703650 VO Parallel Systems WS2019/2020
Expanding Horizons: Additional Programming Models

Philipp Gschwandtner

Overview

- general discussion on programming models
  - characteristics
  - categorization
- examples
  - Pthreads, C++ STL threads, TBB, HPX, AllScale, OpenCL/CUDA, SYCL, Chapel, X10, Matlab

Motivation

- functional portability
  - write once, run anywhere
  - guaranteed by MPI, OpenMP and alike – but is there more?

- performance portability
  - move optimization away from the program into the toolchain
  - enables automatic optimization

- "separation of concerns"
  - domain science experts should focus on their domain, not deal with HPC specifics
    - e.g. I should add memory padding for optimal cache usage?
    - What's the cache line size? What's a cache?
  - computer science experts should know computer science

A Simple Loop

```
// increment every element of
// an array with values 0-9
for(int i = 0; i < 10; i++) {
  A[i] += i;
}
```

A Simple Parallel Loop

```
int rank, size;
MPI_Com_rank(COM,&rank)
MPI_Com_size(COM,&size)
int p = 10/size;
MPI_Scatter(A,...)
for(int i = p*rank; i < p*rank+p; i++) {
  A[i] += i;
}
MPI_Gather(A,...)
```

end of iterator range

start of iterator range

pfor operator
(generic function)

body function
(C++ lambda)

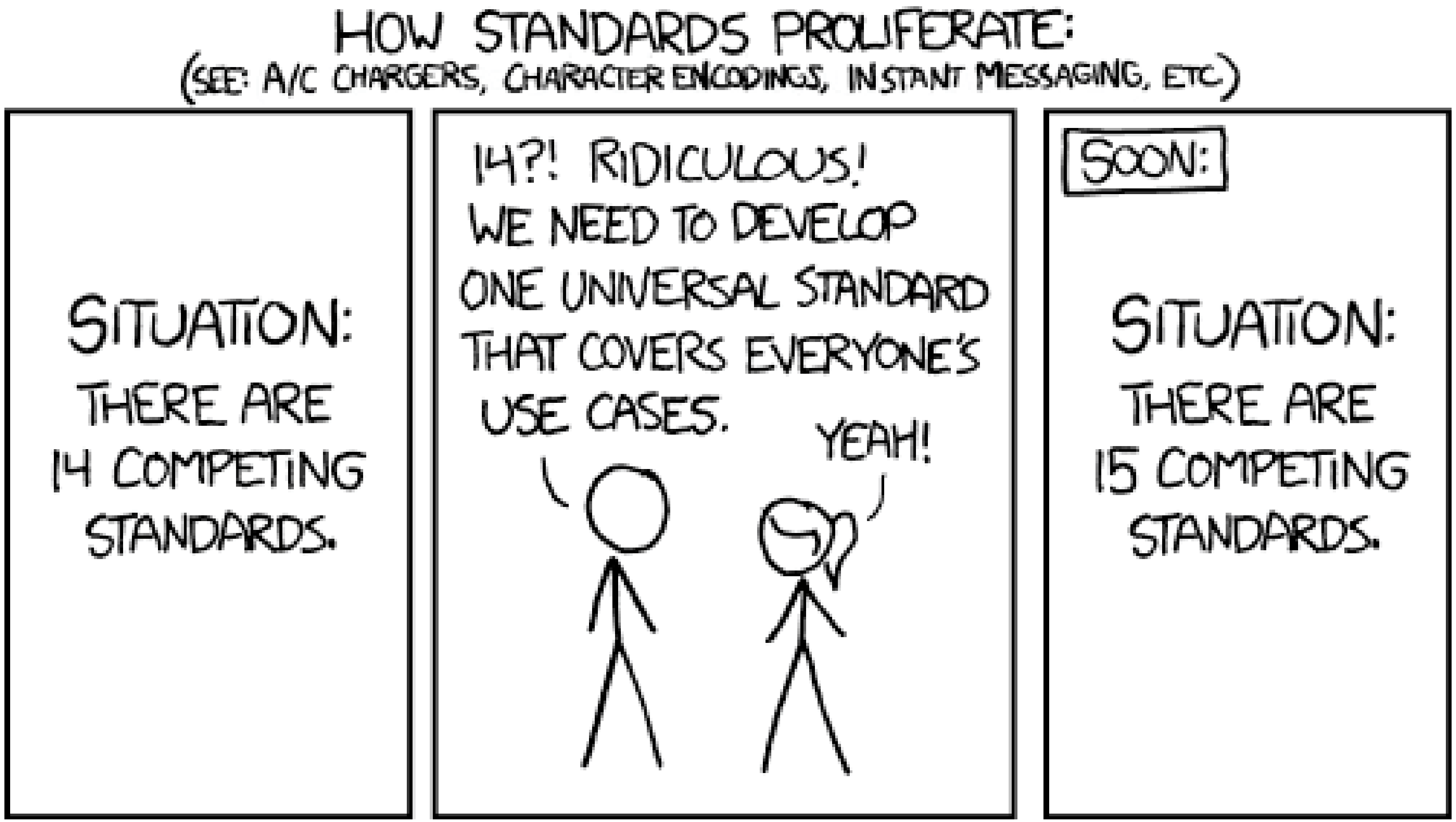
```
pfor(0,10,[&](int i) {
    A[i] += i;
});
```

