LMU LUDWIG-MAXIMILIANS-UNIVERSITÄT MÜNCHEN

HLRS High-Performance Computing Center | Stuttgart

DASH: A C++ PGAS Library for Distributed Data Structures and Parallel Algorithms

www.dash-project.org

Karl Fürlinger

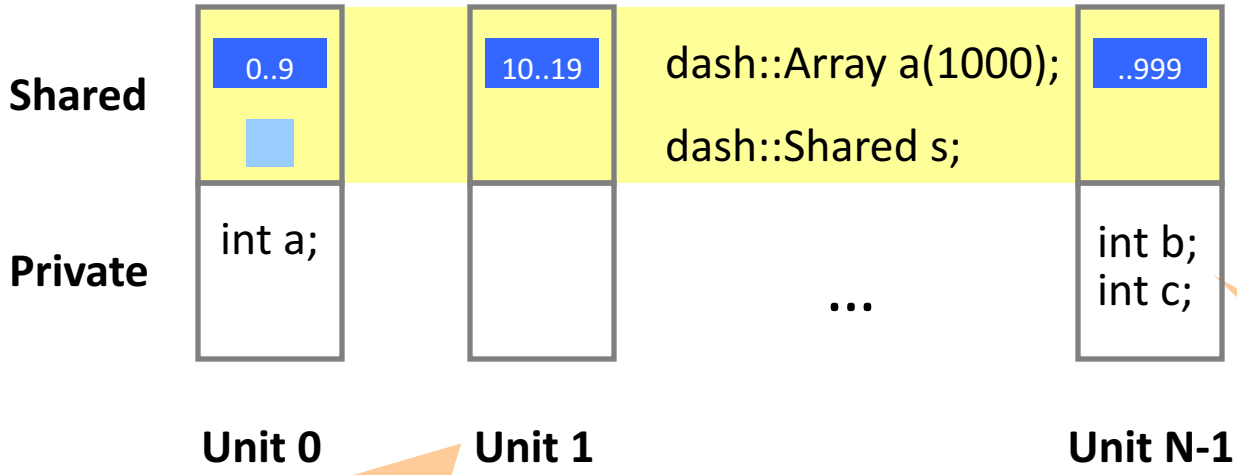
Ludwig-Maximilians-Universität München

José Gracia

High Performance Computing Center Stuttgart (HLRS)

DASH - Overview

- DASH is a C++ template library that offers
  - Distributed data structures and parallel algorithms
  - A complete PGAS (part. global address space) programming system without a custom (pre-)compiler
- Terminology

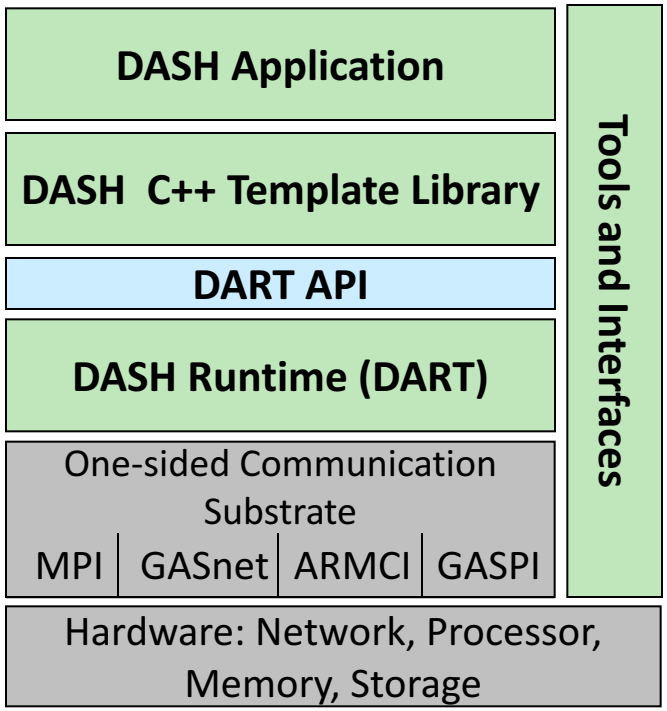


Shared data: managed by DASH in a virtual global address space

Private data: managed by regular C/C++ mechanisms

Unit: The individual participants in a DASH program, usually full OS processes.

DASH Project Structure



	"HA" Phase I (2013-2015)	"Smart-DASH" Phase II (2016-2018)
LMU Munich	Project management, C++ template library	Project management, C++ tempalte library, DASH data dock
TU Dresden	Libraries and interfaces, tools support	Smart data structures, resilience
HLRS Stuttgart	DART runtime	DART runtime
KIT Karlsruhe	Application case studies	
IHR Stuttgart		Smart deployment, Application case studies

www.dash-project.org

SPPEXA

DASH is one of 16 SPPEXA projects

DASH Geography

DART: The DASH Runtime

- The DART Interface
  - Plain-C based interface (“dart.h”)
  - Follows the SPMD execution model
  - Provides global memory abstraction and global pointers
  - Defines one-sided access operations (put and get) and synchronization operations

- Several implementations
  - **DART-SHMEM**: shared-memory based implementation
  - **DART-CUDA:** supports GPUs, based on DART-SHMEM
  - **DART-GASPI**: Initial implementation using GASPI
  - **DART-MPI**: MPI-3 RMA based “workhorse” implementation

Hello World in DASH


```
#include <iostream>
#include <libdash.h>

using namespace std;

int main(int argc, char* argv[])
{
  pid_t pid; char buf[100];

  dash::init(&argc, &argv);
  auto myid = dash::myid();
  auto size = dash::size();
  gethostname(buf, 100); pid = getpid();

  cout<<"'Hello world' from unit "<<myid<<
    " of "<<size<<" on "<<buf<<" pid="<<pid<<endl;

  dash::finalize();
}
```

