

Easy Programming of Linear Algebra Operations on Hybrid CPU-GPU Platforms

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Index

- The libflame library



- The StarSs framework



GPU support

Disclaimer



- Not a course on low-level programming of dense linear algebra kernels on GPUs!

- V. Volkov, J. Demmel. “Benchmarking GPUs to tune dense linear algebra”, SC08
- L-S. Chien, “Hand-tuned SGEMM on GT200 GPU”, TR Tsing Hua Univ., Taiwan

+



- Sorry if the performance numbers of some “products” do not look so good...

Initial considerations

- No low level programming: assume there is a tuned BLAS for GPU/general-purpose cores
- High level approach: minimal changes to existing codes/solutions
 - Abstract programmer from data transfers, without losing performance
- Runtime-based solution for multi-GPU platforms

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- The libflame library

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2. Creating your own algorithm
3. FLAME runtime
4. Clusters of GPUs

- The StarSs framework

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- The libflame library

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- The StarSs framework

What is libflame?

- A library?
- A framework?
- A repository of algorithmic variants?

Who are the targets?

- Newcomers
- Current users of BLAS, LAPACK
- Some PLAPACK/ScaLAPACK users whose problems are too small

Current Coverage

- Level-1, -2, and -3 BLAS
 - No banded support
- Basic LAPACK operations
 - No SVD/EVD support (yet)
- Operations not implemented by LAPACK
 - Example: up-and-downdating
- Supporting utility functions

Key Features

- Formally derived algorithms
- Object-based API (abstraction!)
- High performance
- Storage: column-, row-major, AND general
 - Or a mixture!
- Dependency-aware multithreading
- Build system(s)
 - GNU and Windows

libflame → A user's view → Introduction

Where is libflame available?

- FLAME website
 - www.cs.utexas.edu/users/flame/libflame/
 - Milestone releases
 - Nightly snapshots
 - Available as free software under LGPL

libflame for GNU/Linux

- Software requirements
 - C compiler
 - GNU bash (2.0 or later)
 - GNU make
 - BLAS library
 - OpenMP-aware C compiler (optional)
- Build system
 - `./configure; make; make install`

libflame for Windows

- Software requirements
 - C compiler
 - Python (2.6 or later)
 - Microsoft nmake
 - BLAS library
 - OpenMP-aware C compiler (optional)
- Build system
 - `.\configure.cmd; nmake; nmake install`

libflame → A user's view → Configuration

Options

- Static/dynamic library generation
- lapack2flame compatibility layer
- Multithreading: POSIX threads or OpenMP
- GPU support
- Memory alignment
- Internal error checking

libflame → A user's view → Operation status

A sampling of functionality

operation	Classic FLAME	FLASH/SM	lapack2flame
Level-3 BLAS	y	y	n/a
Cholesky	y	y	y
LU with partial pivoting	y	y	y
LU with incremental pivoting	y	y	*
QR (UT)	y	y	y
LQ (UT)	y	y	y
SPD/HPD inversion	y	y	y
Triangular inversion	y	y	y
Triangular Sylvester	y	y	y
Lyapunov	y	y	y
Up-and-downdate (UT)	y	y	*
SVD	planned		
EVD	planned		

* Not present in LAPACK

Types of interfaces

- Classic
 - Matrix type: flat
 - Task-level parallelism: no
 - Suitable for multithreaded BLAS
- FLASH
 - Matrix type: hierarchical
 - Task-level parallelism: SuperMatrix
 - Sequential execution is optional

External buffers

```
FLA_Obj A;  
  
// Initialize conventional matrix: buffer, m, rs, cs  
  
FLA_Init();  
  
FLA_Obj_create_without_buffer( FLA_DOUBLE, m, m, &A );  
FLA_Obj_attach_buffer( buffer, rs, cs, &A );  
  
FLA_Chol( FLA_LOWER_TRIANGULAR, A );  
  
FLA_Obj_free_without_buffer( &A );  
  
FLA_Finalize();
```

Native objects

```
FLA_Obj A;  
  
// Initialize conventional matrix: buffer, m, rs, cs  
  
FLA_Init();  
  
FLA_Obj_create( FLA_DOUBLE, m, m, 0, 0, &A );  
FLA_Copy_buffer_to_object( FLA_NO_TRANSPOSE, m, m,  
                           buffer, rs, cs, 0, 0, A );  
  
FLA_Chol( FLA_LOWER_TRIANGULAR, A );  
  
FLA_Obj_free( &A );  
  
FLA_Finalize();
```

libflame → A user's view → Examples

Storage-by-blocks (seq)

```
FLA_Obj A;  
  
// Initialize conventional matrix: buffer, m, rs, cs  
// Obtain storage blocksize b.  
  
FLA_Init();  
  
FLASH_Obj_create( FLA_DOUBLE, m, m, 1, &b, &A );  
FLASH_Copy_buffer_to_hier( m, m, buffer, rs, cs,  
                           0, 0, A );  
  
FLASH_Queue_disable();  
FLASH_Chol( FLA_LOWER_TRIANGULAR, A );  
  
FLASH_Obj_free( &A );  
  
FLA_Finalize();
```

Storage-by-blocks (MT)

```
FLA_Obj A;

// Initialize conventional matrix: buffer, m, rs, cs
// Obtain storage blocksize, # of threads: b, n_threads

FLA_Init();

FLASH_Obj_create( FLA_DOUBLE, m, m, 1, &b, &A );
FLASH_Copy_buffer_to_hier( m, m, buffer, rs, cs,
                           0, 0, A );
FLASH_Queue_set_num_threads( n_threads );
FLASH_Chol( FLA_LOWER_TRIANGULAR, A );

FLASH_Obj_free( &A );

FLA_Finalize();
```

Solving a system via LU

```
FLA_Obj A, p, b, x;

FLA_Obj_create( FLA_DOUBLE, m, m, 0, 0, &A );
FLA_Obj_create( FLA_DOUBLE, m, 1, 0, 0, &b );
FLA_Obj_create( FLA_DOUBLE, m, 1, 0, 0, &x );
FLA_Obj_create( FLA_INT,      m, 1, 0, 0, &p );

// Initialize A, b, x.

FLA_LU_piv( A, p );
FLA_LU_piv_solve( A, p, b, x );

FLA_Obj_free( &A );
FLA_Obj_free( &b );
FLA_Obj_free( &x );
FLA_Obj_free( &p );
```

Solving a system via QR

```
FLA_Obj A, T, b, x;

FLA_Obj_create( FLA_DOUBLE, m, n, 0, 0, &A );
FLA_Obj_create( FLA_DOUBLE, m, 1, 0, 0, &b );
FLA_Obj_create( FLA_DOUBLE, n, 1, 0, 0, &x );

// Initialize A, b, x.

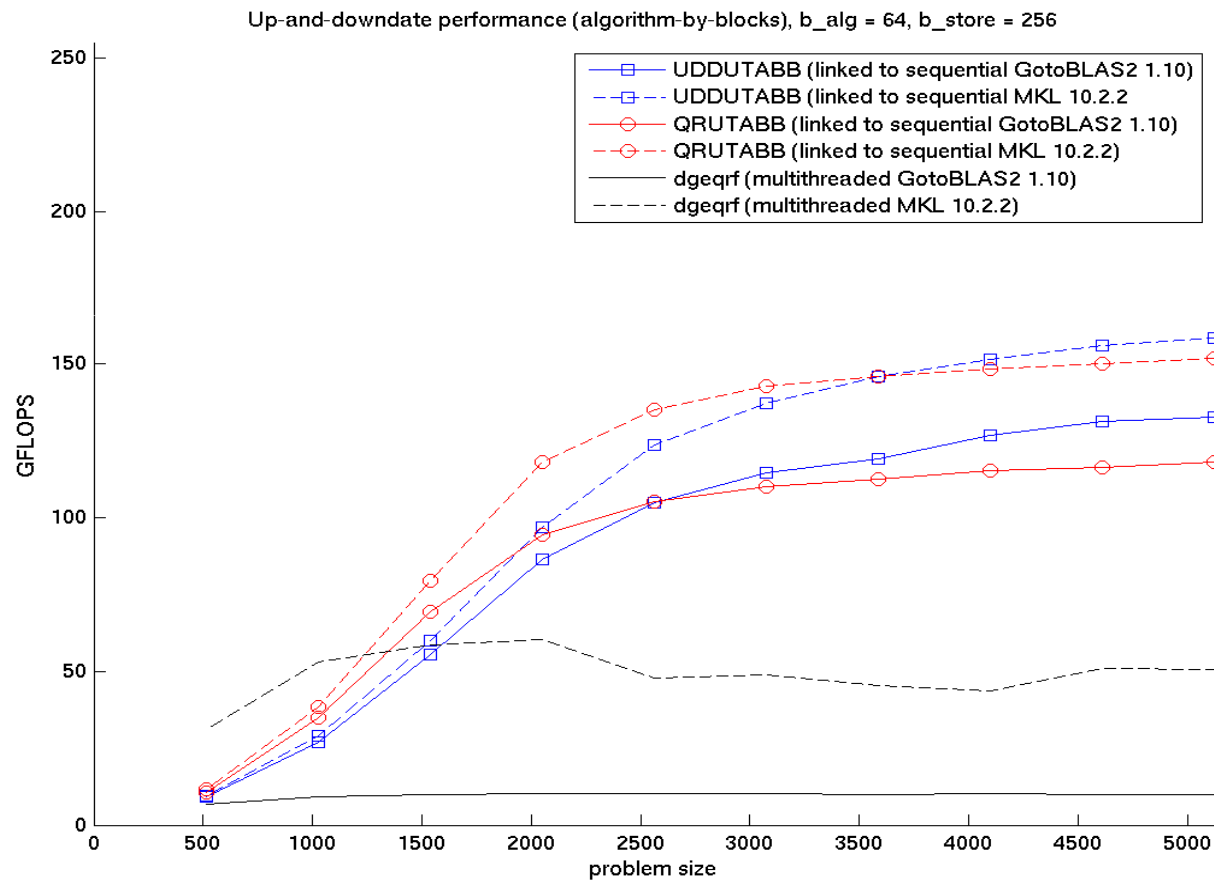
FLA_QR_UT_create_T( A, &T );

FLA_QR_UT( A, T );
FLA_QR_UT_solve( A, T, b, x );

FLA_Obj_free( &A );
FLA_Obj_free( &b );
FLA_Obj_free( &x );
```

libflame → A user's view → Performance

Up-and-Downdate



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1. FLAME notation and algorithms
 2. Spark: from algorithm to code
 3. Running on multicore

- The StarSs framework

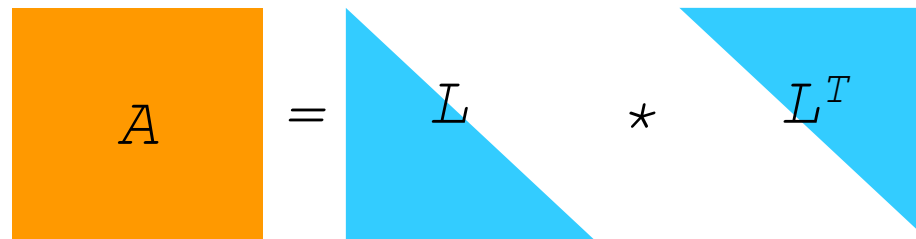
libflame → Creating your own algorithm

The Cholesky factorization

```
FLA_Obj A;  
  
// Initialize conventional matrix: buffer, m, rs, cs  
  
FLA_Init();  
  
FLA_Obj_create_without_buffer( FLA_DOUBLE, m, m, &A );  
FLA_Obj_attach_buffer( buffer, rs, cs, &A );  
  
FLA_Chol( FLA_LOWER_TRIANGULAR, A );  
  
FLA_Obj_free_without_buffer( &A );  
  
FLA_Finalize();
```

The Cholesky factorization

- Lower triangular case:


$$A = L * L^T$$

Key in the solution of s.p.d. linear systems

$$\begin{aligned} A x = b &\equiv (L L^T) x = b \\ L y = b &\Rightarrow y \\ L^T x = y &\Rightarrow x \end{aligned}$$

Algorithm

$$A \rightarrow \begin{pmatrix} \alpha_{11} & * \\ a_{21} & A_{22} \end{pmatrix} \quad L \rightarrow \begin{pmatrix} \lambda_{11} & \\ l_{21} & L_{22} \end{pmatrix}$$

$$A = L * L^T \equiv \begin{pmatrix} \alpha_{11} & * \\ a_{21} & A_{22} \end{pmatrix} = \begin{pmatrix} \lambda_{11} & \\ l_{21} & L_{22} \end{pmatrix} * \begin{pmatrix} \lambda_{11} & \\ l_{21} & L_{22} \end{pmatrix}^T \rightarrow$$

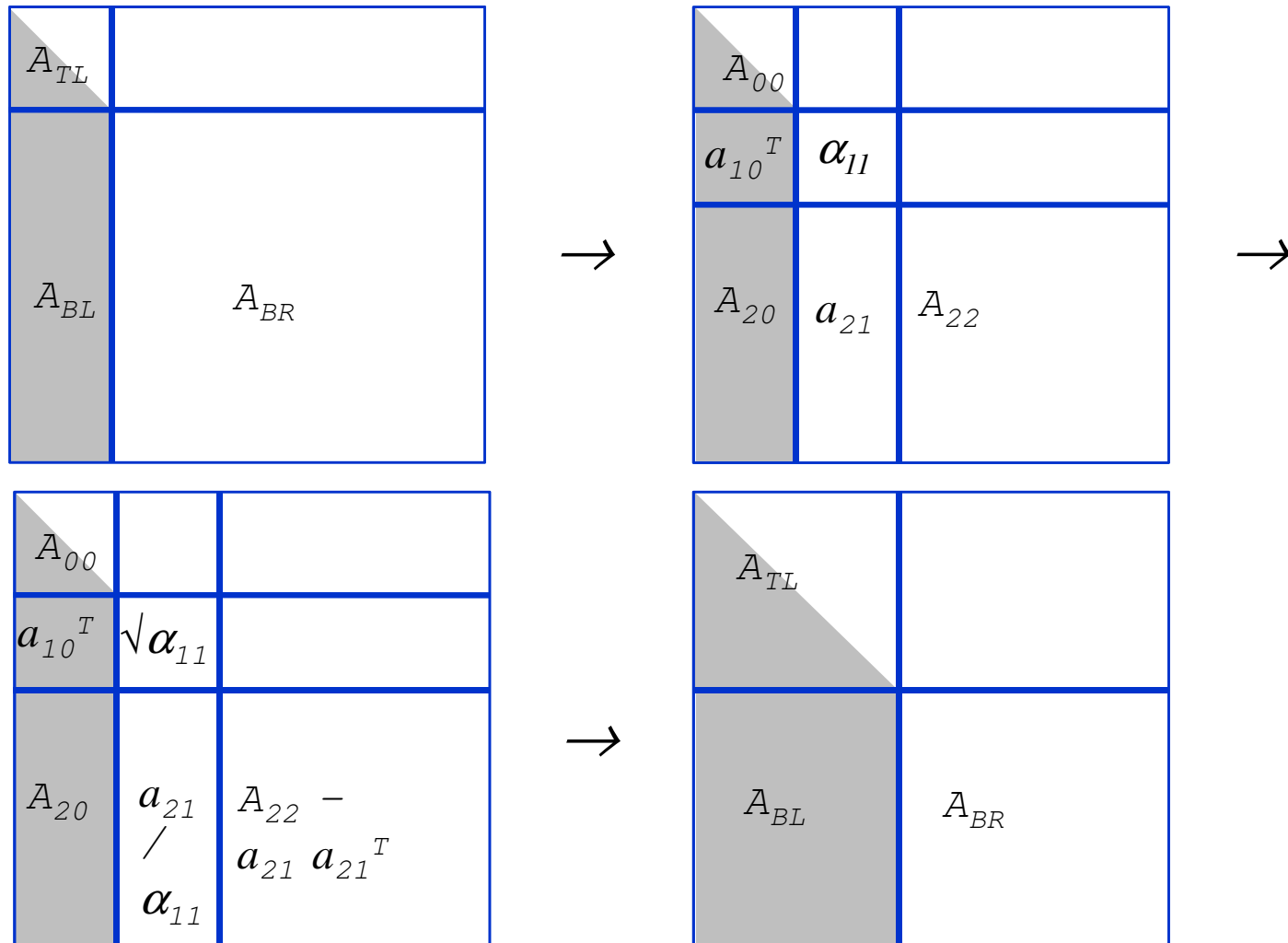
$$\alpha_{11} = \lambda_{11} \lambda_{11}^T \rightarrow \lambda_{11} = \sqrt{\alpha_{11}}$$

$$a_{21} = l_{21} \lambda_{11} \rightarrow l_{21} = a_{21} / \lambda_{11}$$

$$A_{22} = L_{22} L_{22}^T + a_{21} a_{21}^T \rightarrow (A_{22} - a_{21} a_{21}^T) = L_{22} L_{22}^T$$

libflame → Creating your own algorithm → FLAME notation and algorithms

Algorithm loop: repartition+operation+merging



libflame → Creating your own algorithm → FLAME notation and algorithms

Algorithm loop: repartition

A_{TL}	
A_{BL}	A_{BR}

→

A_{00}		
a_{10}^T	α_{11}	
A_{20}	a_{21}	A_{22}

Algorithm: $A := \text{CHOLL_UNB_VAR3}(A)$

Partition $A \rightarrow \left(\begin{array}{c|c} A_{TL} & A_{TR} \\ \hline A_{BL} & A_{BR} \end{array} \right)$

where A_{TL} is 0×0

while $m(A_{TL}) < m(A)$ **do**

Repartition

$\left(\begin{array}{c|c} A_{TL} & A_{TR} \\ \hline A_{BL} & A_{BR} \end{array} \right) \rightarrow \left(\begin{array}{c|c|c} A_{00} & a_{01} & A_{02} \\ \hline a_{10}^T & \alpha_{11} & a_{12}^T \\ \hline A_{20} & a_{21} & A_{22} \end{array} \right)$

where α_{11} is 1×1

$\alpha_{11} := \sqrt{\alpha_{11}}$

$a_{21} := a_{21}/\alpha_{11}$

$A_{22} := A_{22} - \text{TRIL}(a_{21}a_{21}^T)$

Continue with

$\left(\begin{array}{c|c} A_{TL} & A_{TR} \\ \hline A_{BL} & A_{BR} \end{array} \right) \leftarrow \left(\begin{array}{c|c|c} A_{00} & a_{01} & A_{02} \\ \hline a_{10}^T & \alpha_{11} & a_{12}^T \\ \hline A_{20} & a_{21} & A_{22} \end{array} \right)$

endwhile

Indexing operations

libflame → Creating your own algorithm → FLAME notation and algorithms

Algorithm loop: operation

A_{00}		
a_{10}^T	α_{11}	
A_{20}	a_{21}	

→

A_{00}		
a_{10}^T	$\sqrt{\alpha_{11}}$	
A_{20}	a_{21} / α_{11}	$A_{22} - a_{21} a_{21}^T$

Algorithm: $A := \text{CHOLL_UNB_VAR3}(A)$

Partition $A \rightarrow \left(\begin{array}{c|c} A_{TL} & A_{TR} \\ \hline A_{BL} & A_{BR} \end{array} \right)$

where A_{TL} is 0×0

while $m(A_{TL}) < m(A)$ **do**

Repartition

$$\left(\begin{array}{c|c} A_{TL} & A_{TR} \\ \hline A_{BL} & A_{BR} \end{array} \right) \rightarrow \left(\begin{array}{c|c|c} A_{00} & a_{01} & A_{02} \\ \hline a_{10}^T & \alpha_{11} & a_{12}^T \\ \hline A_{20} & a_{21} & A_{22} \end{array} \right)$$

where α_{11} is 1×1

$\alpha_{11} := \sqrt{\alpha_{11}}$
 $a_{21} := a_{21} / \alpha_{11}$
 $A_{22} := A_{22} - \text{TRIL}(a_{21} a_{21}^T)$

Continue with

$$\left(\begin{array}{c|c} A_{TL} & A_{TR} \\ \hline A_{BL} & A_{BR} \end{array} \right) \leftarrow \left(\begin{array}{c|c|c} A_{00} & a_{01} & A_{02} \\ \hline a_{10}^T & \alpha_{11} & a_{12}^T \\ \hline A_{20} & a_{21} & A_{22} \end{array} \right)$$

endwhile

Real computation

libflame → Creating your own algorithm → FLAME notation and algorithms

Algorithm loop: merging

A_{00}		
a_{10}^T	$\sqrt{\alpha_{11}}$	
A_{20}	a_{21} / α_{11}	$A_{22} -$ $a_{21} a_{21}^T$