iterator variable

A captured by reference

loop body

The Sad Truth



How to Categorize Programming Models

- type of API/user interface
  - language? language extension? library?
- domain specificity
  - single use-case only? generic?
- target platform
  - distributed memory? shared memory? accelerators?
- features
  - intra-node scheduling? inter-node scheduling? data decomposition? data distribution? work decomposition? work distribution? fault tolerance? nested parallelism? …

Underlying Communication Models

- shared memory
  - single memory address space
  - direct data access, synchronization via shared memory (e.g. locks, semaphores)

- message passing
  - multiple, distinct memory address spaces
  - data transfer and synchronization via message exchange (e.g. send/recv)

- Global Address Space (GAS)
  - single, global memory address space spanning multiple modes
  - remote data access, synchronization similar to shared memory or implicit
  - often support active messages: “at location x, execute function y” (similar to remote procedure calls)

Type of API (Effort-Benefit Tradeoff)

- applications require less code
- optimizations reside in toolchain
  - application developer has little control
  - automatically apply to every program
- toolchain maintenance is large effort

- applications require more code
- optimizations (partially) in application
  - application developer has full control
  - need to be repeated per application
- toolchain maintenance is minimal

Languages

- upside: new/own syntax
  - tailored towards the specific use-case (e.g. parallel task execution) or domain science (e.g. linear algebra) – Domain Specific Language (DSL)
  - stripped down to the required minimum
  - learn once, use intuitively without requiring a base language such as C++

- downside: toolchain support
  - mandatory: compiler, runtime system, debugger, profiler, etc.
  - maintainer’s view: any language optimizations have to separately implemented per programming model
  - no room for manual low-level optimization (e.g. vectorization, inline assembler)