Initialize the programming environment

Determine total number of units and our own unit ID

Print message. Note SPMD model, similar to MPI.

```
$ mpirun -n 4 ./hello
'Hello world' from unit 2 of 4 on nuc03 pid=30964
'Hello world' from unit 0 of 4 on nuc01 pid=25422
'Hello world' from unit 3 of 4 on nuc04 pid=32243
'Hello world' from unit 1 of 4 on nuc02 pid=26304
```

Distributed Data Structures

- DASH offers distributed data structures
  - Support for flexible data distribution schemes
  - Example: dash::Array<T>

```
dash::Array<int> arr(100);

if( dash::myid()==0 ) {
  for( auto i=0; i<arr.size(); i++ )
    arr[i]=i;
}

arr.barrier();
if(dash::myid()==1 ) {
  for( auto el: arr )
    cout<<(int)el<<" ";
  cout<<endl;
}
```

DASH global array of 100 integers, distributed over all units, default distribution is BLOCKED

Unit 0 writes to the array using the global index i. Operator [] is overloaded for the dash::Array.

Unit 1 executes a range-based for loop over the DASH array

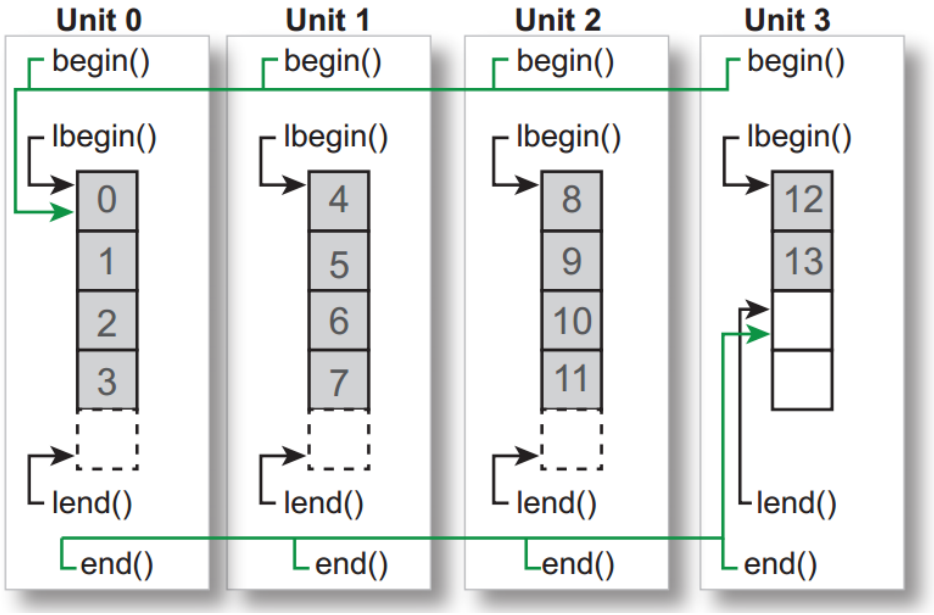
```
$ mpirun -n 4 ./array
0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19
20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36
37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53
54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70
71 72 73 74 75 76 77 78 79 80 81 82 83 84 85 86 87
88 89 90 91 92 93 94 95 96 97 98 99
```

Global-view and Local-view in DASH

- DASH supports both *global-view* and *local-view* semantics

	Global-view	Local-view	LV shorthand
range begin	arr.begin()	arr.local.begin()	arr.lbegin()
range end	arr.end()	arr.local.end()	arr.lend()
# elements	arr.size()	arr.local.size()	arr.lsize()
element access	arr[glob_idx]	arr.local[loc_idx]	

- Example
  - dash::Array with 14 elements, distributed over 4 units
  - default distribution: BLOCKED
  - Blocksize = ceil(14/4)=4



Accessing Local Data

- Access to the local portion of the data is exposed through a local-view proxy object (.local)

```
dash::Array<int> arr(100);

for( auto i=0; i<arr.lsize(); i++ )
  arr.local[i]=dash::myid();

arr.barrier();
if(dash::myid()==dash::size()-1 ) {
  for( auto el: arr )
    cout<<(int)el<<" ";
  cout<<endl;
}
```

.lsize() is short hand for .local.size() and returns the number of local elements

.local is a *proxy object* that represents the part of the data that is local to a unit.

```
$ mpirun -n 4 ./array
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1 1 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
2 2 2 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3
3 3 3 3
```

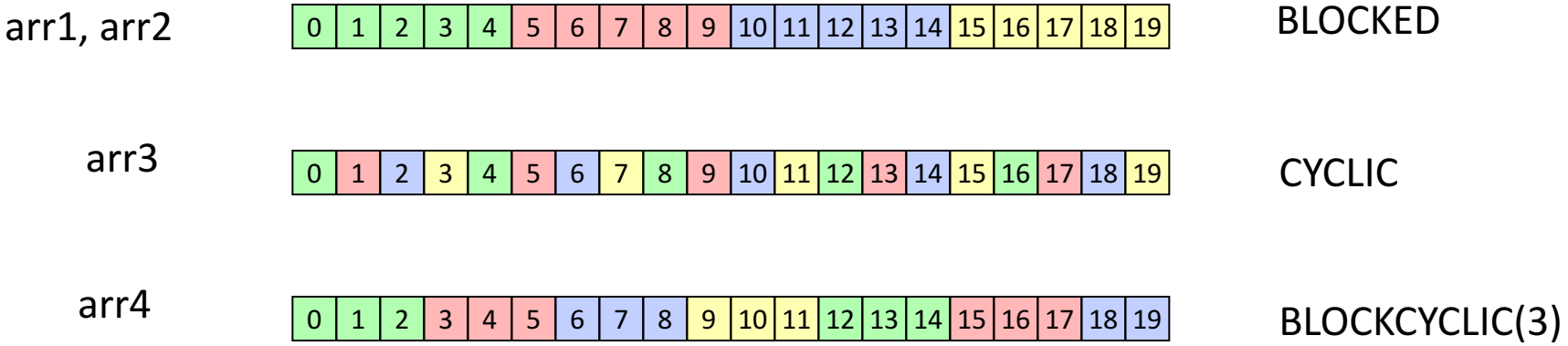
Data Distribution Patterns

- The data distribution pattern is configurable

```
dash::Array<int> arr1(20); // default: BLOCKED

dash::Array<int> arr2(20, dash::BLOCKED)
dash::Array<int> arr3(20, dash::CYCLIC)
dash::Array<int> arr4(20, dash::BLOCKCYCLIC(3))
```

