Pacific Northwest
NATIONAL LABORATORY

SHAD: Productive Programming for High-Performance Systems in Standard C++

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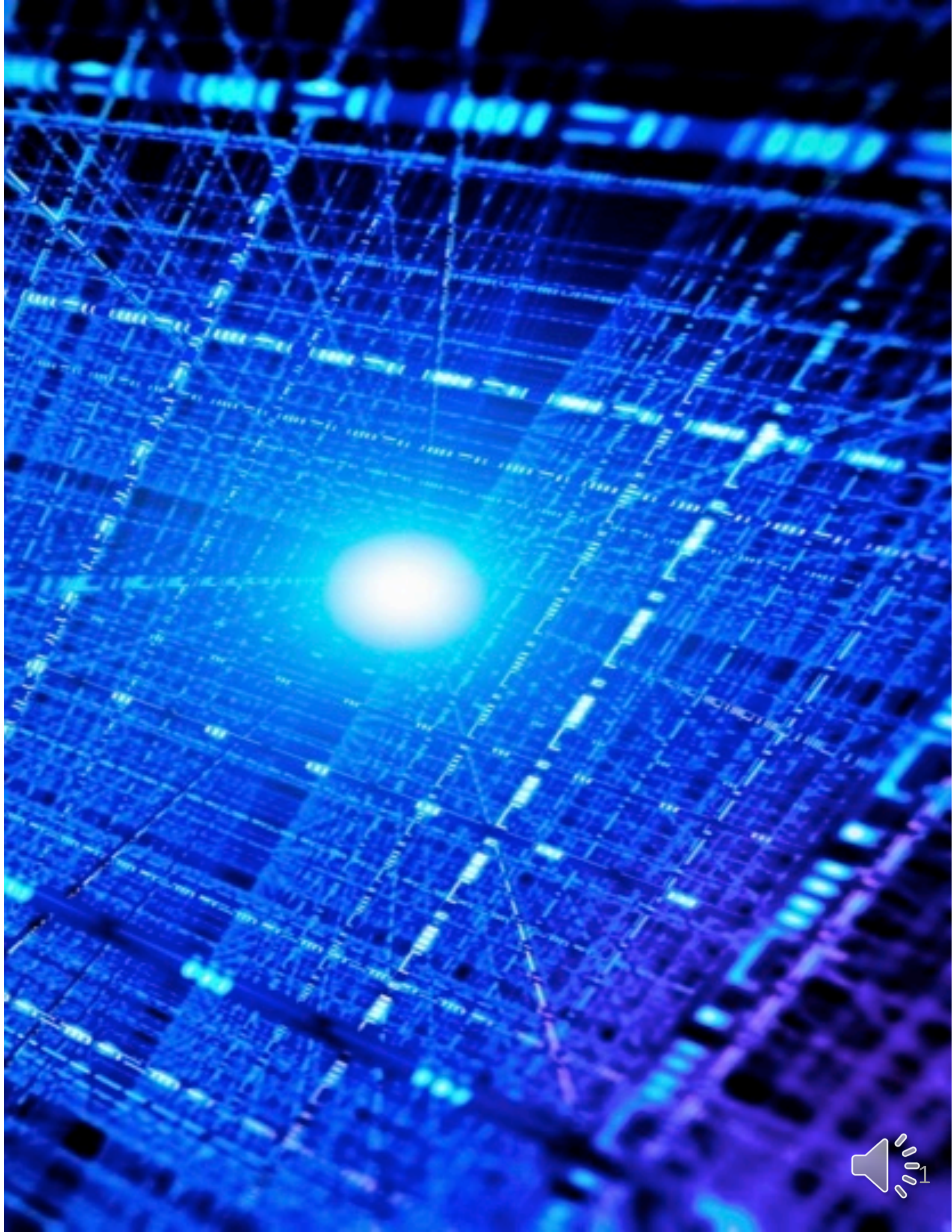
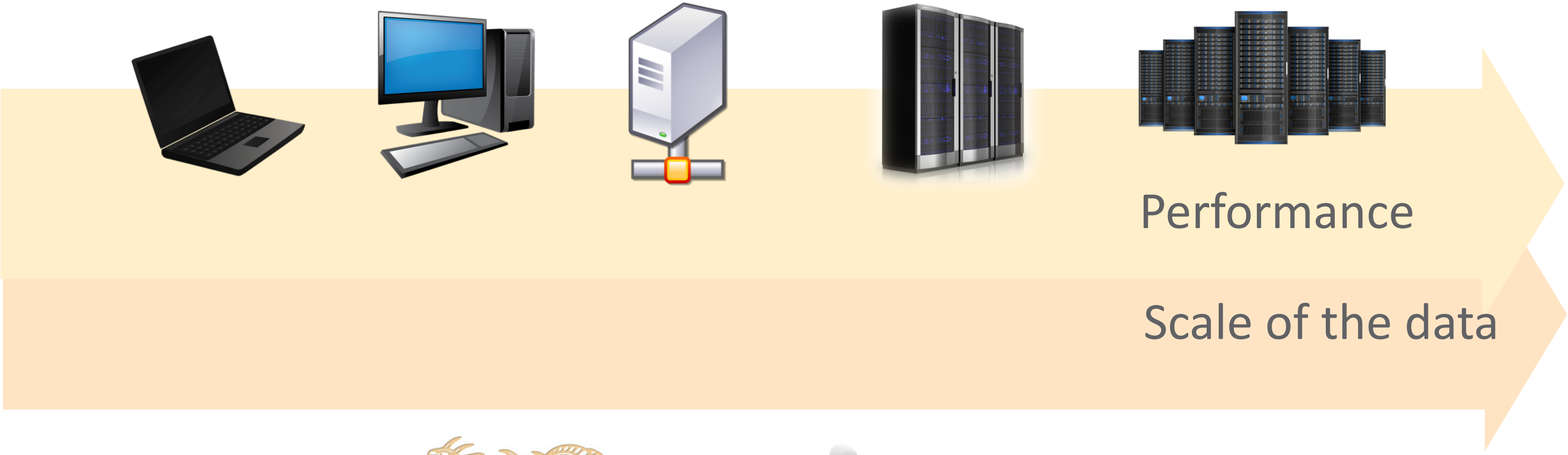