Language Extensions

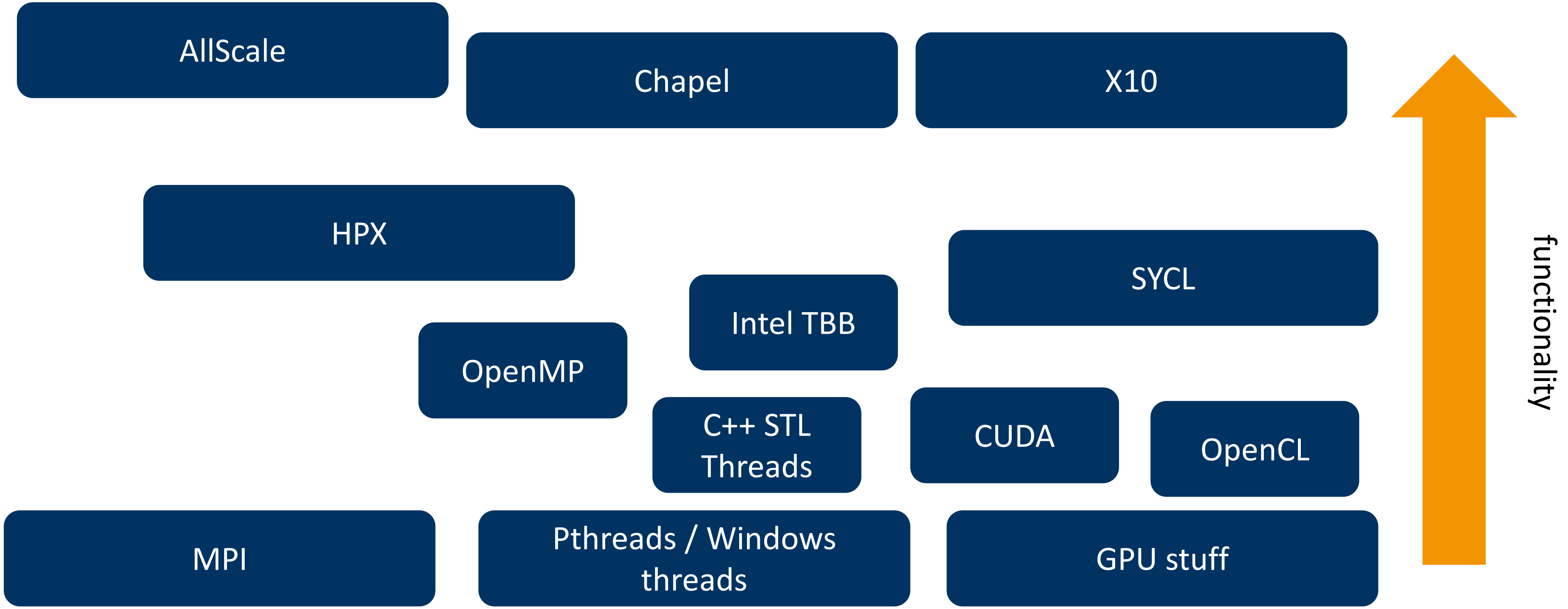
- upside: enrich an existing language with new features
  - builds upon a hopefully mature programming language
  - add use-case- or domain-specific features (e.g. OpenMP)
- downside: toolchain support
  - compiler and other tools need to be extended
  - still needs to partially adhere to base language specification for compatibility

Libraries

- upside: build completely on mature languages
  - toolchain support is already present
  - benefit from new optimizations in e.g. compiler research often without manual effort
- downside: encapsulation required
  - need to wrap the underlying, generic programming language (e.g. prevent accidental `double`-to-`int` conversions)
  - offer a (semi-)fixed-syntax API to the programmer
  - often requires measures to decrease debugging complexity (e.g. templated C++)

Programming Model Tetris

Technological Readiness Level (TRL)



Disclaimer

I have not previously worked with all of the following programming models.

Hence, although (most of) the following code examples are functional, there are very likely faster/prettier solutions.

More sophisticated models offer multiple ways of constructing a solution for a given problem – the implementations shown here are selected to facilitate a quick glance on the model and are not necessarily optimal.

Libraries: Pthreads

- C library for thread-based parallelism
  - API for creating and destroying threads, synchronization and cancellation handling
  - not domain-specific, can be used for any type of program
  - is usually the underlying machinery for e.g. OpenMP

- targets shared memory only
  - no support for distributed memory or accelerators
  - no support for automatic work or data distribution, scheduling, etc.
  - no support for fault tolerance