→

A_{TL}	
A_{BL}	A_{BR}

Algorithm: $A := \text{CHOLL_UNB_VAR3}(A)$

Partition $A \rightarrow \left(\begin{array}{c|c} A_{TL} & A_{TR} \\ \hline A_{BL} & A_{BR} \end{array} \right)$

where A_{TL} is 0×0

while $m(A_{TL}) < m(A)$ **do**

Repartition

$\left(\begin{array}{c|c} A_{TL} & A_{TR} \\ \hline A_{BL} & A_{BR} \end{array} \right) \rightarrow \left(\begin{array}{c|c|c} A_{00} & a_{01} & A_{02} \\ \hline a_{10}^T & \alpha_{11} & a_{12}^T \\ \hline A_{20} & a_{21} & A_{22} \end{array} \right)$

where α_{11} is 1×1

$\alpha_{11} := \sqrt{\alpha_{11}}$

$a_{21} := a_{21} / \alpha_{11}$

$A_{22} := A_{22} - \text{TRIL}(a_{21} a_{21}^T)$

Continue with

$\left(\begin{array}{c|c} A_{TL} & A_{TR} \\ \hline A_{BL} & A_{BR} \end{array} \right) \leftarrow \left(\begin{array}{c|c|c} A_{00} & a_{01} & A_{02} \\ \hline a_{10}^T & \alpha_{11} & a_{12}^T \\ \hline A_{20} & a_{21} & A_{22} \end{array} \right)$

endwhile

Indexing operation

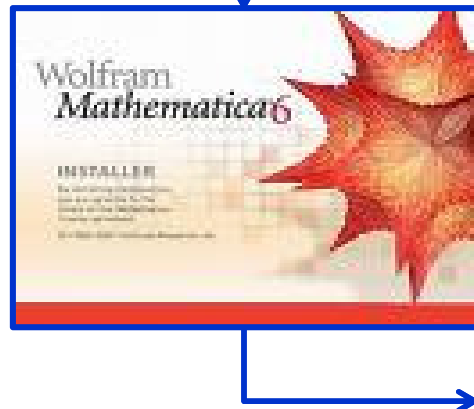
libflame → Creating your own algorithm → FLAME notation and algorithms

Algorithm

- Automatic development from math. specification

$$A = L * L^T$$

Mechanical
procedure



Algorithm: $A := \text{CHOLL_UNB_VAR3}(A)$

Partition $A \rightarrow \left(\begin{array}{c|c} A_{TL} & A_{TR} \\ \hline A_{BL} & A_{BR} \end{array} \right)$

where A_{TL} is 0×0

while $m(A_{TL}) < m(A)$ **do**

Repartition

$$\left(\begin{array}{c|c} A_{TL} & A_{TR} \\ \hline A_{BL} & A_{BR} \end{array} \right) \rightarrow \left(\begin{array}{c|c|c} A_{00} & a_{01} & A_{02} \\ \hline a_{10}^T & \alpha_{11} & a_{12}^T \\ \hline A_{20} & a_{21} & A_{22} \end{array} \right)$$

where α_{11} is 1×1

$$\alpha_{11} := \sqrt{\alpha_{11}}$$

$$a_{21} := a_{21} / \alpha_{11}$$

$$A_{22} := A_{22} - \text{TRIL}(a_{21} a_{12}^T)$$

Continue with

$$\left(\begin{array}{c|c} A_{TL} & A_{TR} \\ \hline A_{BL} & A_{BR} \end{array} \right) \leftarrow \left(\begin{array}{c|c|c} A_{00} & a_{01} & A_{02} \\ \hline a_{10}^T & \alpha_{11} & a_{12}^T \\ \hline A_{20} & a_{21} & A_{22} \end{array} \right)$$

endwhile

libflame → Creating your own algorithm → Spark: from algorithm to code

APIs

Algorithm: $A := \text{CHOLL_UNB_VAR3}(A)$

Partition $A \rightarrow \left(\begin{array}{c|c} A_{TL} & A_{TR} \\ \hline A_{BL} & A_{BR} \end{array} \right)$

where A_{TL} is 0×0

while $m(A_{TL}) < m(A)$ **do**

Repartition

$$\left(\begin{array}{c|c} A_{TL} & A_{TR} \\ \hline A_{BL} & A_{BR} \end{array} \right) \rightarrow \left(\begin{array}{c|c|c} A_{00} & a_{01} & A_{02} \\ \hline a_{10}^T & \alpha_{11} & a_{12}^T \\ \hline A_{20} & a_{21} & A_{22} \end{array} \right)$$

where α_{11} is 1×1

$$\alpha_{11} := \sqrt{a_{11}}$$

$$a_{21} := a_{21} / \alpha_{11}$$

$$A_{22} := A_{22} - \text{TRIL}(a_{21} a_{21}^T)$$

Continue with

$$\left(\begin{array}{c|c} A_{TL} & A_{TR} \\ \hline A_{BL} & A_{BR} \end{array} \right) \leftarrow \left(\begin{array}{c|c|c} A_{00} & a_{01} & A_{02} \\ \hline a_{10}^T & \alpha_{11} & a_{12}^T \\ \hline A_{20} & a_{21} & A_{22} \end{array} \right)$$

endwhile

Spark+APIs

C,
F77,
Matlab,
LabView,
LaTeX

libflame → Creating your own algorithm → Spark: from algorithm to code

Spark website

Algorithm: $A := \text{CHOLL_UNB_VAR3}(A)$

Partition $A \rightarrow \left(\begin{array}{c|c} A_{TL} & A_{TR} \\ \hline A_{BL} & A_{BR} \end{array} \right)$

where A_{TL} is 0×0

while $m(A_{TL}) < m(A)$ **do**

Repartition

$$\left(\begin{array}{c|c} A_{TL} & A_{TR} \\ \hline A_{BL} & A_{BR} \end{array} \right) \rightarrow \left(\begin{array}{c|c|c} A_{00} & a_{01} & A_{02} \\ \hline a_{10}^T & \alpha_{11} & a_{12}^T \\ \hline A_{20} & a_{21} & A_{22} \end{array} \right)$$

where α_{11} is 1×1

$$\alpha_{11} := \sqrt{a_{11}}$$

$$a_{21} := a_{21} / \alpha_{11}$$

$$A_{22} := A_{22} - \text{TRIL}(a_{21}a_{21}^T)$$

Continue with

$$\left(\begin{array}{c|c} A_{TL} & A_{TR} \\ \hline A_{BL} & A_{BR} \end{array} \right) \leftarrow \left(\begin{array}{c|c|c} A_{00} & a_{01} & A_{02} \\ \hline a_{10}^T & \alpha_{11} & a_{12}^T \\ \hline A_{20} & a_{21} & A_{22} \end{array} \right)$$

endwhile

<http://www.cs.utexas.edu/users/flame/Spark/>

libflame → Creating your own algorithm → Spark: from algorithm to code

Example: FLAME@lab

Algorithm: $A := \text{CHOLL_UNB_VAR3}(A)$

Partition $A \rightarrow \left(\begin{array}{c|c} A_{TL} & A_{TR} \\ \hline A_{BL} & A_{BR} \end{array} \right)$

where A_{TL} is 0×0

while $m(A_{TL}) < m(A)$ do

Repartition

$$\left(\begin{array}{c|c} A_{TL} & A_{TR} \\ \hline A_{BL} & A_{BR} \end{array} \right) \rightarrow \left(\begin{array}{c|c|c} A_{00} & a_{01} & A_{02} \\ \hline a_{10}^T & \alpha_{11} & a_{12}^T \\ \hline A_{20} & a_{21} & A_{22} \end{array} \right)$$

where α_{11} is 1×1

$$\alpha_{11} := \sqrt{a_{11}}$$

$$a_{21} := a_{21} / \alpha_{11}$$

$$A_{22} := A_{22} - \text{TRIL}(a_{21} a_{21}^T)$$

Continue with

$$\left(\begin{array}{c|c} A_{TL} & A_{TR} \\ \hline A_{BL} & A_{BR} \end{array} \right) \leftarrow \left(\begin{array}{c|c|c} A_{00} & a_{01} & A_{02} \\ \hline a_{10}^T & \alpha_{11} & a_{12}^T \\ \hline A_{20} & a_{21} & A_{22} \end{array} \right)$$

endwhile

```
[ ATL, ATR, ...
  ABL, ABR ] =
  FLA_Part_2x2( A, 0, 0, 'FLA_TL' );

while ( size( ATL, 1 ) < size( A, 1 ) )
```

```
[ A00, a01, A02, ...
  a10t, alpha11, a12t, ...
  A20, a21, A22 ] =
  FLA_Repart_2x2_to_3x3( ATL, ATR, ...
                        ABL, ABR, ...
                        1, 1, 'FLA_BR' );
```

% ----- %

% :

% ----- %

```
[ ATL, ATR, ...
  ABL, ABR ] = ...
  FLA_Cont_with_3x3_to_2x2( A00, a01, A02, ...
                          a10t, alpha11, a12t, ...
                          A20, a21, A22, ...
                          'FLA_TL' );
```

end

libflame → Creating your own algorithm → Spark: from algorithm to code

Example: FLAME@lab

Algorithm: $A := \text{CHOLL_UNB_VAR3}(A)$

Partition $A \rightarrow \left(\begin{array}{c|c} A_{TL} & A_{TR} \\ \hline A_{BL} & A_{BR} \end{array} \right)$

where A_{TL} is 0×0

while $m(A_{TL}) < m(A)$ **do**

Repartition

$$\left(\begin{array}{c|c} A_{TL} & A_{TR} \\ \hline A_{BL} & A_{BR} \end{array} \right) \rightarrow \left(\begin{array}{c|c|c} A_{00} & a_{01} & A_{02} \\ \hline a_{10}^T & \alpha_{11} & a_{12}^T \\ \hline A_{20} & a_{21} & A_{22} \end{array} \right)$$

where α_{11} is 1×1

$$\begin{aligned} \alpha_{11} &:= \sqrt{a_{11}} \\ a_{21} &:= a_{21} / \alpha_{11} \\ A_{22} &:= A_{22} - \text{TRIL}(a_{21} a_{21}^T) \end{aligned}$$

Continue with

$$\left(\begin{array}{c|c} A_{TL} & A_{TR} \\ \hline A_{BL} & A_{BR} \end{array} \right) \leftarrow \left(\begin{array}{c|c|c} A_{00} & a_{01} & A_{02} \\ \hline a_{10}^T & \alpha_{11} & a_{12}^T \\ \hline A_{20} & a_{21} & A_{22} \end{array} \right)$$

endwhile

Manually fill-in operations

```
[...] = FLA_Part_2x2(...);

while ( size( ATL, 1 ) < size( A, 1 ) )

    [...] = FLA_Repart_2x2_to_3x3(...);

    %-----%
    alpha11 = sqrt( alpha11 );
    a21      = a21 / alpha11;
    A22      = A22 - tril( a21*a21' );
    %-----%

    [...] = FLA_Cont_with_3x3_to_2x2(...);

end
```

libflame → Creating your own algorithm → Running on multicore

Example: FLAMEC

Algorithm $A := \text{CHOL_L_UNB_NAB3}(A)$

Partition $A \Rightarrow \left(\begin{array}{c|c} A_{FL} & A_{FR} \\ \hline A_{BL} & A_{BR} \end{array} \right)$
 where A_{FL} is 0×0
while $m(A_{BL}) < m(A)$ **do**

Repartition

$$\left(\begin{array}{c|c} A_{FL} & A_{FR} \\ \hline A_{BL} & A_{BR} \end{array} \right) \Rightarrow \left(\begin{array}{c|c|c} A_{00} & a_{01} & A_{02} \\ \hline a_{10}^t & \alpha_{11} & a_{12}^t \\ \hline A_{20} & a_{21} & A_{22} \end{array} \right)$$

where α_{11} is 1×1

$\alpha_{11} := \sqrt{a_{11}}$
 $a_{21} := a_{21} / \alpha_{11}$
 $A_{22} := A_{22} - \text{TRIL}(a_{21} a_{11}^T)$

Continue with

$$\left(\begin{array}{c|c} A_{FL} & A_{FR} \\ \hline A_{BL} & A_{BR} \end{array} \right) \Rightarrow \left(\begin{array}{c|c|c} A_{00} & a_{01} & A_{02} \\ \hline a_{10}^t & \alpha_{11} & a_{12}^t \\ \hline A_{20} & a_{21} & A_{22} \end{array} \right)$$

endwhile

```
FLA_Part_2x2( A, &ATL, &ATR,
              &ABL, &ABR, 0, 0, FLA_TL );

while ( FLA_Obj_length( ATL ) < FLA_Obj_length( A ) ){

  b = min( FLA_Obj_length( ABR ), nb_alg );

  FLA_Repart_2x2_to_3x3( ATL, /**/ ATR,          &A00, /**/ &a01, &A02,
                        /* ***** */ /* ***** */
                        ABL, /**/ ABR,          &a10t, /**/ &alpha11, &a12t,
                        1, 1, FLA_BR );

  /*-----*/
  /*                               :                               */
  /*-----*/

  FLA_Cont_with_3x3_to_2x2( &ATL, /**/ &ATR,      A00,  a01,      /**/ A02,
                           /* ***** */ /* ***** */
                           &ABL, /**/ &ABR,      A20,  a21,      /**/ A22,
                           FLA_TL );

}
```

libflame → Creating your own algorithm → Running on multicore

Example: FLAMEC

Algorithm: $A := \text{CHOLL_UNB_VAR3}(A)$

Partition $A \rightarrow \left(\begin{array}{c|c} A_{TL} & A_{TR} \\ \hline A_{BL} & A_{BR} \end{array} \right)$

where A_{TL} is 0×0

while $m(A_{TL}) < m(A)$ **do**

Repartition

$$\left(\begin{array}{c|c} A_{TL} & A_{TR} \\ \hline A_{BL} & A_{BR} \end{array} \right) \rightarrow \left(\begin{array}{c|c|c} A_{00} & a_{01} & A_{02} \\ \hline a_{10}^T & \alpha_{11} & a_{12}^T \\ \hline A_{20} & a_{21} & A_{22} \end{array} \right)$$

where α_{11} is 1×1

$$\alpha_{11} := \sqrt{a_{11}}$$

$$a_{21} := a_{21} / \alpha_{11}$$

$$A_{22} := A_{22} - \text{TRIL}(a_{21}a_{21}^T)$$

Continue with

$$\left(\begin{array}{c|c} A_{TL} & A_{TR} \\ \hline A_{BL} & A_{BR} \end{array} \right) \leftarrow \left(\begin{array}{c|c|c} A_{00} & a_{01} & A_{02} \\ \hline a_{10}^T & \alpha_{11} & a_{12}^T \\ \hline A_{20} & a_{21} & A_{22} \end{array} \right)$$

endwhile

- libflame employs external BLAS:
GotoBLAS, MKL, ACML, ATLAS, netlib

```
FLA_Part_2x2(...);

while ( FLA_Obj_length(ATL) < FLA_Obj_length(A) ){

  FLA_Repart_2x2_to_3x3(...);

  /*-----*/
  FLA_Sqrt( alpha11 );
  FLA_Inv_scal( alpha11, a21 );
  FLA_Syr( FLA_LOWER_TRIANGULAR, FLA_NO_TRANSPOSE,
           FLA_MINUS_ONE, a21, A22 );
  /*-----*/

  FLA_Cont_with_3x3_to_2x2(...);

}
```

Index

- The libflame library

1. A user's view
2. Creating your own algorithm
3. FLAME runtime
4. Cluster of GPUs

- 
1. Task parallelism
 2. SuperMatrix
 3. GPU support

- The SMPs/GPUSs framework

Data-flow parallelism? Dynamic scheduling? Run-time?

- Surely not a new idea...
 - Cilk
 - StarSs (GridSs)
 - StarPU
 - ...
- “An Efficient Algorithm for Exploiting Multiple Arithmetic Units”,
R. M. Tomasulo, IBM J. of R&D, Volume 11, Number 1, Page
25 (1967)

The basis for exploitation of ILP
on current superscalar processors!

The TEXT project

- Towards Exaflop applicaTions



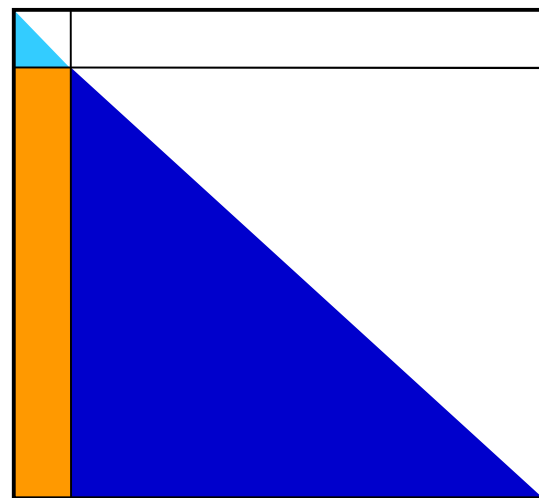
- Demonstrate that **Hybrid MPI/SMPs** addresses the Exascale challenges in a productive and efficient way.
 - Deploy at supercomputing centers: Julich, EPCC, HLRS, BSC
 - Port Applications (HLA, SPECfem3d, PEPC, PSC, BEST, CPMD, LS1 MarDyn) and develop algorithms.
 - Develop additional environment capabilities
 - tools (debug, performance)
 - improvements in runtime systems (load balance and GPUSs)
 - Support other users
 - Identify users of TEXT applications
 - Identify and support interested application developers
 - Contribute to Standards (OpenMP ARB, PERI-XML)

libflame → FLAME runtime → Task parallelism

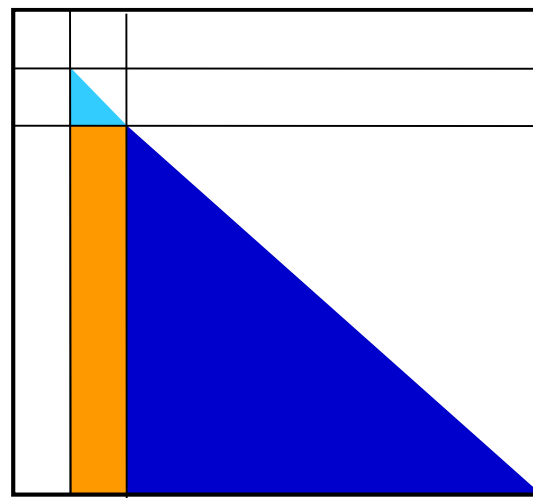
Blocked algorithms

- Cholesky factorization

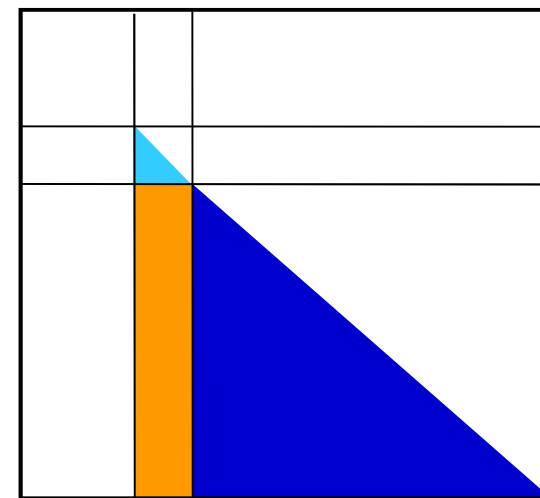
$$\begin{aligned} A_{11} &= L_{11} L_{11}^T \\ A_{21} &:= L_{21} = A_{21} L_{11}^{-T} \\ A_{22} &:= A_{22} - L_{21} L_{21}^T \end{aligned}$$



1st iteration



2nd iteration



3rd iteration

...

libflame → FLAME runtime → Task parallelism

Blocked algorithms

■ Cholesky factorization

$$A = L * L^T$$



Algorithm: $A = \text{CHOL}(L, \text{UNB_VARS}(A))$

Partition $A \rightarrow \begin{pmatrix} A_{TL} & A_{TR} \\ A_{BL} & A_{BR} \end{pmatrix}$
 where A_{TL} is 9×9
 while $m(A_{TR}) < m(A)$ do
 Repartition
 $\begin{pmatrix} A_{TL} & A_{TR} \\ A_{BL} & A_{BR} \end{pmatrix} \leftarrow \begin{pmatrix} A_{00} & a_{01} & A_{02} \\ a_{10}^T & \alpha_{11} & a_{12}^T \\ A_{20} & a_{21} & A_{22} \end{pmatrix}$
 where α_{11} is 1×1
 $\alpha_{11} := \sqrt{a_{11}}$
 $a_{21} := a_{21} / \alpha_{11}$
 $A_{22} := A_{22} - \text{TRIL}(a_{21} a_{12}^T)$
 Continue with
 $\begin{pmatrix} A_{TL} & A_{TR} \\ A_{BL} & A_{BR} \end{pmatrix} \leftarrow \begin{pmatrix} A_{00} & a_{01} & A_{02} \\ a_{10}^T & \alpha_{11} & a_{12}^T \\ A_{20} & a_{21} & A_{22} \end{pmatrix}$
 endwhile