- Assume 4 units

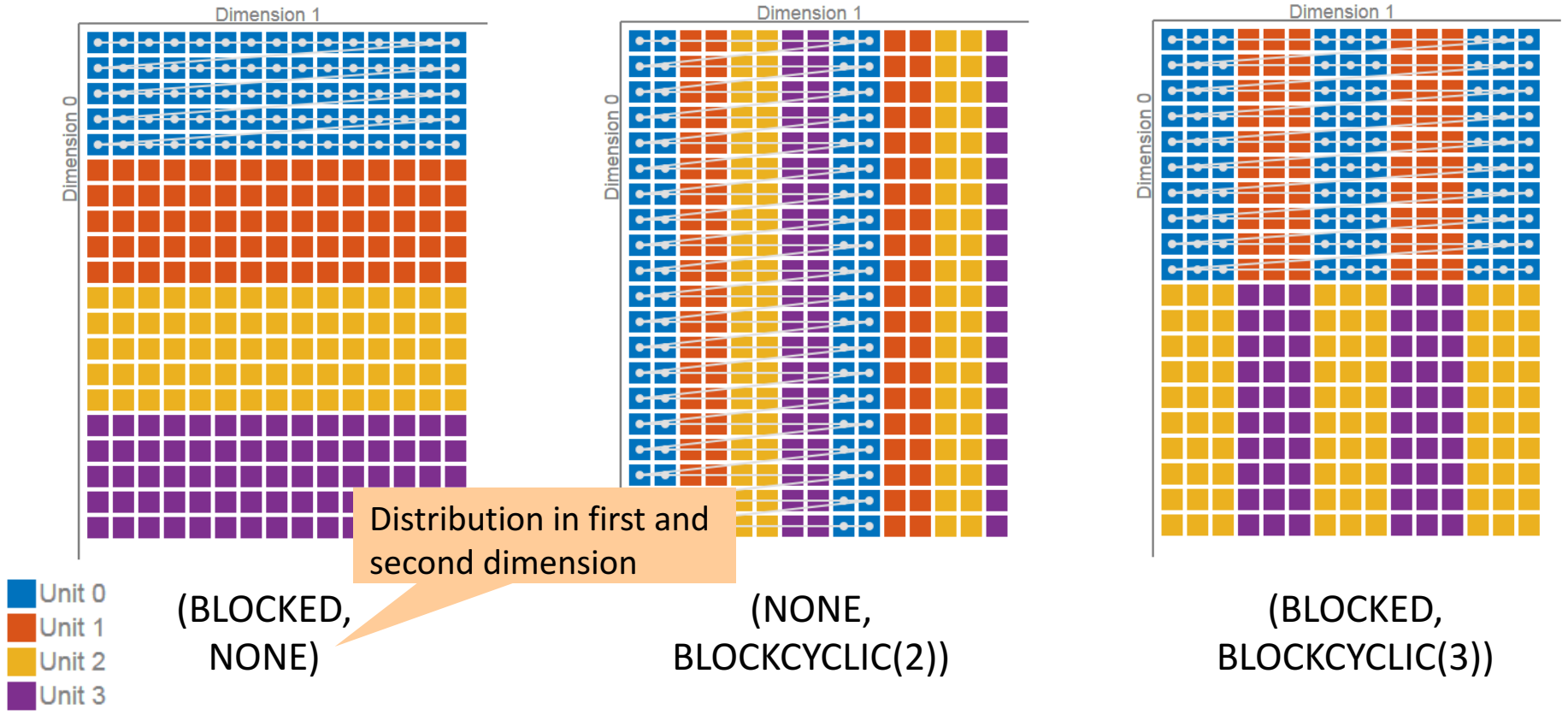


Multidimensional Data Distribution (1)

- dash::Pattern<N> specifies N-dim data distribution
  - Blocked, cyclic, and block-cyclic in multiple dimensions

Pattern<2>(20, 15)

Extent in first and second dimension



Distribution in first and second dimension

(BLOCKED, NONE)

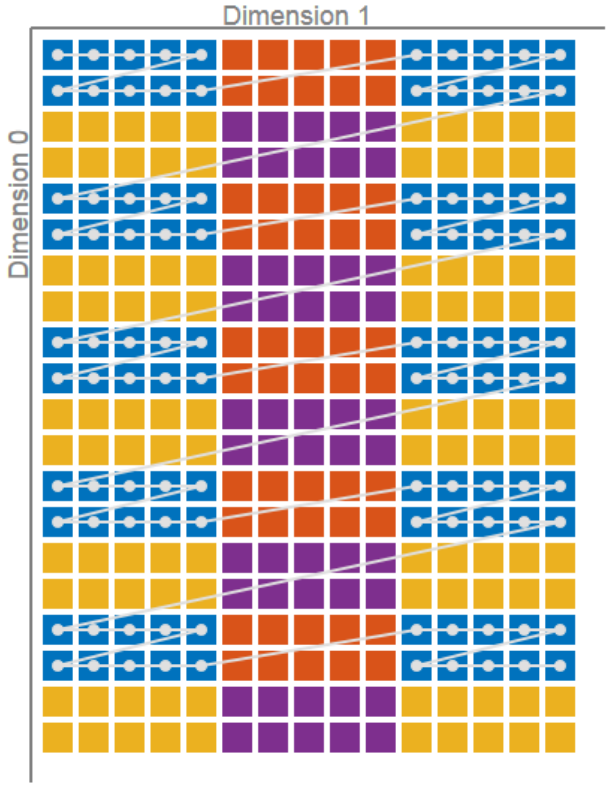
(NONE, BLOCKCYCLIC(2))