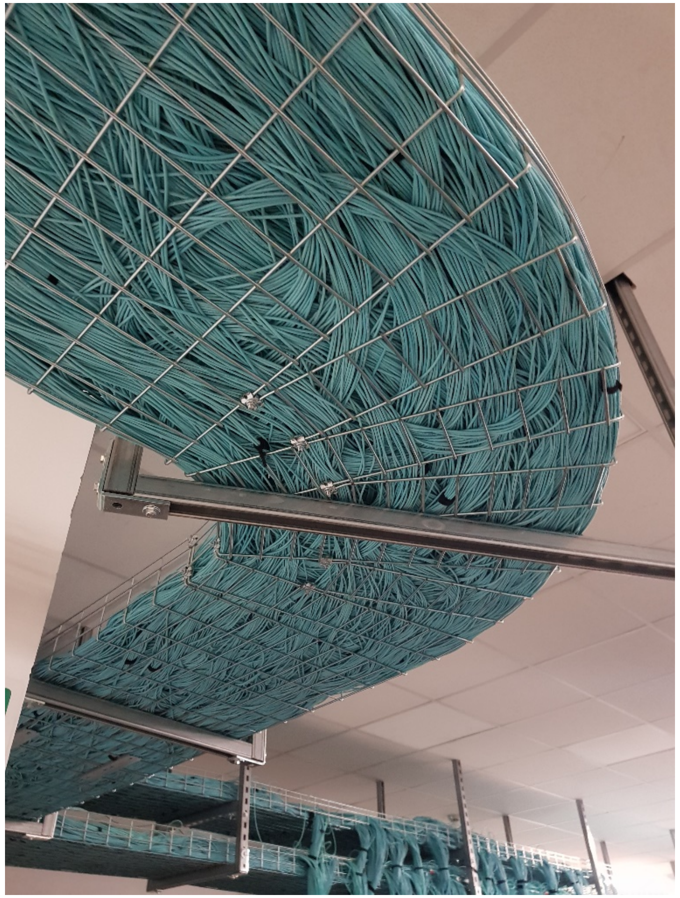
Libraries: Pthreads Example (Optimized Sum)

```c
#define NTHREADS 4
#define SIZE 1000000
#define N (SIZE/NTHREADS)
double sum = 0.0;
pthread_mutex_t sum_mutex;
void *partialSum(void *tid) {
  double mySum = 0.0;
  int start = (*((int*)tid)) * N);
  int end = start + N;
  for(int i = start; i < end ; i++) {
    mySum++; // local sum without lock
  }
  // global sum requires lock
  pthread_mutex_lock(&sum_mutex);
  sum += mySum;
  pthread_mutex_unlock(&sum_mutex);
  pthread_exit(NULL);
}
```

```c
int main(int argc, char *argv[]) {
  int tids[NTHREADS];
  pthread_t threads[NTHREADS];
  pthread_attr_t attr;
  pthread_mutex_init(&sum_mutex, NULL);
  pthread_attr_init(&attr);
  pthread_attr_setdetachstate(&attr,
    PTHREAD_CREATE_JOINABLE);
  for(int i = 0; i < NTHREADS; i++) {
    tids[i] = i;
    pthread_create(&threads[i], &attr, partialSum,
      (void *)&tids[i]); // start threads
  }
  for(int i = 0; i<NTHREADS; i++) {
    pthread_join(threads[i], NULL); // wait
  }
  printf("Done. Sum= %e \n", sum);
  /* cleanup ... */
}
```

Side-Note: Why Care About Fault Tolerance?

- MARCONI @ CINECA, Bologna
  - 250k cores
  - 20 Petaflop/s
- approx. 10.000 optical fibers connecting their HPC infrastructure
- approx. 1 cable failure per day!



Libraries: C++ STL Threads

- thread-based parallelism part of the STL since C++11
  - API similar to Pthreads with convenience functions and type safety
  - e.g. C++17 hint for avoiding false sharing
    `constexpr std::size_t hardware_destructive_interference_size`
  - also features mutex, semaphores, condition variables, futures, etc.

- targets shared memory only
  - no support for distributed memory or accelerators
  - no support for automatic work or data distribution, scheduling, etc.
  - no support for fault tolerance

Libraries: C++ STL Threads Example (Optimized Sum)

```cpp
using DataType = unsigned long long;
using indexType = int;
constexpr DataType size = 100000;
constexpr indexType numThreads = 4;
std::mutex myMutex;

void partialSum(DataType& sum,
  indexType beg, indexType end) {
  DataType mySum{};
  for (auto i = beg; i < end; ++i) {
    mySum++;
  }
  std::lock_guard<std::mutex> lockGuard(myMutex);
  sum += mySum;
} // end of scope, lockGuard releases mutex
```

```cpp
int main() {
  DataType sum{};
  std::vector<std::thread> threads;

  for (int i = 0; i < numThreads; ++i) {
    threads.push_back(std::thread(partialSum,
      std::ref(sum), size/numThreads*i,
      size/numThreads * (i+1)));
  }

  for (auto& t : threads) {
    t.join();
  }

  std::cout << "Result: " << sum << std::endl;
}
```

Libraries: Intel TBB

- thread-based parallelism library
  - higher-level API that offers frequently-used programming patterns
    `parallel_for, parallel_reduce, parallel_scan, parallel_sort`
  - concurrent data structures for vectors, queues, maps, etc.
  - advantage over OpenMP: data structures & no compiler support required

