 1);
            dgemm(A[k][n], A[m][n], A[m][k]);
        }
    }
}

```

- ★ Work partitioned in one dimension (by block-rows).
- ★ Cyclic assignment of work across all steps of the factorization (pipelining of factorization steps).
- ★ Process tracking by a global progress table.
- ★ Stall on dependencies (busy waiting).



# Outline

## 1. Tile Algorithms

- Cholesky Factorization
- QR (&LU) Factorizations

## 2. Experimental environment

- Libraries
- Hardware
- Metrics

## 3. Tuning

- PLASMA

## 4. Comparison against other libraries

- Experiments on few cores
- Experiments on a large number of cores
- PLASMA scalability

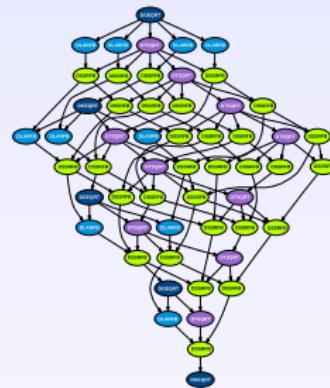
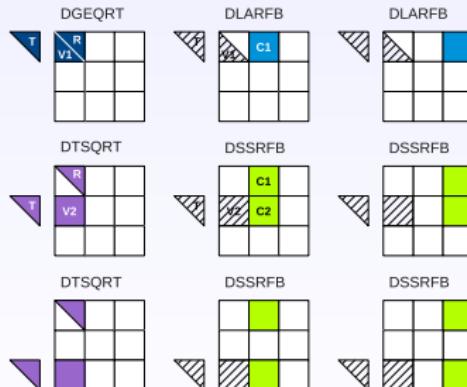
## 5. Conclusion and current work

# Tile QR (&LU) Factorization

```

FOR k = 0..TILES-1
  A[k][k], T[k][k]  $\leftarrow$  DGRQRT(A[k][k])
FOR m = k+1..TILES-1
  A[k][k], A[m][k], T[m][k]  $\leftarrow$  DTSQRT(A[k][k], A[m][k], T[m][k])
FOR n = k+1..TILES-1
  A[k][n]  $\leftarrow$  DLARFB(A[k][k], T[k][k], A[k][n])
FOR m = k+1..TILES-1
  A[k][n], A[m][n]  $\leftarrow$  DSSRFB(A[m][k], T[m][k], A[k][n], A[m][n])

```



- ★ Different from the block algorithm.
- ★ Derived from out-of-core algorithm.
- ★ Input matrix stored and processed by square tiles.
- ★ Complex DAG.

# Tile QR Factorization - Static pipeline

```

void dgearqf(double *RV1, double *T);
void dtsqrqf(double *R, double *V2, double *T);
void dlarfb(double *V1, double *T, double *C1);
void dssrbf(double *V2, double *T, double *C1, double *C2);

k = 0; n = my_core_id;
void dgearqf(double *RV1, double *T);
void dtsqrqf(double *R, double *V2, double *T);
void dlarfb(double *V1, double *T, double *C1);
void dssrbf(double *V2, double *T, double *C1, double *C2);

while (n >= TILES) {
    k++;
    n = n-TILES+k;
    m = k;

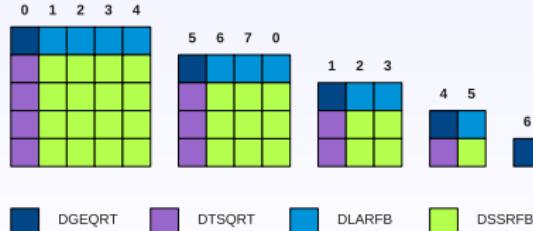
    while (k < TILES && n < TILES) {
        next_n = n; next_m = m; next_k = k;

        next_m++;
        if (next_m == TILES) {
            next_n += cores_num;
            while (next_n >= TILES && next_k < TILES) {
                next_k++; next_n = next_n-TILES+next_k;
            } next_m = next_k;
        }

        if (n == k) {
            if (m == k) {
                while(progress[k][k] != k-1);
                dgearqf(A[k][k], T[k][k]);
                progress[k][k] = k;
            }
            else{
                while(progress[m][k] != k-1);
                dtsqrqf(A[k][k], A[m][k], T[m][k]);
                progress[m][k] = k;
            }
        }
        else {
            if (m == k) {
                while(progress[k][k] != k);
                while(progress[k][n] != k-1);
                dlarfb(A[k][k], T[k][k], A[k][n], A[m][n]);
                progress[m][n] = k;
            }
        }
        n = next_n; m = next_m; k = next_k;
    }
}

```

- ★ Work partitioned in one dimension (by block-rows).
- ★ Cyclic assignment of work across all steps of the factorization (pipelining of factorization steps).
- ★ Process tracking by a global progress table.
- ★ Stall on dependencies (busy waiting).



# Outline

## 1. Tile Algorithms

- Cholesky Factorization
- QR (&LU) Factorizations

## 2. Experimental environment

- Libraries
- Hardware
- Metrics

## 3. Tuning

- PLASMA

## 4. Comparison against other libraries

- Experiments on few cores
- Experiments on a large number of cores
- PLASMA scalability

## 5. Conclusion and current work

# Outline

## 1. Tile Algorithms

- Cholesky Factorization
- QR (&LU) Factorizations

## 2. Experimental environment

- Libraries
- Hardware
- Metrics

## 3. Tuning

- PLASMA

## 4. Comparison against other libraries

- Experiments on few cores
- Experiments on a large number of cores
- PLASMA scalability

## 5. Conclusion and current work

# Libraries

## ★ LAPACK:

- ▶ LAPACK 3.2 on Intel machine;
- ▶ LAPACK 3.1.1 on IBM machine;

## ★ SCALAPACK:

- ▶ SCALAPACK 1.8.0;

## ★ Vendor libraries:

- ▶ Intel MKL 10.1;
- ▶ IBM ESSL 4.3;
- ▶ IBM PESSL 3.3;

## ★ Tile algorithms:

- ▶ PLASMA ;
- ▶ TBLAS.

# Libraries

## ★ LAPACK:

- ▶ LAPACK 3.2 on Intel machine;
- ▶ LAPACK 3.1.1 on IBM machine;

## ★ SCALAPACK:

- ▶ SCALAPACK 1.8.0;

## ★ Vendor libraries:

- ▶ Intel MKL 10.1;
- ▶ IBM ESSL 4.3;
- ▶ IBM PESSL 3.3;

## ★ Tile algorithms:

- ▶ **PLASMA** ;
- ▶ TBLAS.

# Outline

## 1. Tile Algorithms

- Cholesky Factorization
- QR (&LU) Factorizations

## 2. Experimental environment

- Libraries
- Hardware
- Metrics

## 3. Tuning

- PLASMA

## 4. Comparison against other libraries

- Experiments on few cores
- Experiments on a large number of cores
- PLASMA scalability

## 5. Conclusion and current work

# Intel Xeon - 16 cores machine

- ★ Node:
  - ▶ quad-socket quad-core Intel64 processors (16 cores).
- ★ Intel Xeon processor:
  - ▶ quad-core;
  - ▶ Frequency: 2,4 GHz.
- ★ Theoretical peak:
  - ▶ 9.6 Gflop/s/core;
  - ▶ 153.6 Gflop/s/node.
- ★ System and compilers:
  - ▶ Linux 2.6.25;
  - ▶ Intel Compilers 11.0.

# IBM Power6 - 32 cores machine

- ★ Node:
  - ▶ 16 dual-core Power6 processors (32 cores).
- ★ Power6 processor:
  - ▶ dual-core;
  - ▶ each core 2-way SMT;
  - ▶ L1: 64kB data + 64 kB instructions;
  - ▶ L2: 4 MB per core, accessible by the other core;
  - ▶ L3: 32 MB per processor, one controller per core (80 MB/s).
  - ▶ Frequency: 4.7 GHz.
- ★ Theoretical peak:
  - ▶ 18.8 Gflop/s/core;
  - ▶ 601.6 Gflop/s/node.
- ★ System and compilers:
  - ▶ AIX 5.3;
  - ▶ xlf version 12.1;
  - ▶ xlc version 10.1.

# Outline

## 1. Tile Algorithms

- Cholesky Factorization
- QR (&LU) Factorizations

## 2. Experimental environment

- Libraries
- Hardware
- Metrics

## 3. Tuning

- PLASMA

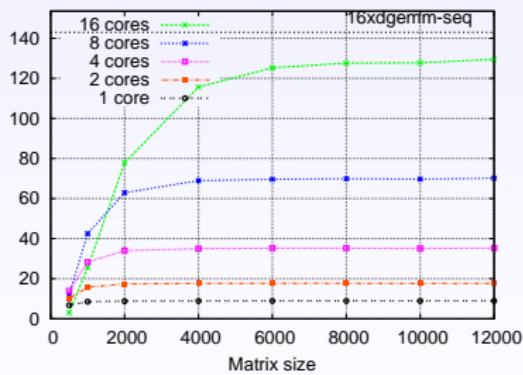
## 4. Comparison against other libraries

- Experiments on few cores
- Experiments on a large number of cores
- PLASMA scalability

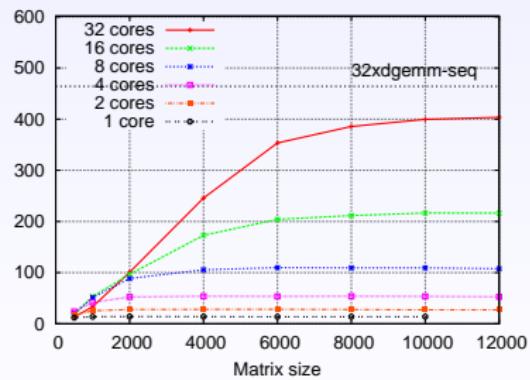
## 5. Conclusion and current work

# Performance metrics (How to read the graphs)

- ★ Performance: Gflop/s (y-axis).
- ★ Plots scaled to the theoretical peak.
- ★ Parallel DGEMM.
- ★ Upper bound: embarrassingly parallel fastest core kernel:
  - ▶ DPOTRF ( $LL^T$ ) → dgemm;
  - ▶ DGEQRF ( $QR$ ) → dssrfb;
  - ▶ DGETRF ( $LU$ ) → dsssm.



Intel64- DGEMM



Power6- DGEMM

# Outline

## 1. Tile Algorithms

- Cholesky Factorization
- QR (&LU) Factorizations

## 2. Experimental environment

- Libraries
- Hardware
- Metrics

## 3. Tuning

- PLASMA

## 4. Comparison against other libraries

- Experiments on few cores
- Experiments on a large number of cores
- PLASMA scalability

## 5. Conclusion and current work

# Outline

## 1. Tile Algorithms

- Cholesky Factorization
- QR (&LU) Factorizations

## 2. Experimental environment

- Libraries
- Hardware
- Metrics

## 3. Tuning

- PLASMA

## 4. Comparison against other libraries

- Experiments on few cores
- Experiments on a large number of cores
- PLASMA scalability

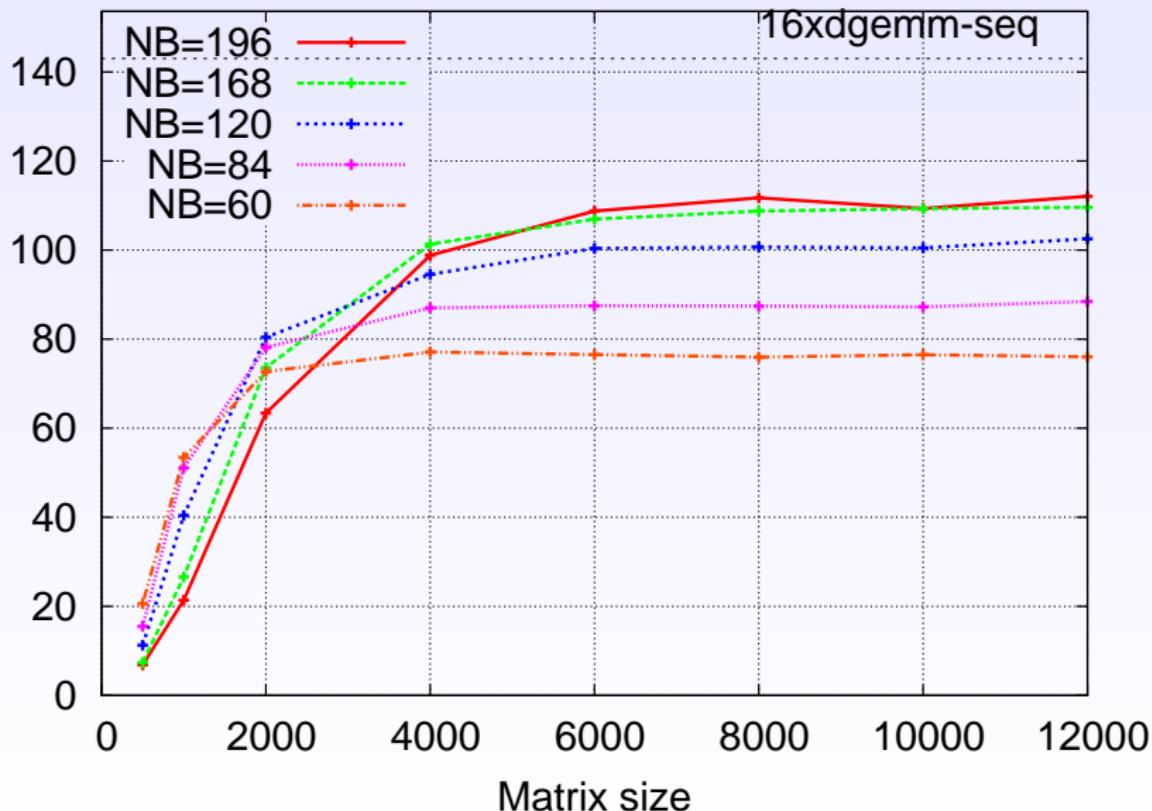
## 5. Conclusion and current work

# Degrees of freedom

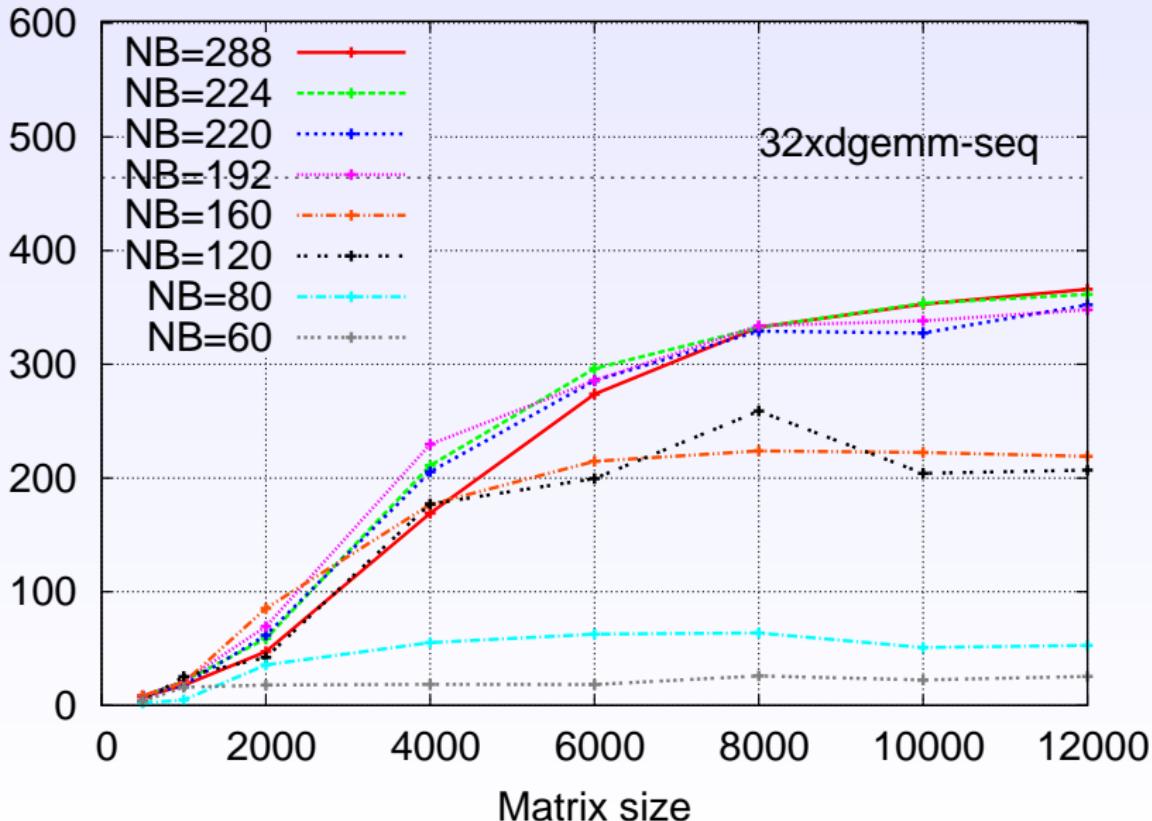
Input parameters of the serial core kernels:

- ★ **NB**: tile size;
- ★ **IB**: internal blocking (for dssrfb and dssssm only).