Performance, Portability, and Productivity



Performance

Scale of the data

Teaser

Tackling the Stock Market with HPC – it’s all about money

- Problem: find the **highest price** in a set of **stock options**
  - Input: ~134 millions of stock-option descriptors
  - Output: the max-priced option
- Black-Scholes formula
  - Input: a stock-option descriptor
  - Output: its price
  - 127-line black-box C function, plenty of <`math.`h> stuff
  - [C. Bienia *et al.*, PARSEC Benchmark Suite, PACT,08]

“Old school” C++

```
price_t max_price(std::array<option_t, n> &a) {
  auto m = std::numeric_limits<price_t>::min();
  for (auto it = a.begin(); it != a.end(); ++it)
    m = std::max(res, blck_schls(*it));
  return m;
}
```

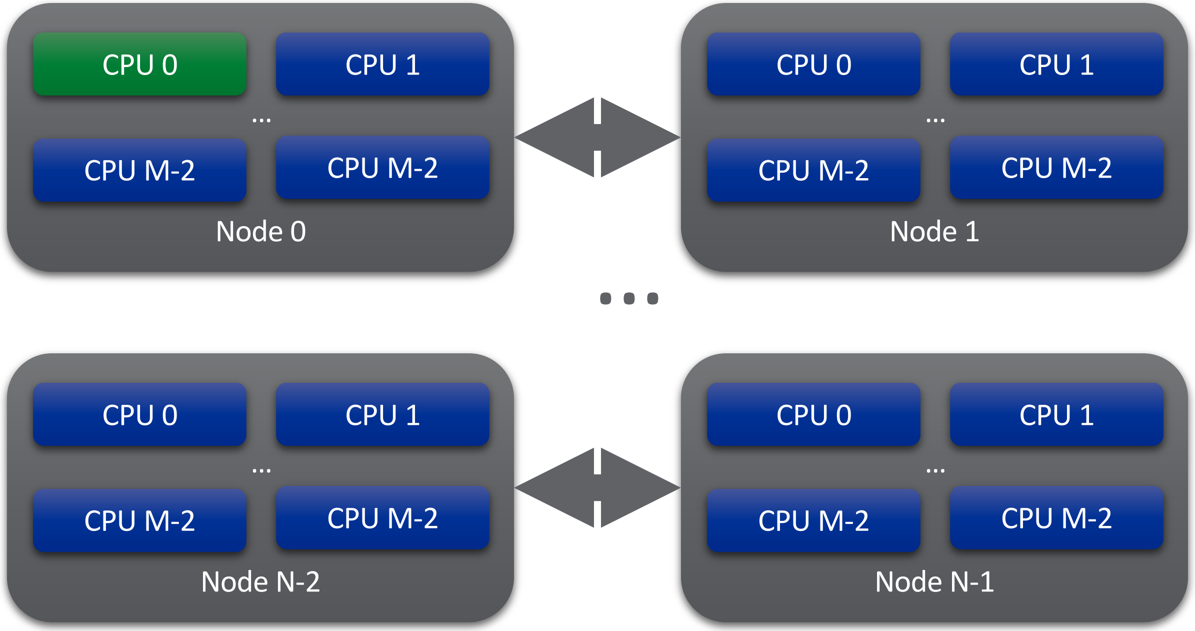
STL Containers + STL Iterators + for loop