(BLOCKED, BLOCKCYCLIC(3))

Multidimensional Data Distribution (2)

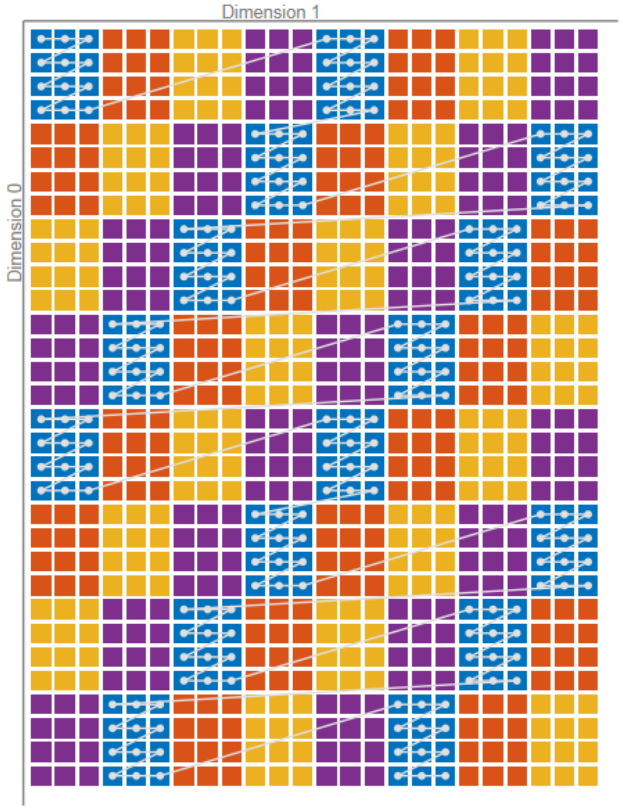
- Tiled data distribution and tile-shifted distribution

TilePattern<2>(20, 15)



(TILE(2), TILE(5))

ShiftTilePattern<2>(32, 24)

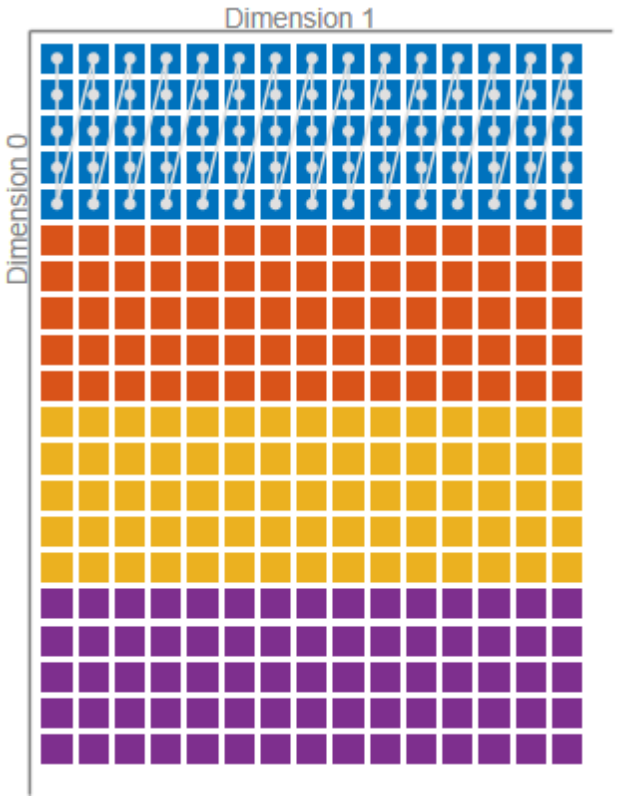


(TILE(4), TILE(3))

Multidimensional Data Distribution (3)

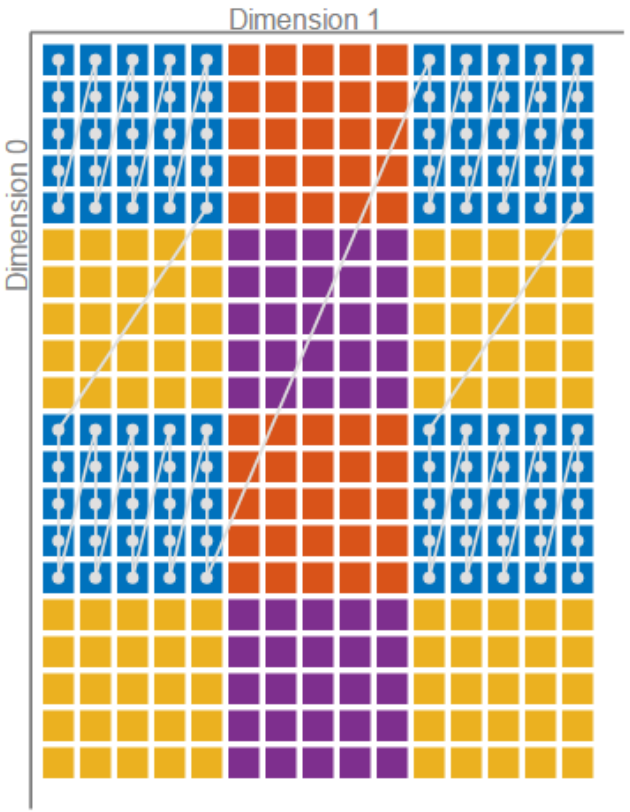
- Row-major and column-major storage

Pattern<2, COL_MAJOR>(20, 15)



(BLOCKED, NONE)