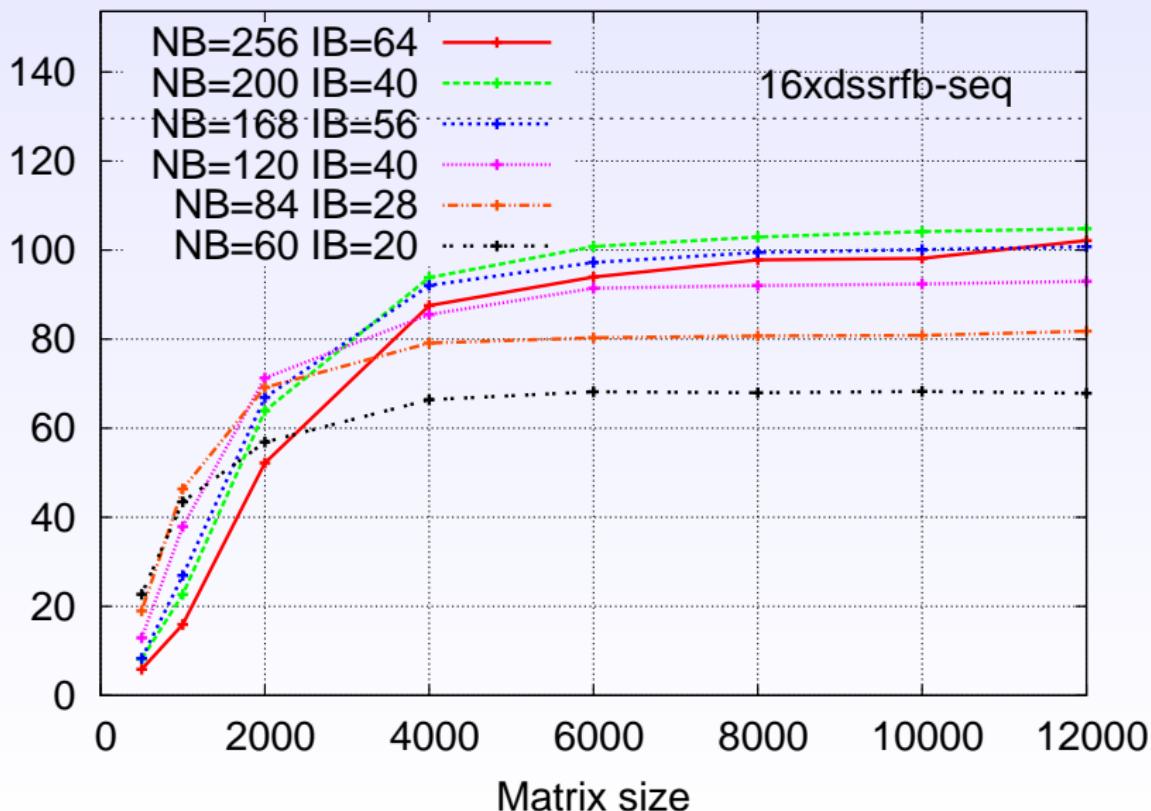
# Impact of NB - DPOTRF- Intel64- 16 cores



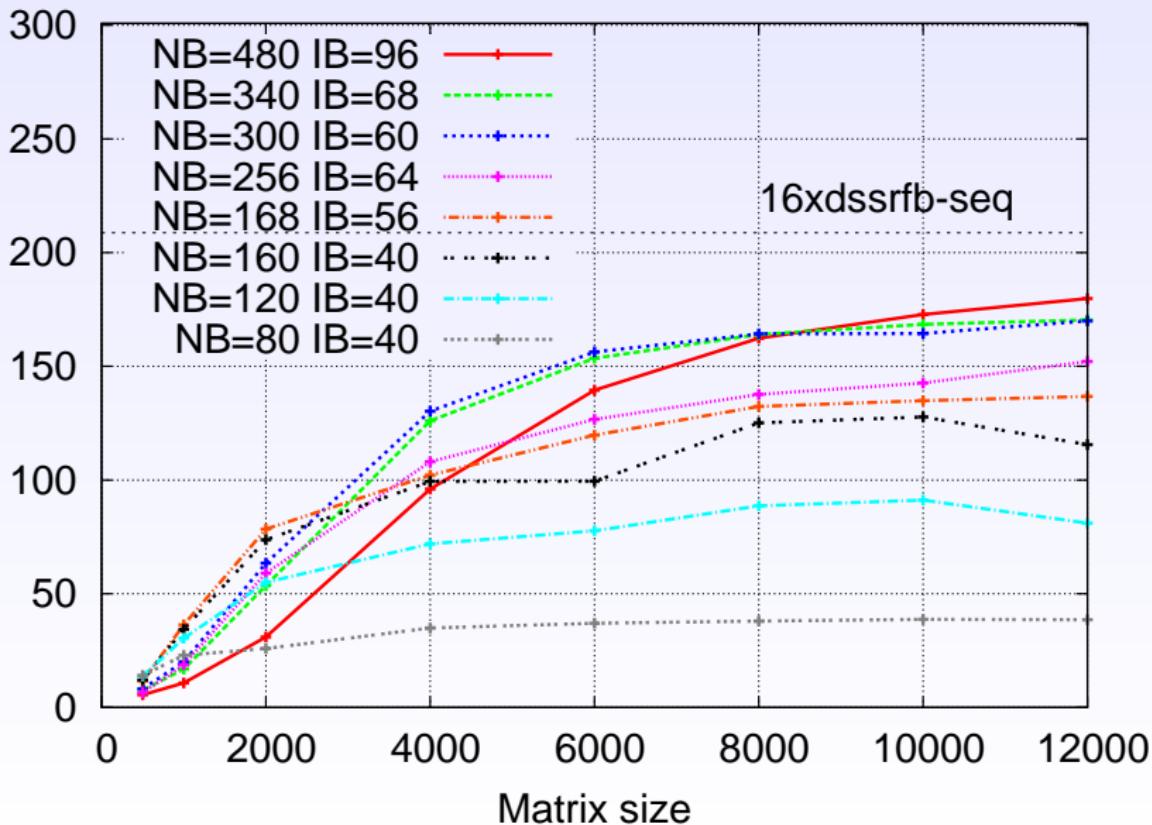
# Impact of NB - DPOTRF- Power6- 32 cores



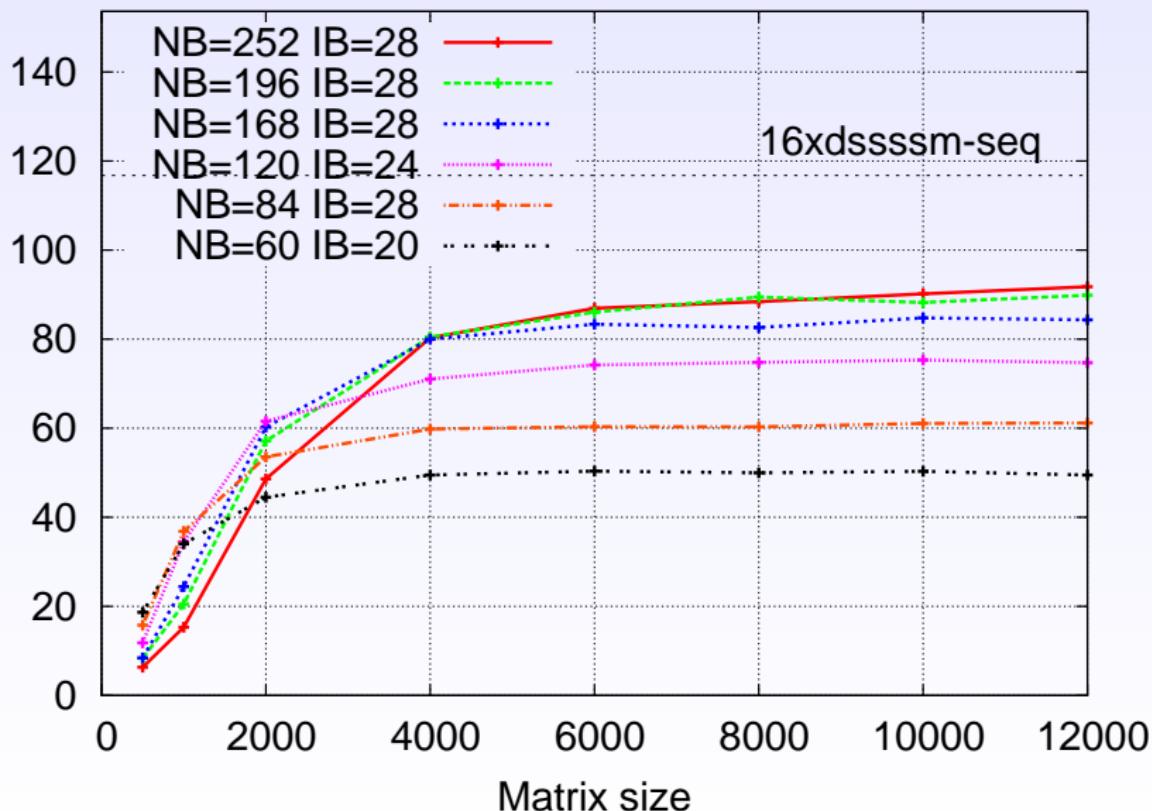
# Impact of NB/IB - DGEQRF- Intel64- 16 cores



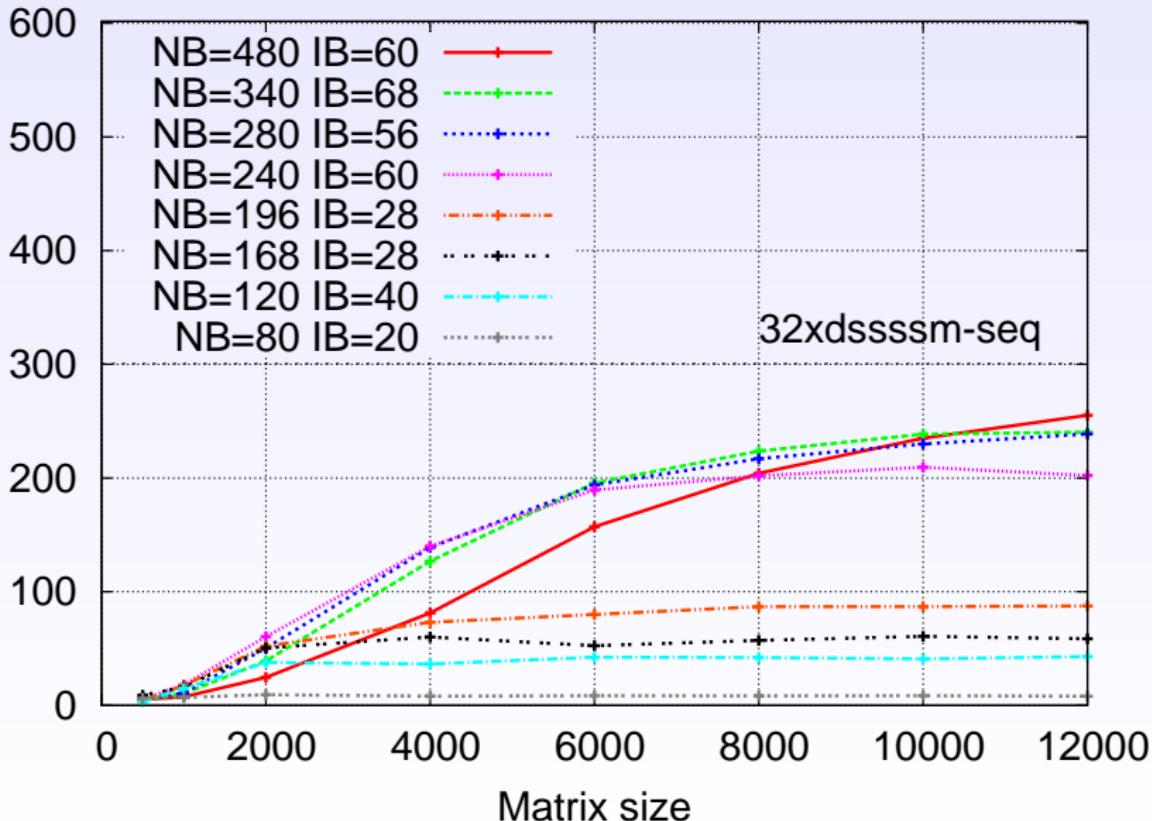
# Impact of NB/IB - DGEQRF- Power6- 32 cores



# Impact of NB/IB - DGETRF- Intel64- 16 cores



# Impact of NB/IB - DGETRF- Power6- 32 cores



# Exhaustive search

For "each" matrix size and number of cores:

1. Time PLASMA on all NB/IB samples;
2. Select the best sample.

## Number of samples

- ★  $|\{(IB, NB) \mid IB|NB, 40 \leq NB \leq 500, 4 \leq IB \leq NB\}| = 1352$ ;
- ★ all combinations cannot be explored on large executions;

→ need for a pruned search.

# Exhaustive search

For "each" matrix size and number of cores:

1. Time PLASMA on all NB/IB samples;
2. Select the best sample.

## Number of samples

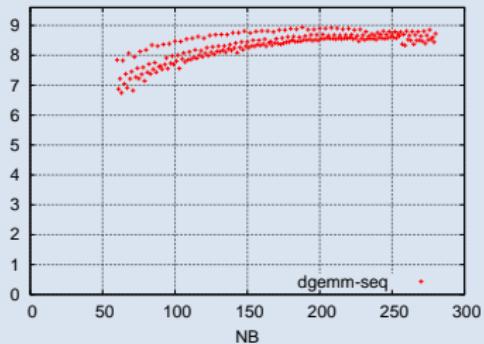
- ★  $|\{(IB, NB) \mid IB|NB, 40 \leq NB \leq 500, 4 \leq IB \leq NB\}| = 1352$ ;
- ★ all combinations cannot be explored on large executions;

→ need for a pruned search.

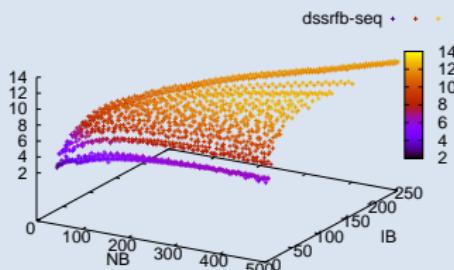
# Pruned search

## Method

1. Time serial core kernels (dgemm, dssrfb, dssssm).



Intel64 - dgemm



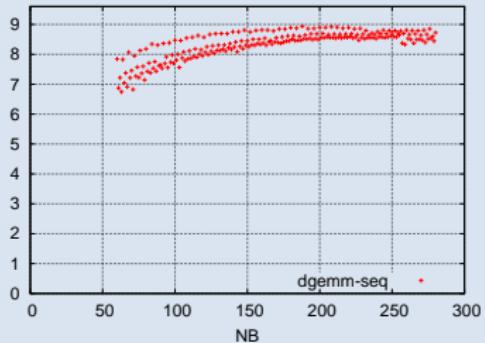
Power6 - dssrfb

2. Pick up the "best" NB or NB/IB samples (**pruning**);
3. Select one per matrix size and number of cores.

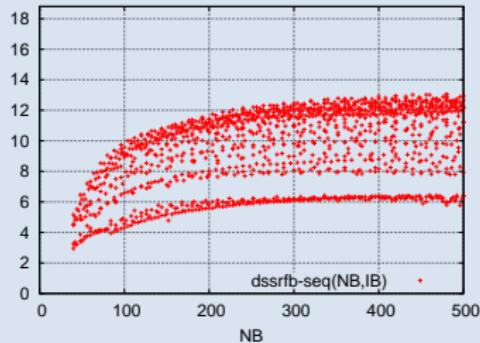
# Pruned search

## Method

1. Time serial core kernels (dgemm, dssrfb, dssssm).



Intel64 - dgemm



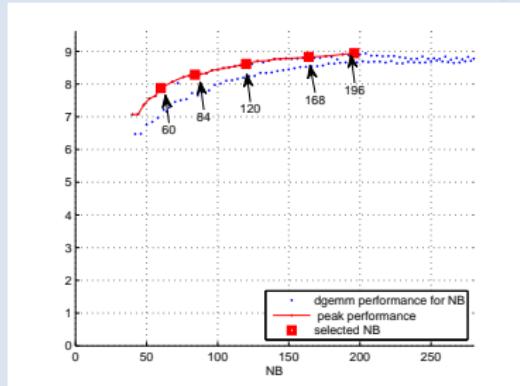
Power6 - dssrfb

2. Pick up the "best" NB or NB/IB samples ([pruning](#));
3. Select one per matrix size and number of cores.

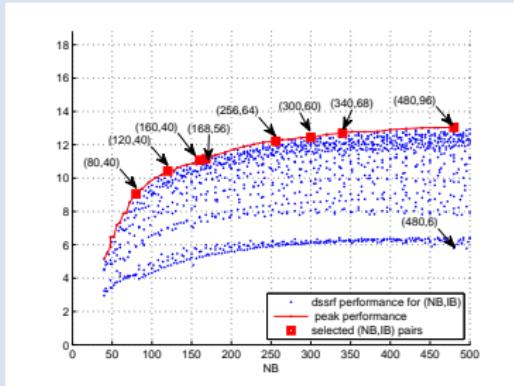
# Pruned search

## Method

1. Time serial core kernels (dgemm, dssrfb, dssssm).



Intel64 - dgemm

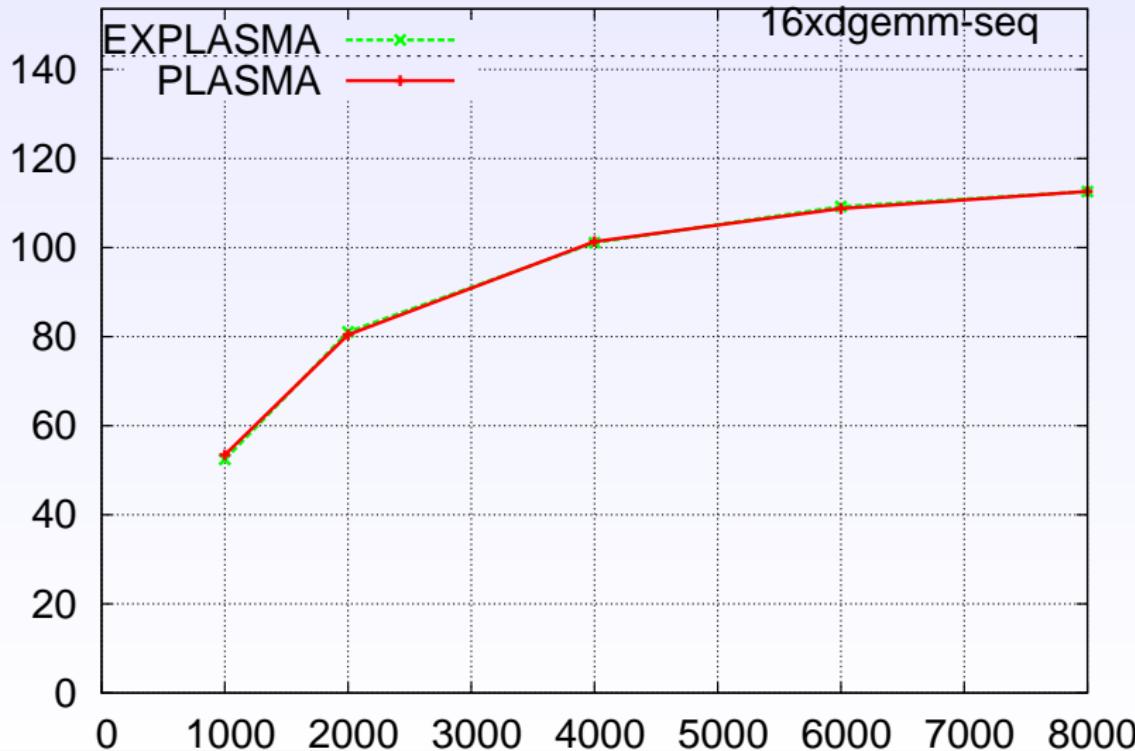


Power6 - dssrfb

2. Pick up the "best" NB or NB/IB samples (**pruning**);
3. Select one per matrix size and number of cores.

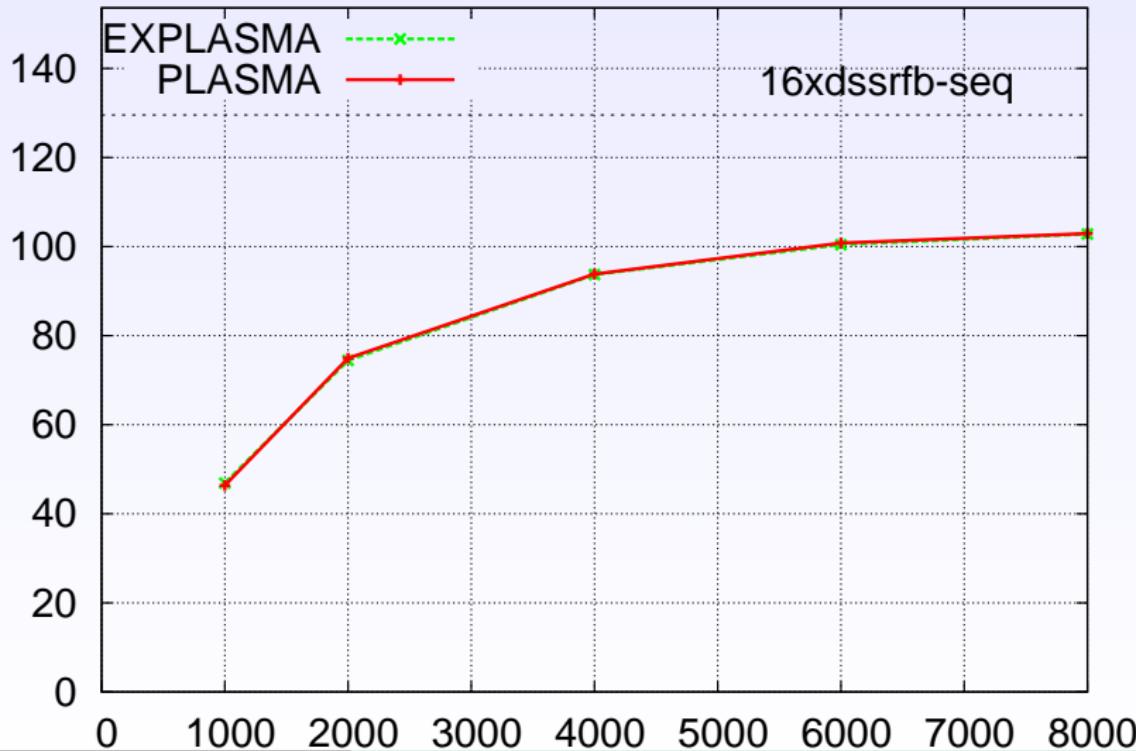
# Exhaustive search VS pruned search

## Intel64- 16 cores - DPOTRF



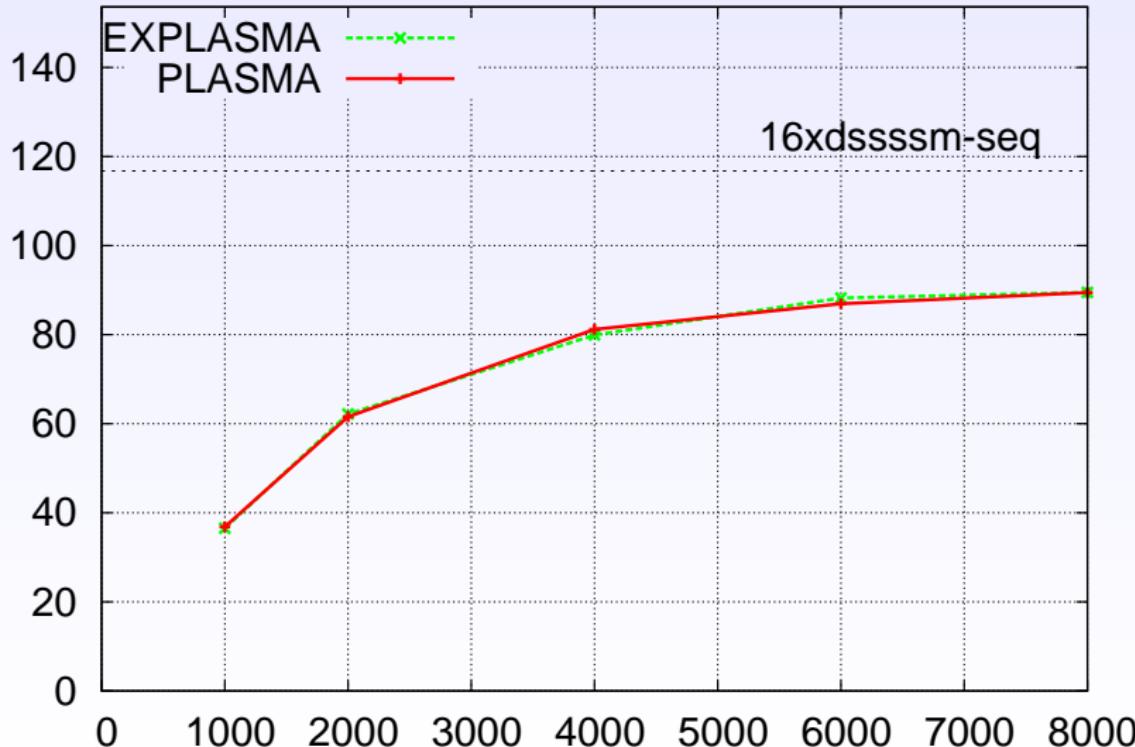
# Exhaustive search VS pruned search

## Intel64- 16 cores - DGEQRF



# Exhaustive search VS pruned search

Intel64- 16 cores - DGETRF



# Other software

- ★ PLASMA: pruned search.