- targets shared memory only
  - no support for distributed memory or accelerators
  - supports automatic work decomposition & distribution
  - no support for fault tolerance

Libraries: Intel TBB Example (Optimized Sum)

```cpp
using namespace tbb;
constexpr int size = 100000;

struct SumFunctor {
  float mySum;
  void operator()(
      const blocked_range<size_t>& r) {
    for(auto i = r.begin(); i != r.end(); ++i)
      mySum++;
  }
  SumFunctor(SumFunctor&, split) : mySum(0) {}
  void join(const SumFunctor& y) {
    mySum += y.mySum;
  }
  SumFunctor() : mySum(0) {}
};
```

```cpp
int main() {
  SumFunctor sf;
  parallel_reduce(
    blocked_range<size_t>(0,size), sf);
  std::cout << sf.mySum << std::endl;
}
```

Libraries: HPX

- GAS-based library for distributed memory
  - shared memory parallelism programming style
  - supports data and task parallelism
  - offers control over data distribution, scheduling, etc.

- targets shared and distributed memory systems
  - limited automatic support for distributed memory (explicit user code changes)
  - support for automatic work/data decomposition and distribution
  - no support for fault tolerance

Libraries: HPX Example (Squaring Distributed Vector Elements)

```
char const* const vec_name = "vec";
char const* const latch_name = "latch";
hpx::partitioned_vector<int> v; // create vec
hpx::lcos::latch l; // synchronization object
if(0 == hpx::get_locality_id()) { // root
  std::vector<hpx::id_type> localities =
    hpx::find_all_localities();
  v = hpx::partitioned_vector<int>(10000,
    hpx::container_layout(localities));
  v.register_as(vec_name);
  l = hpx::lcos::latch(localities.size());
  l.register_as(latch_name);
}
```

```
else { // connect to data at root
  hpx::future<void> f1 =
    v.connect_to(vec_name);
  l.connect_to(latch_name);
  f1.get();
}
partitioned_vector_view<int> view(v);
hpx::parallel::for_each( // square array data
    hpx::parallel::execution::par,
    view.begin(), view.end(),
    [](int& val) { val *= val; });
l.count_down_and_wait(); // wait
return hpx::finalize();
```

Extension: AllScale

- GAS-based language (embedded DSL)
  - shared memory parallelism programming style
  - supports data, task and nested parallelism
  - offers control over data distribution, scheduling, etc.

- targets shared and distributed memory systems
  - limited automatic support for distributed memory (explicit user code changes)
  - support for process-level fault tolerance

Extension: AllScale Example (2D Stencil)

```
const int N = 200;
const int T = 100;
using Grid = data::StaticGrid<double, N, N>;
using Point = allscale::utils::Vector<int, 2>;
Grid temp;

allscale::api::user::algorithm::stencil(temp, T,
  [k,T,N](time_t, const Point& p, const Grid& temp)->double { // inner elements
    return temp[p] + k*(temp[p+Point{-1,0}] + temp[p+Point{+1,0}] +
                      temp[p+Point{0,-1}] + temp[p+Point{0,+1}] + (-4)*temp[p]);
  },
  [k,T,N](time_t, const Point&, const Grid&)->double { // boundary cells
    return 0; // boundaries are constants
  });
```

Languages: OpenCL

- C-like language + library for accelerator programming
  - use library to communicate with OpenCL driver on the host
  - use OpenCL-language to run code on the accelerator
    - is compiled by OpenCL compiler at execution
  - requires OpenCL toolchain (compiler, debugger, etc…)
  - similar to CUDA

- targets specifically accelerators
  - no support for distributed memory
  - no support for automatic work/data decomposition & distribution
  - no support for fault tolerance

Languages: OpenCL Example (Matrix Multiplication)

```
// this code runs on the host computer
clGetPlatformIDs(...); // setup environment
clGetDeviceIDs(...); // setup env
clCreateContext(...); // setup env
clCreateCommandQueue(...); // setup env
clCreateBuffer(...); // allocate gpu memory
clEnqueueWriteBuffer(...); // copy data to GPU
clCreateProgramWithSource(...); // build exe
clGetProgramBuildInfo(...); // build exe
clCreateKernel(...); // build exe
clEnqueueNDRangeKernel(...); // run kernel
clEnqueueReadBuffer(...); // get data from GPU
/* cleanup ... */
```

```
// this code runs on the GPU
__kernel void matrix_mul(
    __global float *matrix_A,
    __global float *matrix_B,
    __global float *matrix_C) {
  int i = get_global_id(0);
  int j = get_global_id(1);
  float sum = 0.0;
  for(int k = 0; k < M; ++k) {
    sum += matrix_A[N*i+k] * matrix_B[M*k+j];
  }
  matrix_C[N*i+j] = sum;
}
```