APIs + Tools

```
FLA_Part_2x2 (...);

while ( FLA_Obj_length(ATL) < FLA_Obj_length(A) ){

  FLA_Repart_2x2_to_3x3 (...);

  /*-----*/
  FLA_Chol( FLA_LOWER_TRIANGULAR, A11 );
  FLA_Trsm( FLA_RIGHT, FLA_LOWER_TRIANGULAR,
            FLA_TRANSPOSE, FLA_NONUNIT_DIAG,
            FLA_ONE, A11, A21 );
  FLA_Syrk( FLA_LOWER_TRIANGULAR, FLA_NO_TRANSPOSE,
            FLA_MINUS_ONE, A21, FLA_ONE, A22 );
  /*-----*/

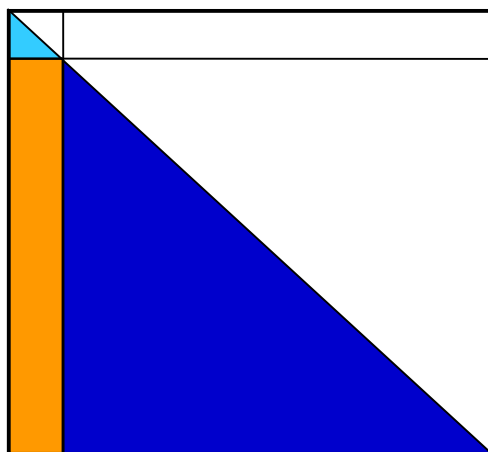
  FLA_Cont_with_3x3_to_2x2 (...);

}
```

libflame → FLAME runtime → Task parallelism

Blocked algorithms

- Simple parallelization:
link with MT BLAS



$$A_{11} = L_{11} L_{11}^T$$

$$A_{21} := L_{21} = A_{21} L_{11}^{-T}$$

$$A_{22} := A_{22} - L_{21} L_{21}^T$$

```
FLA_Part_2x2 (...);

while ( FLA_Obj_length(ATL) < FLA_Obj_length(A) ){

    FLA_Repart_2x2_to_3x3 (...);

    /*-----*/
    FLA_Chol( FLA_LOWER_TRIANGULAR, A11 );
    FLA_Trsm( FLA_RIGHT, FLA_LOWER_TRIANGULAR,
              FLA_TRANSPOSE, FLA_NONUNIT_DIAG,
              FLA_ONE, A11, A21 );
    FLA_Syrk( FLA_LOWER_TRIANGULAR, FLA_NO_TRANSPOSE,
              FLA_MINUS_ONE, A21, FLA_ONE, A22 );
    /*-----*/

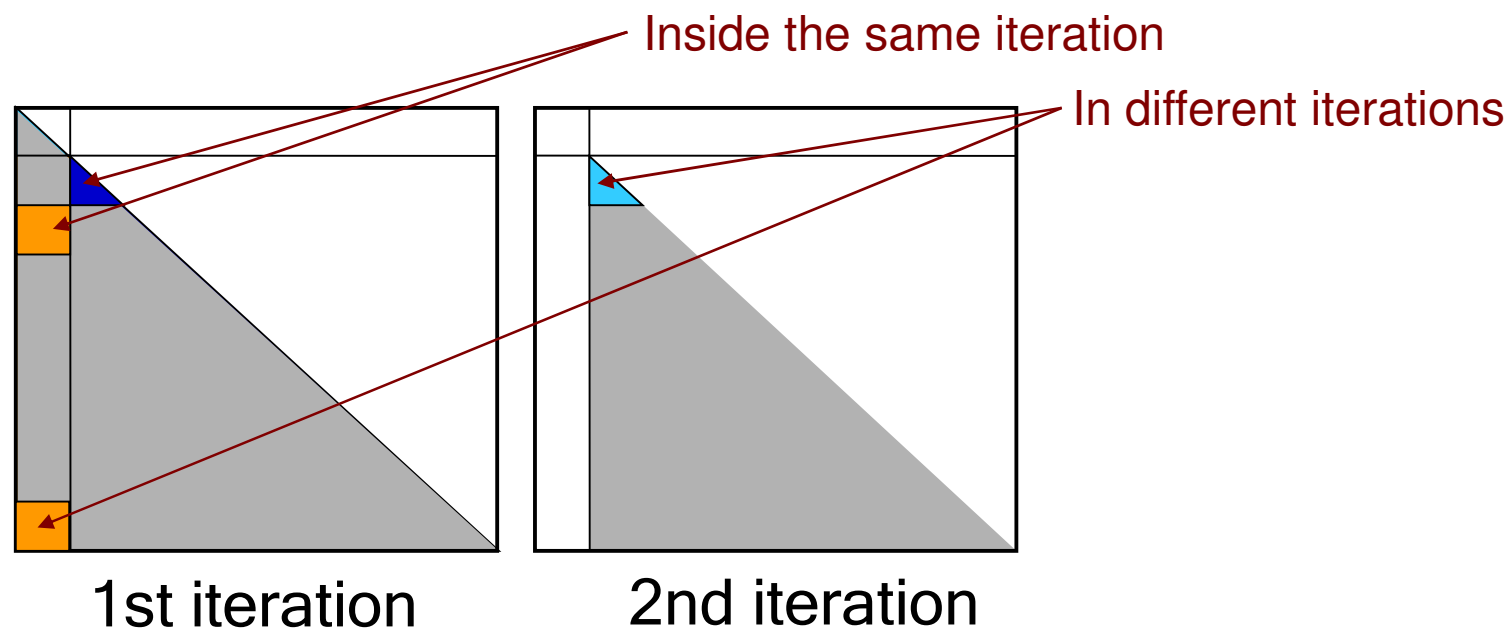
    FLA_Cont_with_3x3_to_2x2 (...);

}
```

libflame $\rightarrow$ FLAME runtime $\rightarrow$ Task parallelism

Blocked algorithms

- There is more parallelism!



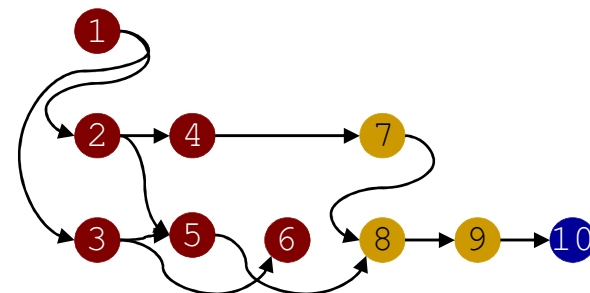
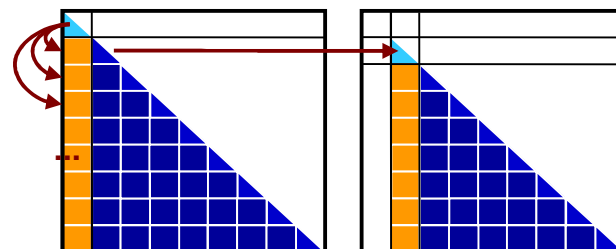
libflame $\rightarrow$ FLAME runtime $\rightarrow$ SuperMatrix

Exploiting task-level parallelism

```

Algorithm  $A := \text{CHOL}_L\text{-UNB\_NAB3}(A)$ 
Partition  $A \mapsto \begin{pmatrix} A_{FL} & A_{FR} \\ A_{BL} & A_{BR} \end{pmatrix}$ 
  where  $A_{FL}$  is  $0 \times 0$ 
  while  $m(A_{BL}) < m(A)$  do
    Repartition
     $\begin{pmatrix} A_{FL} & A_{FR} \\ A_{BL} & A_{BR} \end{pmatrix} \mapsto \begin{pmatrix} A_{00} & a_{01} & A_{02} \\ a_{10}^T & a_{11} & a_{12}^T \\ A_{20} & a_{21} & A_{22} \end{pmatrix}$ 
    where  $a_{11}$  is  $1 \times 1$ 
     $a_{11} := \sqrt{a_{11}}$ 
     $a_{21} := a_{21}/a_{11}$ 
     $A_{22} := A_{22} - \text{TRIL}(a_{21}a_{11}^T)$ 
    Continue with
     $\begin{pmatrix} A_{FL} & A_{FR} \\ A_{BL} & A_{BR} \end{pmatrix} \leftarrow \begin{pmatrix} A_{00} & a_{01} & A_{02} \\ a_{10}^T & a_{11} & a_{12}^T \\ A_{20} & a_{21} & A_{22} \end{pmatrix}$ 
  endwhile
  
```

- SuperMatrix: automatic identification of tasks/dependencies



libflame → FLAME runtime → SuperMatrix

Exploiting task-level parallelism

Algorithm $A := \text{CHOL_UNB_NAB3}(A)$

Partition $A \mapsto \begin{pmatrix} A_{FL} & A_{FR} \\ A_{BL} & A_{BR} \end{pmatrix}$
 where A_{FL} is 0×0
while $m(A_{BL}) < m(A)$ **do**

Repartition

$$\begin{pmatrix} A_{FL} & A_{FR} \\ A_{BL} & A_{BR} \end{pmatrix} \rightarrow \begin{pmatrix} A_{00} & a_{01} & A_{02} \\ a_{10}^T & a_{11} & a_{12}^T \\ A_{20} & a_{21} & A_{22} \end{pmatrix}$$

where a_{11} is 1×1

$a_{11} := \sqrt{a_{11}}$
 $a_{21} := a_{21}/a_{11}$
 $A_{22} := A_{22} - \text{TRIL}(a_{21}a_{11}^T)$

Continue with

$$\begin{pmatrix} A_{FL} & A_{FR} \\ A_{BL} & A_{BR} \end{pmatrix} \leftarrow \begin{pmatrix} A_{00} & a_{01} & A_{02} \\ a_{10}^T & a_{11} & a_{12}^T \\ A_{20} & a_{21} & A_{22} \end{pmatrix}$$

endwhile

- SuperMatrix: automatic identification of tasks/dependencies

HOW?



- Input/output/input-output operands and order of operations in code determine dependencies
- Direction of operands is defined as part of BLAS specification

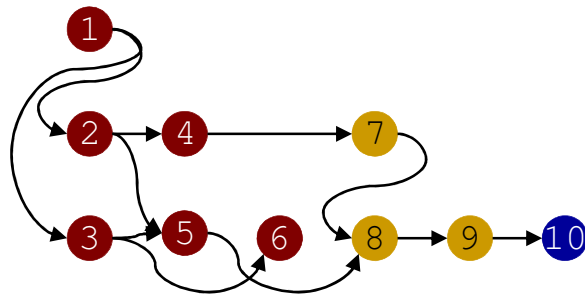
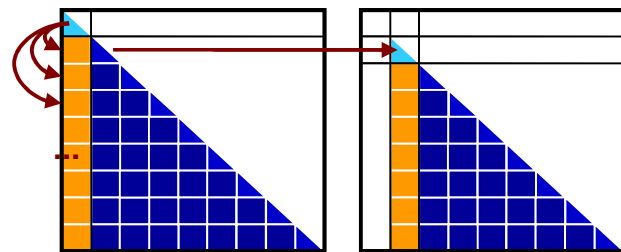
```

/*-----*/
FLA_Chol( FLA_LOWER_TRIANGULAR, A11 );
FLA_Trsm( FLA_RIGHT, FLA_LOWER_TRIANGULAR,
          FLA_TRANSPOSE, FLA_NONUNIT_DIAG,
          FLA_ONE, A11, A21 );
FLA_Syrk( FLA_LOWER_TRIANGULAR, FLA_NO_TRANSPOSE,
          FLA_MINUS_ONE, A21, FLA_ONE, A22 );
/*-----*/

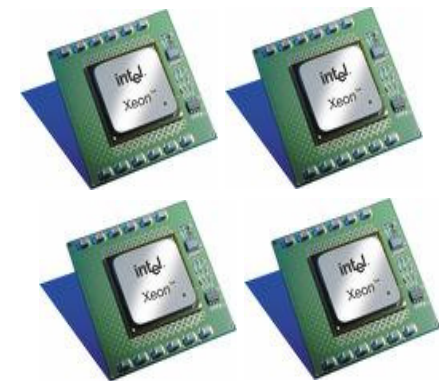
```

libflame → FLAME runtime → SuperMatrix

Exploiting task-level parallelism

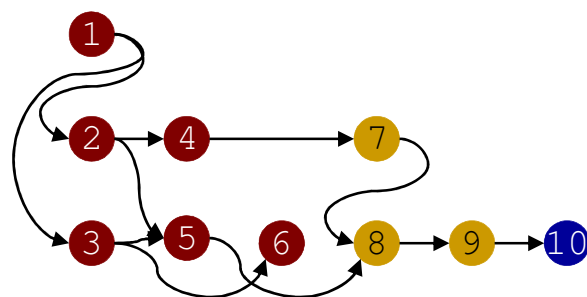
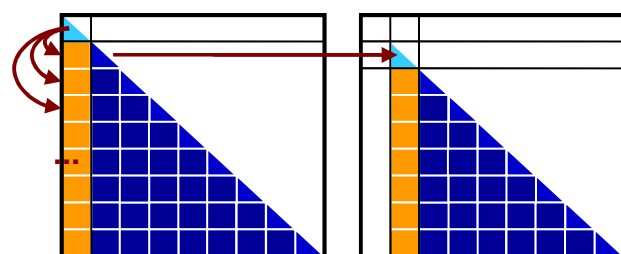


- SuperMatrix: scheduling of tasks to cores



libflame → FLAME runtime → SuperMatrix

Exploiting task-level parallelism



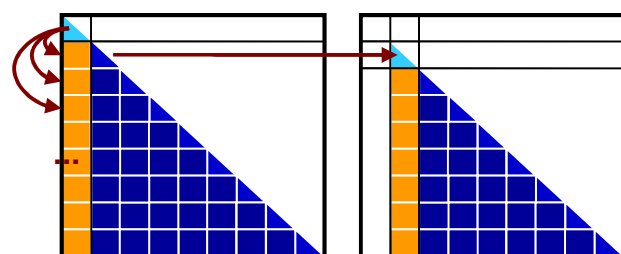
- SuperMatrix: scheduling of tasks to cores

HOW?

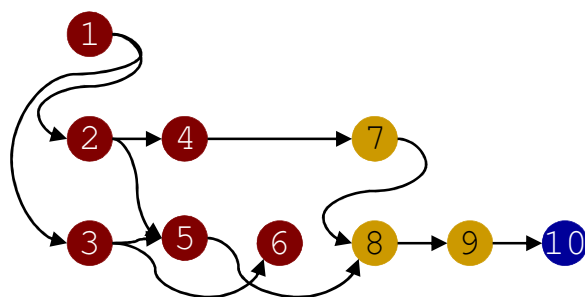
- List of ready tasks
- One thread per core
 1. Centralized list
 2. One list per-thread
 3. One list per-thread and work-stealing

libflame → FLAME runtime → GPU support

Single GPU



- SuperMatrix: Dealing with data transfers between host (CPU)/device (GPU) memory spaces



libflame → FLAME runtime → GPU support

Single GPU: a user's view

```
FLA_Obj A;

// Initialize conventional matrix: buffer, m, rs, cs
// Obtain storage blocksize, # of threads: b, n_threads

FLA_Init();

FLASH_Obj_create( FLA_DOUBLE, m, m, 1, &b, &A );
FLASH_Copy_buffer_to_hier( m, m, buffer, rs, cs,
                           0, 0, A );
FLASH_Queue_set_num_threads( n_threads );
FLASH_Queue_enable_gpu();
FLASH_Chol( FLA_LOWER_TRIANGULAR, A );

FLASH_Obj_free( &A );

FLA_Finalize();
```

libflame → FLAME runtime → GPU support

Single GPU: under the cover

```
FLA_Part_2x2 (...); ←  
  
while ( FLA_Obj_length(ATL) < FLA_Obj_length(A) ){  
  
    FLA_Repart_2x2_to_3x3 (...) ←  
  
    /*-----*/  
    FLASH_Chol( FLA_LOWER_TRIANGULAR, A11 );  
    FLASH_Trsm( FLA_RIGHT, FLA_LOWER_TRIANGULAR,  
                FLA_TRANSPOSE, FLA_NONUNIT_DIAG,  
                FLA_ONE, A11, A21 );  
    FLASH_Syrk( FLA_LOWER_TRIANGULAR, FLA_NO_TRANSPOSE,  
                FLA_MINUS_ONE, A21, FLA_ONE, A22 );  
    /*-----*/  
  
    FLA_Cont_with_3x3_to_2x2 (...) ←  
  
}
```

Indexing operations (with
addresses in device
memory)

libflame → FLAME runtime → GPU support

Single GPU: under the cover

```
FLA_Part_2x2(...);

while ( FLA_Obj_length(ATL) < FLA_Obj_length(A) ){

  FLA_Repart_2x2_to_3x3(...);

  /*-----*/
  FLASH_Chol( FLA_LOWER_TRIANGULAR, A11 );
  FLASH_Trsm( FLA_RIGHT, FLA_LOWER_TRIANGULAR,
              FLA_TRANSPOSE, FLA_NONUNIT_DIAG,
              FLA_ONE, A11, A21 );
  FLASH_Syrk( FLA_LOWER_TRIANGULAR, FLA_NO_TRANSPOSE,
              FLA_MINUS_ONE, A21, FLA_ONE, A22 );
  /*-----*/

  FLA_Cont_with_3x3_to_2x2(...);
}
```



Real computation:
Runtime keeps track of data in
host/device memory and
performs the necessary
transfers, reducing #copies

libflame → FLAME runtime → GPU support

Single GPU: under the cover

```
FLA_Part_2x2 (...);  
  
while ( FLA_Obj_length(ATL) < FLA_Obj_length(A) ){  
    FLA_Repart_2x2_to_3x3 (...);  
  
    /*-----*/  
    FLASH_Chol( FLA_LOWER_TRIANGULAR, A11 );  
    FLASH_Trsm( FLA_RIGHT, FLA_LOWER_TRIANGULAR,  
                FLA_TRANSPOSE, FLA_NONUNIT_DIAG,  
                FLA_ONE, A11, A21 );  
    FLASH_Syrk( FLA_LOWER_TRIANGULAR, FLA_NO_TRANSPOSE,  
                FLA_MINUS_ONE, A21, FLA_ONE, A22 );  
    /*-----*/  
  
    FLA_Cont_with_3x3_to_2x2 (...);  
}
```



1. Copy matrix to GPU memory before algorithm commences

libflame → FLAME runtime → GPU support

Single GPU: under the cover

```
FLA_Part_2x2 (...);  
  
while ( FLA_Obj_length(ATL) < FLA_Obj_length(A) ){  
  
    FLA_Repart_2x2_to_3x3 (...);  
  
    /*-----*/  
    FLASH_Chol( FLA_LOWER_TRIANGULAR, A11 );  
    FLASH_Trsm( FLA_RIGHT, FLA_LOWER_TRIANGULAR,  
                FLA_TRANSPOSE, FLA_NONUNIT_DIAG,  
                FLA_ONE, A11, A21 );  
    FLASH_Syrk( FLA_LOWER_TRIANGULAR, FLA_NO_TRANSPOSE,  
                FLA_MINUS_ONE, A21, FLA_ONE, A22 );  
    /*-----*/  
  
    FLA_Cont_with_3x3_to_2x2 (...);  
  
}
```



2. Copy block **A11** from device to host before its factorization

libflame → FLAME runtime → GPU support

Single GPU: under the cover

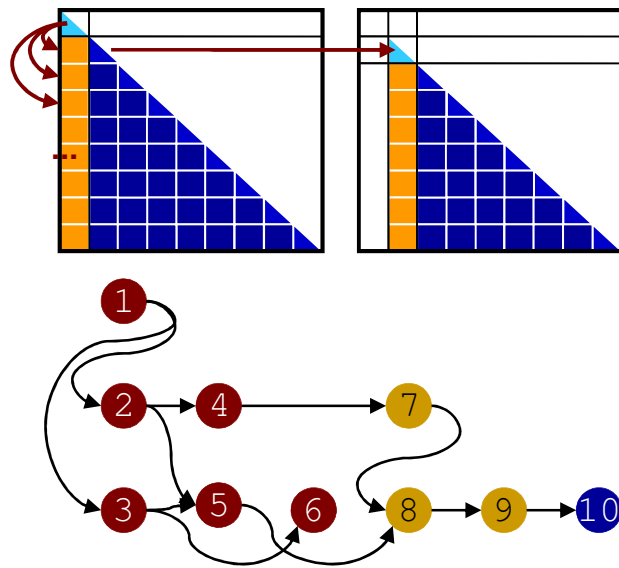
```
FLA_Part_2x2(...);  
  
while ( FLA_Obj_length(ATL) < FLA_Obj_length(A) ){  
  
    FLA_Repart_2x2_to_3x3(...);  
  
    /*-----*/  
    FLASH_Chol( FLA_LOWER_TRIANGULAR, A11 );  
    FLASH_Trsm( FLA_RIGHT, FLA_LOWER_TRIANGULAR,  
                FLA_TRANSPOSE, FLA_NONUNIT_DIAG,  
                FLA_ONE, A11, A21 );  
    FLASH_Syrk( FLA_LOWER_TRIANGULAR, FLA_NO_TRANSPOSE,  
                FLA_MINUS_ONE, A21, FLA_ONE, A22 );  
    /*-----*/  
  
    FLA_Cont_with_3x3_to_2x2(...);  
  
}
```