- ★ TBLAS: exhaustive search.
- ★ SCALAPACK, PESSL: exhaustive search.
- ★ LAPACK, MKL, ESSL: tuned by vendor.

# Outline

## 1. Tile Algorithms

- Cholesky Factorization
- QR (&LU) Factorizations

## 2. Experimental environment

- Libraries
- Hardware
- Metrics

## 3. Tuning

- PLASMA

## 4. Comparison against other libraries

- Experiments on few cores
- Experiments on a large number of cores
- PLASMA scalability

## 5. Conclusion and current work

# Outline

## 1. Tile Algorithms

- Cholesky Factorization
- QR (&LU) Factorizations

## 2. Experimental environment

- Libraries
- Hardware
- Metrics

## 3. Tuning

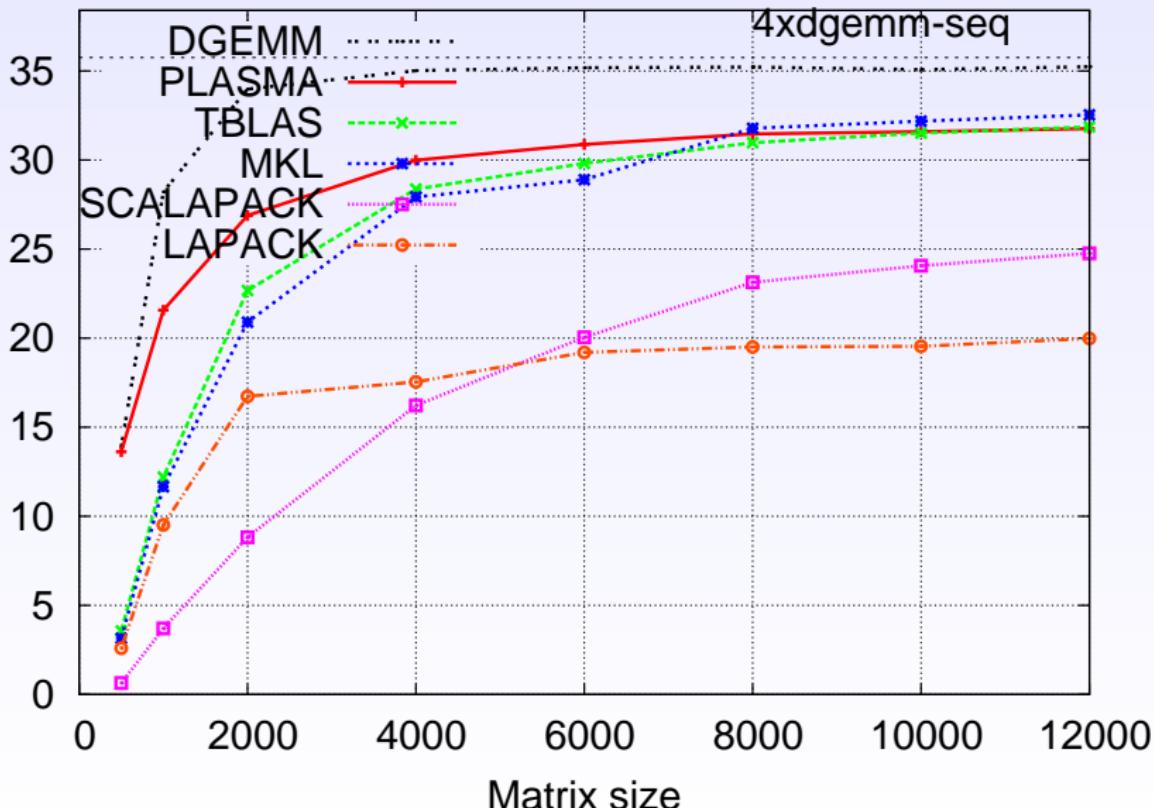
- PLASMA

## 4. Comparison against other libraries

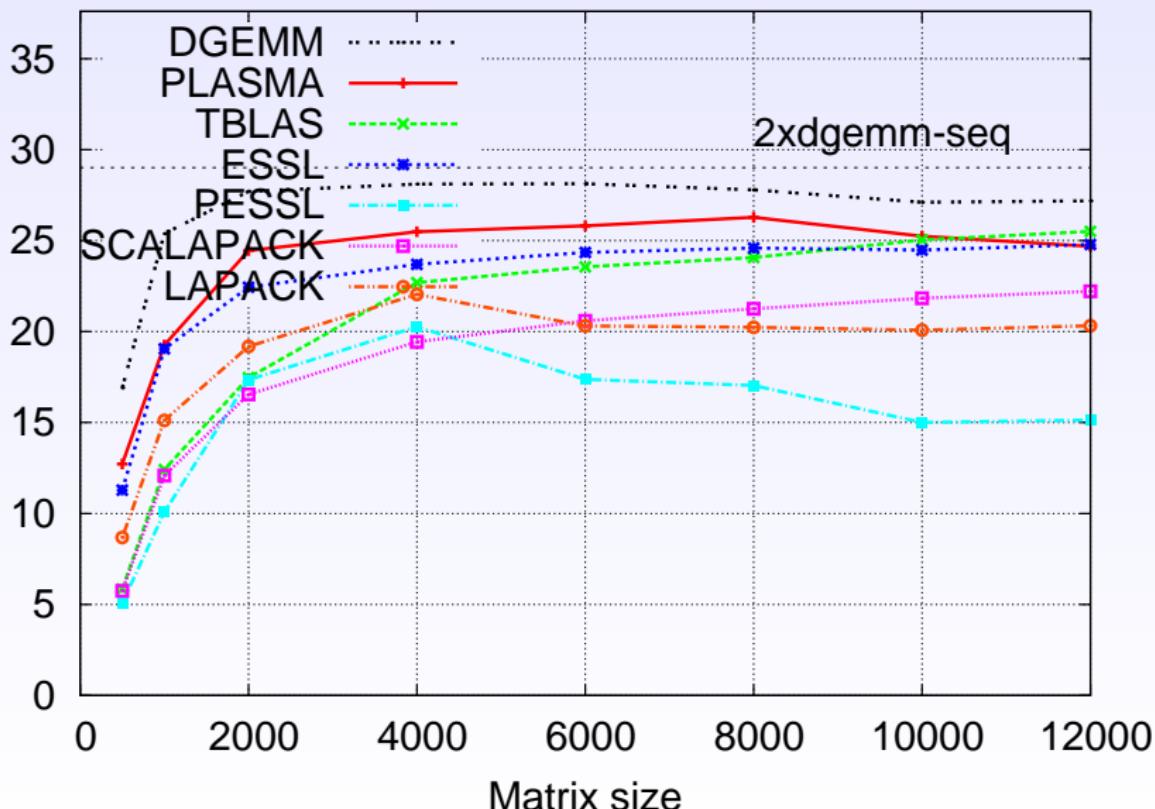
- Experiments on few cores
- Experiments on a large number of cores
- PLASMA scalability

## 5. Conclusion and current work

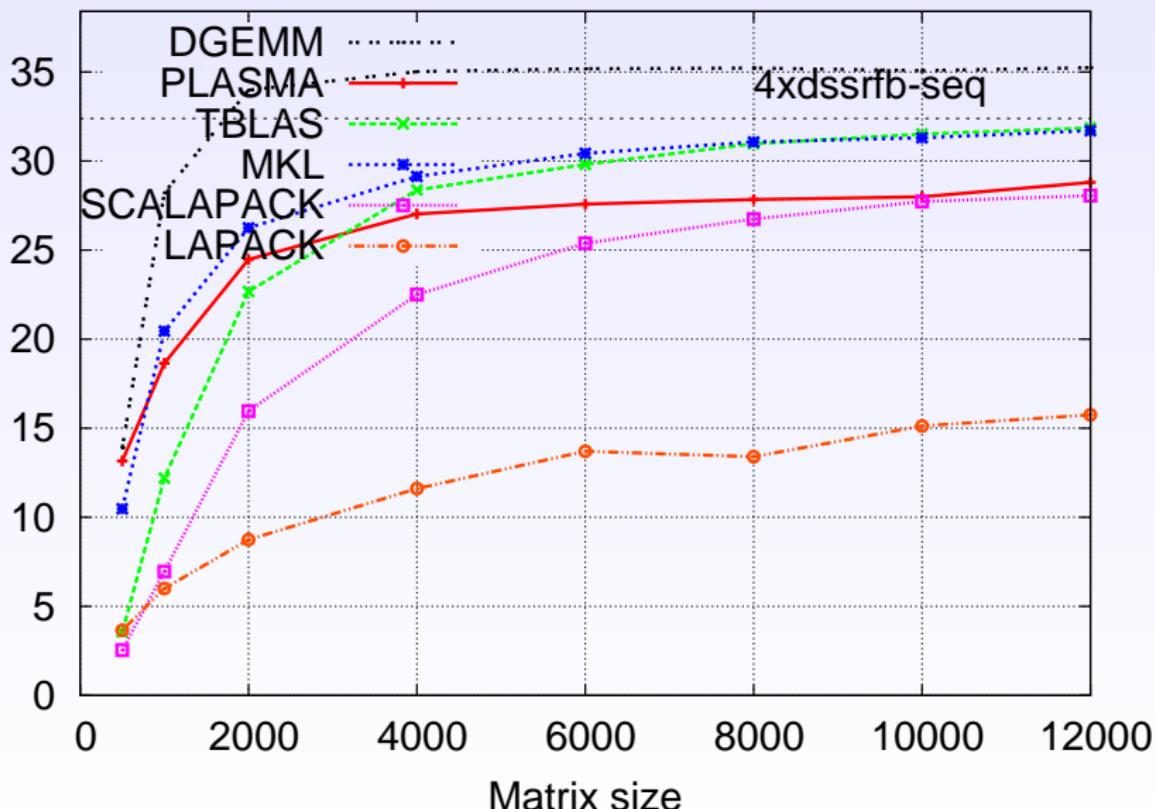
## DPOTRF- Intel64- 4 cores



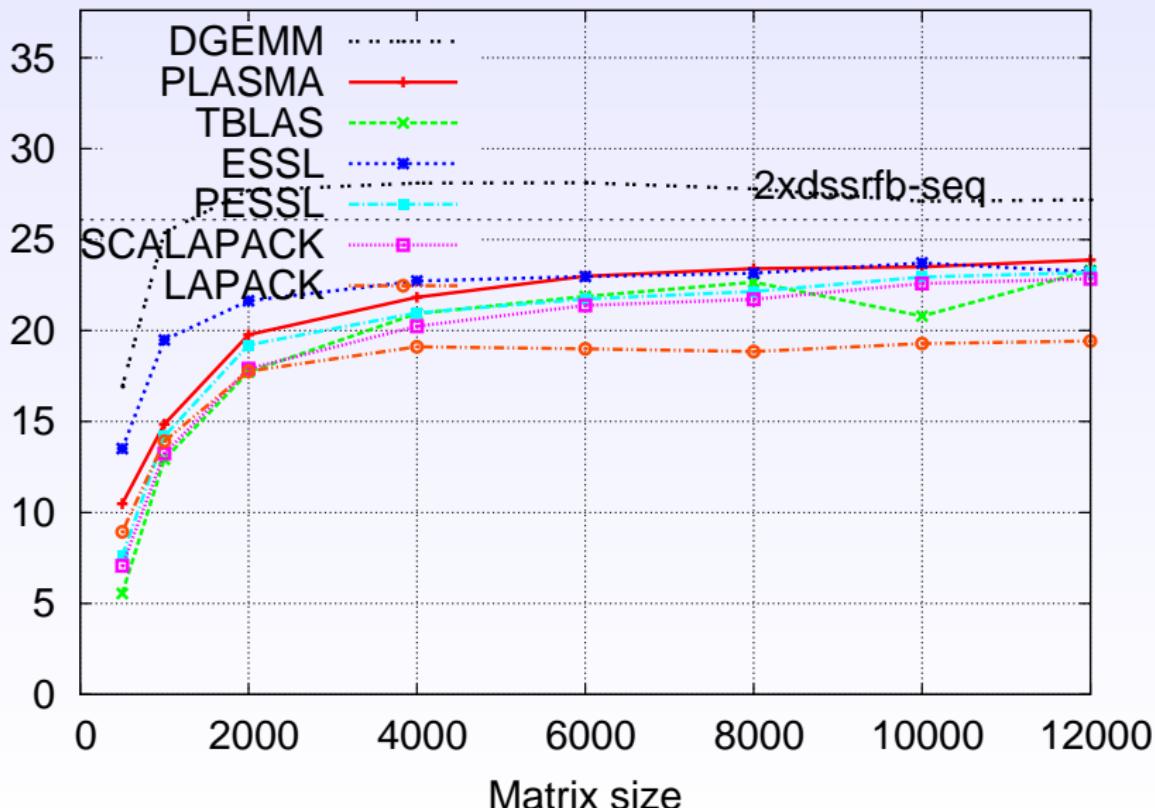
## DPOTRF- Power6- 2 cores



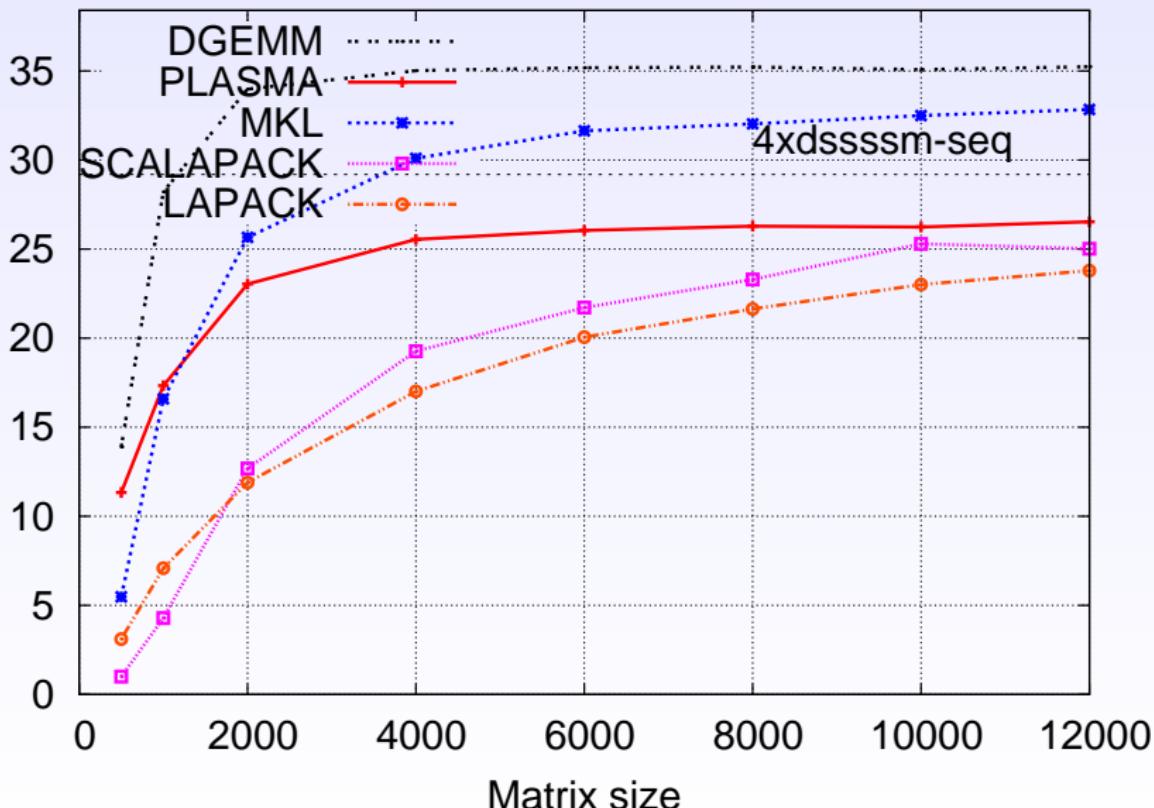
## DGEQRF- Intel64- 4 cores



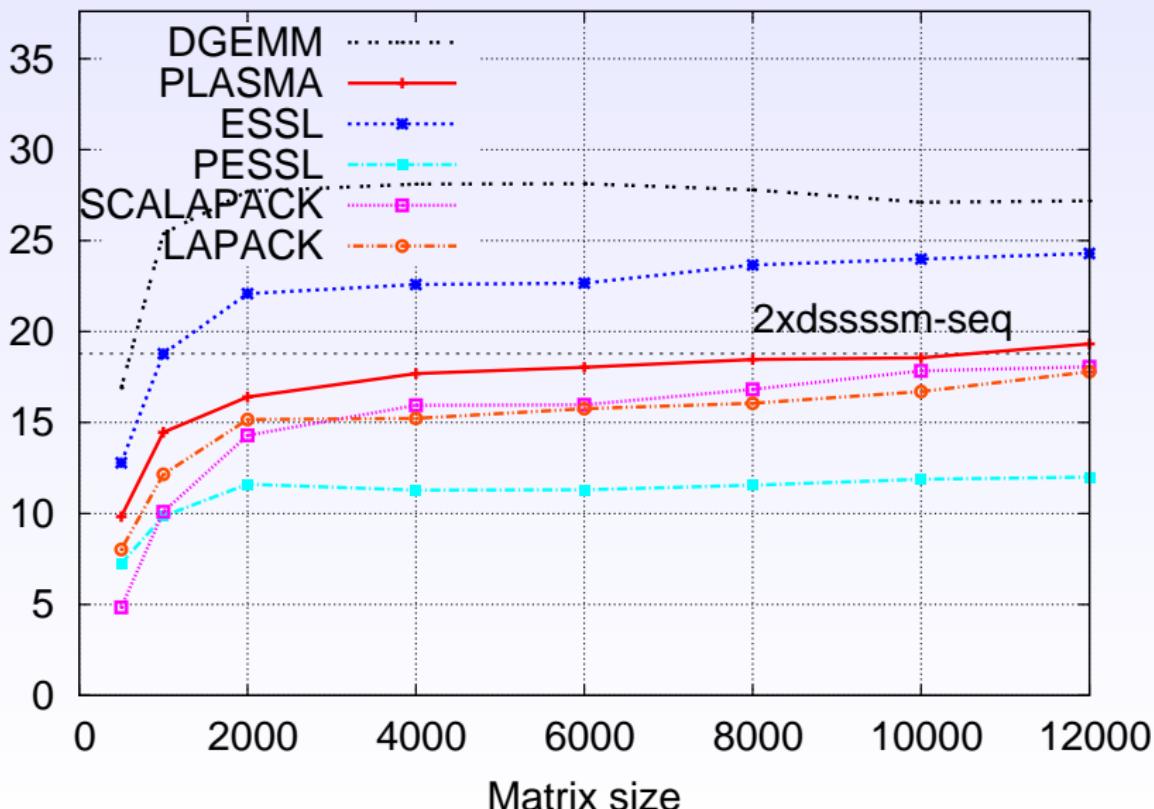
## DGEQRF- Power6- 2 cores



## DGETRF- Intel64- 4 cores



## DGETRF- Power6- 2 cores



# Outline

## 1. Tile Algorithms

- Cholesky Factorization