Languages: SYCL

- C++-based DSL for accelerators with advantages over OpenCL/CUDA
  - type safety and more advantages of a C++ API
  - single source that runs on CPU or accelerators (debugging!)
  - not vendor-specific
  - minimum amount of boilerplate code

- targets CPUs and accelerators (shared memory only)
  - no support for distributed memory (➔ CELERITY @ DPS Group ☺)
  - limited support for automatic work/data decomposition and distribution
  - no support for fault tolerance

Languages: SYCL Example (Vector Add)

```
using namespace cl::sycl;
#define LENGTH (1024)

std::vector h_a(LENGTH);
std::vector h_b(LENGTH);
std::vector h_r(LENGTH);

/* initialize a and b... */

buffer d_a(h_a); // input buffer
buffer d_b(h_b); // input buffer
buffer d_r(h_r); // output buffer
queue myQueue;
```

```
command_group(myQueue, [&]() {
  // Data accessors
  auto a = d_a.get_access<access::read>();
  auto b = d_b.get_access<access::read>();
  auto r = d_r.get_access<access::write>();
  // Kernel
  parallel_for(count, kernel_functor(
      [=](id<> item) {
    int i = item.get_global(0);
    r[i] = a[i] + b[i];
  }));
});
```

Languages: Chapel

- GAS-based language developed by Cray
  - shared memory parallelism programming style
    - processes are called “*locales*”, and can have multiple “*threads*”
  - supports data, task and nested parallelism, offers distributed data structures
  - offers explicit control over data distribution, scheduling, etc.
  - advantage over OpenMP: supports distributed memory
  - advantage over MPI: no explicit message passing required

- targets shared and distributed memory systems
  - limited automatic support for distributed memory (explicit user code changes)
  - support for process-level fault tolerance

Languages: Chapel Examples (Opt. Sum, Shared and Distributed)

```
// automatically synchronized
var sum : sync int = 0;
// forall starts a thread per core
forall i in 1..1000000 {
  sum += 1; // no race condition!
}
// workaround due to a bug
var res = sum;
// print result
writeln(res);
```

```
// assign work in round-robin fashion
use CyclicDist;
// index space for distributed memory
const IndexSpace = {1..100000} dmapped
  Cyclic(startIdx=1);
var sum : sync int = 0;
// distribute iterations among localities
forall i in IndexSpace {
  sum += 1;
}
var res = sum;
writeln(res);
```

Languages: X10

- GAS-based language developed by IBM
  - distributed memory
  - quite similar Chapel (but more object-orientation and Java-adherence, also offers garbage collection!)
- targets distributed memory incl. accelerators
  - limited automatic support for distributed memory (explicit user code changes)
  - support for process-level fault tolerance

Languages: X10 Example: Optimized Sum

```
import x10.array.*;

public class DistArraySum {
  static N = 10;

  static def sum(a:DistArray[Double]):Double {
    var sum:Double = 0;
    for(pt in a) sum += at(a.place(pt)) a(pt);
    return sum;
  }
  public static def main(Rail[String]) {
    val a = new DistArray_BlockBlock_2[Double](N, N, (i:Long,j:Long)=>(i+j) as Double);
    Console.OUT.println("Sum: " + sum(a));
  }
}
```

Languages: Matlab

- domain-specific language for math applications
  - offers index-notation, syntax for matrix- and element-wise operations, etc.
  - offers built-in visualization tools

- offers various forms of parallelism
  - vectorization via specific functions implemented using the Intel MKL
  - distributed memory and accelerator parallelism via the Parallel Computing Toolbox and the Matlab Parallel Server
    - supports multi-process parallelism and GPUs via MPI and CUDA
    - offers interface to call MPI and CUDA from within Matlab code