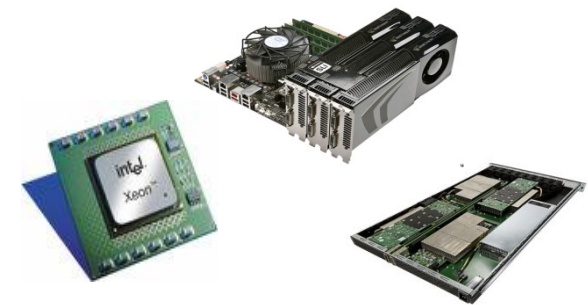
3. Copy block **A11** from host to device before using it in subsequent computations

libflame → FLAME runtime → GPU support

Multi-GPU



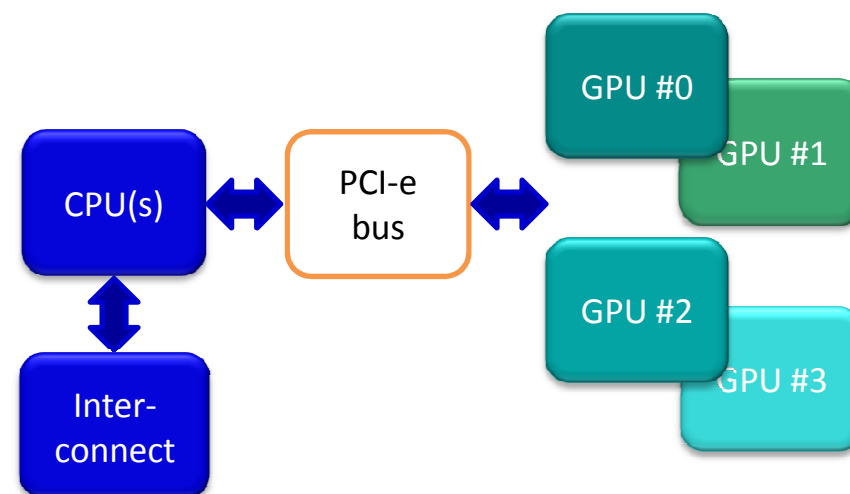
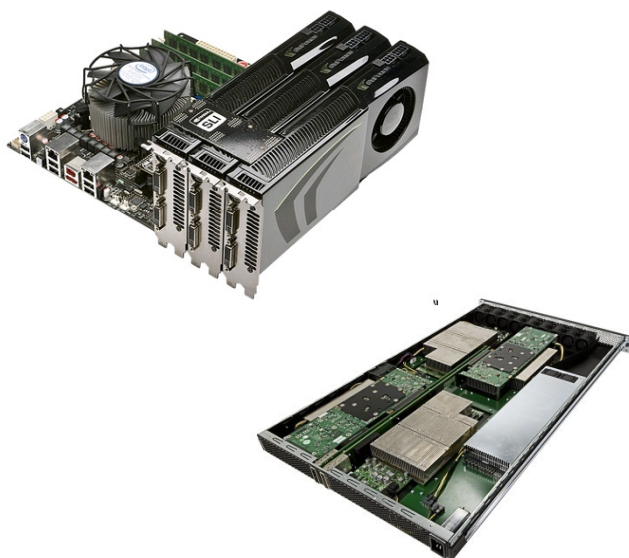
- SuperMatrix: Dealing with data transfers between host (CPU)/device (GPU) memory spaces



libflame → FLAME runtime → GPU support

Multi-GPU

- How do we program these?



libflame → FLAME runtime → GPU support

Multi-GPU: a user's view

```
FLA_Obj A;

// Initialize conventional matrix: buffer, m, rs, cs
// Obtain storage blocksize, # of threads: b, n_threads

FLA_Init();

FLASH_Obj_create( FLA_DOUBLE, m, m, 1, &b, &A );
FLASH_Copy_buffer_to_hier( m, m, buffer, rs, cs,
                          0, 0, A );
FLASH_Queue_set_num_threads( n_threads );
FLASH_Queue_enable_gpu();
FLASH_Chol( FLA_LOWER_TRIANGULAR, A );

FLASH_Obj_free( &A );

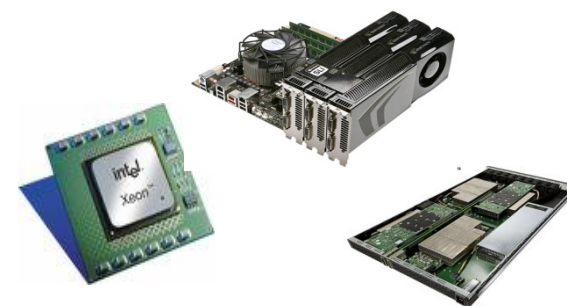
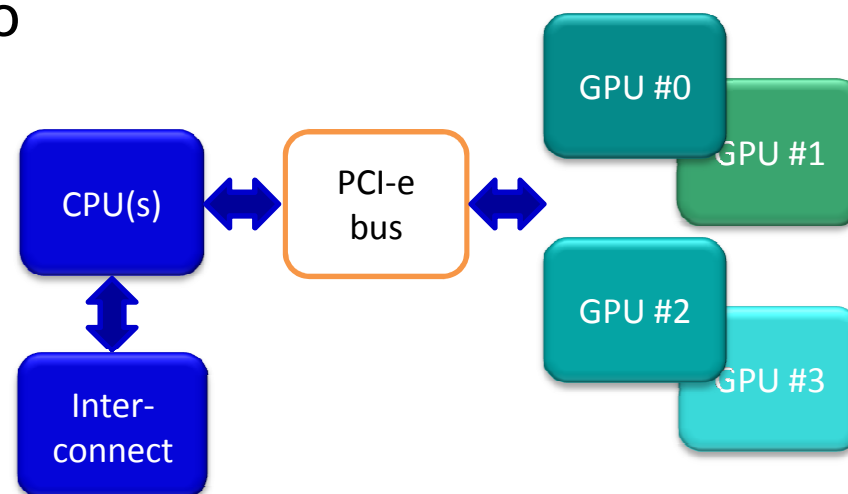
FLA_Finalize();
```

libflame → FLAME runtime → GPU support

Multi-GPU: under the cover

- Naïve approach:
- Before execution, transfer data to device
- Upon completion, retrieve results back to host

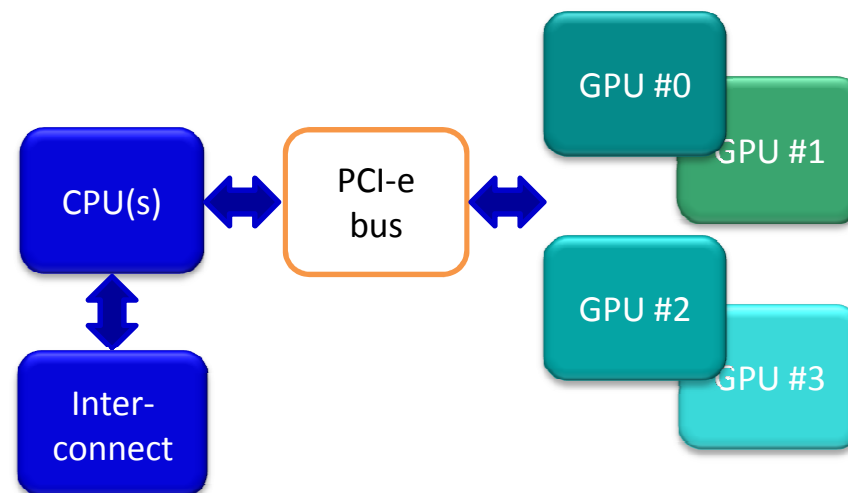
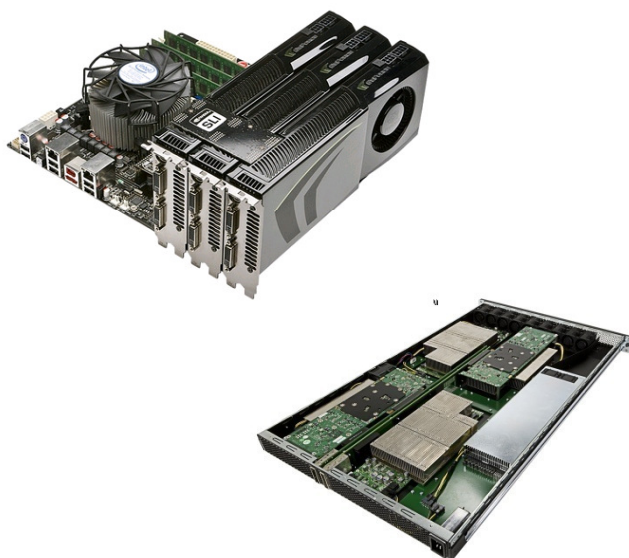
→ poor data locality



libflame → FLAME runtime → GPU support

Multi-GPU: under the cover

- How do we program these?



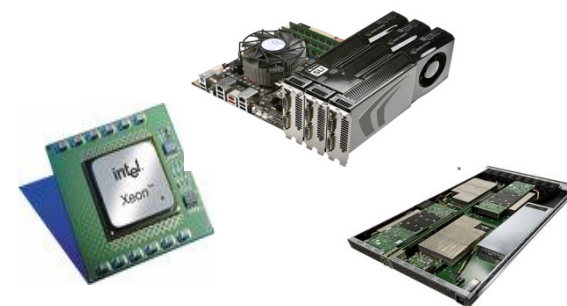
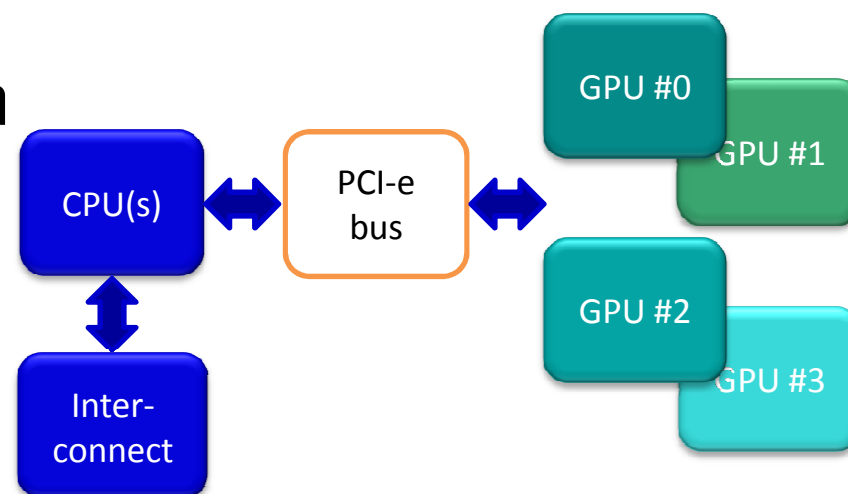
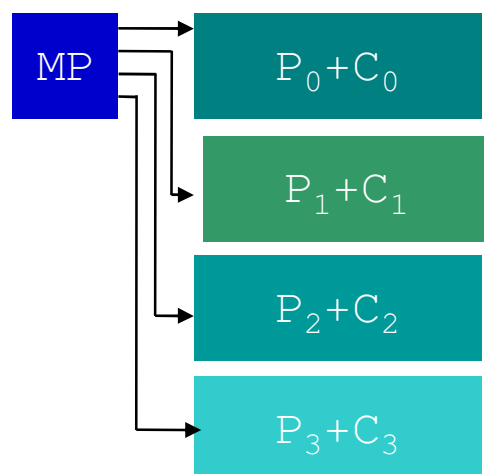
View as a...

- Shared-memory multiprocessor + DSM

libflame → FLAME runtime → GPU support

Multi-GPU: under the cover

- View system as a shared-memory multiprocessors (multi-core processor with hw. coherence)



Multi-GPU: under the cover

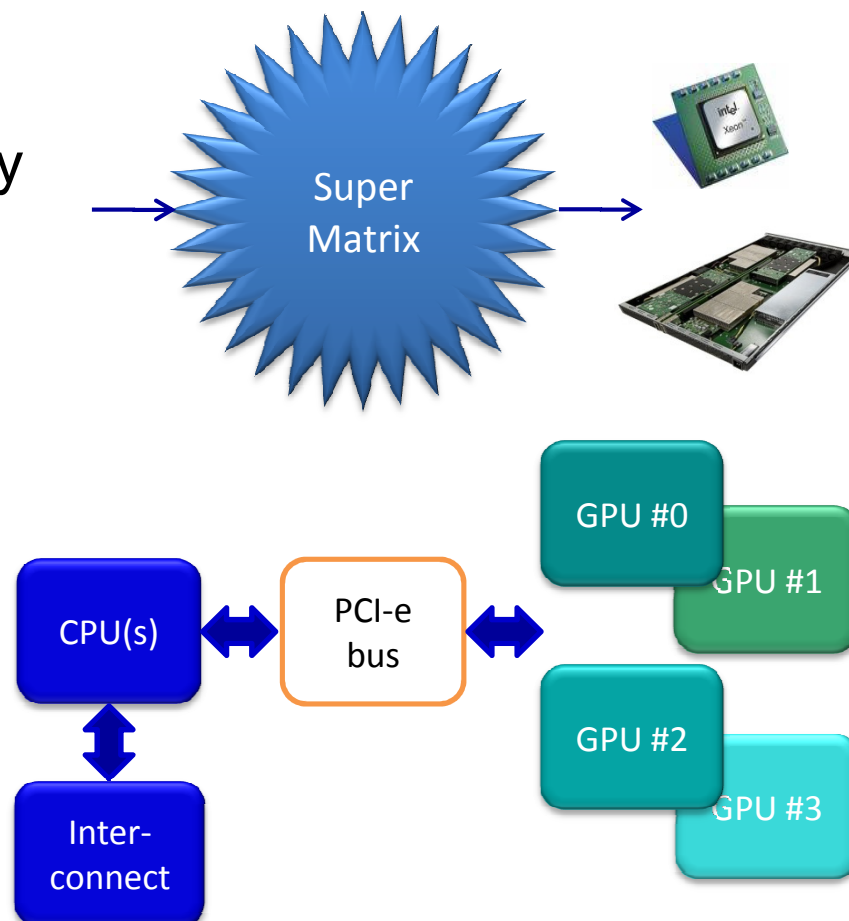
- Software Distributed-Shared Memory (DSM)
 - Software: flexibility vs. efficiency
 - Underlying distributed memory hidden from the users
 - Reduce memory transfers using write-back, write-invalidate,...
 - Well-known approach, not too efficient as a middleware for general apps.

- Regularity of dense linear algebra operations makes a difference!

libflame → FLAME runtime → GPU support

Multi-GPU: under the cover

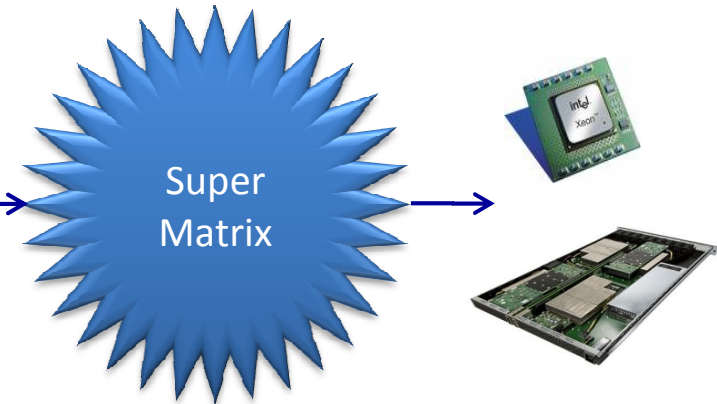
- Reduce #data transfers:
- Run-time handles device memory as a software cache:
 - Operate at block level
 - Software → flexibility
 - *Write-back*
 - *Write-invalidate*



libflame → FLAME runtime → GPU support

Multi-GPU: under the cover

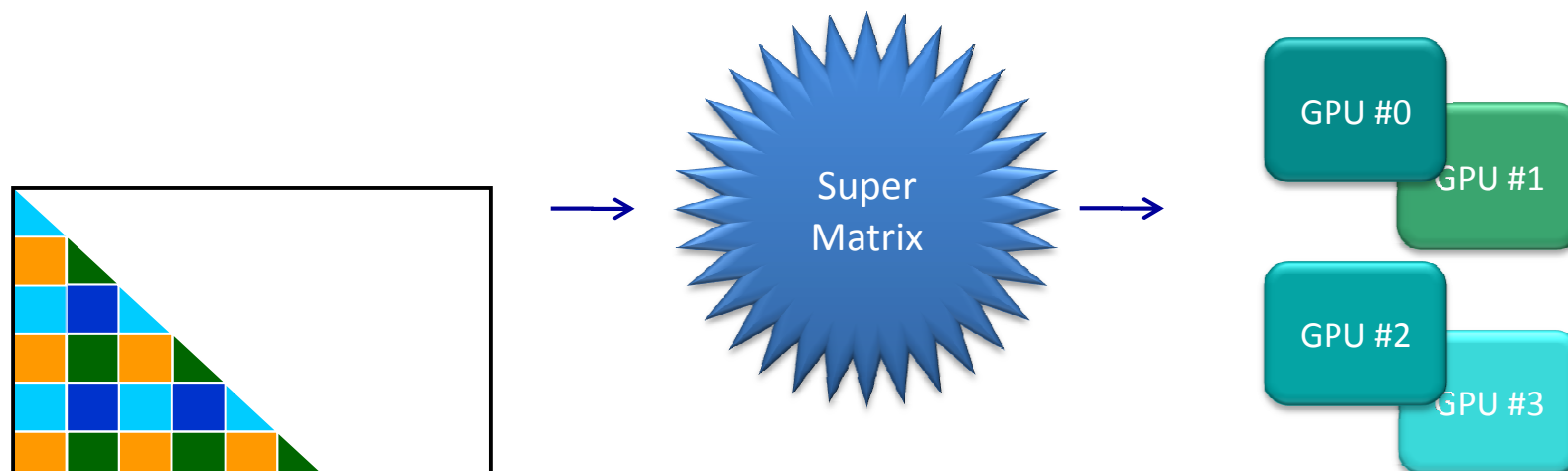
```
FLA_Part_2x2 (...);  
  
while ( FLA_Obj_length(ATL) < FLA_Obj_length(A) ){  
  
    FLA_Repart_2x2_to_3x3 (...);  
  
    /*-----*/  
    FLASH_Chol( FLA_LOWER_TRIANGULAR, A11 );  
    FLASH_Trsm( FLA_RIGHT, FLA_LOWER_TRIANGULAR,  
                FLA_TRANSPOSE, FLA_NONUNIT_DIAG,  
                FLA_ONE, A11, A21 );  
    FLASH_Syrk( FLA_LOWER_TRIANGULAR, FLA_NO_TRANSPOSE,  
                FLA_MINUS_ONE, A21, FLA_ONE, A22 );  
    /*-----*/  
  
    FLA_Cont_with_3x3_to_2x2 (...);  
  
}
```



1. Distribute matrix among GPU memories (2D workload distribution) before algorithm commences

libflame → FLAME runtime → GPU support

Multi-GPU: under the cover

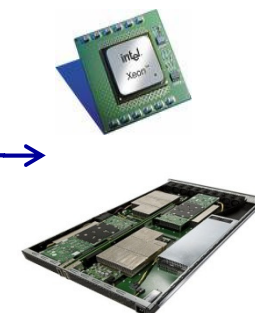


1. Distribute matrix among GPU memories (**2D workload distribution**): owner-computes rule

libflame → FLAME runtime → GPU support

Multi-GPU: under the cover

```
FLA_Part_2x2 (...);  
  
while ( FLA_Obj_length(ATL) < FLA_Obj_length(A) ){  
  
    FLA_Repart_2x2_to_3x3 (...);  
  
    /*-----*/  
    FLASH_Chol( FLA_LOWER_TRIANGULAR, A11 );  
    FLASH_Trsm( FLA_RIGHT, FLA_LOWER_TRIANGULAR,  
                FLA_TRANSPOSE, FLA_NONUNIT_DIAG,  
                FLA_ONE, A11, A21 );  
    FLASH_Syrk( FLA_LOWER_TRIANGULAR, FLA_NO_TRANSPOSE,  
                FLA_MINUS_ONE, A21, FLA_ONE, A22 );  
    /*-----*/  
  
    FLA_Cont_with_3x3_to_2x2 (...);  
  
}
```

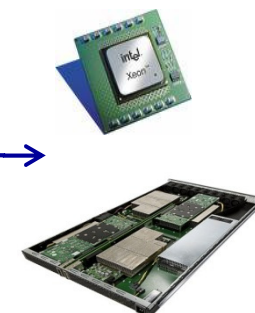


2. Copy block **A11** from corresponding device to host before its factorization

libflame → FLAME runtime → GPU support

Multi-GPU: under the cover

```
FLA_Part_2x2 (...);  
  
while ( FLA_Obj_length(ATL) < FLA_Obj_length(A) ){  
  
    FLA_Repart_2x2_to_3x3 (...);  
  
    /*-----*/  
    FLASH_Chol( FLA_LOWER_TRIANGULAR, A11 );  
    FLASH_Trsm( FLA_RIGHT, FLA_LOWER_TRIANGULAR,  
                FLA_TRANSPOSE, FLA_NONUNIT_DIAG,  
                FLA_ONE, A11, A21 );  
    FLASH_Syrk( FLA_LOWER_TRIANGULAR, FLA_NO_TRANSPOSE,  
                FLA_MINUS_ONE, A21, FLA_ONE, A22 );  
    /*-----*/  
  
    FLA_Cont_with_3x3_to_2x2 (...);  
  
}
```