- QR (&LU) Factorizations

## 2. Experimental environment

- Libraries
- Hardware
- Metrics

## 3. Tuning

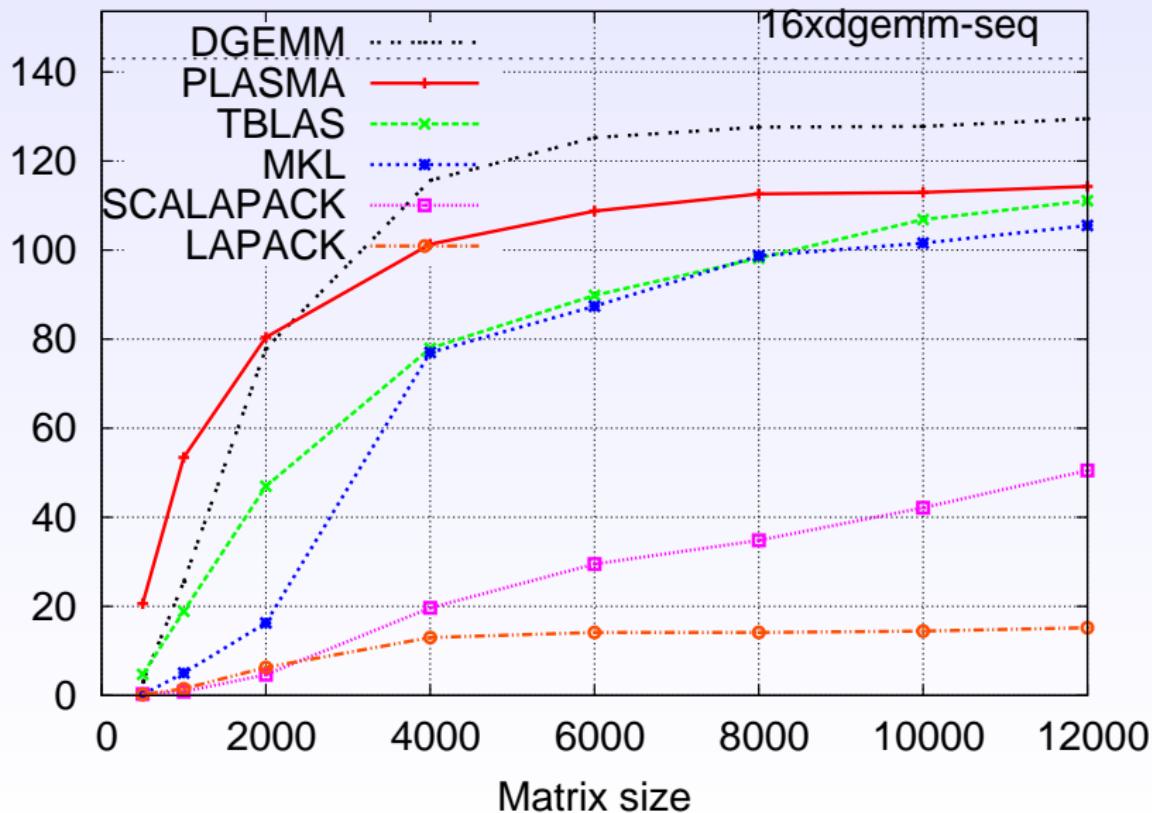
- PLASMA

## 4. Comparison against other libraries

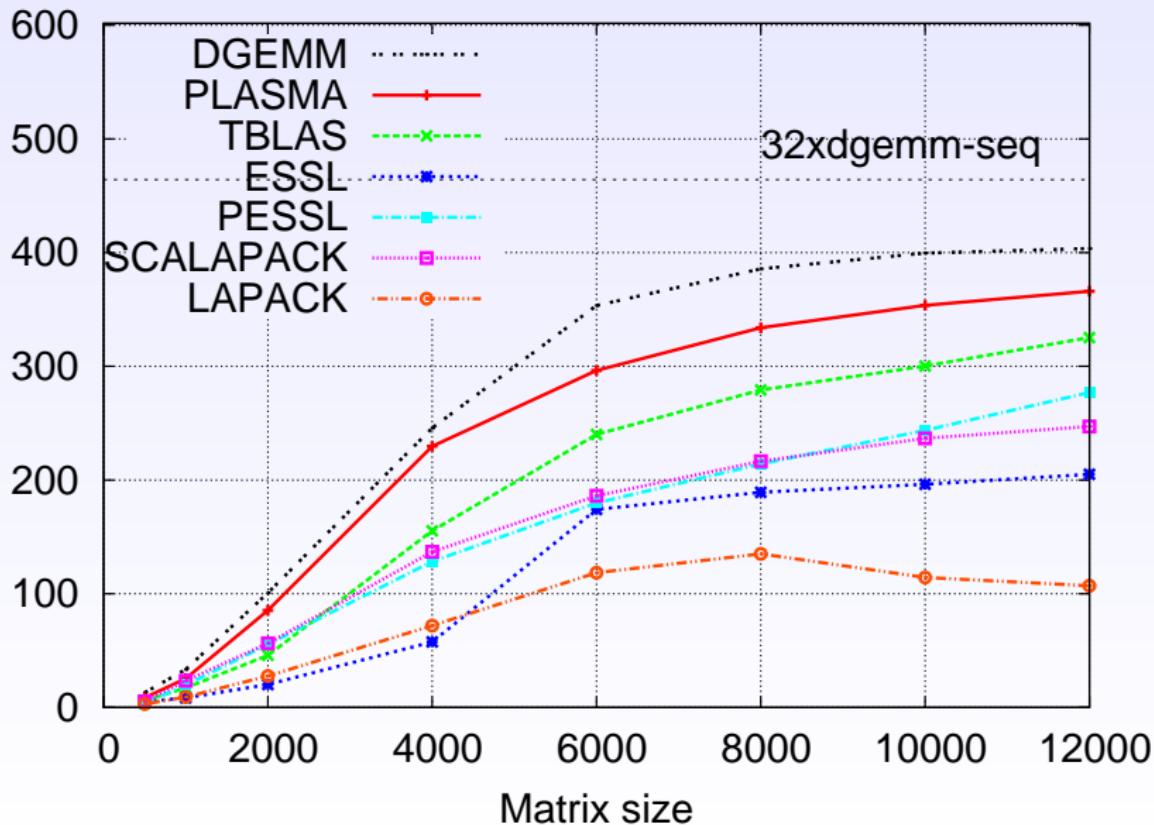
- Experiments on few cores
- Experiments on a large number of cores
- PLASMA scalability

## 5. Conclusion and current work

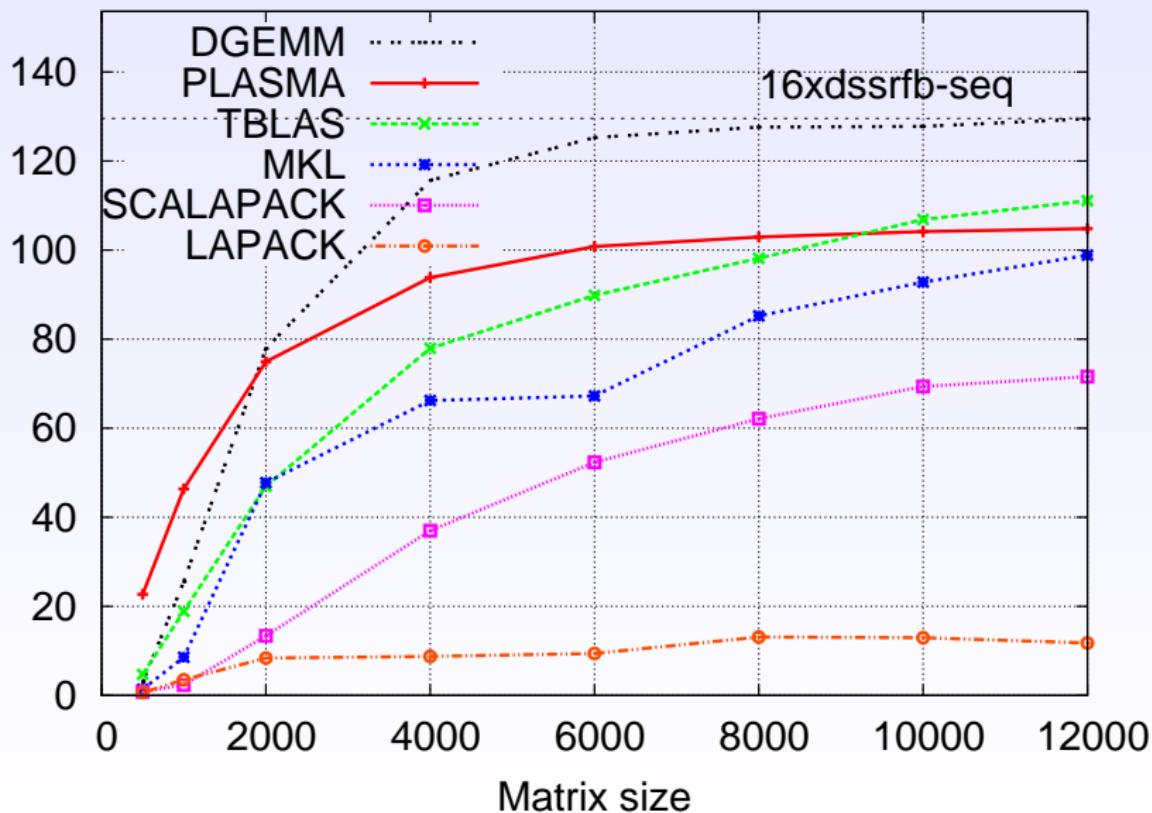
## DPOTRF- Intel64- 16 cores



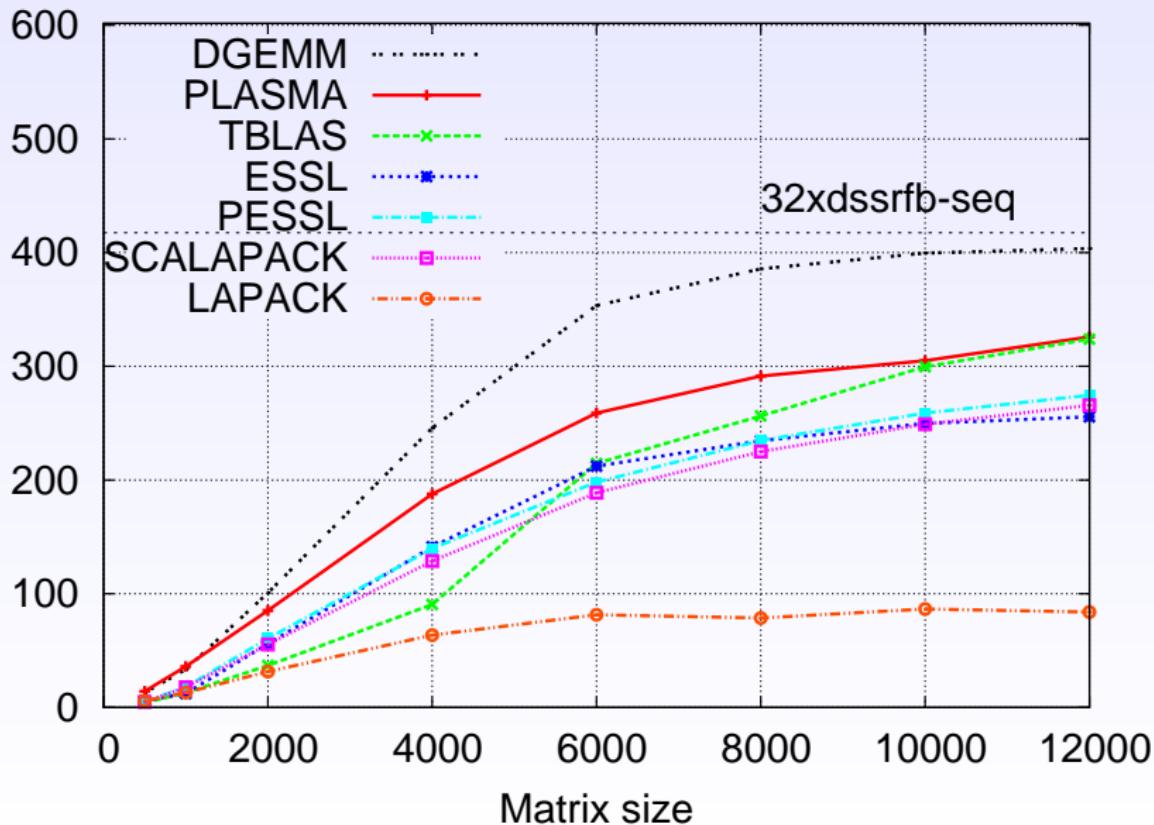
## DPOTRF- Power6- 32 cores



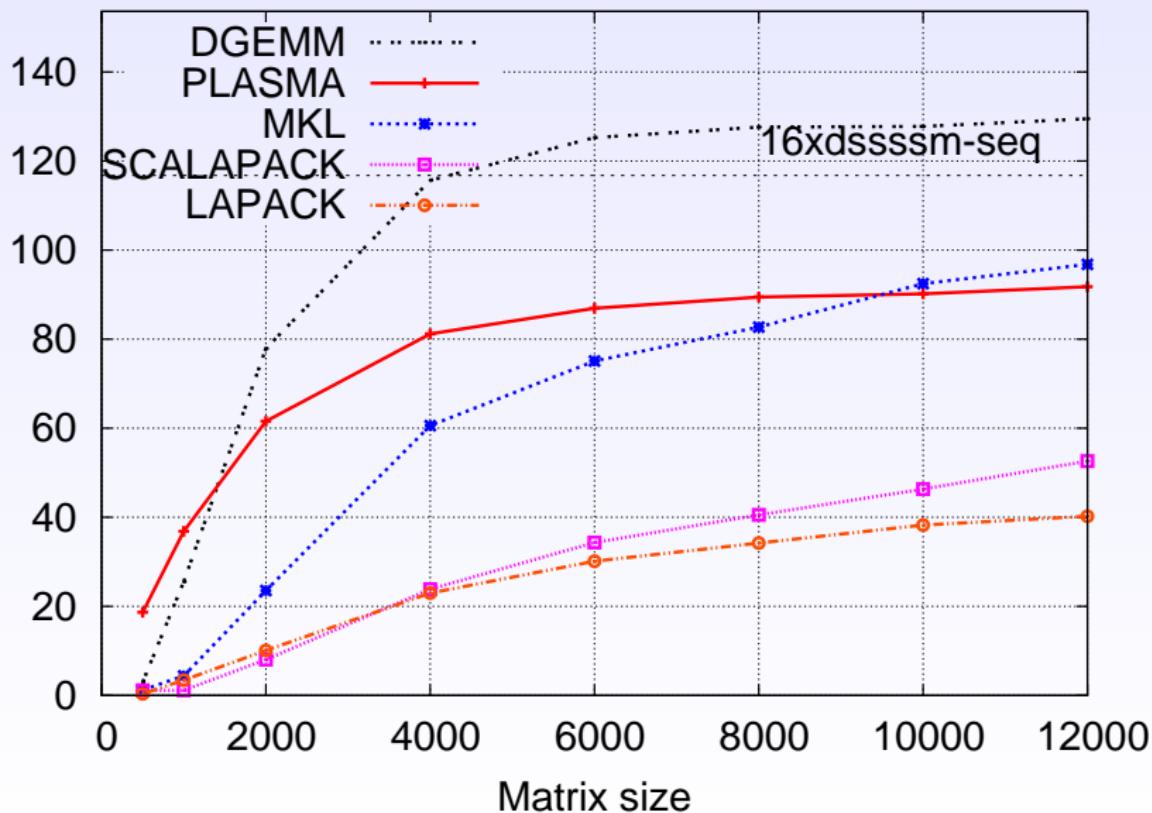
## DGEQRF- Intel64- 16 cores



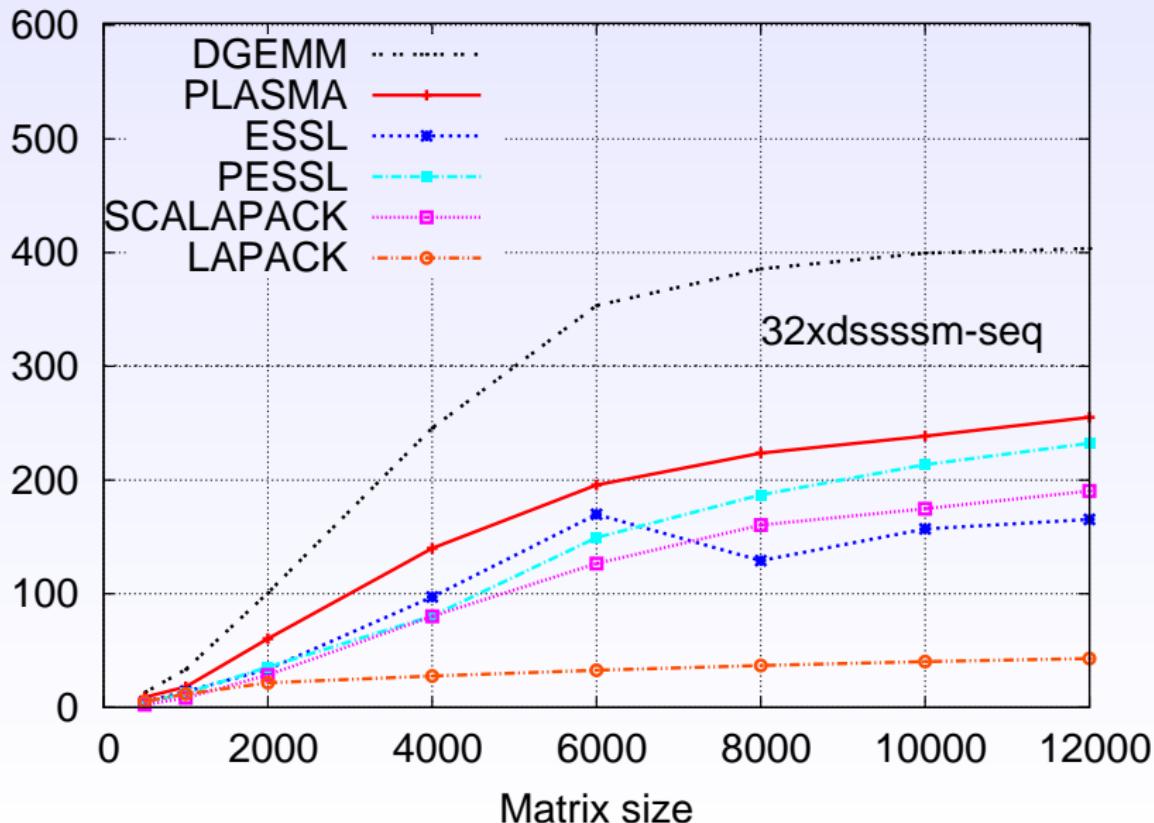
## DGEQRF- Power6- 32 cores



## DGETRF- Intel64- 16 cores



## DGETRF- Power6- 32 cores



# Outline

## 1. Tile Algorithms

- Cholesky Factorization
- QR (&LU) Factorizations

## 2. Experimental environment

- Libraries
- Hardware
- Metrics

## 3. Tuning

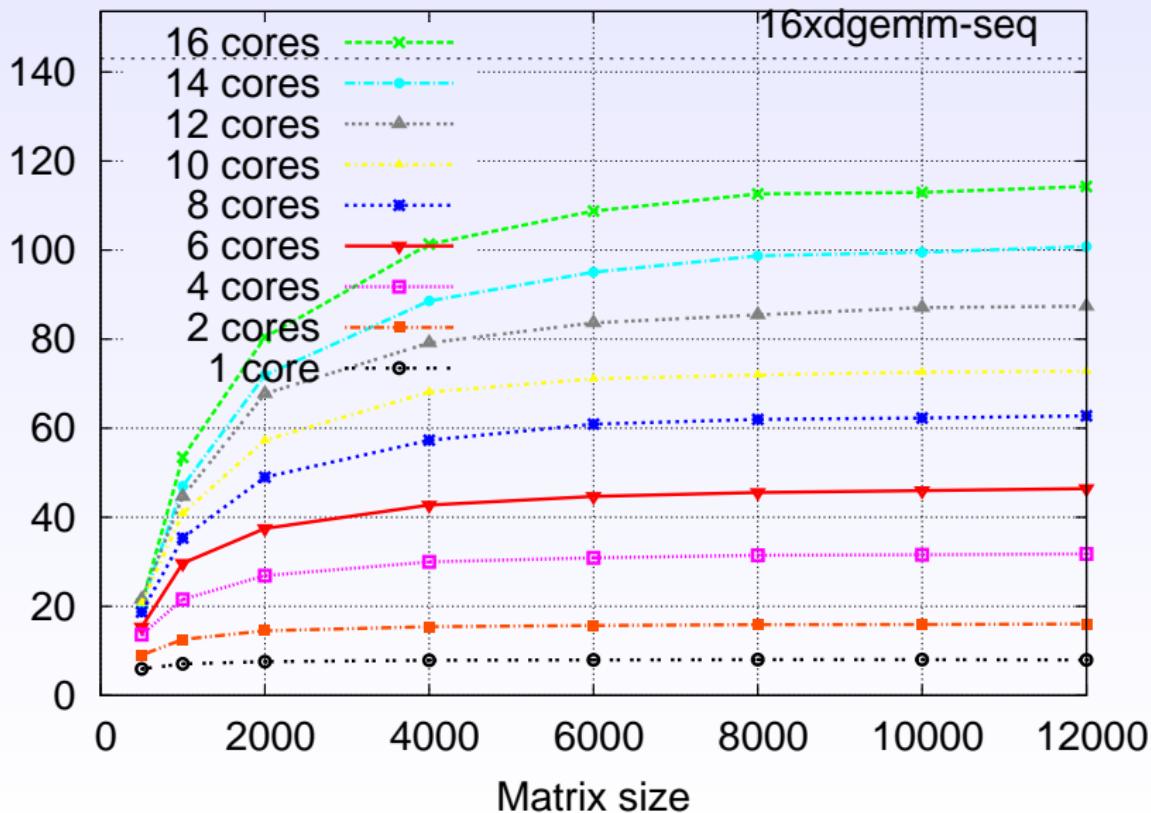
- PLASMA

## 4. Comparison against other libraries

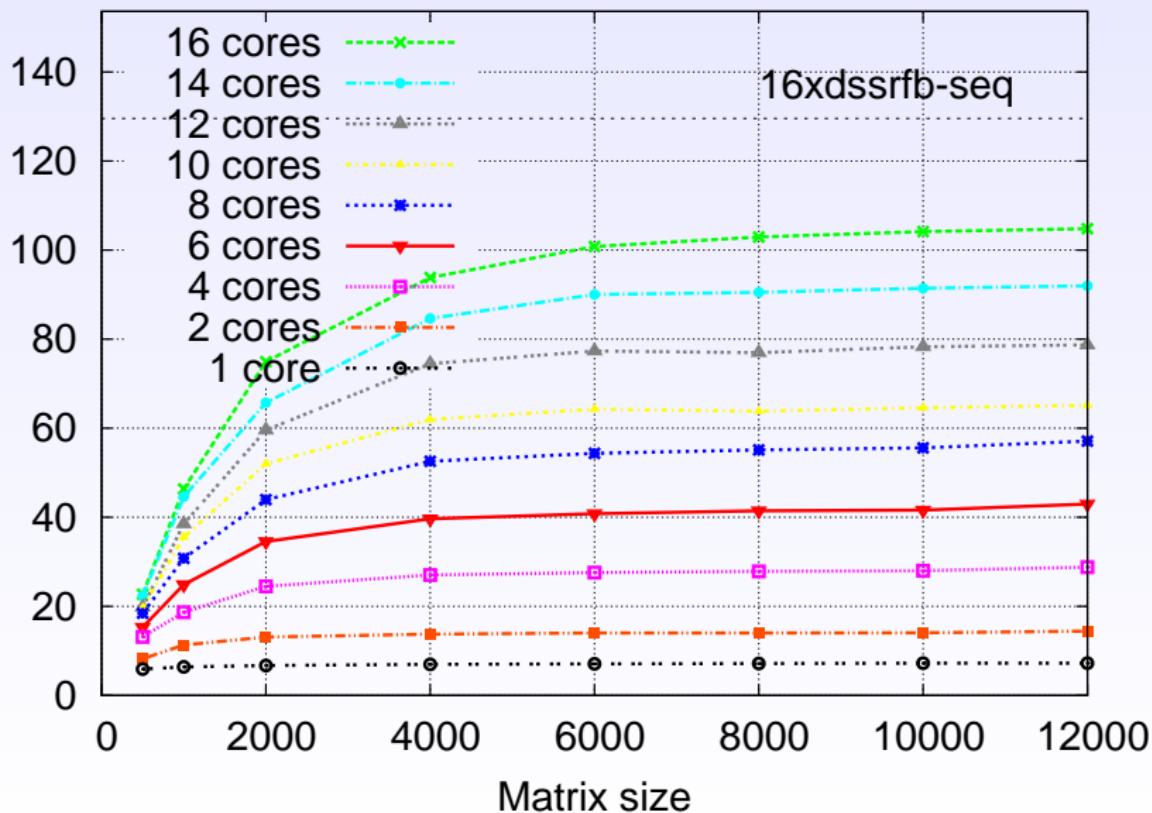
- Experiments on few cores
- Experiments on a large number of cores
- **PLASMA scalability**

## 5. Conclusion and current work

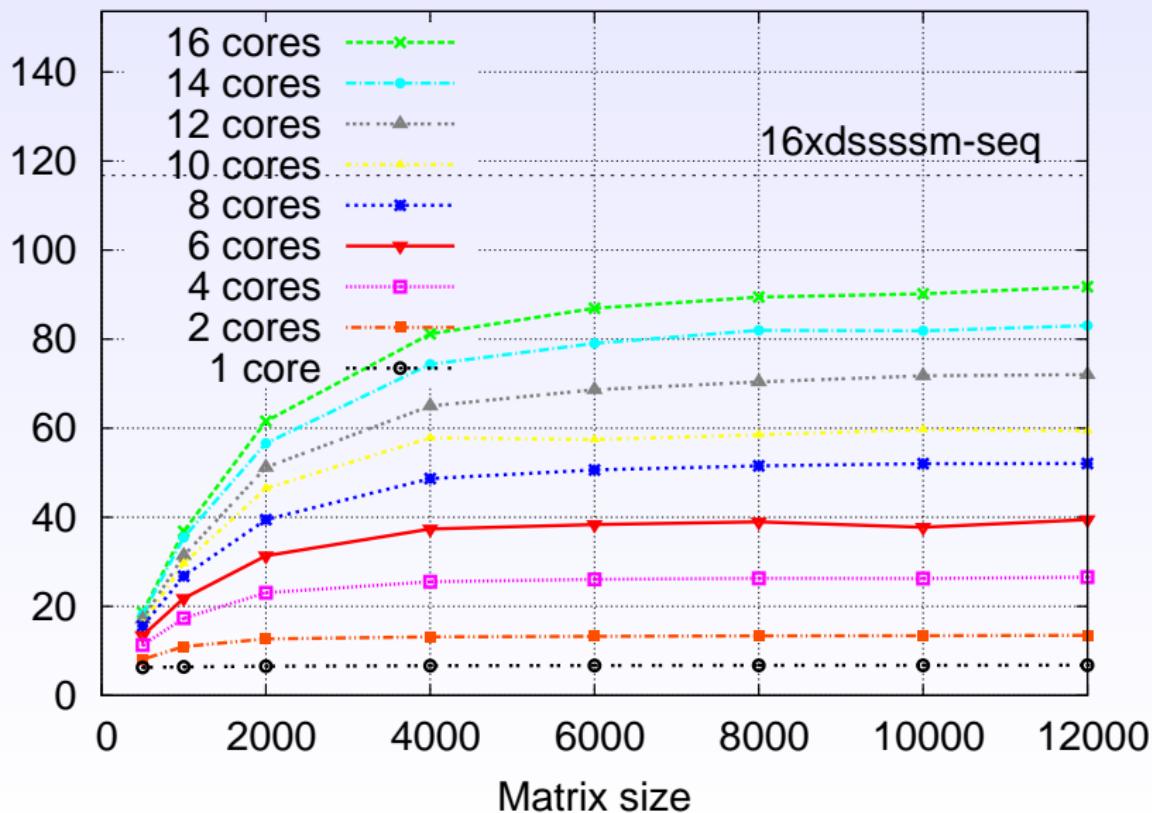