Languages: Matlab Examples: SPMD & GPUs

```matlab
% start a pool with 3 workers
parpool(3);
% run program in parallel
spmd
  q = magic(labindex + 2);
end
% plot the data
figure
subplot(1,3,1), imagesc(q{1});
subplot(1,3,2), imagesc(q{2});
subplot(1,3,3), imagesc(q{3});
```

```matlab
% start a pool with all GPUs
parpool(gpuDeviceCount);
numSamples = 100;
% initialize data on the GPUs
X = zeros(numSamples,N,'gpuArray');
% distribute computation accross GPUs
parfor i = 1:numSamples
    X(i,:) = rand(1,N,'gpuArray');
    for n=1:numIterations
        X(i,:) = r.*X(i,:).*(1-X(i,:));
    end
end
```

Overview of State-of-the-art Programming Models

	Architectural			Task System				Management				Eng.	
	Communication Model	Distributed Memory	Heterogeneity	Graph Structure	Task Partitioning	Result Handling	Task Cancellation	Worker Management	Resilience Management	Work Mapping	Synchronization	Technological Readiness	Implementation Type
C++ STL	smem	×	×	dag	×	i/e	×	i	×	i/e	e	9	Library
TBB	smem	×	×	tree	×	i	✓	i	×	i	i	8	Library
HPX	gas	i	e	dag	✓	e	✓	i/e	×	i/e	e	6	Library
Legion	gas	i	e	tree	✓	e	×	i	×	i/e	e	4	Library
PaRSEC	msg	e	e	dag	×	e	✓	i	✓	i/e	i	4	Library
OpenMP	smem	×	i	dag	×	i	✓	e	×	i	i/e	9	Extension
Charm++	gas	i	e	dag	✓	i/e	×	i	✓	i/e	e	6	Extension
OmpSs	smem	×	i	dag	×	i	×	i	✓	i	i/e	5	Extension
AllScale	gas	i	i	dag	✓	i/e	×	i	✓	i	i/e	3	Extension
StarPU	msg	e	e	dag	✓	i	×	i	×	i/e	e	5	Extension
Cilk Plus	smem	×	×	tree	×	i	×	i	×	i	e	8	Lang.
Chapel	gas	i	i	dag	✓	i	×	i	×	i/e	e	5	Lang.
X10	gas	i	i	dag	✓	i	×	i	✓	i/e	e	5	Lang.

Where is the Research Going?

- everybody talks about increasing the "separation of concerns"
  - let computer science guys master the computer science
  - let domain science guys master their domain sciences
- everybody talks about "portability"
  - large efforts in creating DSLs that allow running on any architecture (e.g. Intel "One API")
  - write code once, compile and run on GPU, GPU, FPGA, etc.
  - often blurry line of distinction between libraries and extensions
- everybody talks about "performance portability"
  - nobody knows how to define it accurately
  - nobody knows how to achieve it properly

Considerations for Application Developers

- Which platform should I target?
  - shared memory, distributed memory, accelerators, ...
- Which features and degree of control do I need?
  - automatic work and data decomposition and distribution, scheduling, fault tolerance, ...
  - porting legacy codes might constrain you to using libraries (or possibly language extensions)
- How much support do I need?
  - consider maturity and long-term support of the language/extension/library
- Which programming language do I know?
  - check libraries or embedded DSLs of languages you already master

Considerations for System Developers

- Which features do I want to offer?
  - e.g. automatic data decomposition & distribution often requires data flow analysis and hence a compiler

- What do I require my application developers to master?
  - build upon widely-used programming languages
  - choosing a library-based model often decreases adoption barriers

- How much effort can I spend on this? How many people are in my workforce?
  - languages and their toolchains take an immense (!) amount of effort if done properly
  - only move away from library-only solutions if necessary
  - even then, consider language extensions first

Summary

- choose your weapon wisely
  - feature set / target architecture / effort
- glimpse into the world of DSLs
  - Pthreads, C++ STL threads, TBB, HPX, AllScale, OpenCL/CUDA, SYCL, Chapel, X10, Matlab

Read up on the feature sets of each library / extension / etc. you are going to use!

Image Sources

- Standards: https://xkcd.com/927/
- State-of-the-Art Overview: https://link.springer.com/content/pdf/10.1007%2Fs11227-018-2238-4.pdf