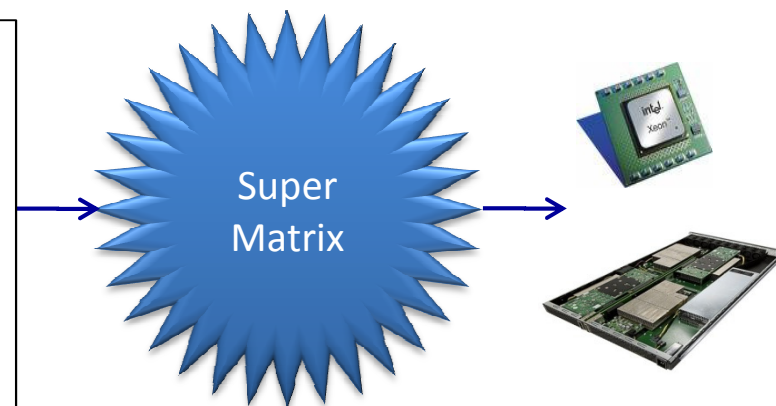


3. Broadcast block `A11` from host to appropriate devices before using it in subsequent computations (write-update)

libflame → FLAME runtime → GPU support

Multi-GPU: under the cover

```
FLA_Part_2x2 (...);  
  
while ( FLA_Obj_length(ATL) < FLA_Obj_length(A) ){  
  
    FLA_Repart_2x2_to_3x3 (...);  
  
    /*-----*/  
    FLASH_Chol( FLA_LOWER_TRIANGULAR, A11 );  
    FLASH_Trsm( FLA_RIGHT, FLA_LOWER_TRIANGULAR,  
                FLA_TRANSPOSE, FLA_NONUNIT_DIAG,  
                FLA_ONE, A11, A21 );  
    FLASH_Syrk( FLA_LOWER_TRIANGULAR, FLA_NO_TRANSPOSE,  
                FLA_MINUS_ONE, A21, FLA_ONE, A22 );  
    /*-----*/  
  
    FLA_Cont_with_3x3_to_2x2 (...);  
  
}
```

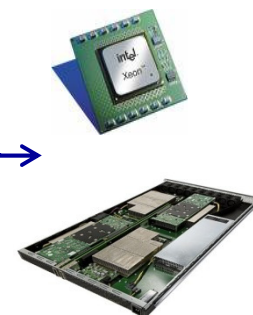


4. Keep `A11` in receiving device(s) in case needed in subsequent computations (cache)

libflame → FLAME runtime → GPU support

Multi-GPU: under the cover

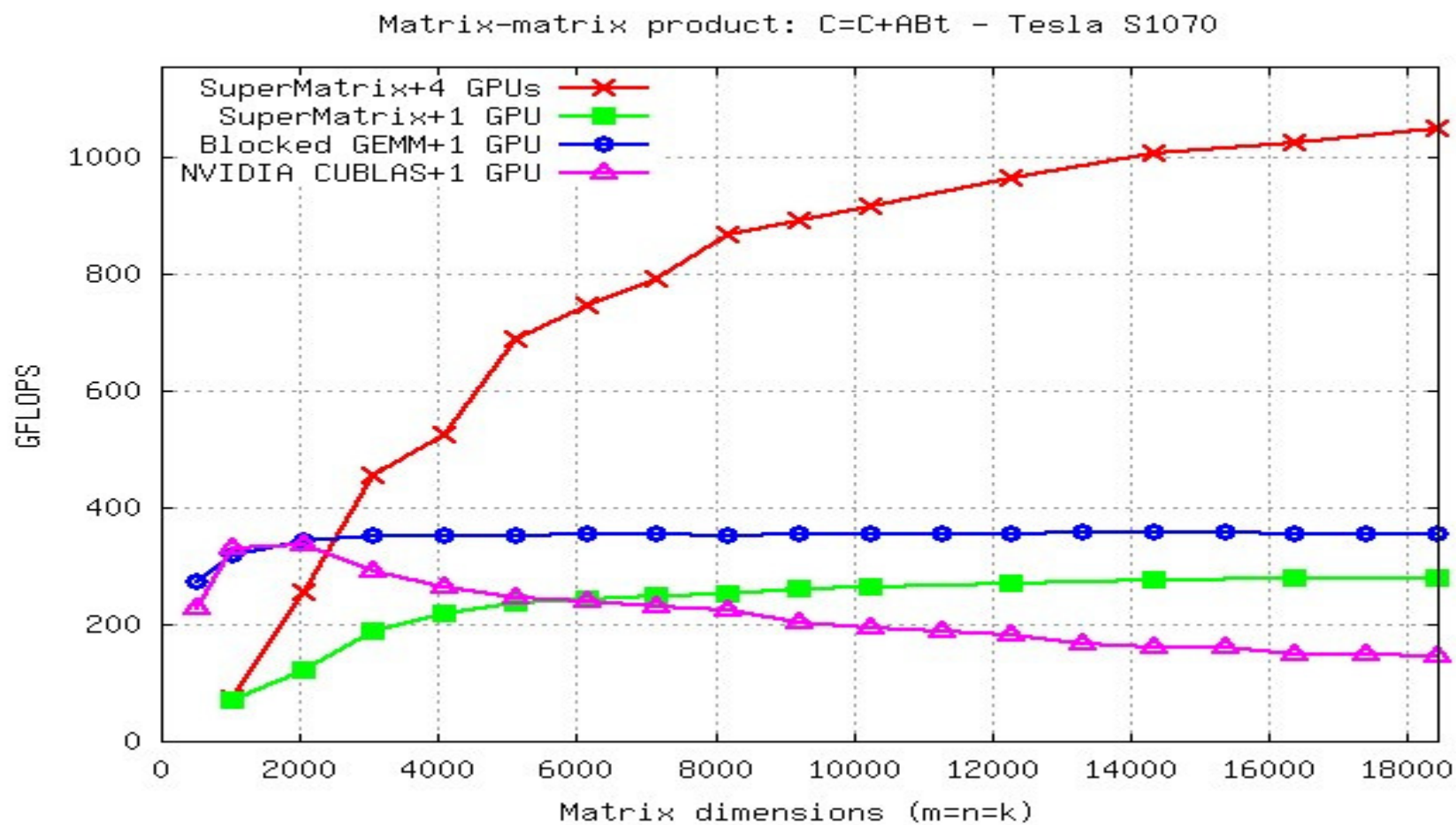
```
FLA_Part_2x2 (...);  
  
while ( FLA_Obj_length(ATL) < FLA_Obj_length(A) ){  
  
    FLA_Repart_2x2_to_3x3 (...);  
  
    /*-----*/  
    FLASH_Chol( FLA_LOWER_TRIANGULAR, A11 );  
    FLASH_Trsm( FLA_RIGHT, FLA_LOWER_TRIANGULAR,  
                FLA_TRANSPOSE, FLA_NONUNIT_DIAG,  
                FLA_ONE, A11, A21 );  
    FLASH_Syrk( FLA_LOWER_TRIANGULAR, FLA_NO_TRANSPOSE,  
                FLA_MINUS_ONE, A21, FLA_ONE, A22 );  
    /*-----*/  
  
    FLA_Cont_with_3x3_to_2x2 (...);  
  
}
```



5. Keep updated **A21** in
device till replaced (write-
back)

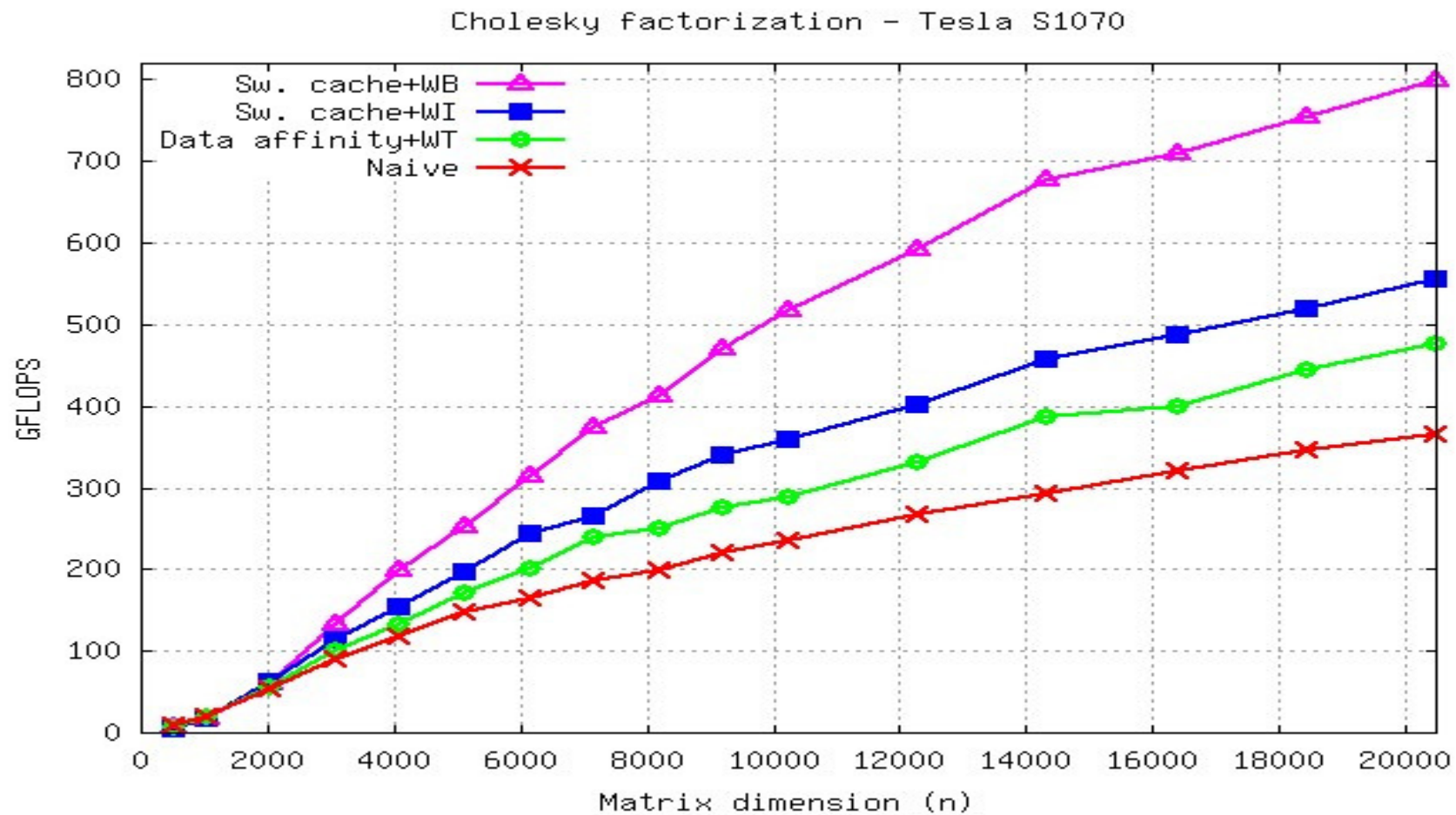
libflame → FLAME runtime → GPU support

Performance



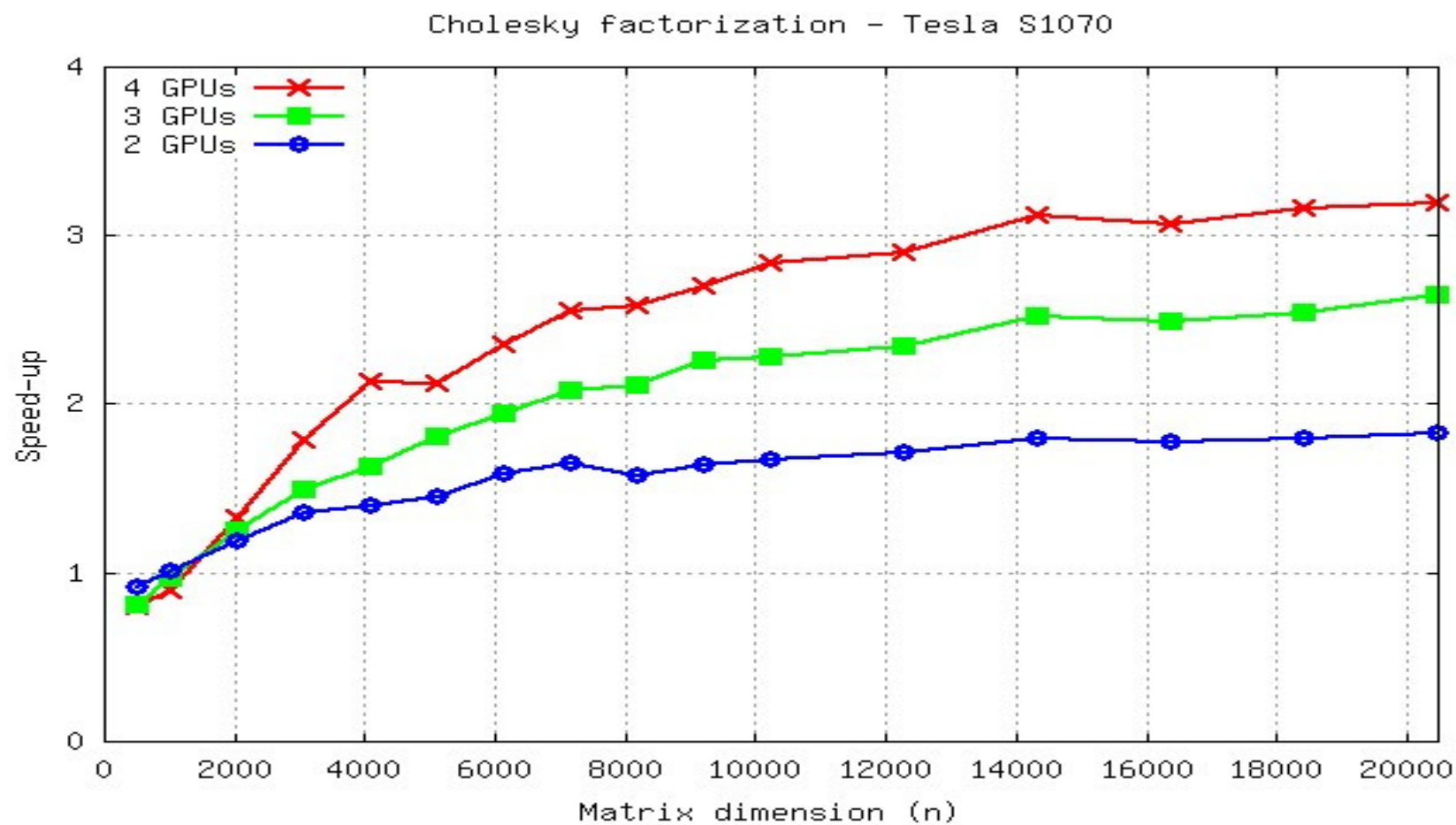
libflame → FLAME runtime → GPU support

Performance



libflame → FLAME runtime → GPU support

Performance



Index

- The libflame library

1. A user's view
2. Creating your own algorithm
3. FLAME runtime
4. Clusters of GPUs

- 
1. DLA for clusters
 2. Host-centric view
 3. Device-centric view

- The StarSs framework

libflame → Clusters of GPUs → DLA for clusters

libflame-like libraries

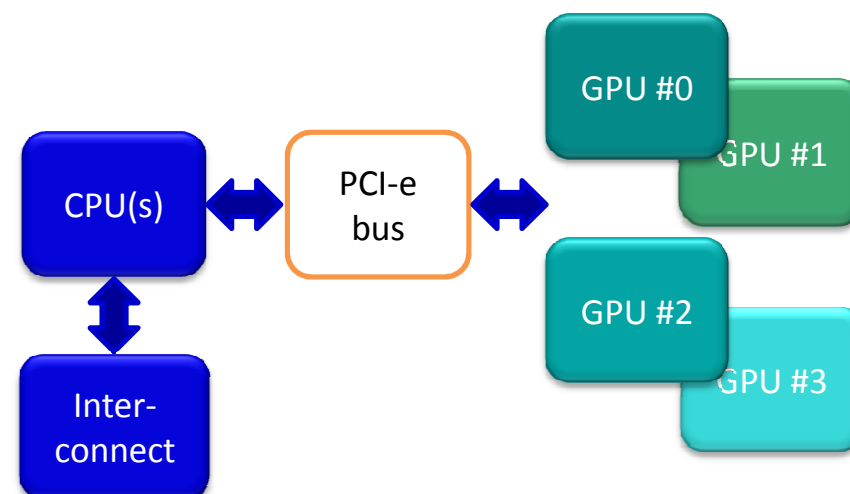
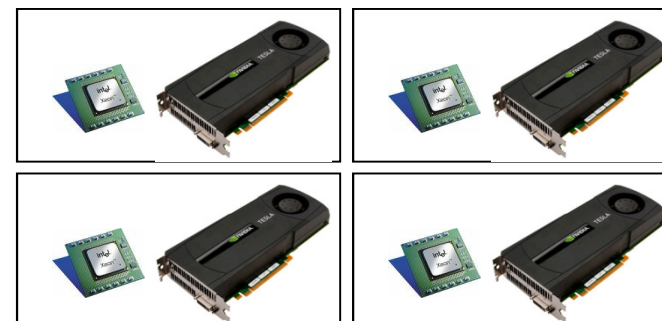
- PLAPACK (UT@Austin)
 - Use of objects (`PLA_Obj`), vectors, matrices, projected vectors, etc., with layout embedded
 - PMB distribution
 - Layered and modular design: all communication is done via copies (`PLA_Copy`) and reductions (`PLA_Reduce`) from one object type to another

- Elemental (Jack Poulson)
 - Based on PLAPACK, but C++
 - Element-wise cyclic data layout

libflame → Clusters of GPUs → Host-centric view

Data in host memory

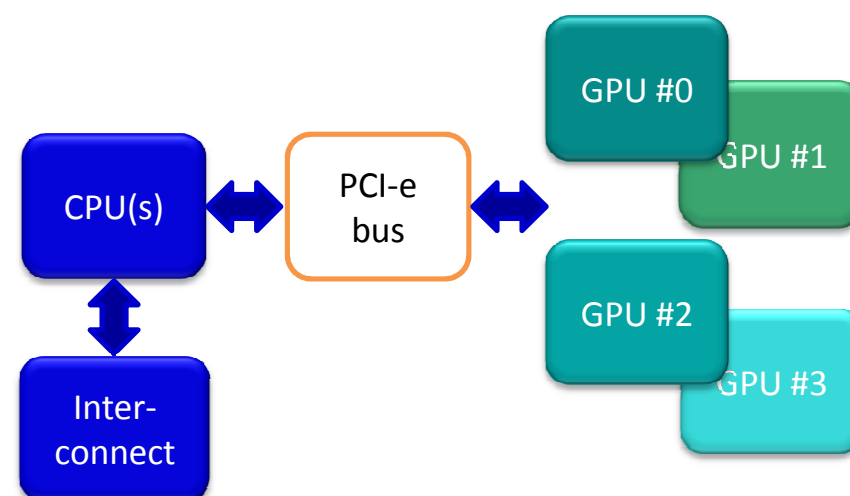
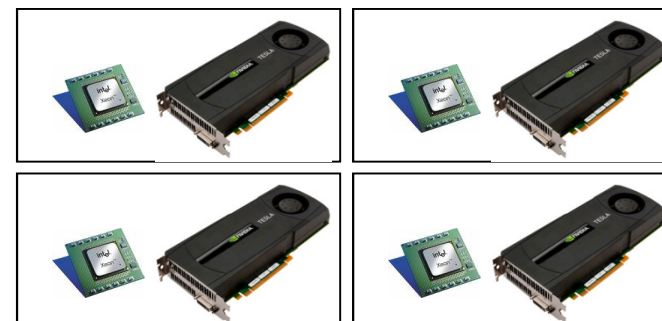
- Before executing a kernel, copy input data to GPU memory
- After execution, retrieve results back to node main memory
- Easy to program (wrappers to kernels)
- Copies linked to kernel execution: $O(n^3)$ transfers between CPU and GPU



libflame → Clusters of GPUs → Device-centric view

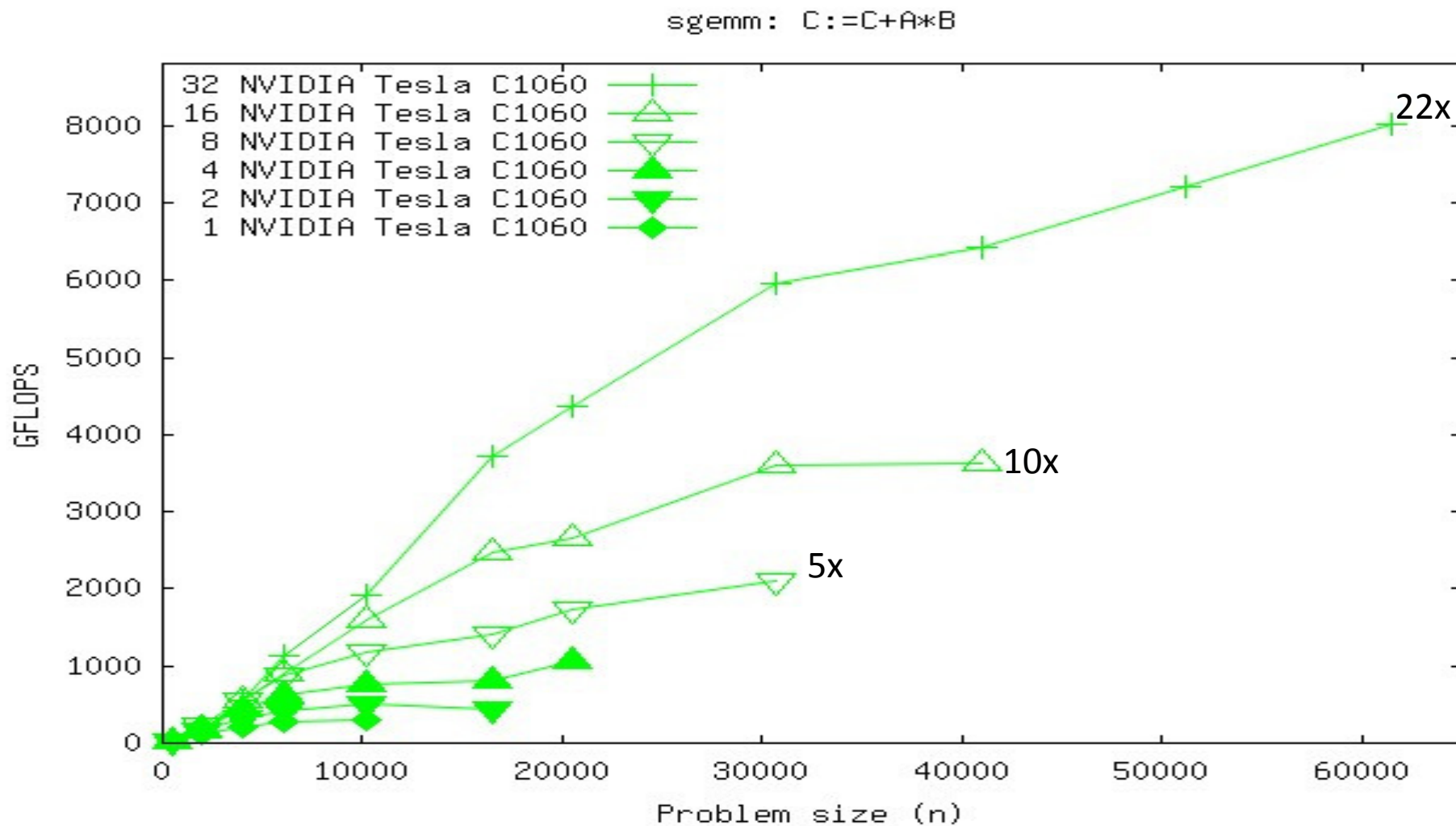
Data in GPU memory

- Before sending a piece of data, retrieve it back to node main memory (compact on the fly)
- After reception, copy contents to GPU memory
- Easy to program (wrappers to MPI calls)
- Copies linked to communication, not kernel execution: $O(n^2)$ transfers between CPU and GPU