## PLASMA- DPOTRF- Intel64



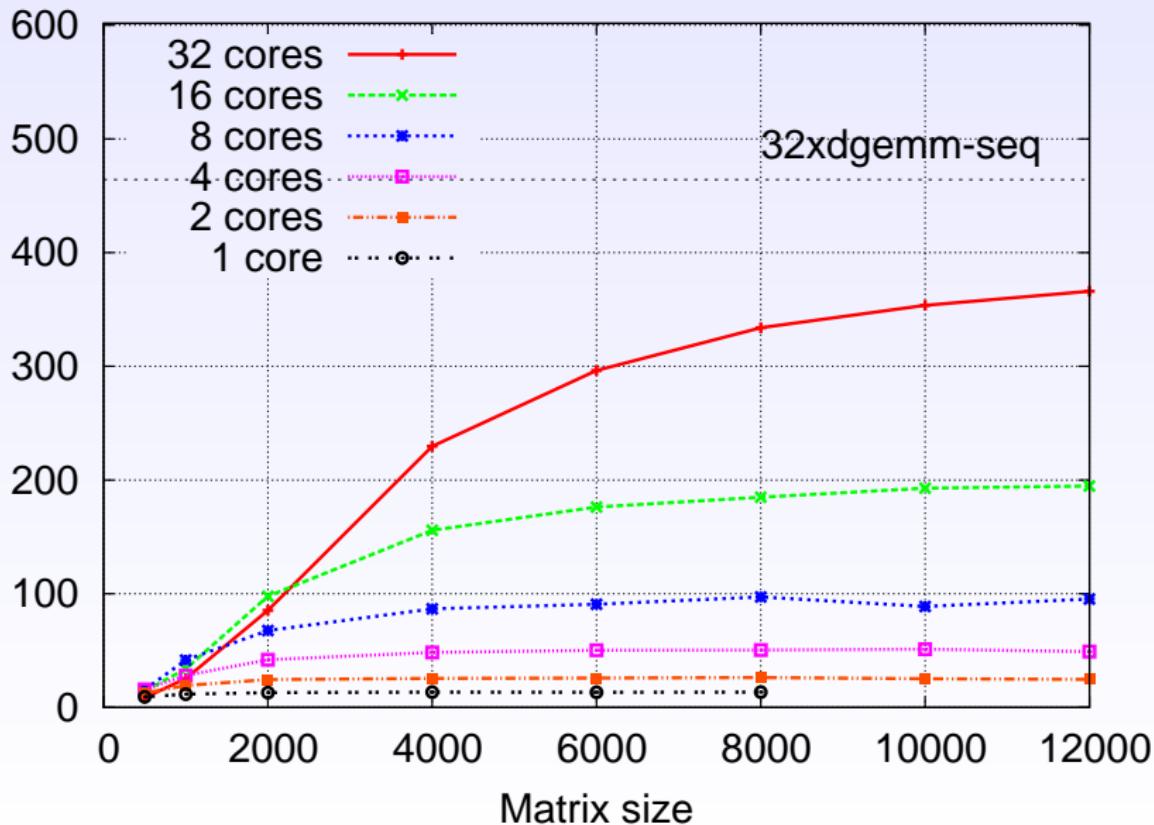
## PLASMA- DGEQRF- Intel64



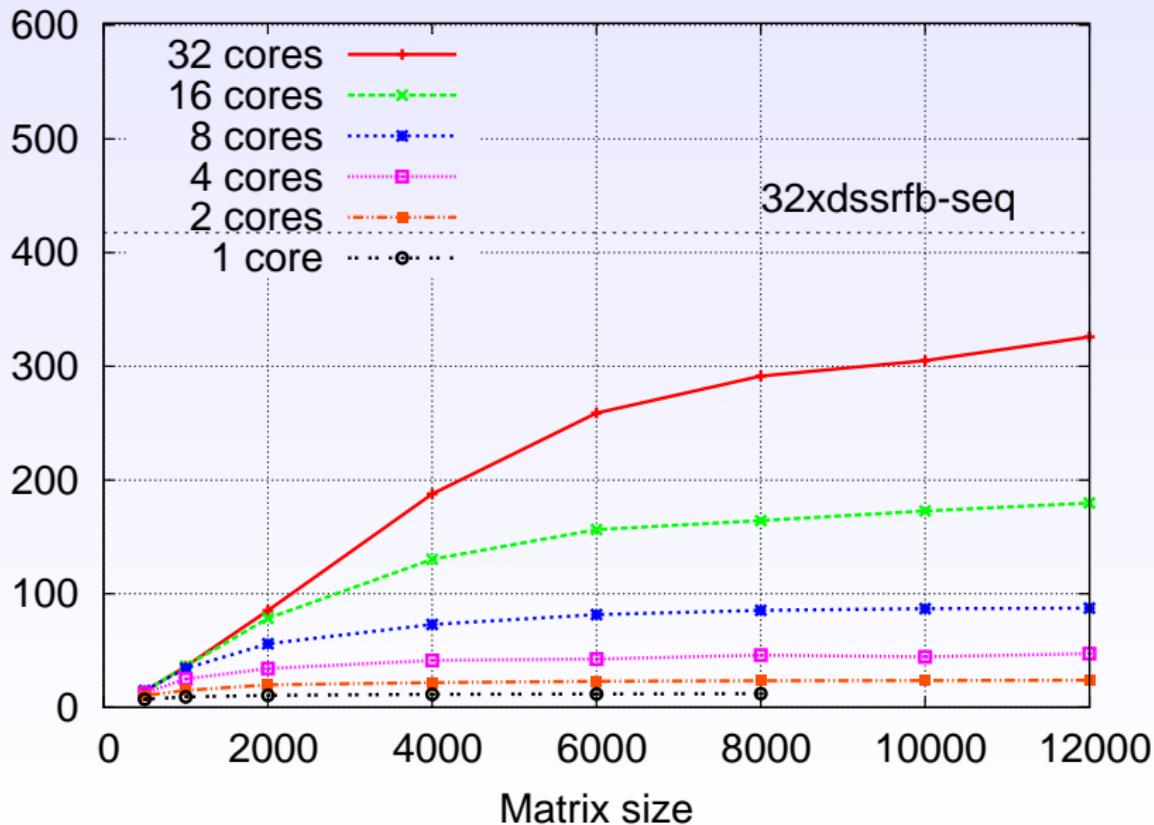
## PLASMA- DGETRF- Intel64



## PLASMA- DPOTRF- Power6



## PLASMA- DGEQRF- Power6



# Outline

## 1. Tile Algorithms

- Cholesky Factorization
- QR (&LU) Factorizations

## 2. Experimental environment

- Libraries
- Hardware
- Metrics

## 3. Tuning

- PLASMA

## 4. Comparison against other libraries

- Experiments on few cores
- Experiments on a large number of cores
- PLASMA scalability

## 5. Conclusion and current work

# Conclusion

- ★ Performance brought by tile algorithms:
  - ⌚ Possible overheads:
    - extra-flops;
    - kernels not optimized.
  - ⌚ Benefits:
    - better data reuse;
    - better scheduling opportunities.
- ★ Better scalability.
- ★ Importance of tuning:
  - efficient pruned search.

# Current work

- ★ Compute-intensive kernels:
  - successive BLAS-3 calls → single BLAS-3 call.
- ★ Dynamic scheduling:
  - Piotr's presentation.
- ★ Improve scalability for small matrix sizes:
  - increase parallelism (tile TSQR).
- ★ Generalization to other linear algebra algorithms:
  - two-sided factorizations.

# Thanks

Questions?