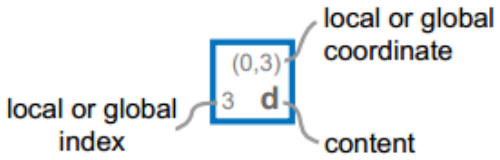
TilePattern<2, COL_MAJOR>(20, 15)



(TILE(5), TILE(5))

DASH NArray Global View and Local View

- Local view works similar to contiguous memory



Global View

(0,0) 0 a	(0,1) 1 b	(0,2) 2 c	(0,3) 3 d
(1,0) 4 e	(1,1) 5 f	(1,2) 6 g	(1,3) 7 h
(2,0) 8 i	(2,1) 9 j	(2,2) 10 k	(2,3) 11 l
(3,0) 12 m	(3,1) 13 n	(3,2) 14 o	(3,3) 15 p
(4,0) 16 q	(4,1) 17 r	(4,2) 18 s	(4,3) 19 t
(5,0) 20 u	(5,1) 21 v	(5,2) 22 w	(5,3) 23 x
(6,0) 24 y	(6,1) 25 z	(6,2) 26 A	(6,3) 27 B

```
dash::NArray<char, 2> mat(7, 4);
cout << mat(2, 1) << endl;  // prints 'j'

if(dash::myid()==0 ) {
  cout << mat.local(2, 1) << endl; // prints 'z'
}
```

Local View (Unit 0)

(0,0) 0 a	(0,1) 1 b	(0,2) 2 c	(0,3) 3 d
(1,0) 4 m	(1,1) 5 n	(1,2) 6 o	(1,3) 7 p
(2,0) 8 y	(2,1) 9 z	(2,2) 10 A	(2,3) 11 B

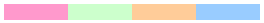
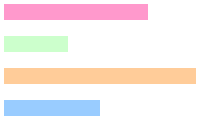
Local View (Unit 1)

(0,0) 0 e	(0,1) 1 f	(0,2) 2 g	(0,3) 3 h
(1,0) 4 q	(1,1) 5 r	(1,2) 6 s	(1,3) 7 t

Local View (Unit 2)

(0,0) 0 i	(0,1) 1 j	(0,2) 2 k	(0,3) 3 l
(1,0) 4 u	(1,1) 5 v	(1,2) 6 w	(1,3) 7 x

DASH Distributed Data Structures Overview

Container	Description	Data distribution
Array<T>	1D Array 	static, configurable
NArray<T, N> **Matrix**<T,N>	N-dim. Array 	static, configurable
Shared<T>	Shared scalar 	fixed (at 0)
Map*<T> **List*** <T>	Variable-size, locally indexed container 	manual
CoArray*<T>	Similar to CAF 	uniform

(*) Under construction

Other DASH Features (1)

- STL concept compatibility
  - Containers, algorithms, iterators, ranges but generalized to the distributed and parallel case
  - Global references, global iterators, global ranges, …
  - Makes it easier for programmers to get started
  - Ensures interoperability with STL algorithms

```
// use STL algorithm to work on local part of data
// arr.lbegin() is short for arr.local.begin()
std::fill(arr.lbegin(), arr.lend();

// use DASH algorithm to work on whole array in parallel
dash::fill(arr.begin(), arr.end();
```

Other DASH Features (2)

- Asynchronous communication
  - Important to overlap communication and computation

```
// async. bulk transfer
auto fut = dash::copy_async(block.begin(), block.end(),
                            local_ptr);
...
fut.wait();

// async element access
int i = arr.async[33];
```

- Parallel I/O
  - Pattern is stored as meta info and can be restored from HDF5

```
// DASH HDF streams mimic C++ streams interface
dash::io::HDFOutputStream os("outfile.hdf5");
os << dash::io::HDF5Dataset("data") << arr1 ;
```

DASH Example: S(R)UMMA Algorithm

- Block matrix-matrix mulitplication algorithm with block prefetching

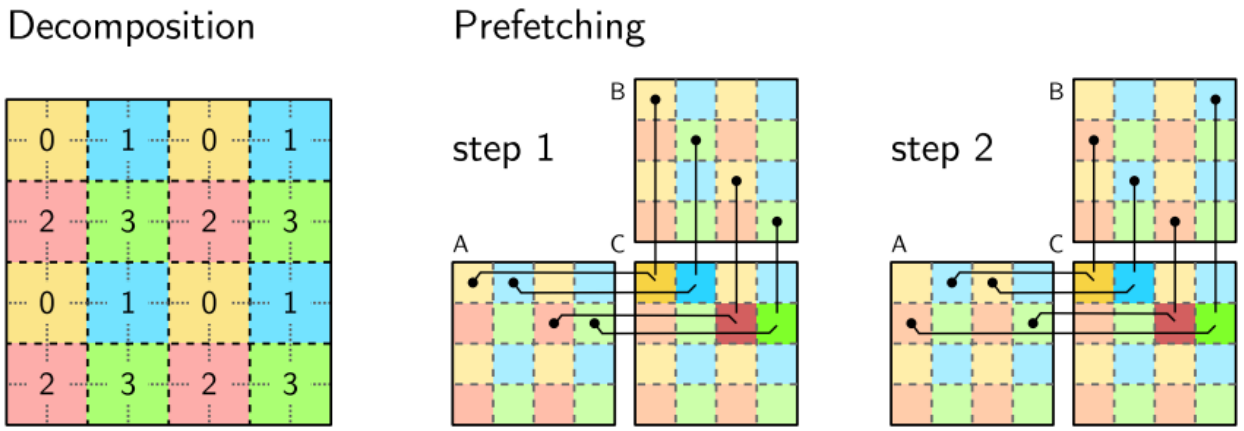


Image source: [1]

```
while(!done) {
  blk_a = ...
  blk_b = ...
  // prefetch
  auto get_a = dash::copy_async(blk_a.begin(), blk_a.end(), lblk_a_get);
  auto get_b = dash::copy_async(blk_b.begin(), blk_b.end(), lblk_b_get);
  // local DGEMM
  dash::multiply(lblk_a_comp, lblk_b_comp, lblk_c_comp);
  // wait for transfer to finish
  get_a.wait(); get_b.wait();
  // swap buffers
  swap(lblk_a_get, lblk_a_comp);  swap(lblk_b_get, lblk_b_comp);
}
```