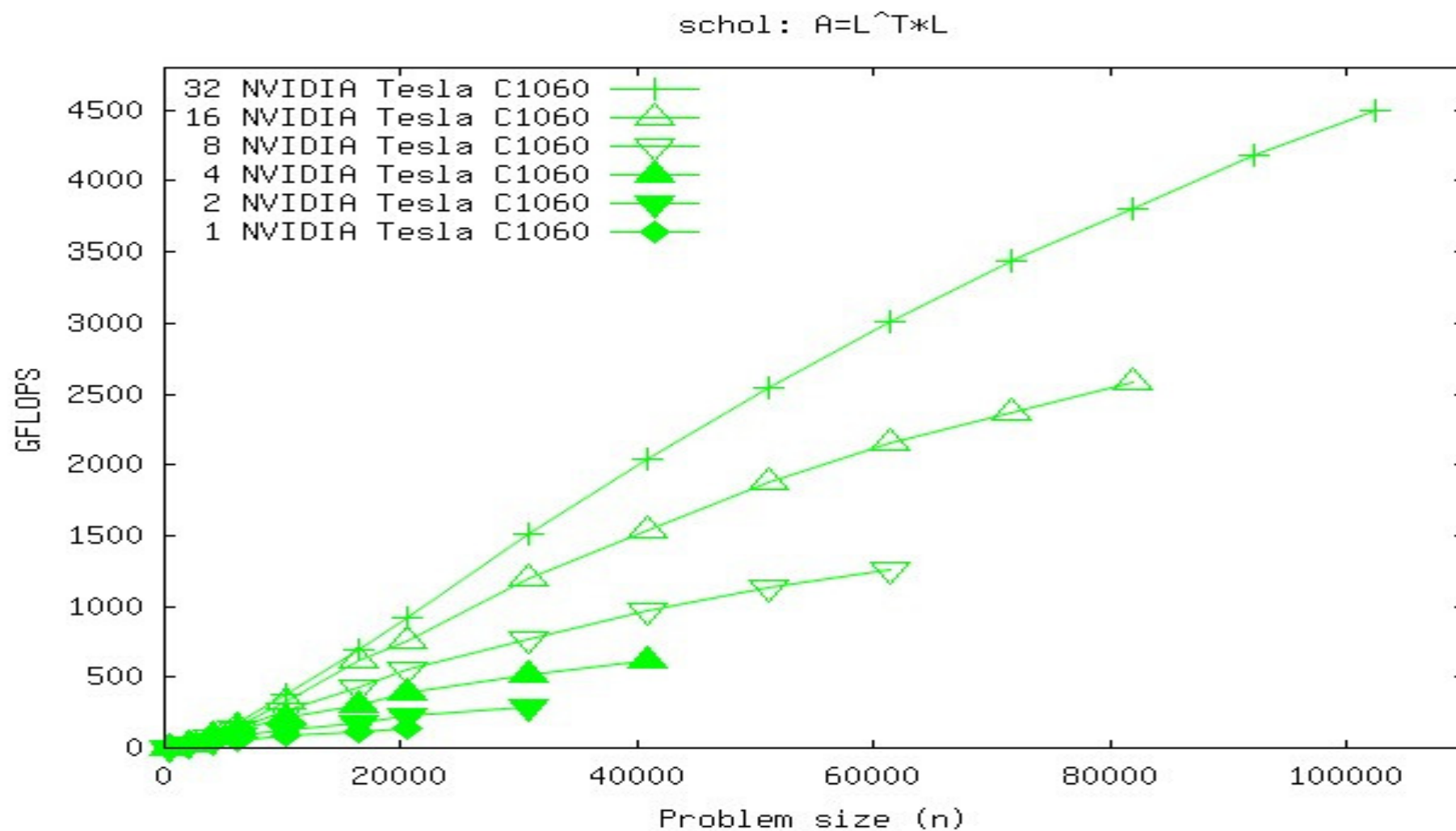
libflame → Clusters of GPUs

Performance



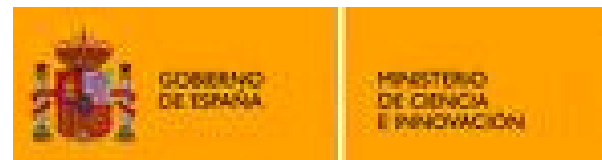
libflame → Clusters of GPUs

Performance



Acknowledgements

- Funding sources



Further information

- Contact:
 - field@cs.utexas.edu
- FLAME project website:
 - www.cs.utexas.edu/users/flame/
- *libflame: The Complete Reference*
 - www.cs.utexas.edu/users/field/docs/
 - Updated nightly
 - www.lulu.com/content/5915632
 - Updated occasionally

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- The libflame library



- The StarSs framework



**Barcelona
Supercomputing
Center**
Centro Nacional de Supercomputación



GPU support

The TEXT project

- Towards Exaflop applicaTions



- Demonstrate that **Hybrid MPI/SMPs** addresses the Exascale challenges in a productive and efficient way.
 - Deploy at supercomputing centers: Julich, EPCC, HLRS, BSC
 - Port Applications (HLA, SPECfem3D, PEPC, PSC, BEST, CPMD, LS1 MarDyn) and develop algorithms.
 - Develop additional environment capabilities
 - tools (debug, performance)
 - improvements in runtime systems (load balance and GPUs)
 - Support other users
 - Identify users of TEXT applications
 - Identify and support interested application developers
 - Contribute to Standards (OpenMP ARB, PERI-XML)

Index

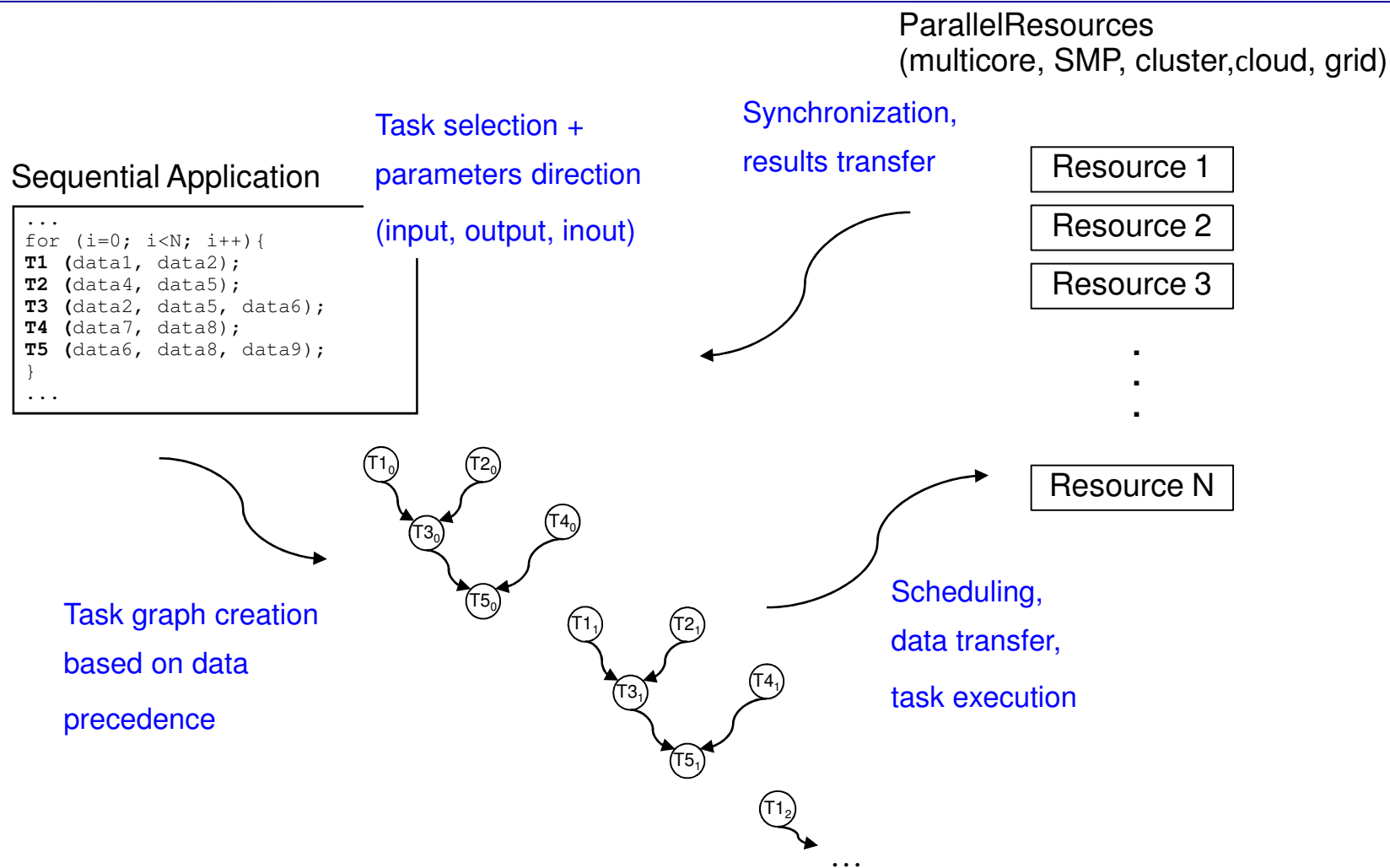
- The libflame library
- The StarSs framework

1. StarSs overview
2. OmpSs

Slides from Rosa M. Badia
Barcelona Supercomputing Center
Thanks!

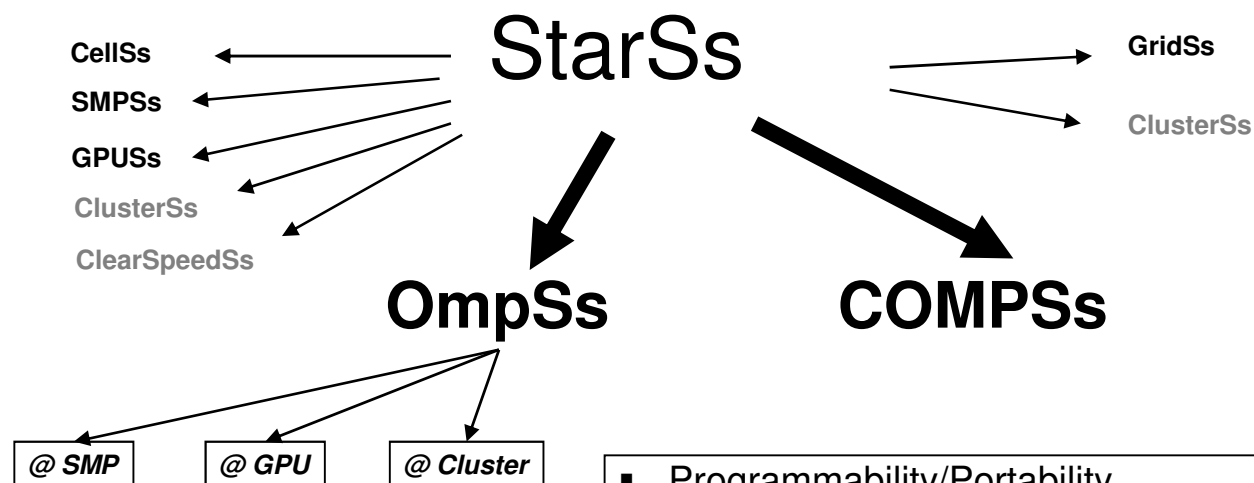
StarSs → StarSs overview

Programming model



StarSs → StarSs overview

Programming model



StarSs

- A “node” level programming model
- Sequential C/Fortran/Java + annotations
- Task based. Asynchrony, data-flow.
- “Simple” linear address space
- Directionality annotations on tasks arguments
- Nicely integrates in hybrid MPI/StarSs
- Natural support for heterogeneity

Programmability/Portability

- Incremental parallelization/restructure
- Separate algorithm from resources
- Disciplined programming
- **“Same” source code runs on “any” machine**
 - Optimized task implementations will result in better performance.

Performance

- Intelligent Runtime
 - Automatically extracts and exploits parallelism
 - Dataflow, workflow
 - Matches computations to specific resources on each type of target platform
- Asynchronous (data-flow) execution and locality awareness

A sequential program...

```
void vadd3 (float A[BS], float B[BS],
           float C[BS]);

void scale_add (float sum, float A[BS],
               float B[BS]);

void accum (float A[BS], float *sum);

for (i=0; i<N; i+=BS)           // C=A+B
    vadd3 ( &A[i], &B[i], &C[i]);
...
for (i=0; i<N; i+=BS)           // sum(C[i])
    accum (&C[i], &sum);
...
for (i=0; i<N; i+=BS)           // B=sum*A
    scale_add (sum, &E[i], &B[i]);
...
for (i=0; i<N; i+=BS)           // A=C+D
    vadd3 (&C[i], &D[i], &A[i]);
...
for (i=0; i<N; i+=BS)           // E=G+F
    vadd3 (&G[i], &F[i], &E[i]);
```

A sequential program... taskified...

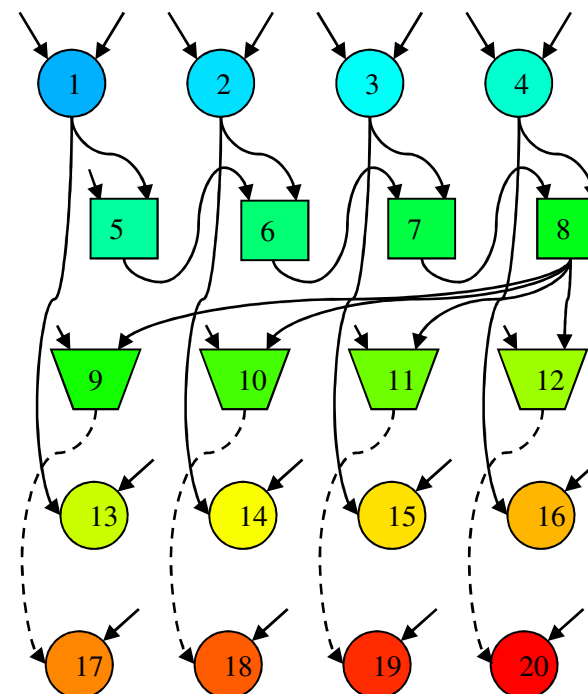
```
#pragma css task input(A, B) output(C)
void vadd3 (float A[BS], float B[BS],
           float C[BS]);

#pragma css task input(sum, A) inout(B)
void scale_add (float sum, float A[BS],
               float B[BS]);

#pragma css task input(A) inout(sum)
void accum (float A[BS], float *sum);

for (i=0; i<N; i+=BS)           // C=A+B
    vadd3 ( &A[i], &B[i], &C[i]);
...
for (i=0; i<N; i+=BS)           // sum(C[i])
    accum (&C[i], &sum);
...
for (i=0; i<N; i+=BS)           // B=sum*A
    scale_add (sum, &E[i], &B[i]);
...
for (i=0; i<N; i+=BS)           // A=C+D
    vadd3 (&C[i], &D[i], &A[i]);
...
for (i=0; i<N; i+=BS)           // E=G+F
    vadd3 (&G[i], &F[i], &E[i]);
```

Compute dependences @ task instantiation time



Color/number: order of task instantiation

Some antidependencies covered by flow dependences not drawn

A sequential program... taskified... with data-flow execution

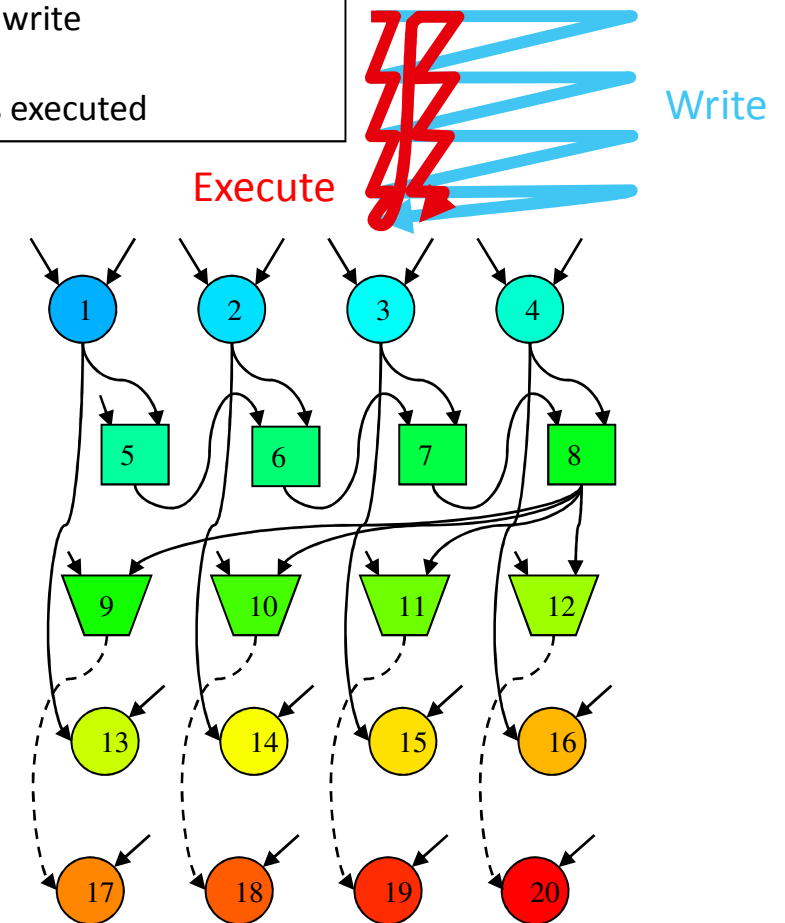
```
#pragma css task input(A, B) output(C)
void vadd3 (float A[BS], float B[BS],
           float C[BS]);

#pragma css task input(sum, A) inout(B)
void scale_add (float sum, float A[BS],
               float B[BS]);

#pragma css task input(A) inout(sum)
void accum (float A[BS], float *sum);

for (i=0; i<N; i+=BS)           // C=A+B
    vadd3 ( &A[i], &B[i], &C[i]);
...
for (i=0; i<N; i+=BS)           // sum(C[i])
    accum (&C[i], &sum);
...
for (i=0; i<N; i+=BS)           // B=sum*A
    scale_add (sum, &E[i], &B[i]);
...
for (i=0; i<N; i+=BS)           // A=C+D
    vadd3 (&C[i], &D[i], &A[i]);
...
for (i=0; i<N; i+=BS)           // E=G+F
    vadd3 (&G[i], &F[i], &E[i]);
```