# Outline

## 1. Scalability of other libraries

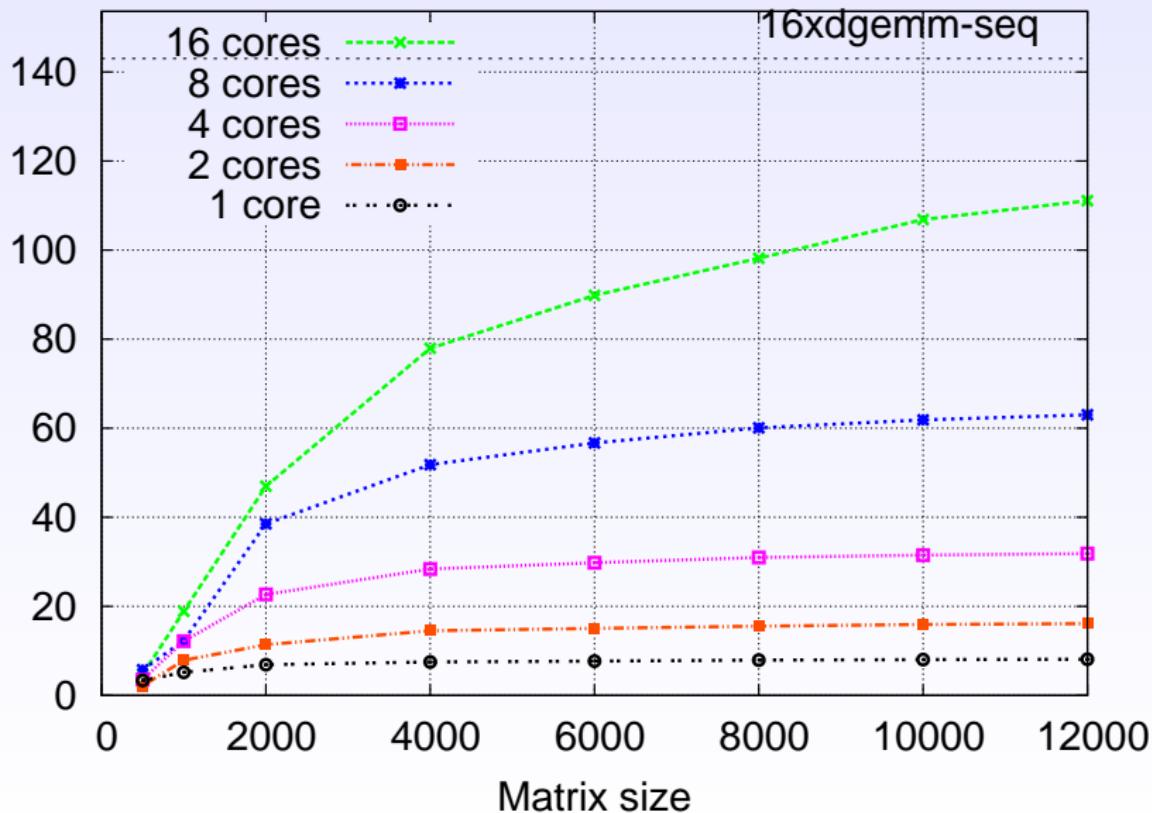
- TBLAS
- MKL- ESSL
- SCALAPACK- PESSL
- LAPACK

# Outline

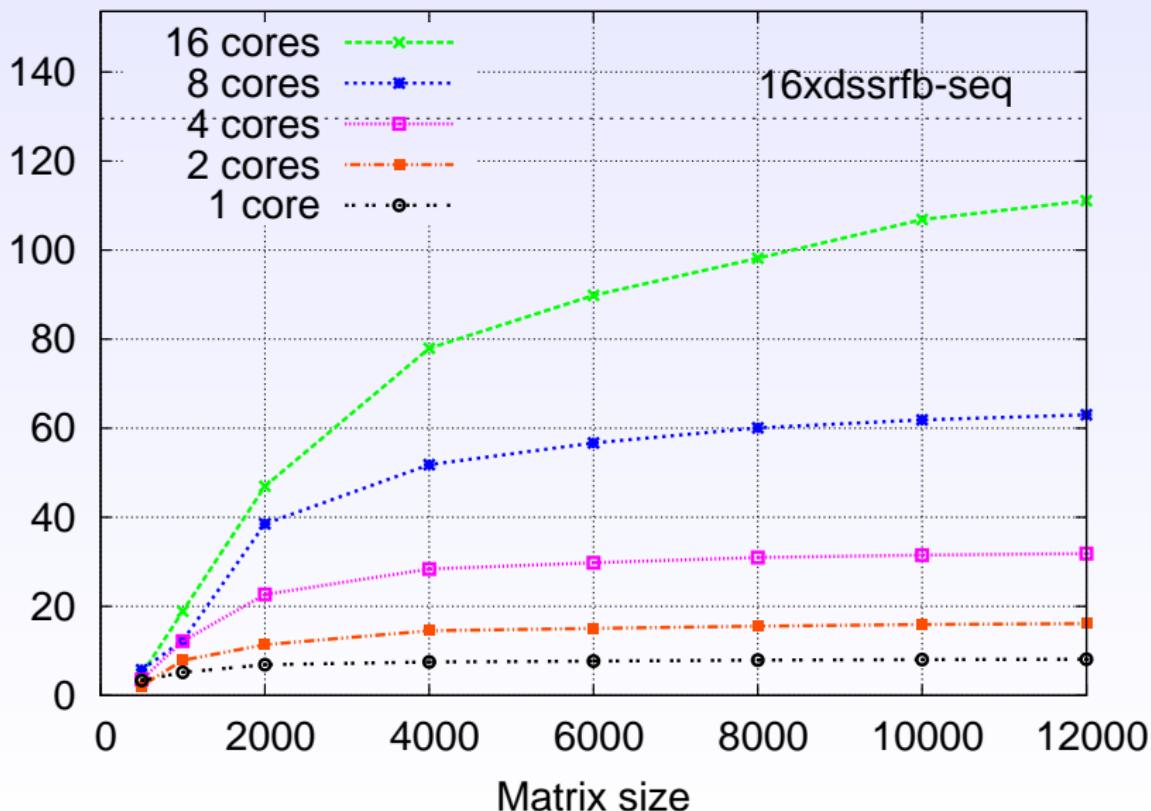
## 1. Scalability of other libraries

- TBLAS
- MKL- ESSL
- SCALAPACK- PESSL
- LAPACK

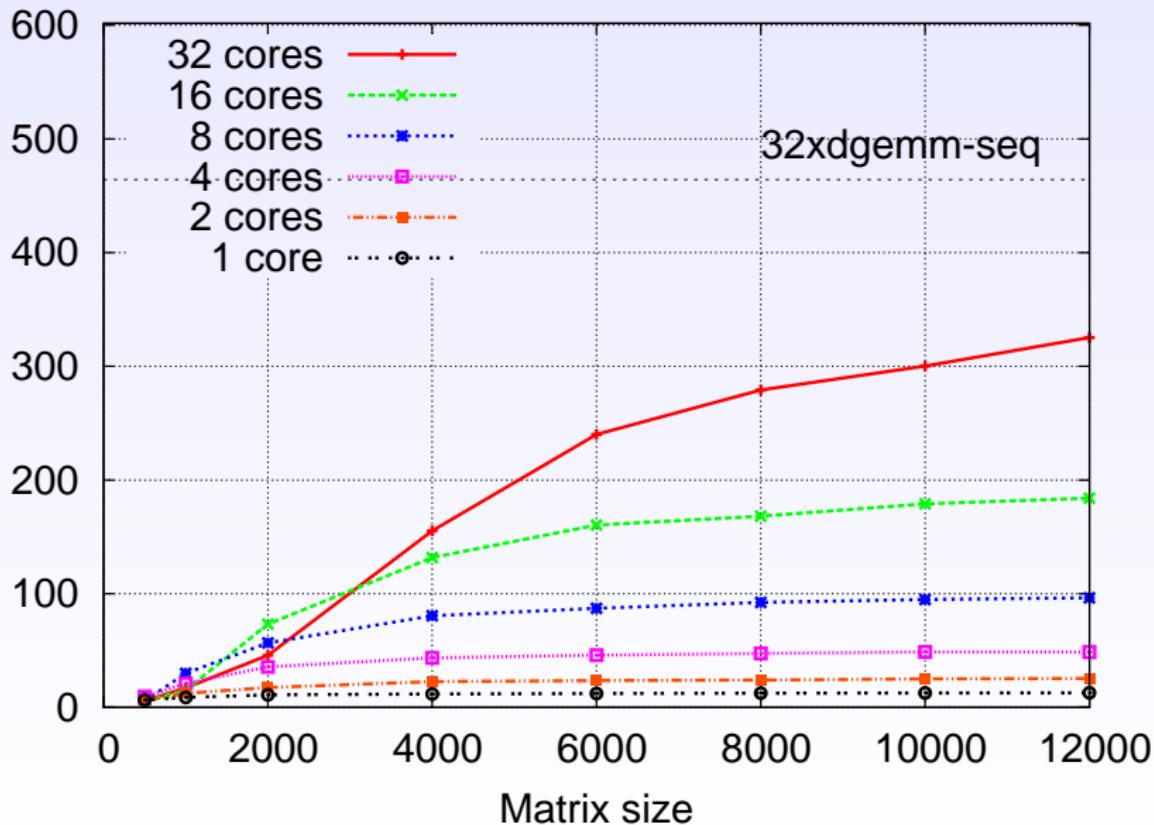
## TBLAS- DPOTRF- Intel64



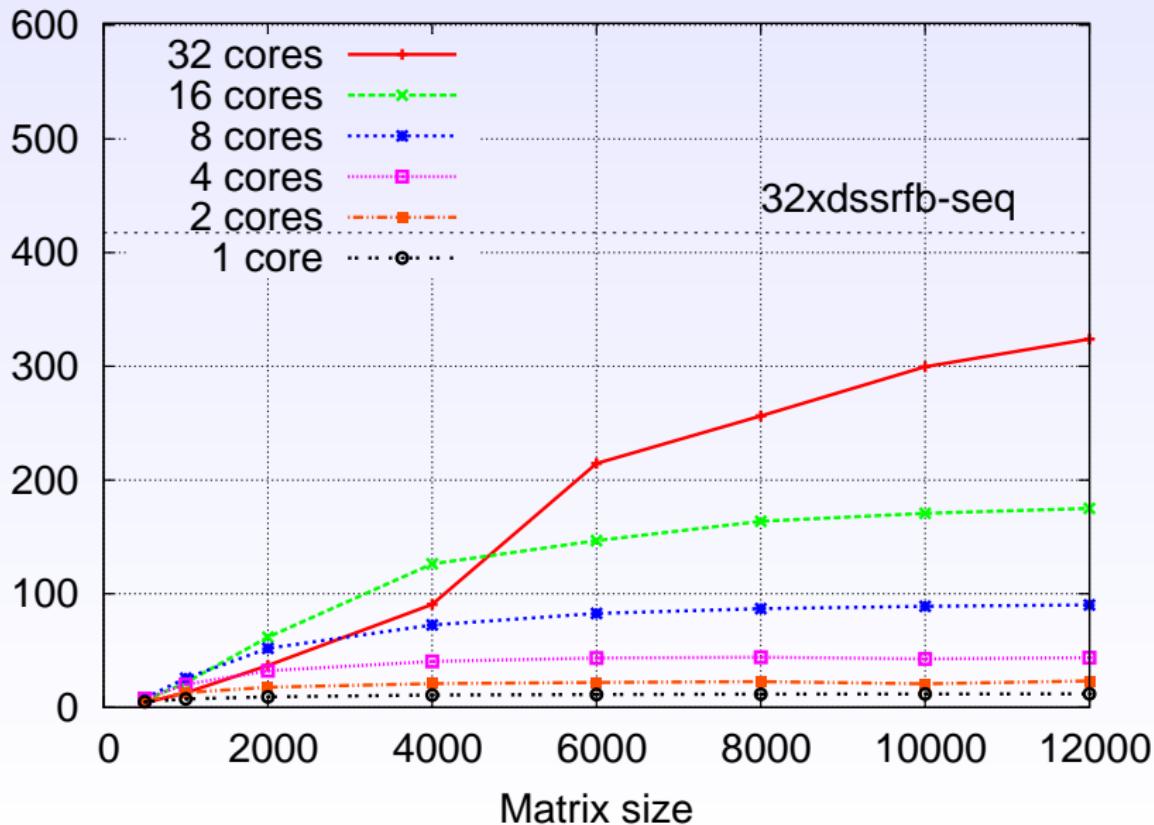
## TBLAS- DGEQRF- Intel64



## TBLAS- DPOTRF- Power6



## TBLAS- DGEQRF- Power6

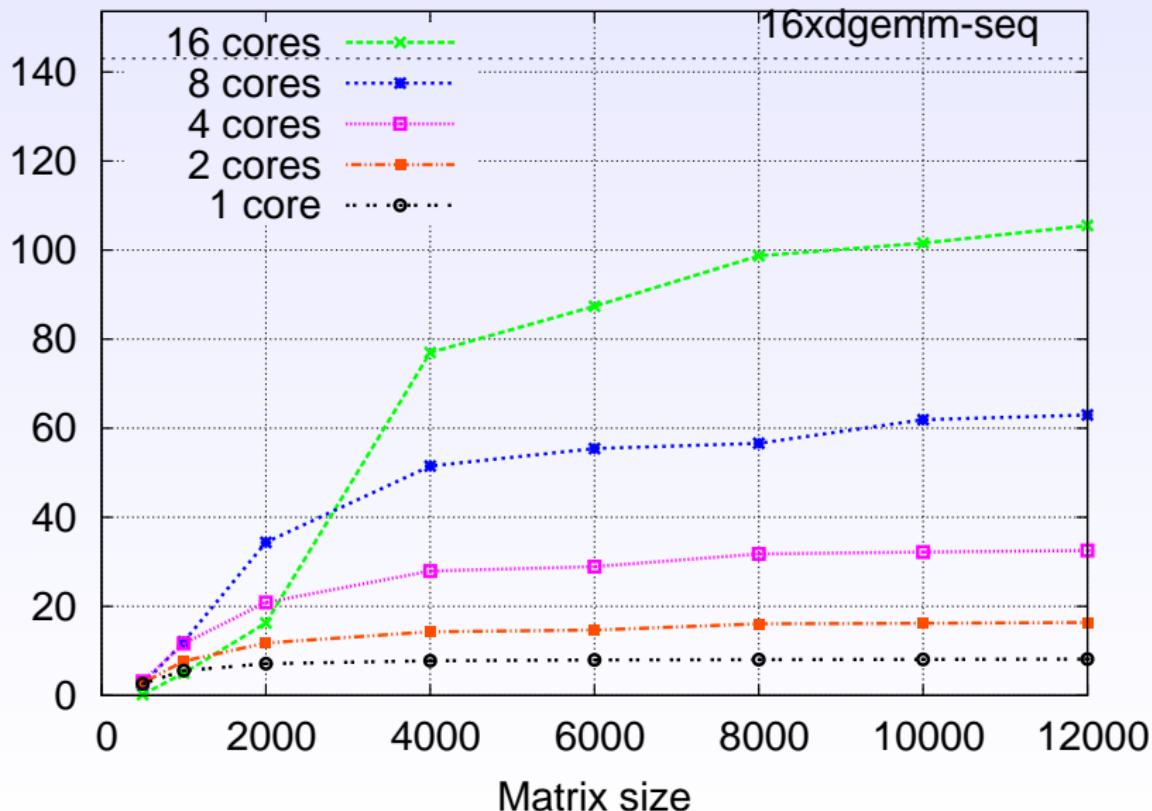


# Outline

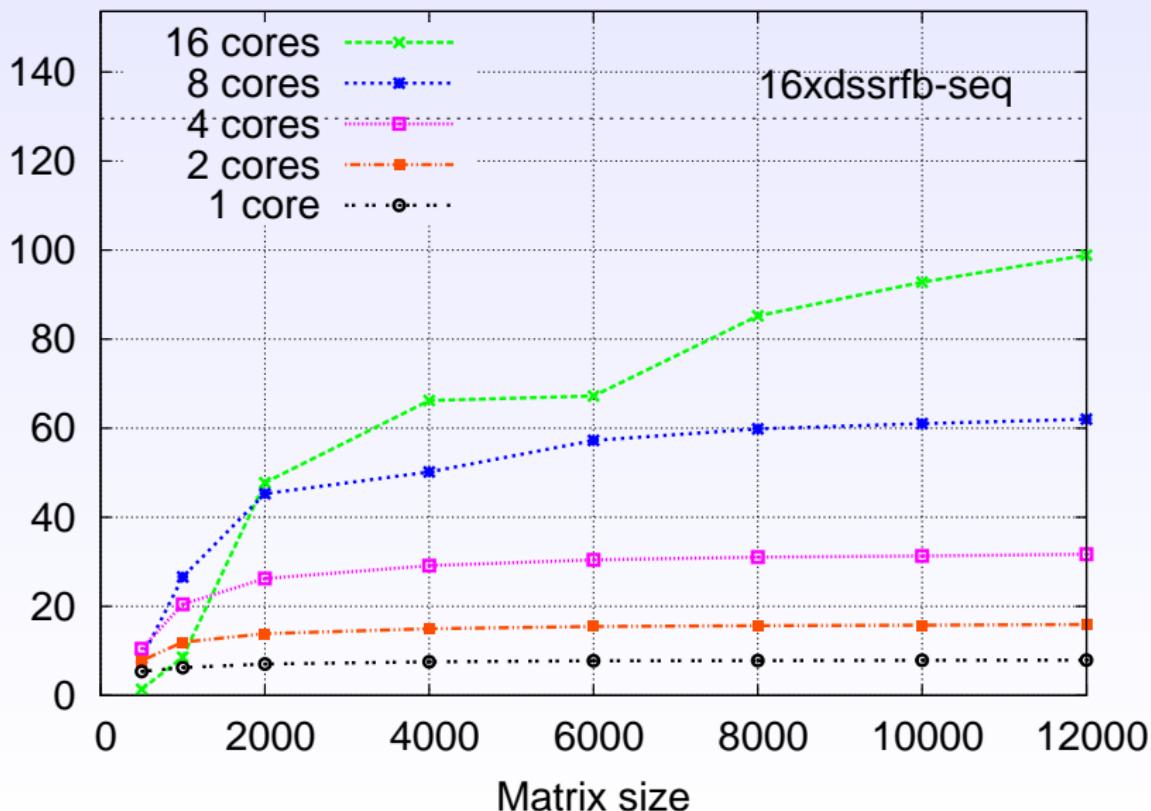
## 1. Scalability of other libraries

- TBLAS
- MKL- ESSL
- SCALAPACK- PESSL
- LAPACK