DGEMM on a Single Shared Memory Node

- LRZ SuperMUC, phase 2: Haswell EP, 1.16 Tflop/sec peak

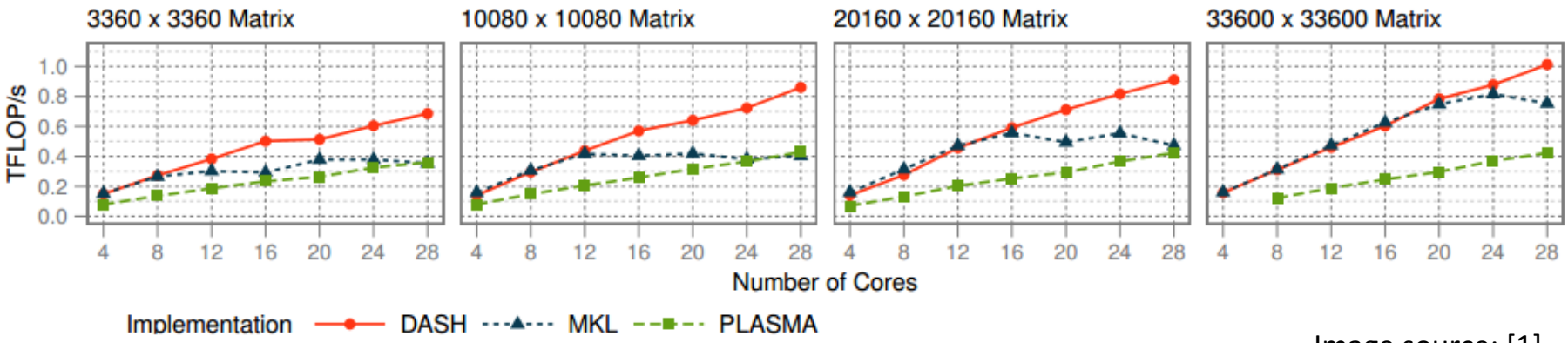


Image source: [1]

- DASH: Multi-process, using one-sided communication and single-threaded MKL
- MKL: Multithreaded, using OpenMP
- PLASMA: Multithreaded tile-algorithms on top of sequential BLAS

[1] T. Fuchs, K. Fürlinger: A Multi-Dimensional Distributed Array Abstraction for PGAS, *HPCC 2016*

PDGEMM: DASH vs. ScaLAPACK Multinode

- Strong scaling on SuperMUC (57344 × 57344 matrix)

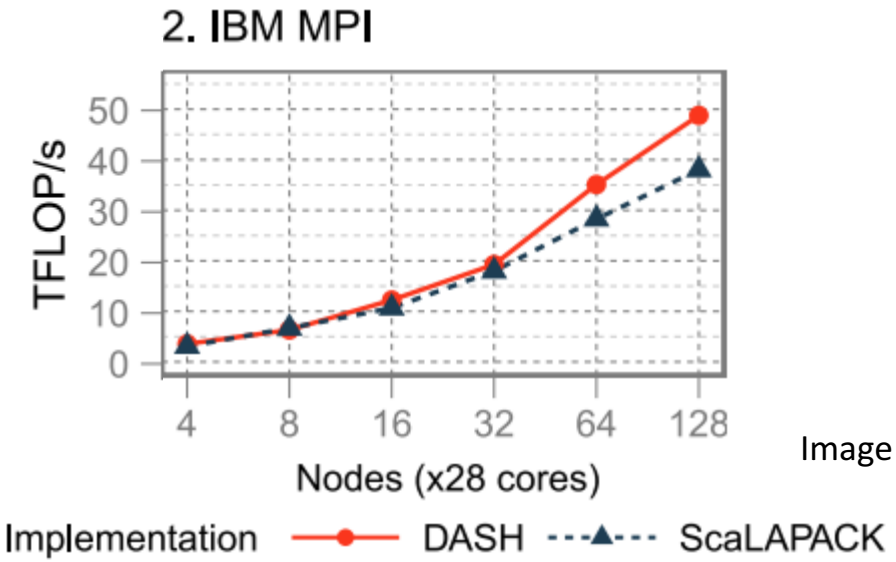


Image source: [1]

- Trace: Overlapping communication and computation

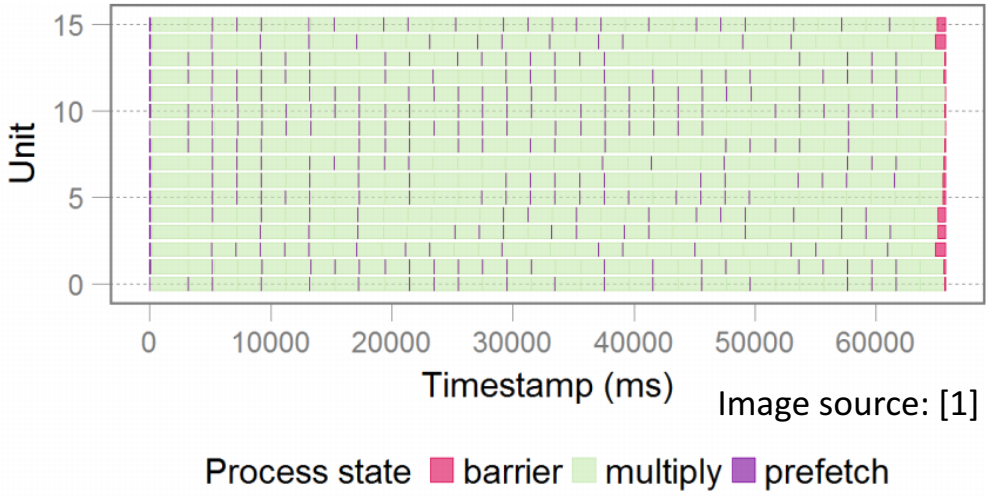


Image source: [1]