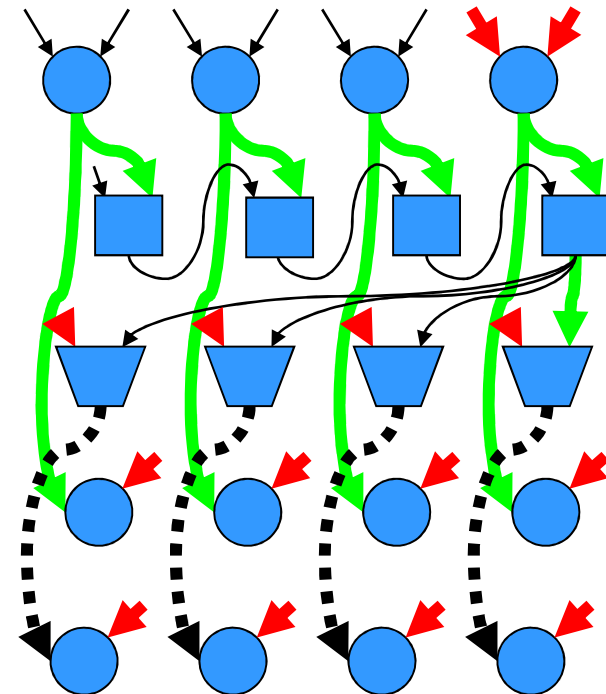
Decouple
how we write
from
how it is executed



Color/number: a possible order of task execution

The potential of data access information

- Flexibility to dynamically traverse dataflow graph “optimizing”
 - Concurrency. Critical path
 - Memory access: data transfers performed by run time
- Opportunities for
 - Prefetch
 - Reuse
 - Eliminate antidependences (rename)
 - Replication management
 - Coherency/consistency handled by the runtime



Index

- The libflame library

- The StarSs framework

1. StarSs overview
2. OmpSs



1. Overview & syntax
2. Compiler
3. Runtime
4. Examples

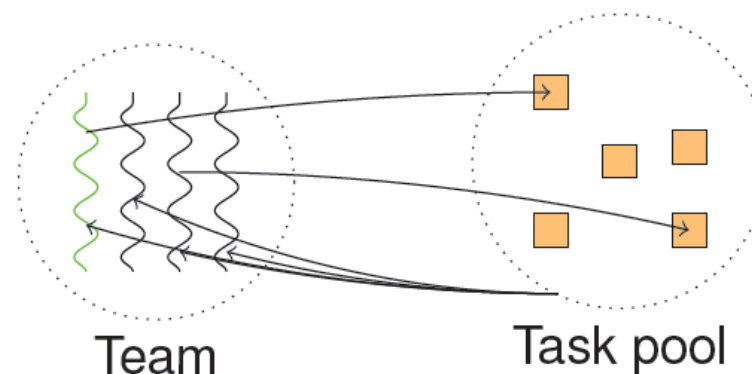
StarSs → OmpSs → Overview & syntax

OmpSs = OpenMP + StarSs extensions

- OmpSs is based on OpenMP with some differences:
 - Different execution model
 - Extended memory model
 - Extensions for point-to-point inter-task synchronizations
 - data dependencies
 - Extensions for heterogeneity
 - Other minor extensions

Execution model

- Thread-pool model
 - OpenMP parallel “ignored”
- All threads created on startup
 - One of them starts executing main
- All get work from a task pool
 - And can generate new work



Memory model

- Two “modes” are allowed:
 - pure SMP:
 - Single address space
 - OpenMP standard memory model is used
 - non-SMP (cluster, GPUs, ...):
 - Multiple address spaces exists
 - Same data may exists in multiple of these
 - Data consistency ensured by the implementation

Main element: Task

- Task: unit of computation
- Task definition
 - Pragmas in lined
 - Pragmas attached to function definition

```
#pragma omp task
void foo (int Y[size], int size) {
    int j;

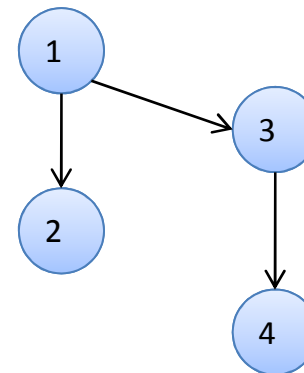
    for (j=0; j<size; j++) Y[j]= j;
}

int main()
{
    int X[100]
    foo (X, 100);
}
```

Defining dependences

- Clauses that express data direction:
 - input
 - output
 - inout
- Dependences computed at runtime taking into account these clauses

```
#pragma omp task output( x )  
x = 5;  
#pragma omp task input( x )  
printf( "%d\n" , x ) ;  
#pragma omp task inout( x )  
x++;  
#pragma omp task input( x )  
printf ( "%d\n" , x ) ;
```



Heterogeneity: the target directive

- Directive to specify device specific information:

#pragma omp target [clauses]

- Clauses:

- device: which device (smp, gpu)
- copy_in, copy_out, copy_inout: data to be moved in and out
- implements: specifies alternate implementations

```
#pragma target device (smp)
#pragma omp task input (Y)
void foo (int Y[size], int size) {
    int j;

    for (j=0; j<size; j++) Y[j]= j;
}

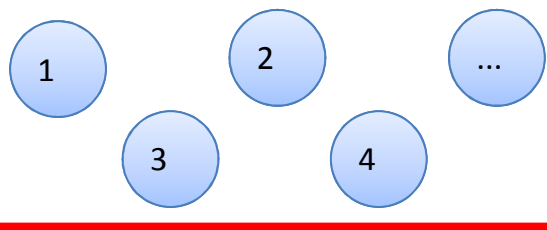
int main()
{
    int X[100]
    foo (X, 100) ;
}
```

Synchronization

#pragma omp task wait

- Suspends the current task until all children tasks are completed
- Just direct children, not descendants

```
void traverse_list ( List l )  
{  
    Element e ;  
    for ( e = l-> first; e ; e = e->next )  
        #pragma omp task  
        process ( e ) ;  
  
    #pragma omp taskwait  
}
```



Hierarchical task graph

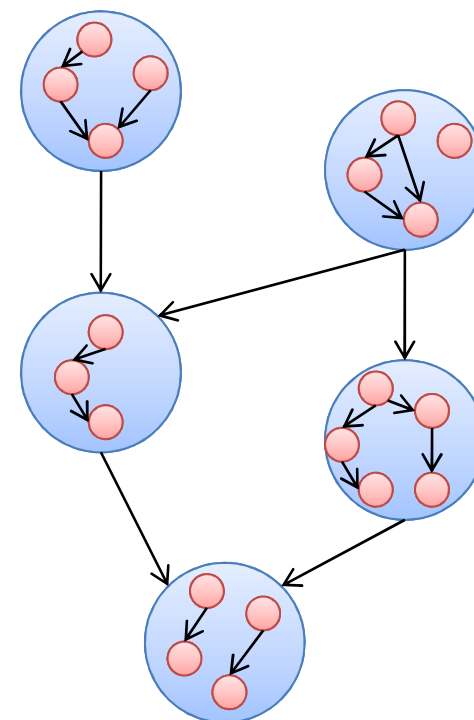
■ Nesting

```
#pragma omp task input([BS][BS]A, [BS][BS]B)\
inout([BS][BS]C)
void small_dgemm(float *C, float *A, float *B);

#pragma omp task input([N][N]A, [N][N] B)\
inout([N][N]C)
void block_dgemm(float *C, float *A, float *B){
    int i, j, k;

    for (i=0; i< N; i+=BS)
        for (j=0; j< N; j+=BS)
            for (k=0; k< N; k+=BS)
                small_dgemm(&C[i][j], &A[i][k], &B[k][j])
}

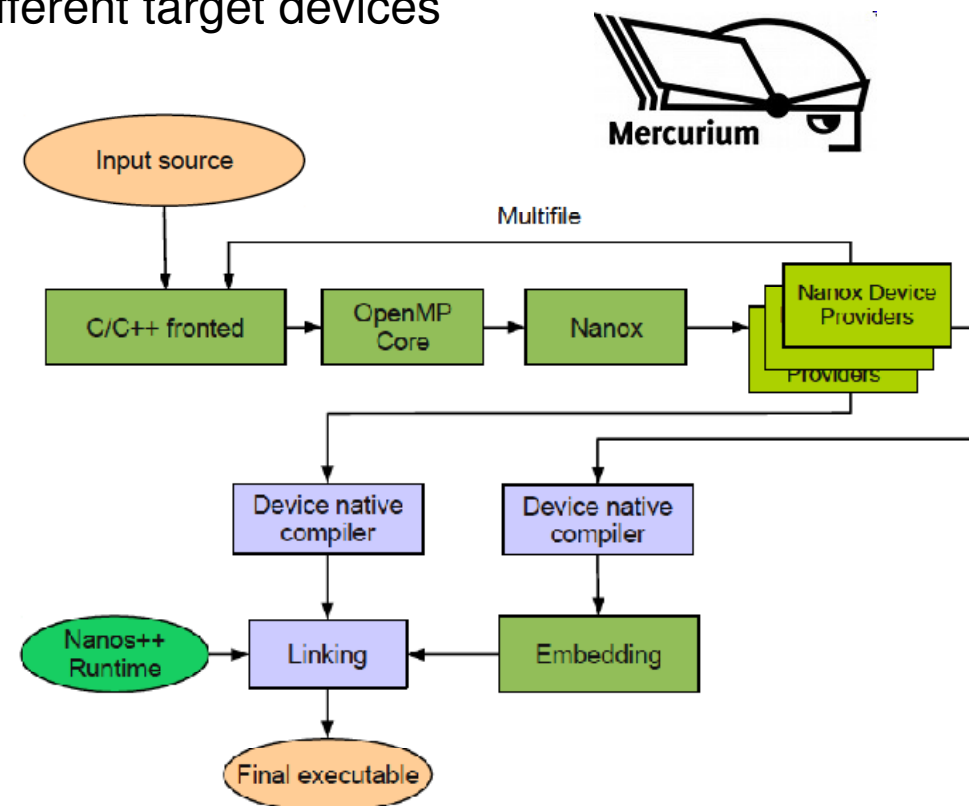
main() {
    ...
    block_dgemm(A,B,C);
    block_dgemm(D,E,F);
    #pragma omp task wait
}
```



StarSs → OmpSs → Compiler

Mercurium

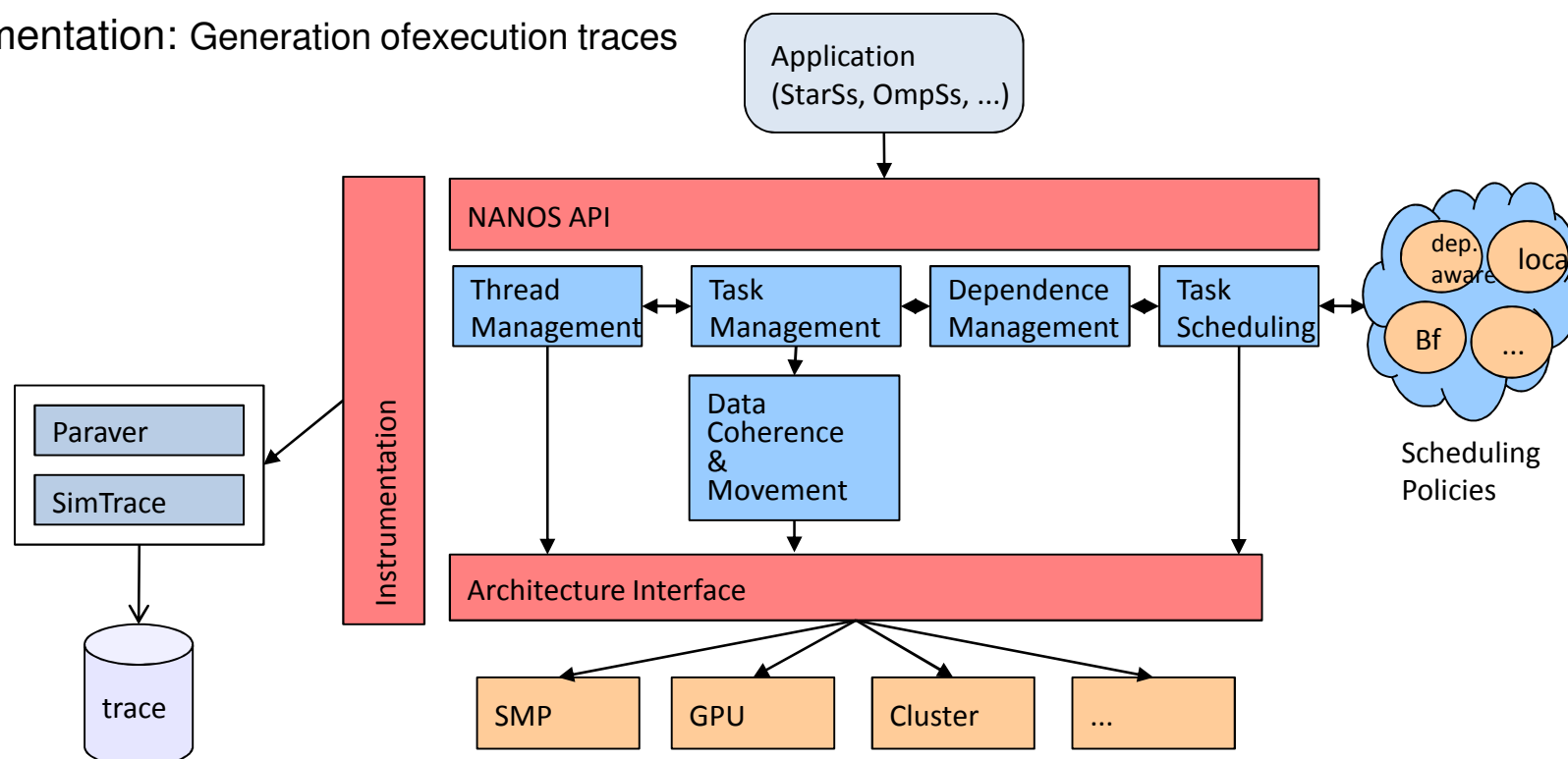
- Minor role
- Recognizes constructs and transforms them to calls to the runtime
- Manages code restructuring for different target devices
 - Device-specific handlers
 - May generate code in a separate file
 - Invokes different back-end compilers
 - nvcc for NVIDIA



StarSs → OmpSs → Runtime

Structure

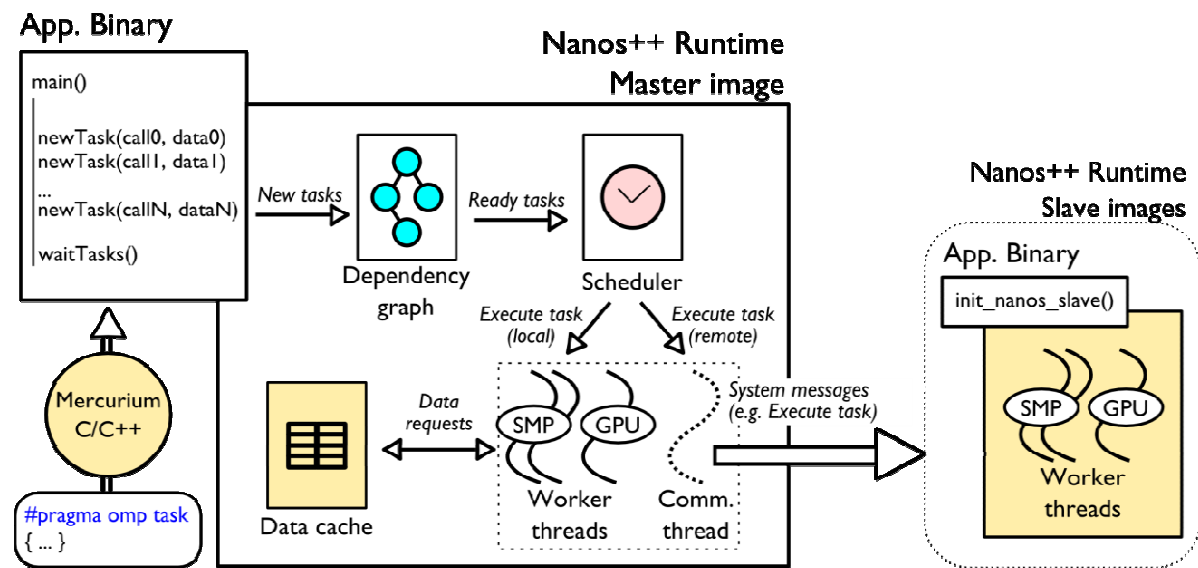
- Support to different programming models: OpenMP (OmpSs), StarSs, Chapel
- Independent components for thread, task, dependence handling, task scheduling, ...
- Most of the runtime independent of the target arch.: SMP, GPU, simulator, cluster
- Support to heterogeneous targets: i.e., threads running tasks in regular cores and GPUs
- Instrumentation: Generation of execution traces



StarSs → OmpSs → Runtime

Structure behaviour: task handling

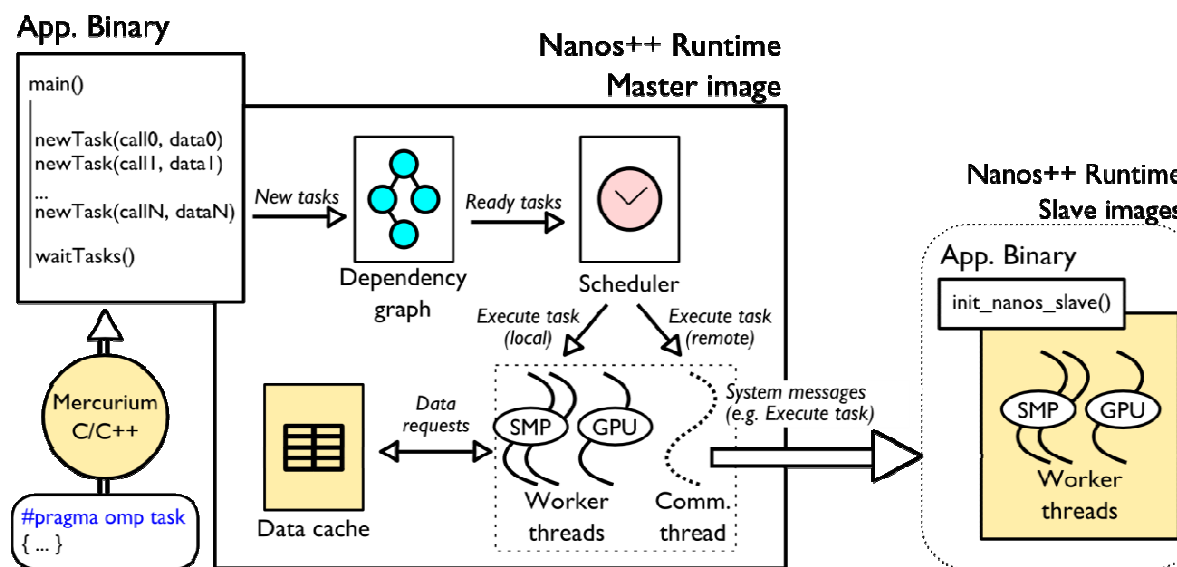
- Task generation
- Data dependence analysis
- Task scheduling



StarSs → OmpSs → Runtime

Structure behaviour: coherence support

- Different address spaces managed with:
 - A hierarchical directory
 - A software cache per each:
 - Cluster node
 - GPU
- Data transfers between different memory spaces only when needed
 - Write-through
 - Write-back



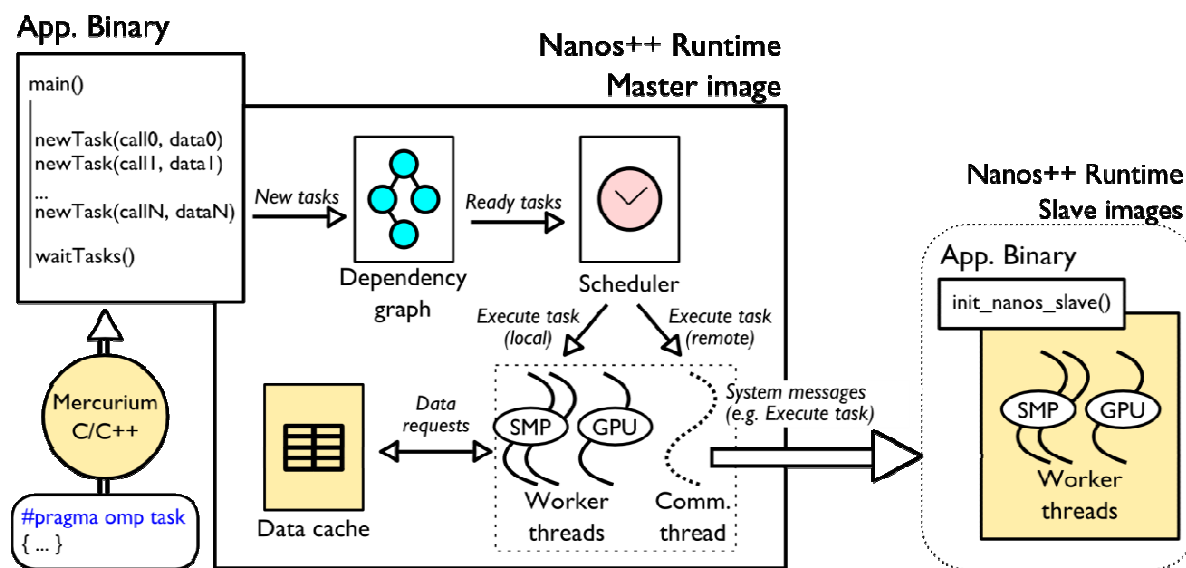
StarSs → OmpSs → Runtime

Structure behaviour: clusters

- One runtime instance per node
 - One master image
 - N-1 worker images
- Low level communication through active messages
- Tasks generated by master
 - Tasks executed by worker threads in the master
 - Tasks delegated to slave nodes through the communication thread