“Old-school” C++ – HPC?

```
price_t max_price(…) {…}
```

STL Containers + STL Algorithms

- 1x CPU core
- Intel(R) Xeon(R) CPU @ 2.80GHz
- gcc 9.1



Node 0: CPU 0, CPU 1, …, CPU M-2, CPU M-2

Node 1: CPU 0, CPU 1, …, CPU M-2, CPU M-2

…

Node N-2: CPU 0, CPU 1, …, CPU M-2, CPU M-2

Node N-1: CPU 0, CPU 1, …, CPU M-2, CPU M-2

8.5 millions
options/sec

Modern(ish) C++

```
price_t max_price(std::array<option_t, n> &a) {
 std::array<price_t, n_options> p;
 std::transform(a.begin(), a.end(), p.begin(),
blck_schls);
 return *std::max_element(p.begin(),
```

STL Containers + STL Algorithms

Modern C++: execution policies may be our friends

```
price_t max_price(std::array<option_t, n> &a) {
 std::array<price_t, n_options> p;
 std::transform(std::execution::seq,
  a.begin(), a.end(), p.begin(), blck_schls);
 return *std::max_element(std::execution::seq,
  p.begin(), p.end());
}
```

STL Execution Policies

Modern C++: execution policies ARE our friends!

```
price_t max_price(std::array<option_t, n> &a) {
 std::array<price_t, n_options> p;
 std::transform(std::execution::par,
  a.begin(), a.end(), p.begin(), blck_schls);
 return *std::max_element(std::execution::par,
  p.begin(), p.end());
}
```