Porting LULESH (Work in Progress)

- LULESH: A shock-hydrodynamics mini-application

```
class Domain // local data
{
private:
std::vector<Real_t> m_x;
// many more...

public:
Domain() { // C'tor
  m_x.resize(numNodes);
  //...
}

Real_t& x(Index_t idx) {
  return m_x[idx];
}
};
```

MPI Version

```
class Domain // global data
{
private:
dash::NArray<Real_t, 3> m_x;
// many more...

public:
Domain() { // C'tor
  dash::Pattern<3> nodePat(
     nx()*px(), ny()*py(), nz()*pz(),
     BLOCKED, BLOCKED, BLOCKED);
  m_x.allocate(nodePat);
}

Real_t& x(Index_t idx) {
  return m_x.lbegin()[idx];
}
};
```

DASH Version

Porting LULESH (goals)

- Remove limitations of MPI domain decomposition
  - Cubic number of MPI processes only (P x P x P)
  - Cubic per-processor grid
  - DASH allows any P x Q x R configuration

- Avoid replication, manual index calculation, bookkeeping

```
if (rowMin | rowMax) {
   /* ASSUMING ONE DOMAIN PER RANK, CONSTANT BLOCK SIZE HERE */
   int sendCount = dx * dz ;

   if (rowMin) {
      destAddr = &domain.commDataSend[pmsg * maxPlaneComm] ;
      for (Index_t fi=0; fi<xferFields; ++fi) {
         Domain_member src = fieldData[fi] ;
         for (Index_t i=0; i<dz; ++i) {
            for (Index_t j=0; j<dx; ++j) {
               destAddr[i*dx+j] = (domain.*src)(i*dx*dy + j) ;
            }
         }
         destAddr += sendCount ;
      }
      destAddr -= xferFields*sendCount ;

      MPI_Isend(destAddr, xferFields*sendCount, baseType,
                myRank - domain.tp(), msgType,
                MPI_COMM_WORLD, &domain.sendRequest[pmsg]) ;
      ++pmsg ;
```

implicit assumptions

manual index calculation

manual bookkeeping

Replicated about 80 times

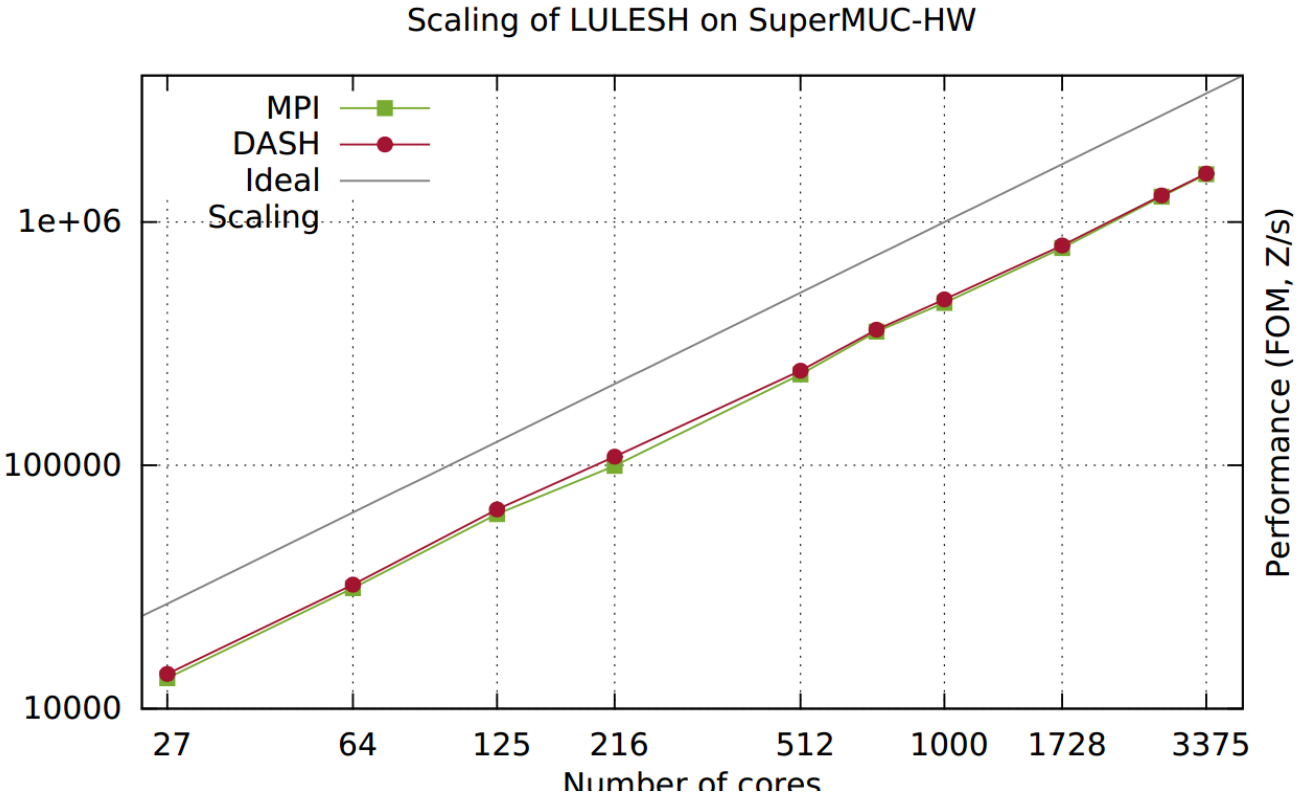
Porting LULESH (options)