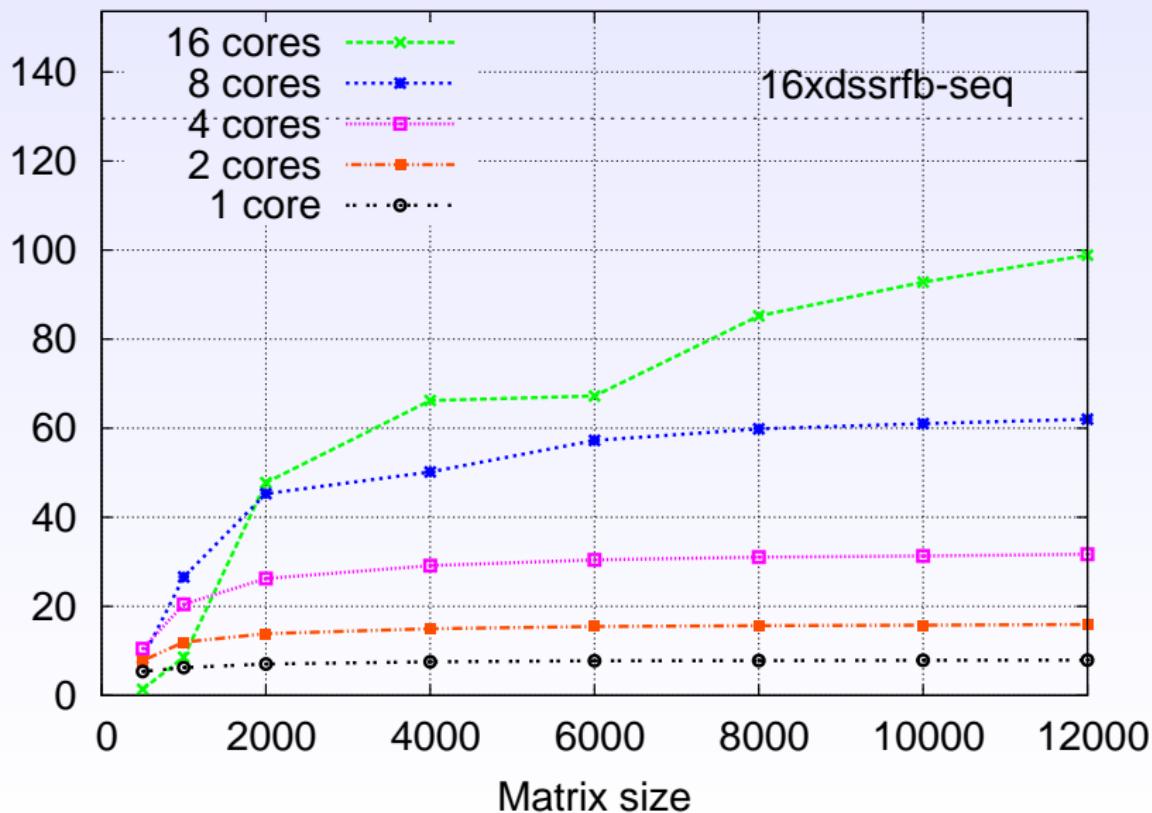
## MKL- DPOTRF- Intel64



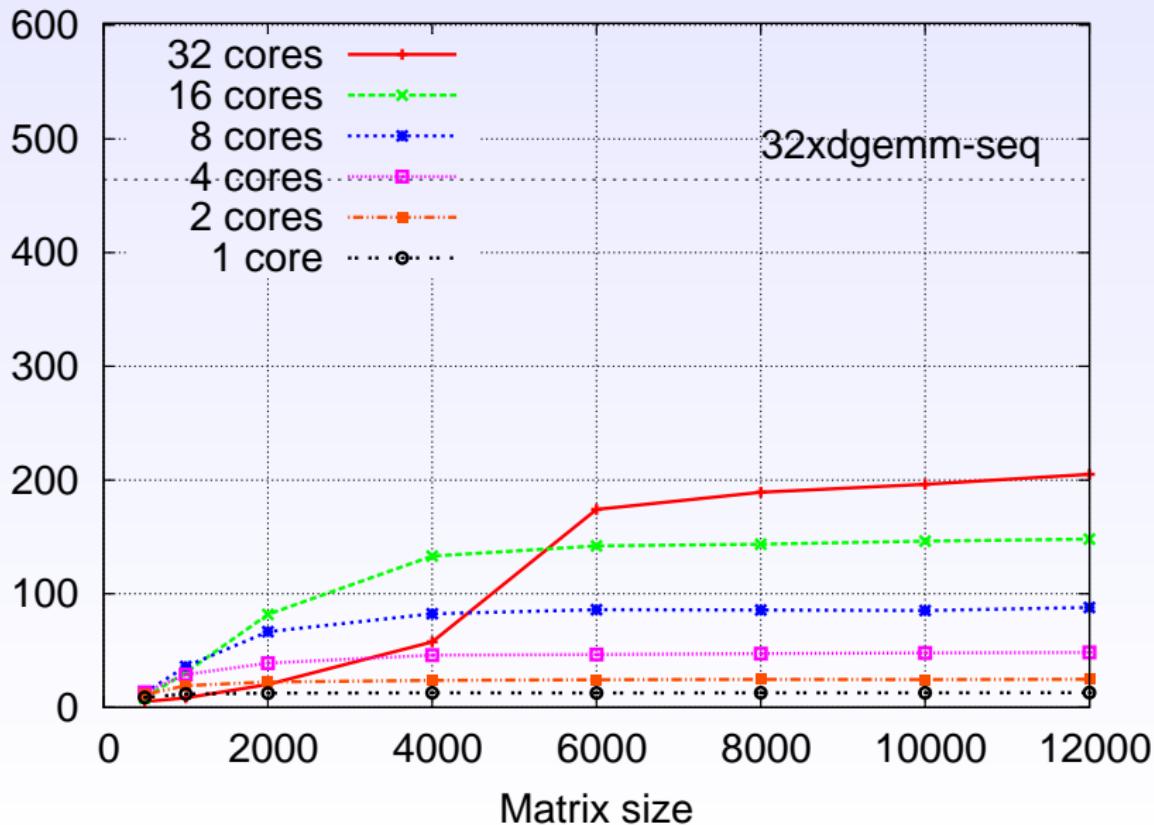
## MKL- DGEQRF- Intel64



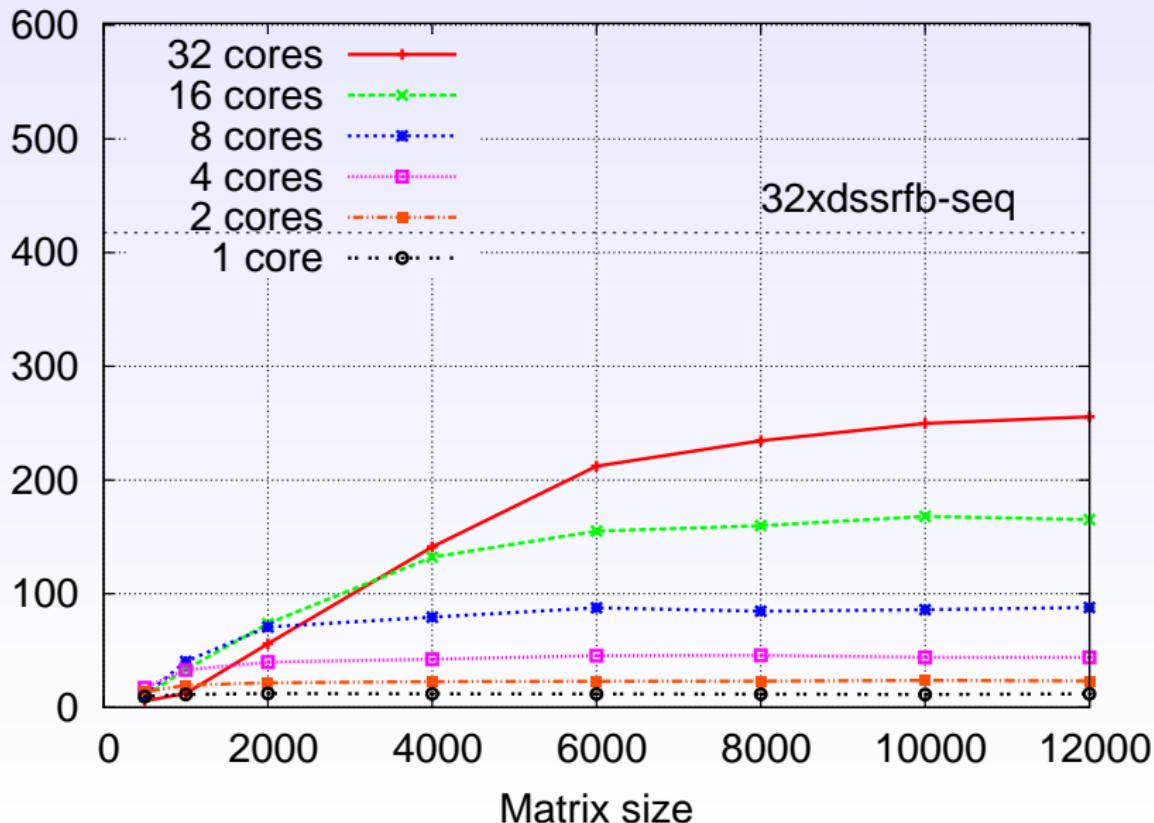
## MKL- DGETRF- Intel64



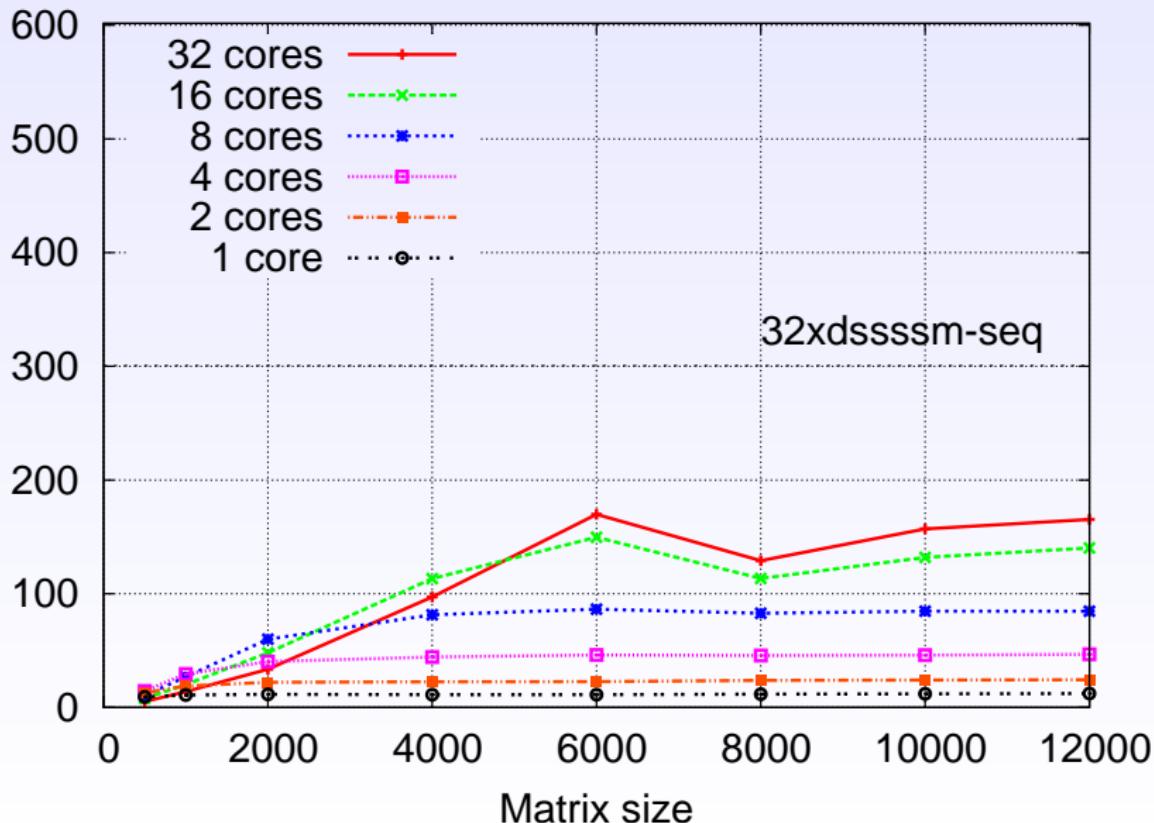
## ESSL- DPOTRF- Power6



## ESSL- DGEQRF- Power6



## ESSL- DGETRF- Power6

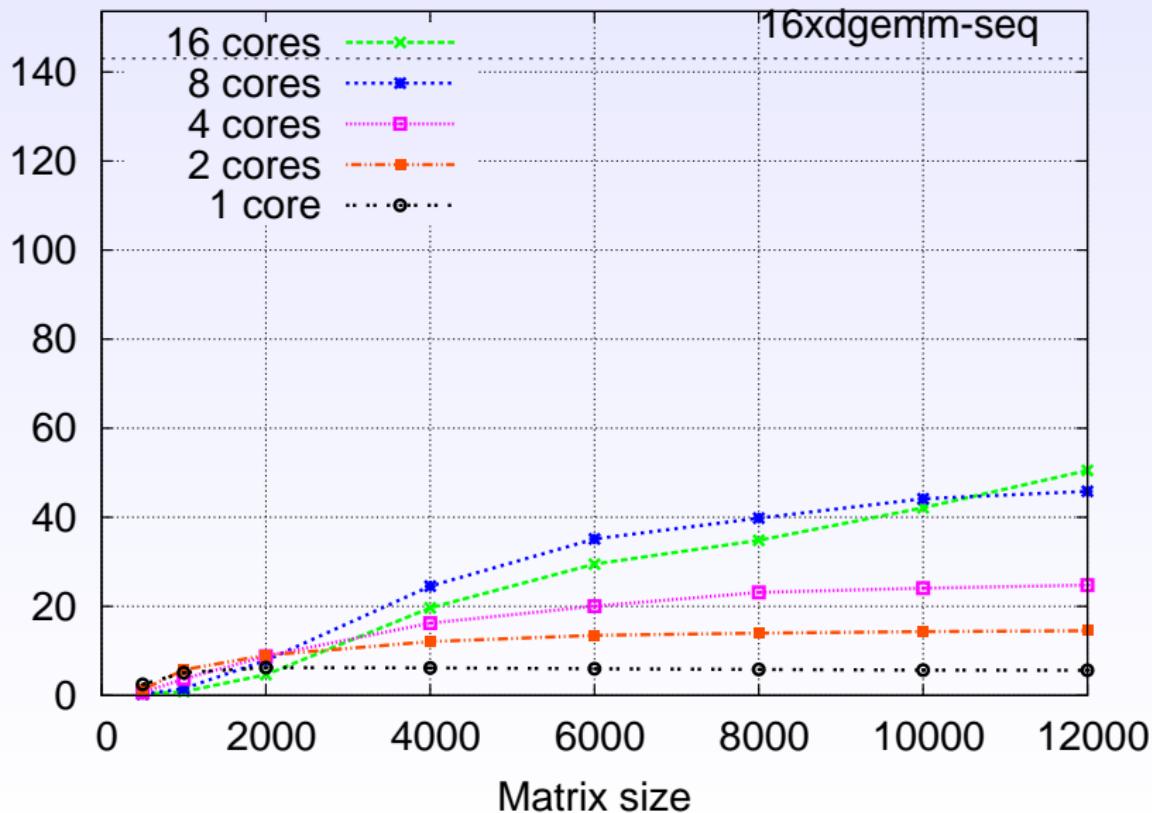


# Outline

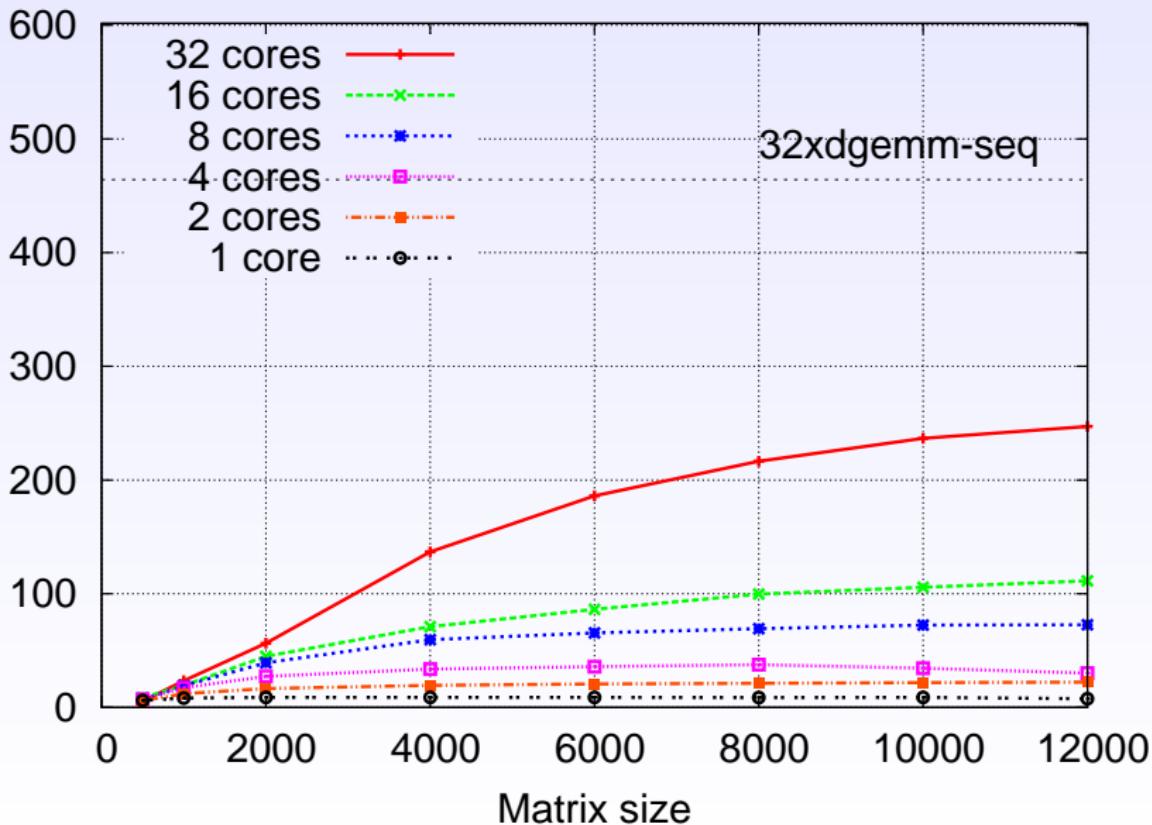
## 1. Scalability of other libraries

- TBLAS
- MKL- ESSL
- SCALAPACK- PESSL
- LAPACK

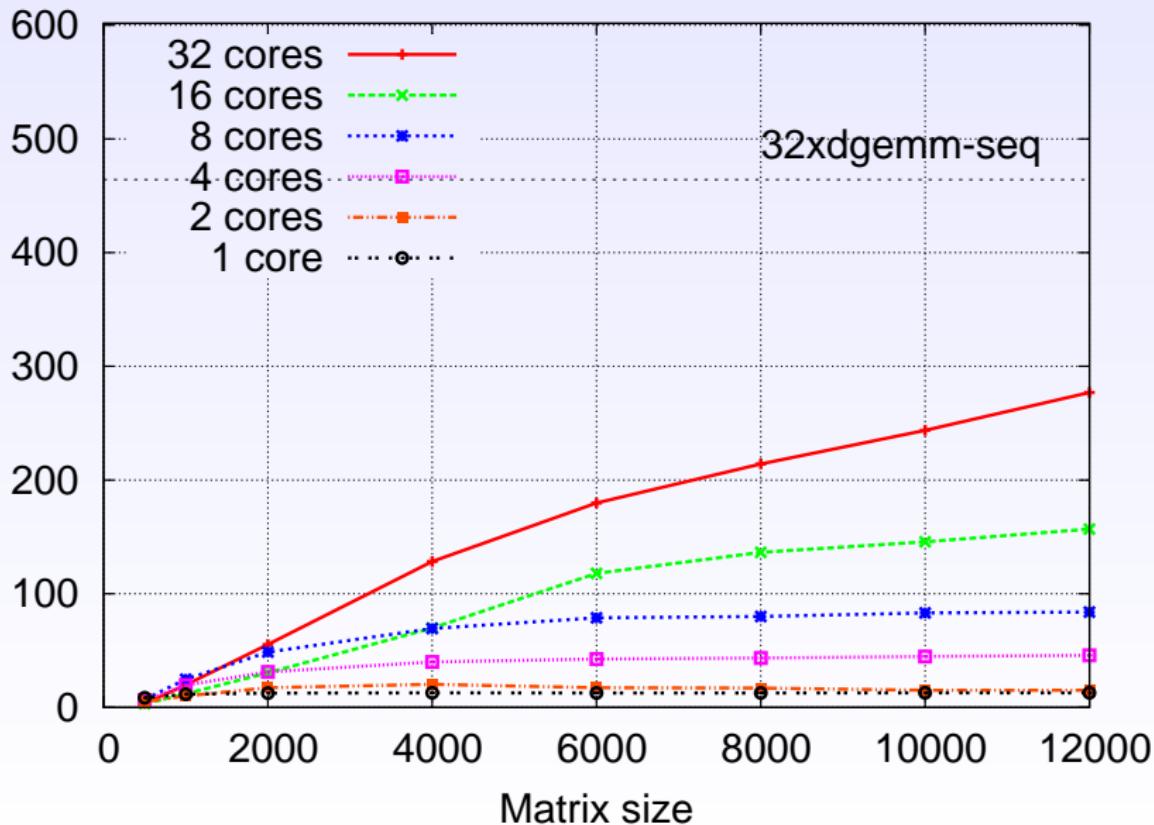
## SCALAPACK- DPOTRF- Intel64



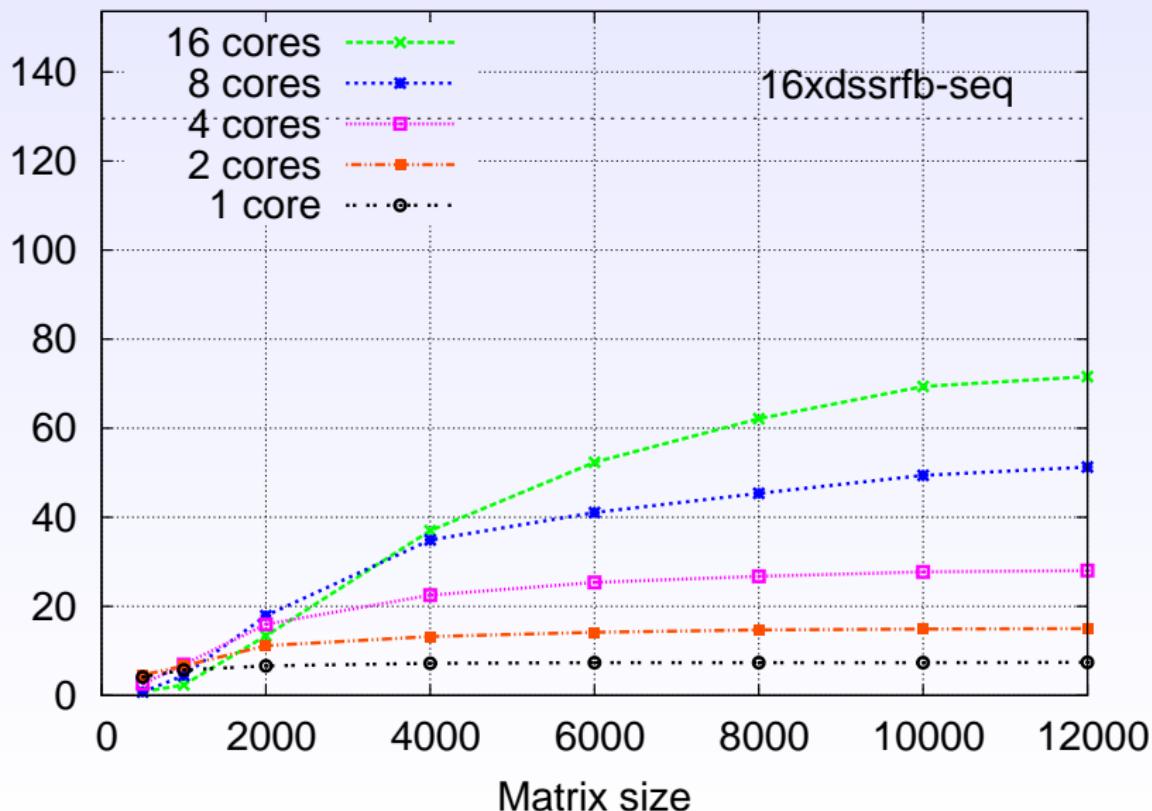