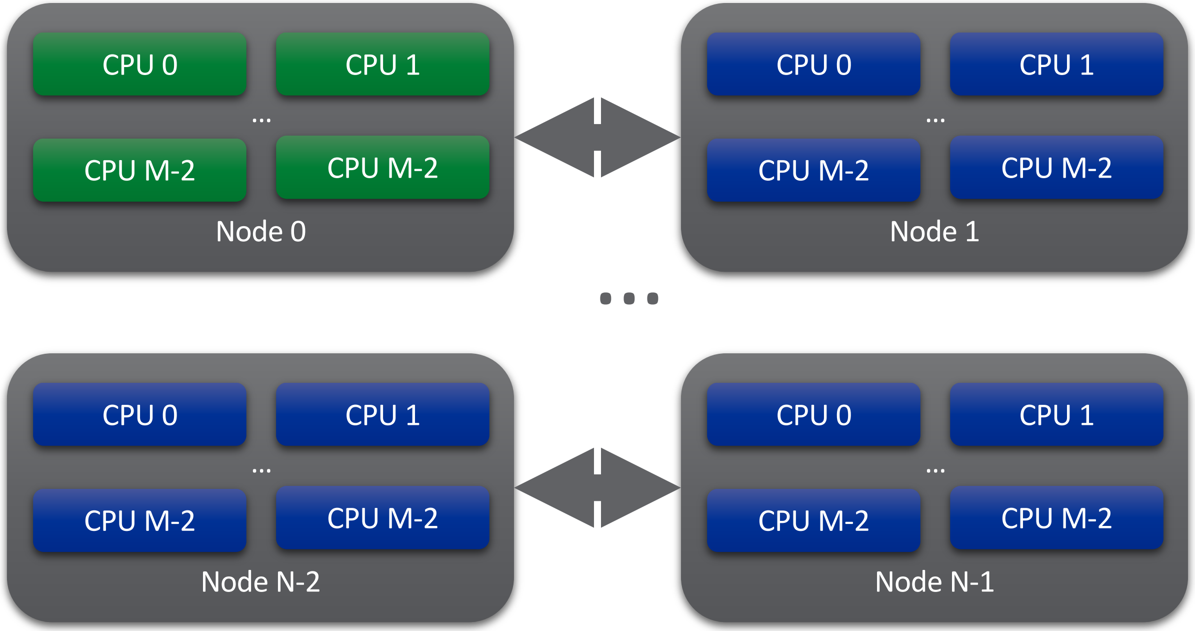
Parallel STL

Modern C++ – HPC?

```
price_t max_price(…) {…}
```

Parallel STL

- 10-core Socket
- Intel(R) Xeon(R) CPU @ 2.80GHz
- gcc 9.1



72.9 millions

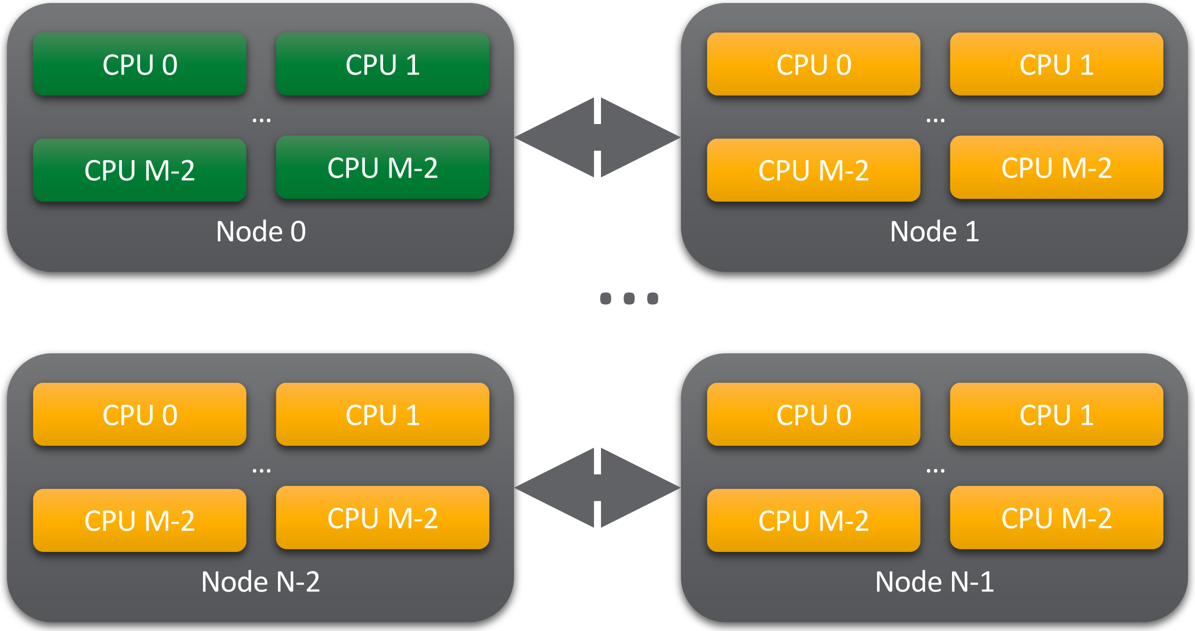
options/sec

~8.5x speedup

What about the other N-1 nodes?

```
price_t max_price(…) {…}
```

?



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SCALABLE
HIGH-PERFORMANCE
ALGORITHMS &
DATA-STRUCTURES

https://github.com/pnnl/SHAD

Here comes the SHAD!

```
price_t max_price(shad::array<option_t, n> &a) {
 shad::array<price_t, n_options> p;
 shad::transform(shad::execution::par,
  a.begin(), a.end(), p.begin(), blck_schls);
 return *shad::max_element(shad::execution::par,
  p.begin(), p.end());
}
```