- DASH can be integrated in existing applications and allows for incremental porting

- Porting options:
  1. Port data structures, but keep communication as-is (using MPI two-sided)
     - Can use HDF5 writer for checkpointing
  2. Keep explicit packing code but use one-sided put instead of MPI_Irecv/MPI_Isend
     - Similar to UPC++ version, potential performance benefit
  3. Use DASH for communication directly (TBD)
     - auto halo = …; dash::swap(halo) …
     - less replicated code, more flexibility
  4. Use dash::HaloNArray (TBD)
     - N-dimensional array with built-in halo areas

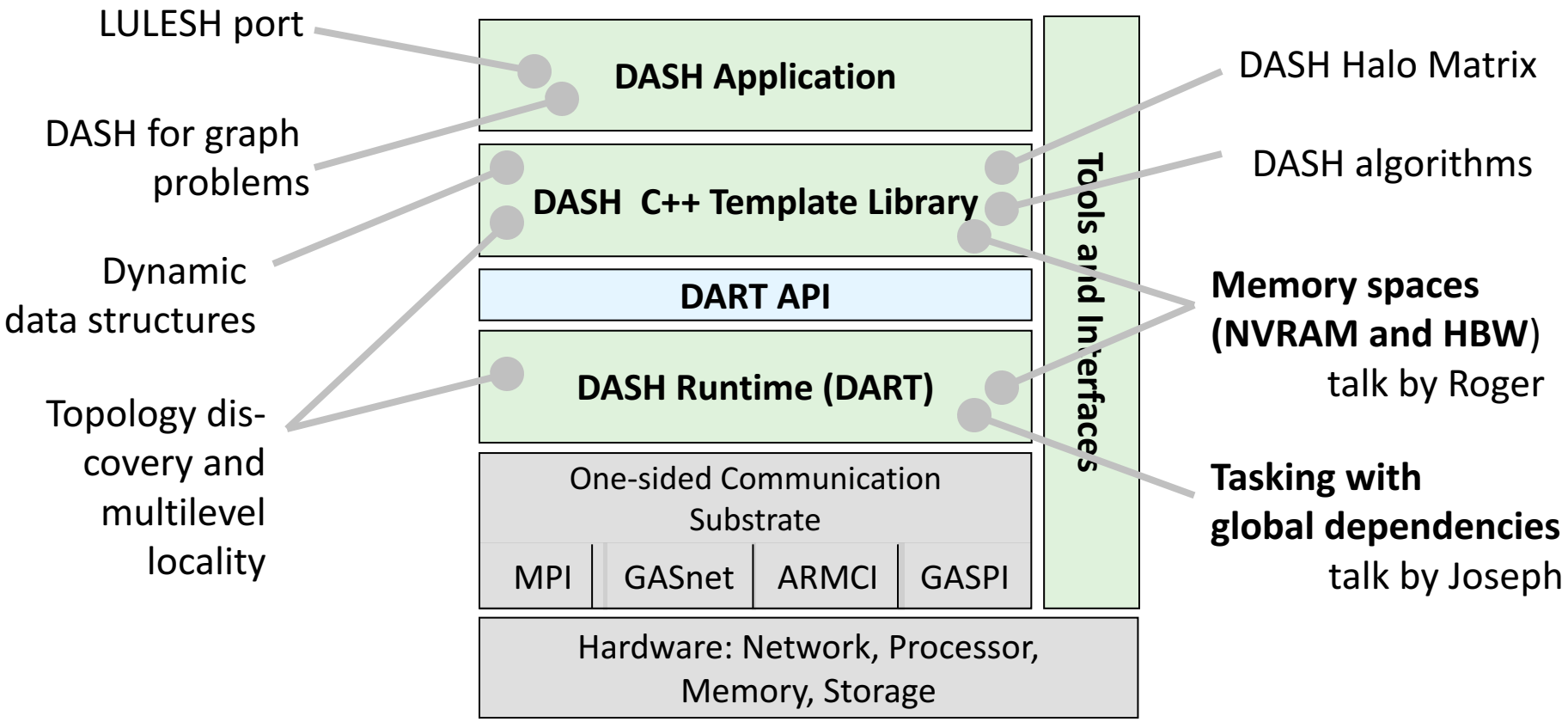
Performance of the DASH Version (using put)

- Performance and scalability (weak scaling) of LULESH, implemented in MPI and DASH



[2] Karl Fürlinger, Tobias Fuchs, and Roger Kowalewski. **DASH: A C++ PGAS Library for Distributed Data Structures and Parallel Algorithms**. In *Proceedings of the 18th IEEE International Conference on High Performance Computing and Communications (HPCC 2016)*. Sydney, Australia, December 2016. accepted for publication.

DASH: On-going and Future Work



Summary

- DASH is
  - A complete data-oriented PGAS programming system (i.e., entire applications can be written in DASH),
  - A library that provides distributed data structures with STL-like semantics,
  - Interoperable with MPI and OpenMP (hybrid applications, incremental transition).

- DASH aims at
  - Running at the largest supercomputers (Linux clusters, CRAY, IBM, K-Computer),
  - Paying negligible overhead for high-level abstractions thus increasing user productivity.

Acknowledgements

- Funding

DFG Deutsche Forschungsgemeinschaft

("HA" and "Smart-DASH")

Bundesministerium für Bildung und Forschung

("MEPHISTO")

- The DASH Team

  T. Fuchs (LMU), **R. Kowalewski (LMU),** D. Hünich (TUD), A. Knüpfer (TUD), **J. Gracia (HLRS),** C. Glass (HLRS), H. Zhou (HLRS), K. Idrees (HLRS), **J. Schuchart (HLRS),** D. Rubio (IHR), F. Mößbauer (LMU), K. Fürlinger (LMU)

- More Information
  - http://www.dash-project.org/
  - https://github.com/dash-project/dash/