## SCALAPACK- DPOTRF- Power6



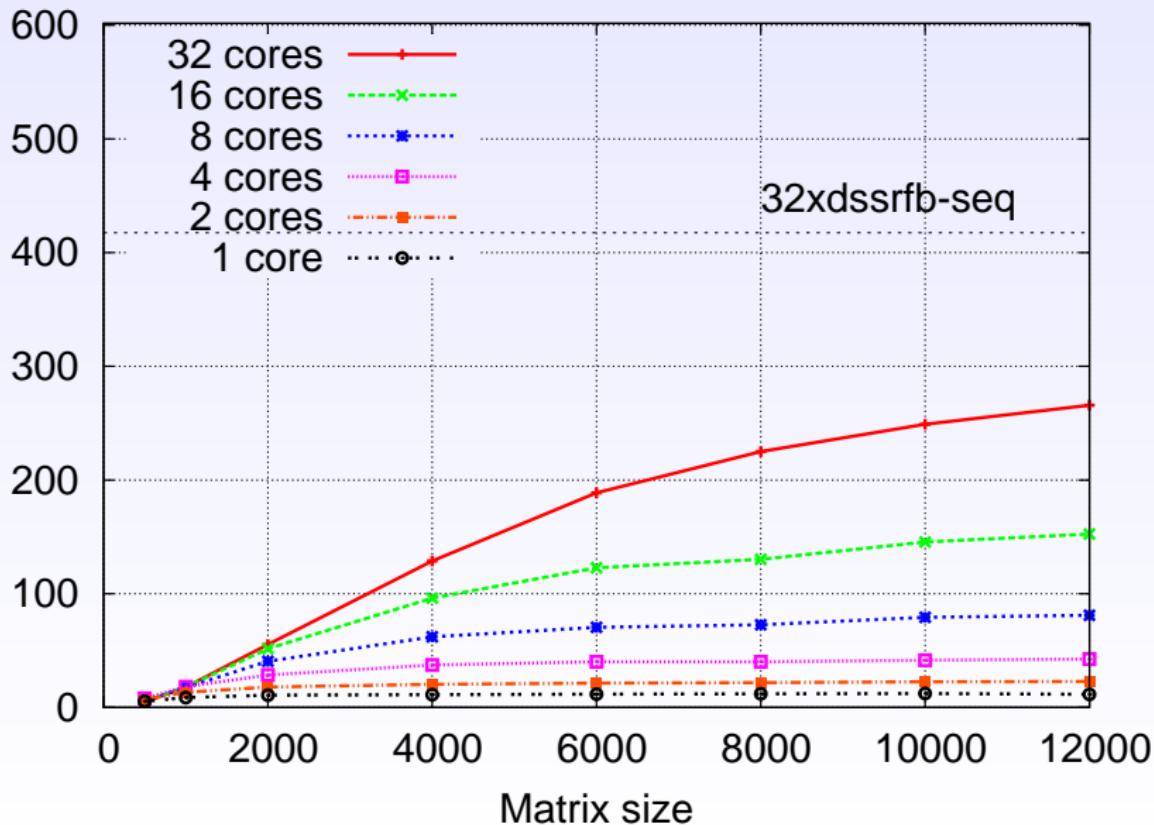
## PESSL- DPOTRF- Power6



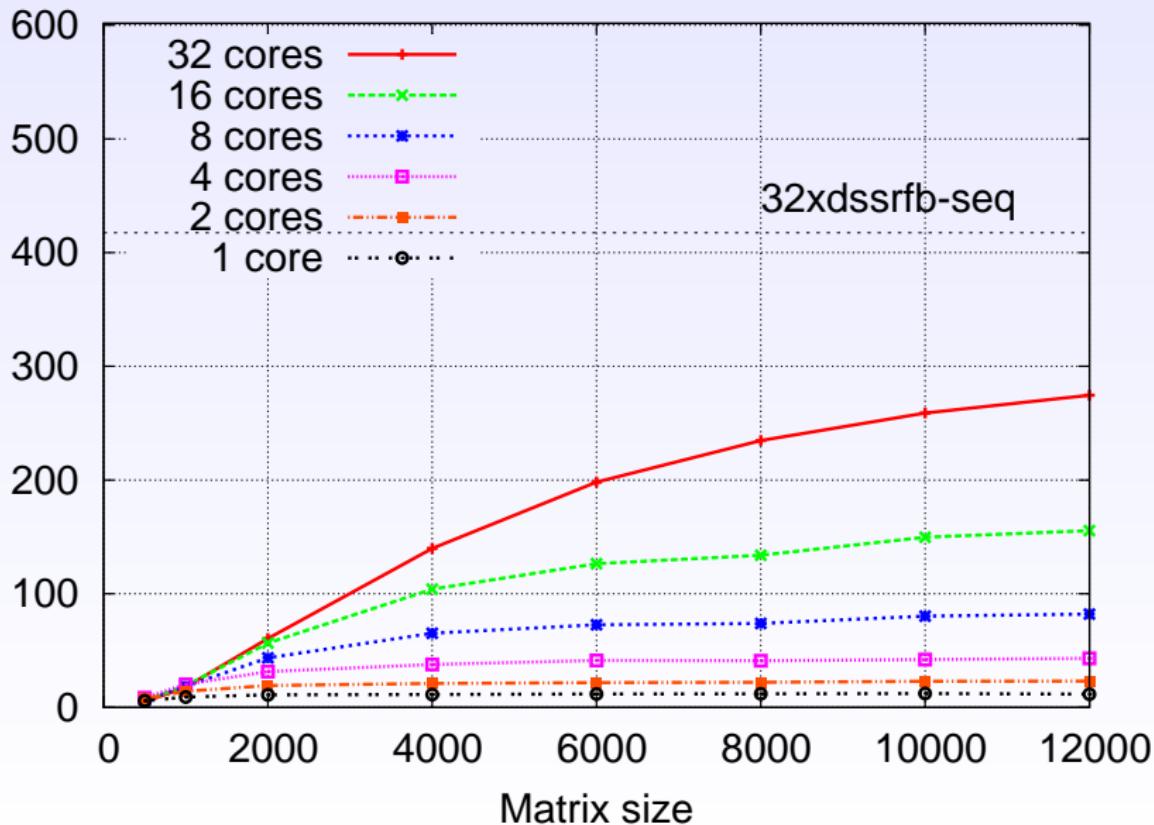
## SCALAPACK- DGEQRF- Intel64



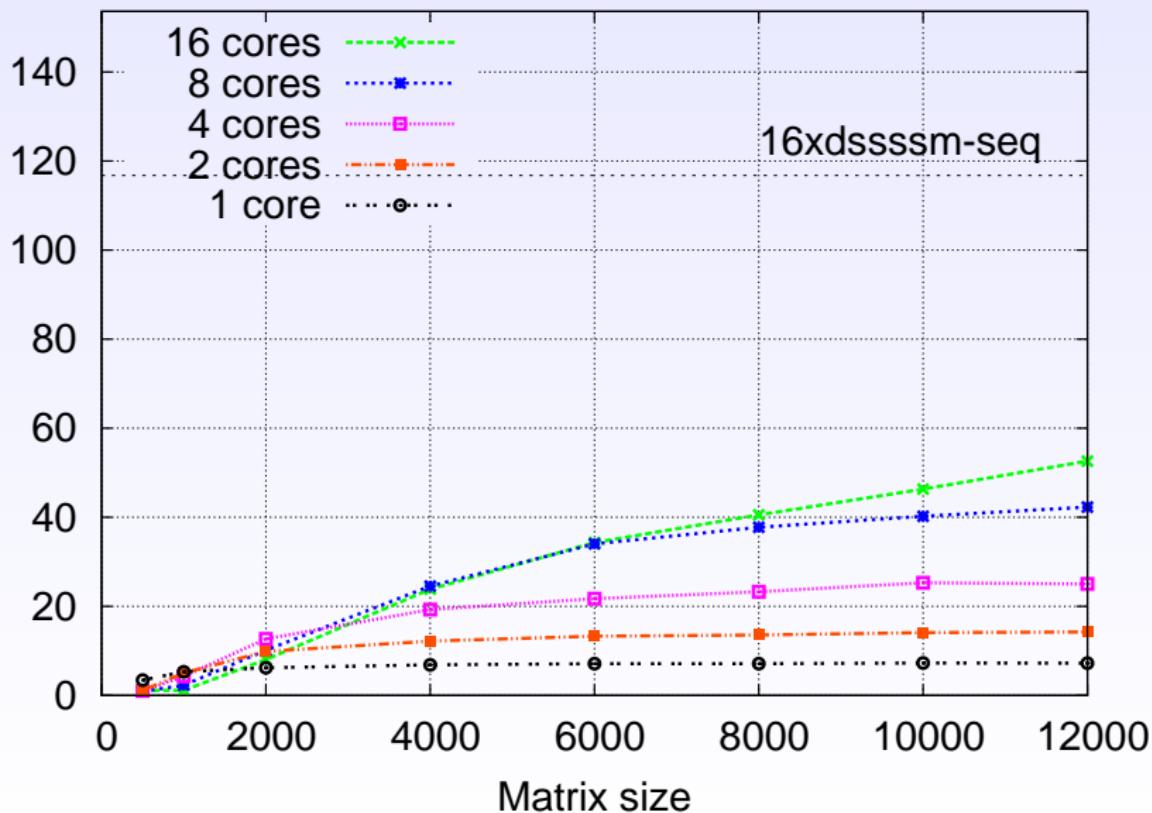
## SCALAPACK- DGETRF- Power6



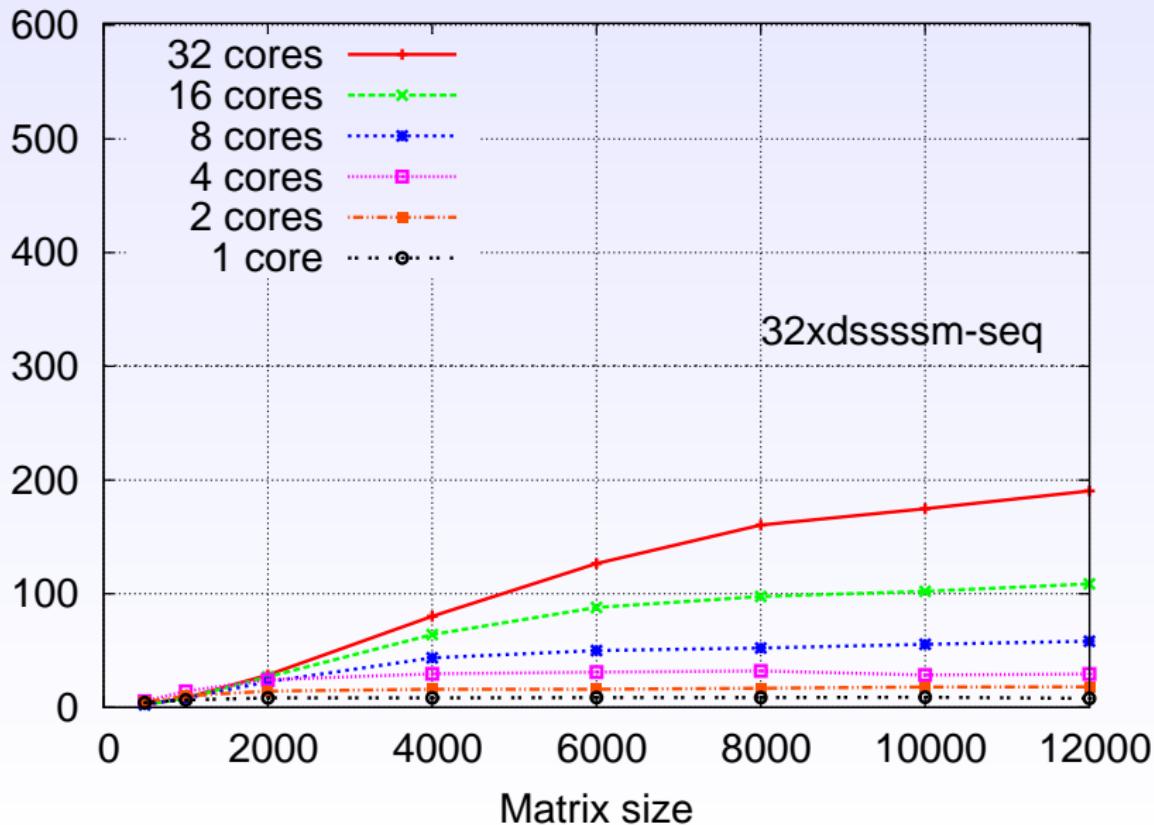
## PESSL- DGEQRF- Power6



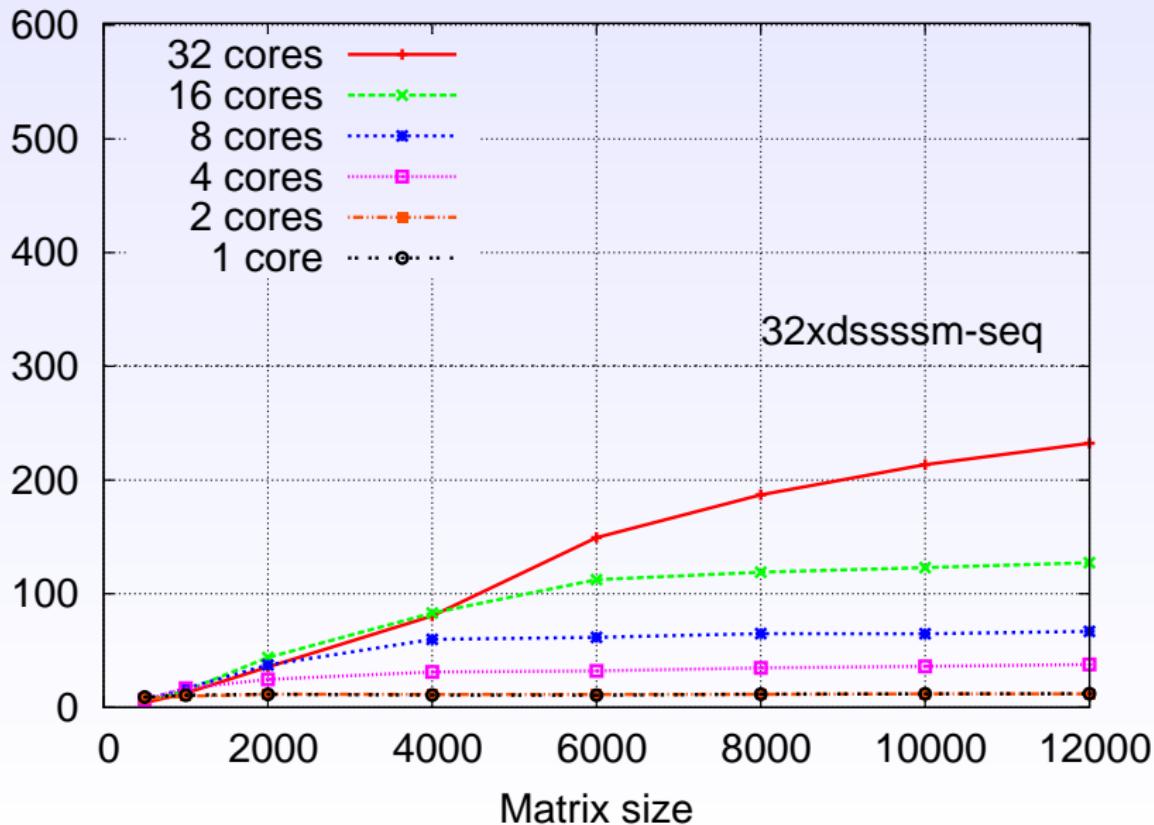
## SCALAPACK- DGETRF- Intel64



## SCALAPACK- DGETRF- Power6



## PESSL- DGETRF- Power6

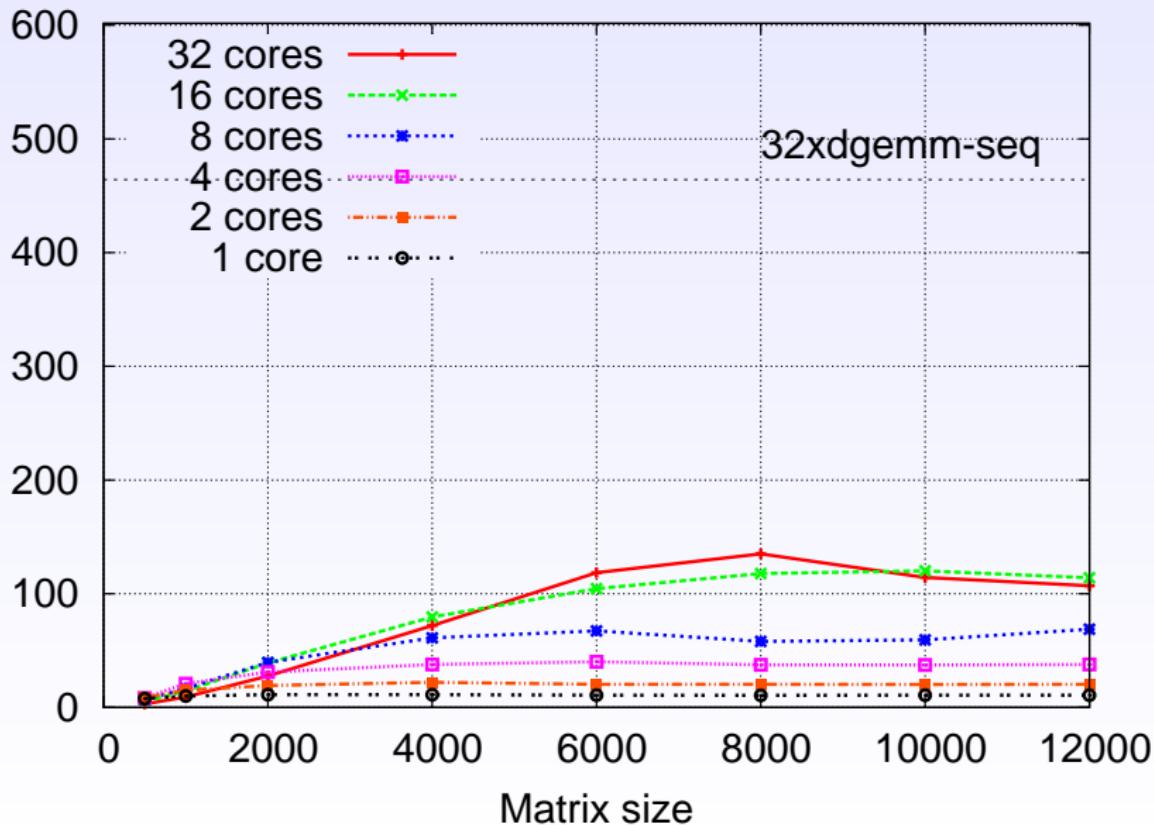


# Outline

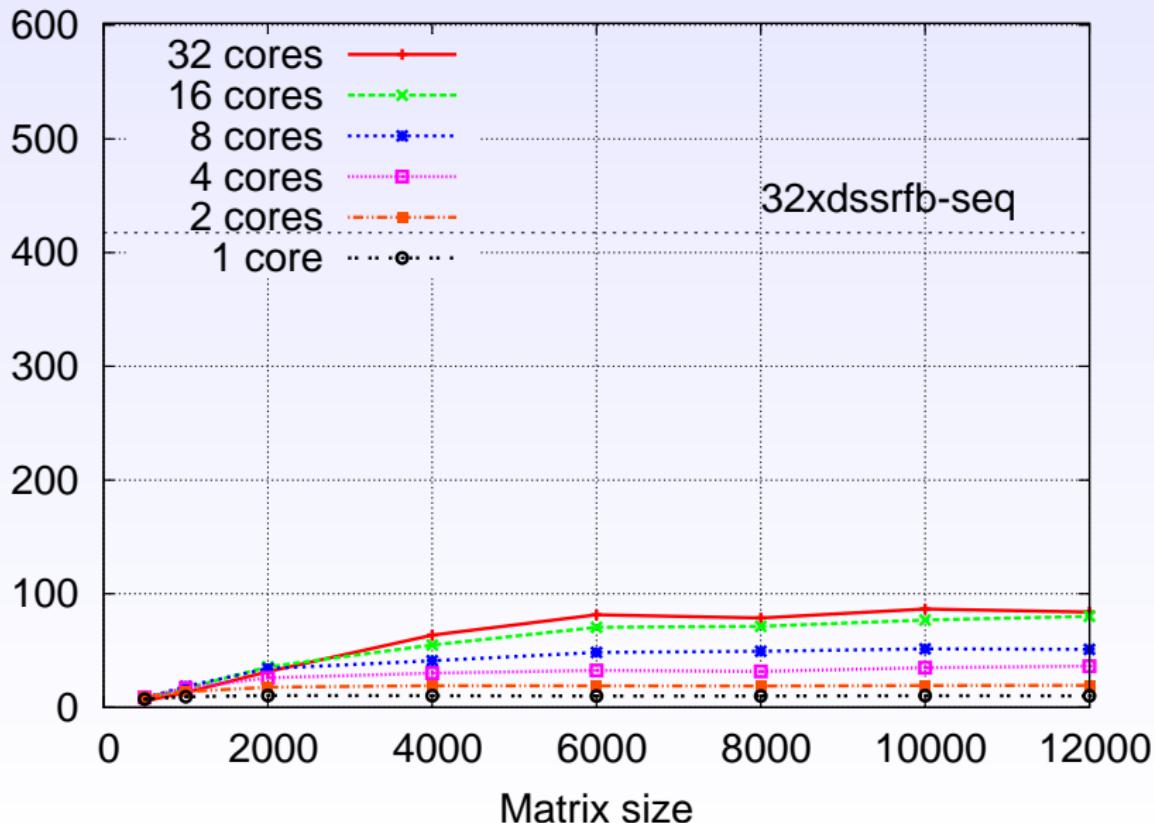
## 1. Scalability of other libraries

- TBLAS
- MKL- ESSL
- SCALAPACK- PESSL
- LAPACK

## LAPACK- DPOTRF



## LAPACK- DGEQRF



## LAPACK- DGETRF