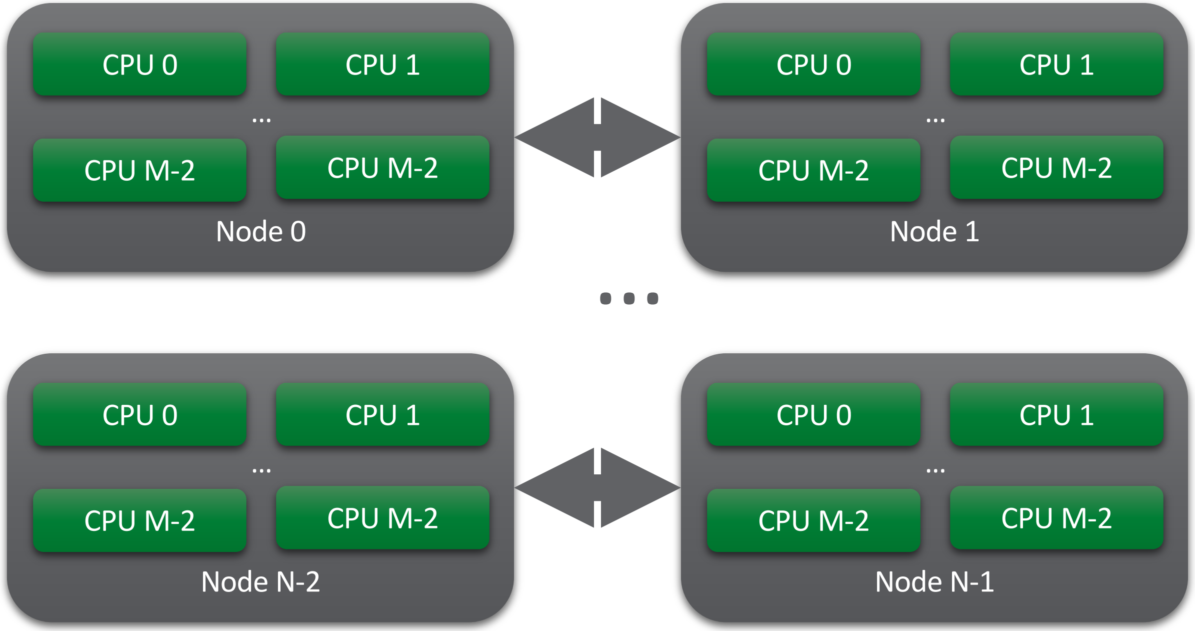
SHAD-powered Distributed STL

Here comes the SHAD! – HPC!

```
price_t max_price(…) {…}
```

SHAD-powered Distributed STL

- 16x 10-core sockets
- Intel(R) Xeon(R) CPU @ 2.80GHz
- gcc 9.1



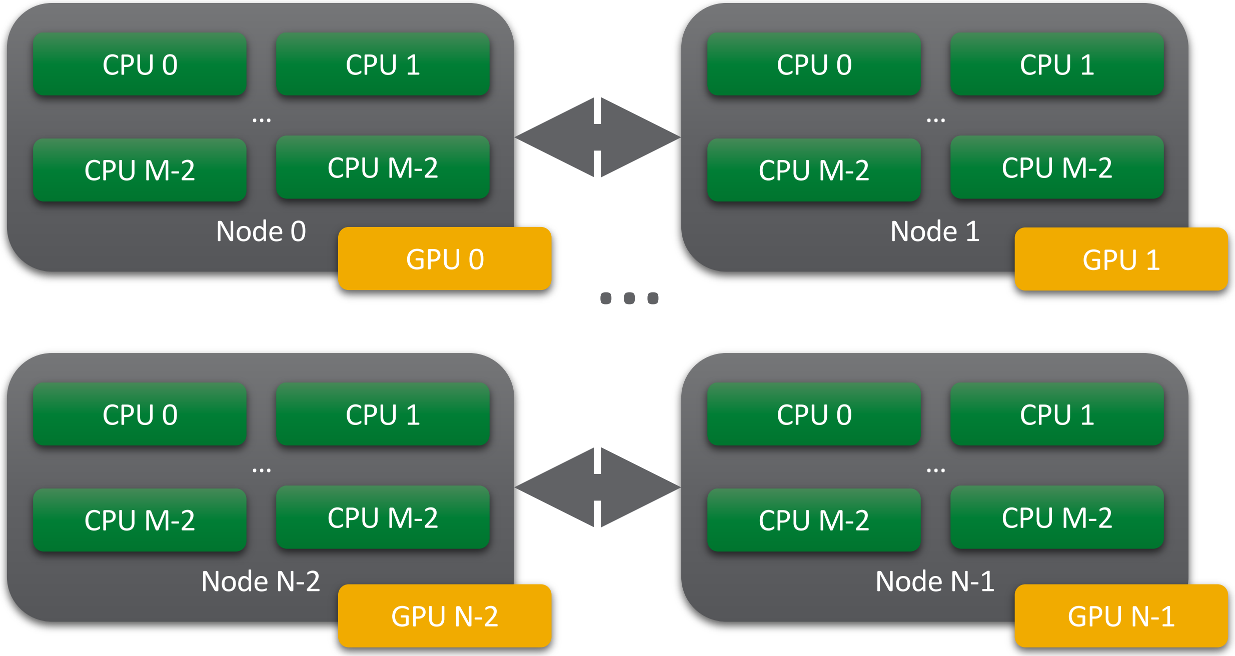
706.7 millions
options/sec

~82.5x speedup
vs plain STL

And what about… The GPUs?!

```
price_t max_price(…) {…}
```

?