- Remote task execution:

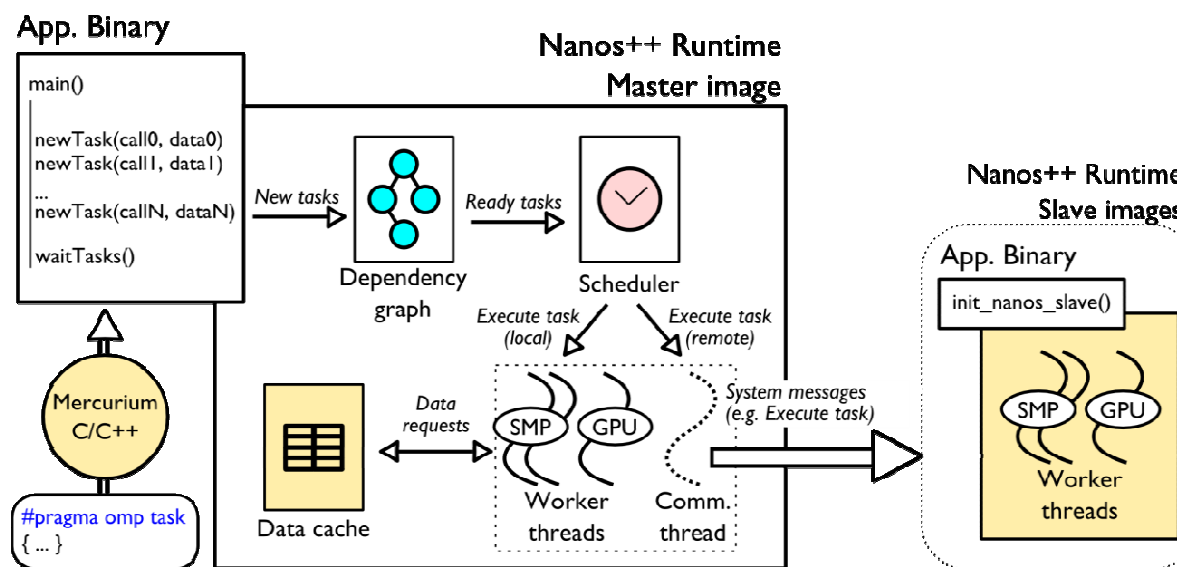
- Data transfer (if necessary)
- Overlap of computation with communication
- Task execution
 - Local scheduler



StarSs → OmpSs → Runtime

Structure behaviour: GPUs

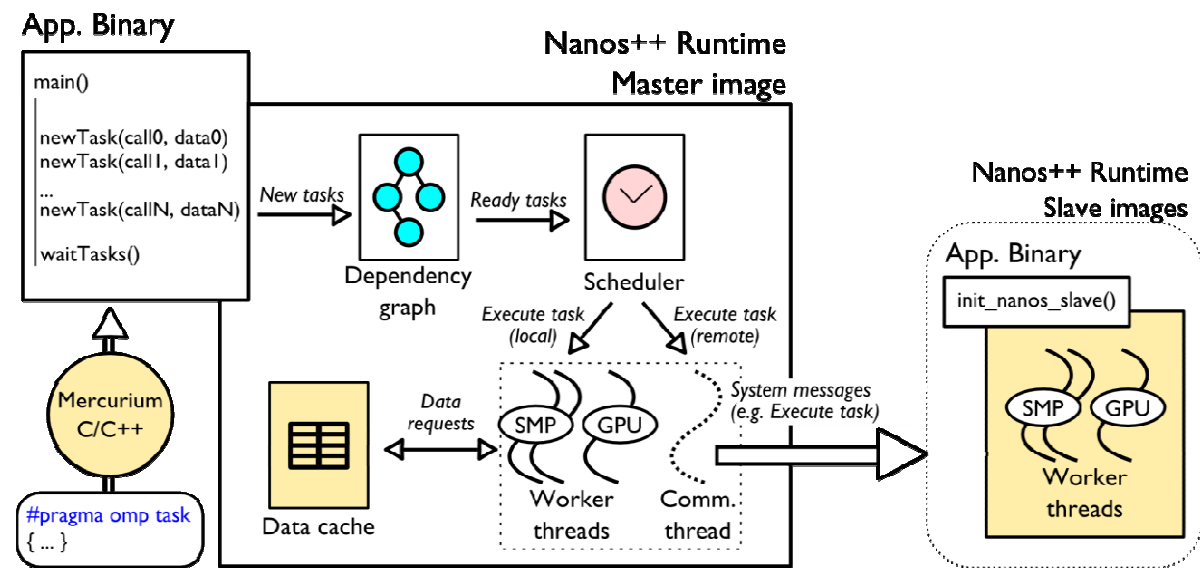
- Automatic handling of Multi-GPU execution
- Transparent data-management on GPU side (allocation, transfers, ...) and synchronization
- One manager thread in the host per GPU. Responsible for:
 - Transferring data from/to GPUs
 - Executing GPU tasks
 - Synchronization
- Overlap of computation and communication
- Data pre-fetch



StarSs → OmpSs → Runtime

Structure behaviour: clusters of GPUs

- Composes previous approaches
- Supports for heterogeneity and hierarchy:
 - Application with homogeneous tasks: SMP or GPU
 - Applications with heterogeneous tasks: SMP and GPU
 - Applications with hierarchical and heterogeneous tasks:
 - I.e., coarser grain SMP tasks
 - Internally generating GPU tasks

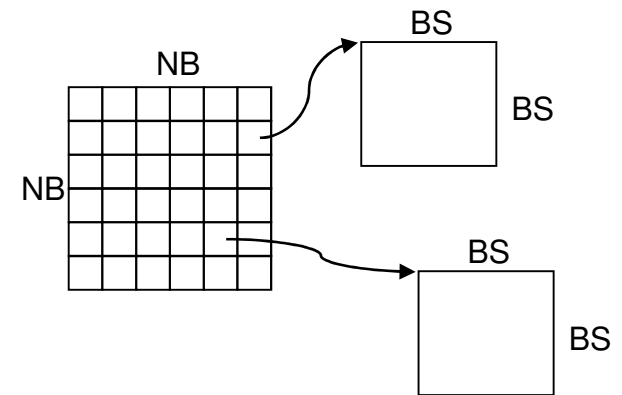


StarSs → OmpSs → Examples

MxM on matrix stored by blocks

```
int main (int argc, char **argv) {
    int i, j, k;
    ...
    initialize(A, B, C);

    for (i=0; i < NB; i++)
        for (j=0; j < NB; j++)
            for (k=0; k < NB; k++)
                mm_tile( C[i][j], A[i][k],
                        B[k][j]);
}
```



Will work on matrices of
any size

Will work on any number of
cores/devices

```
#pragma omp task input ([BS][BS]A, [BS][BS]B) \
inout ([BS][BS]C)
static void mm_tile ( float C[BS][BS],
                     float A[BS][BS],
                     float B[BS][BS]) {

    int i, j, k;

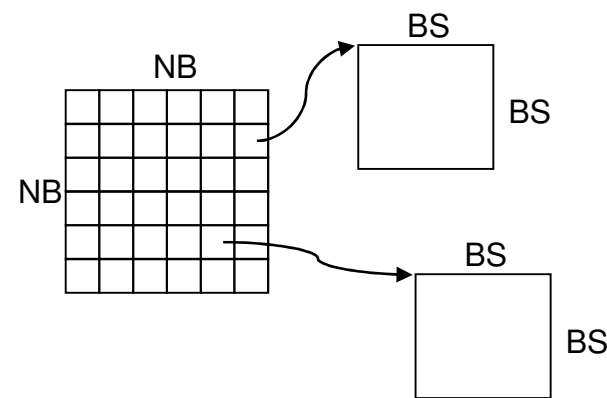
    for (i=0; i < BS; i++)
        for (j=0; j < BS; j++)
            for (k=0; k < BS; k++)
                C[i][j] += A[i][k] * B[k][j];
}
```

StarSs → OmpSs → Examples

MxM on GPUs using CUBLAS kernel

```
int main (int argc, char **argv) {
    int i, j, k;
    ...
    initialize(A, B, C);

    for (i=0; i < NB; i++)
        for (j=0; j < NB; j++)
            for (k=0; k < NB; k++)
                mm_tile( C[i][j], A[i][k],
                        B[k][j]);
}
```

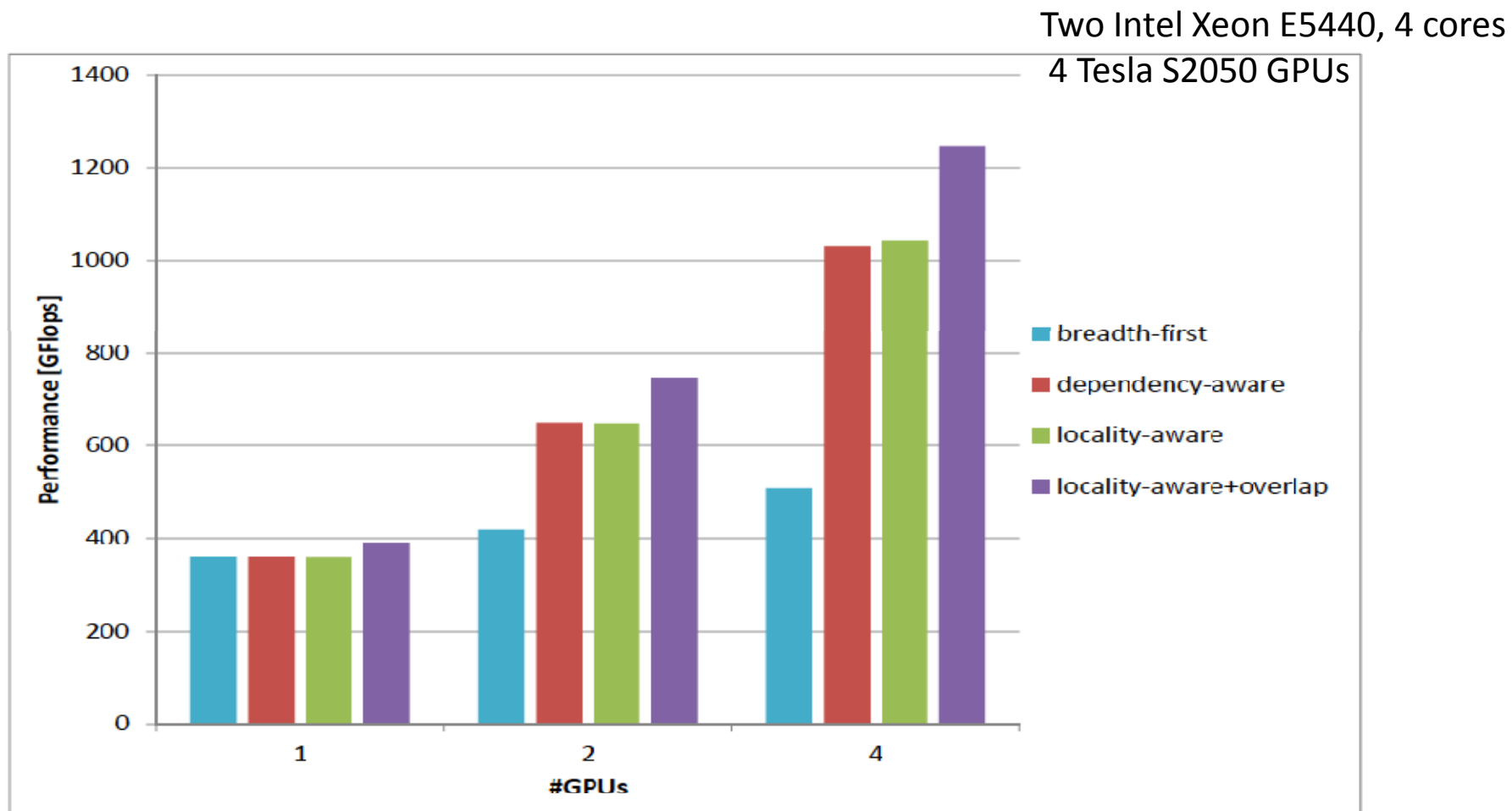


```
#pragma omp target device (cuda) copy_deps
#pragma omp task input([BS][BS]A, [BS][BS]B, BS)\
    inout([BS][BS]C)
void mm_tile(float *A, float *B, float *C, int BS)
{
    unsigned char nt = 'N';
    float sone = 1.0, smone = -1.0;
    float *d_A, *d_B, *d_C;

    cublasSgemm(nt, nt, nt, BS, BS, smone, A,
                BS, B, BS, sone, C, BS);
}
```

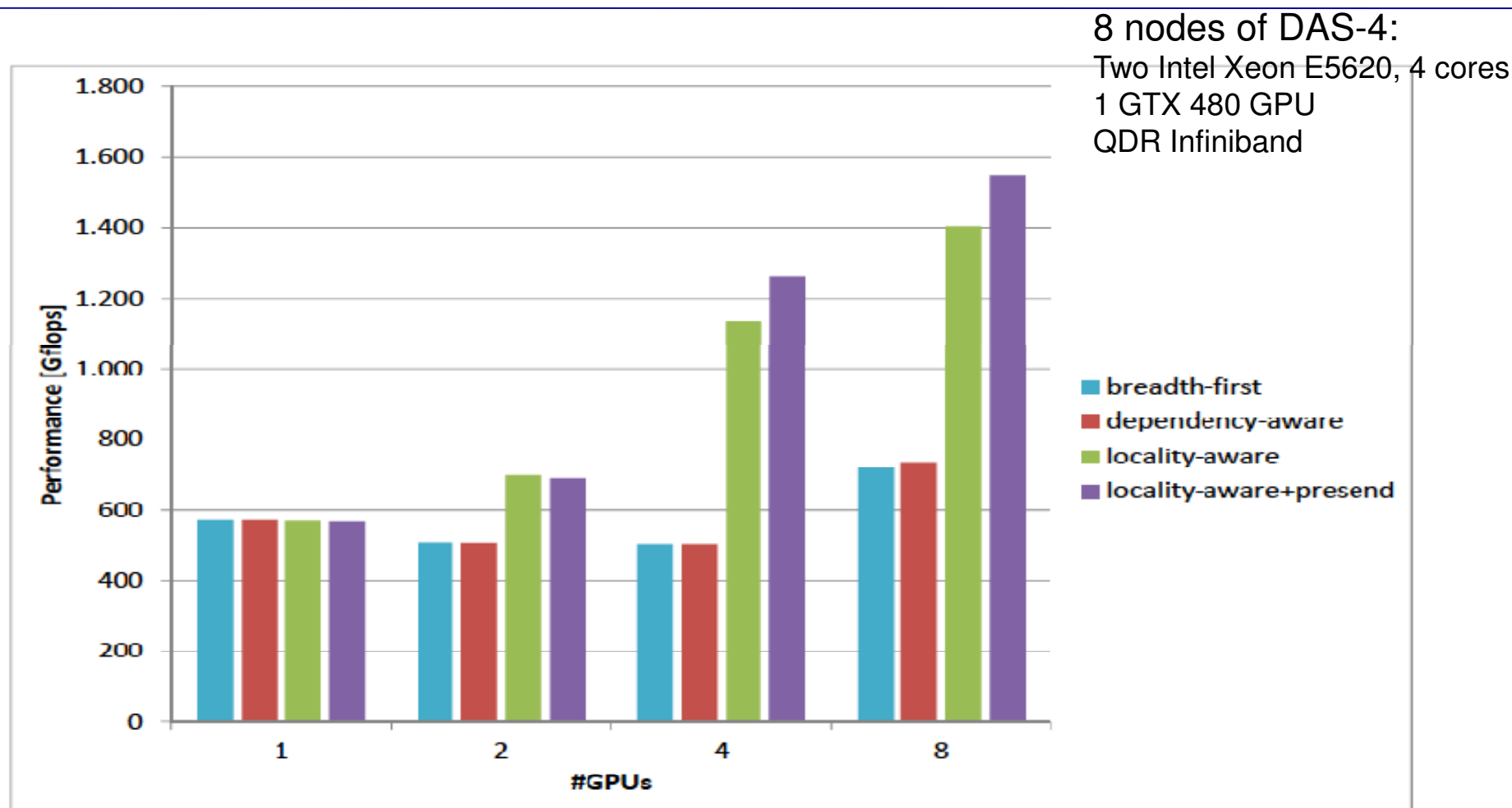
StarSs → OmpSs → Examples

MxM performance on multi-GPU



StarSs → OmpSs → Examples

MxM performance on cluster of GPUs



StarSs → OmpSs → Examples

Cholesky: Block matrix storage on GPU

- Source code independent of # devices

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



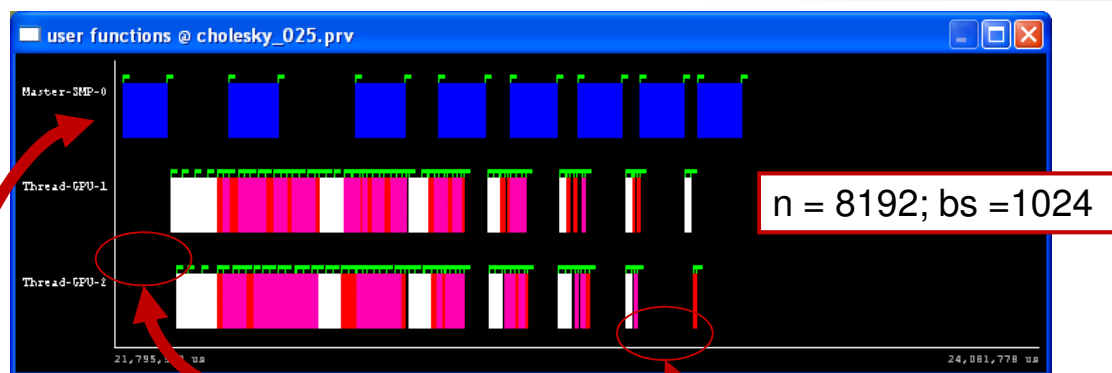
Spotrf:
Slow task @ GPU
In critical path (scheduling problem)

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

StarSs → OmpSs → Examples

Cholesky: Heterogeneous execution

- `spotrf` more efficient at CPU
- Overlap between CPU and GPU



Late start

Lack of overlap

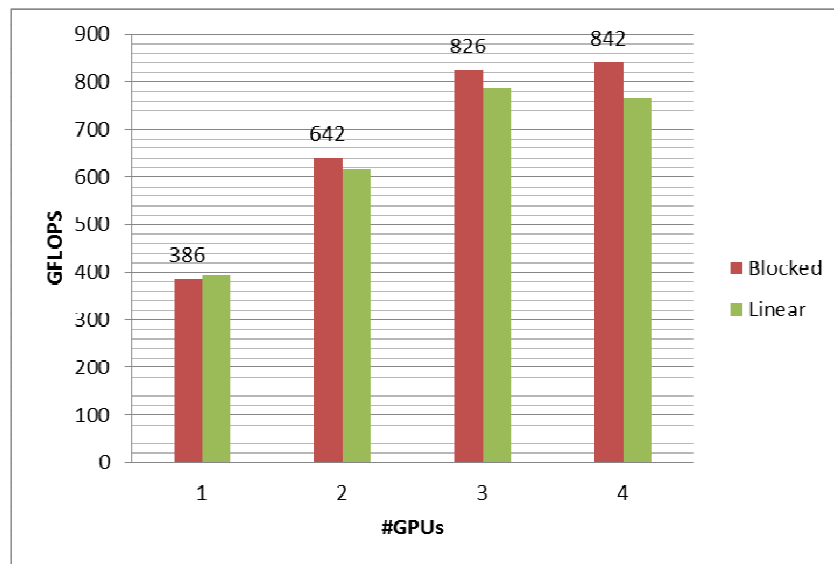
```
#pragma omp target device (smp) copy_deps
#pragma omp task inout([BS][BS]A)
void spotrf_tile(float *A, int BS)
{
    long INFO;
    char L = 'L';

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


StarSs → OmpSs → Examples

Cholesky performance

- Matrixsize: 16K x 16K
- Block size: 2K x 2K
- Storage: Blocked / contiguous
- Tasks:
 - spotrf: MAGMA
 - trsm, syrk, gemm: CUBLAS



Further information

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 - www.bsc.es

Farewell

Thanks for your attention!*



*Hope you enjoyed this as much as Antibes-Sophia's beach