CPU 0
CPU 1
…
CPU M-2
CPU M-2
Node 0
GPU 0

CPU 0
CPU 1
…
CPU M-2
CPU M-2
Node 1
GPU 1

…

CPU 0
CPU 1
…
CPU M-2
CPU M-2
Node N-2
GPU N-2

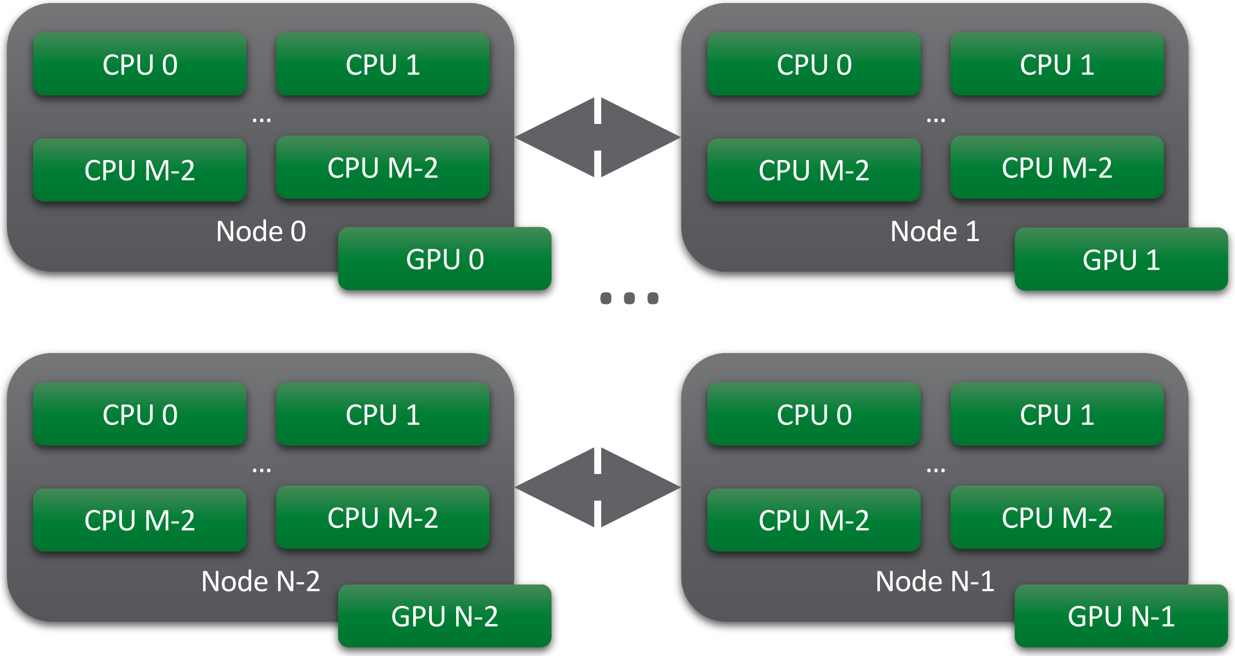
CPU 0
CPU 1
…
CPU M-2
CPU M-2
Node N-1
GPU N-1

Here comes the SHAD again! – HPC!!

```
price_t max_price(…) {…}
```

SHAD-powered Distributed STL

- 4x GPU equipped cluster nodes
- Intel(R) Xeon(R) CPU @ 2.80GHz
  + Nvidia Tesla GPU
- gcc 9.1 + nvcc (CUDA toolkit 9.2)



CPU 0 CPU 1 … CPU M-2 CPU M-2 Node 0 GPU 0

CPU 0 CPU 1 … CPU M-2 CPU M-2 Node 1 GPU 1

…

CPU 0 CPU 1 … CPU M-2 CPU M-2 Node N-2 GPU N-2

CPU 0 CPU 1 … CPU M-2 CPU M-2 Node N-1 GPU N-1

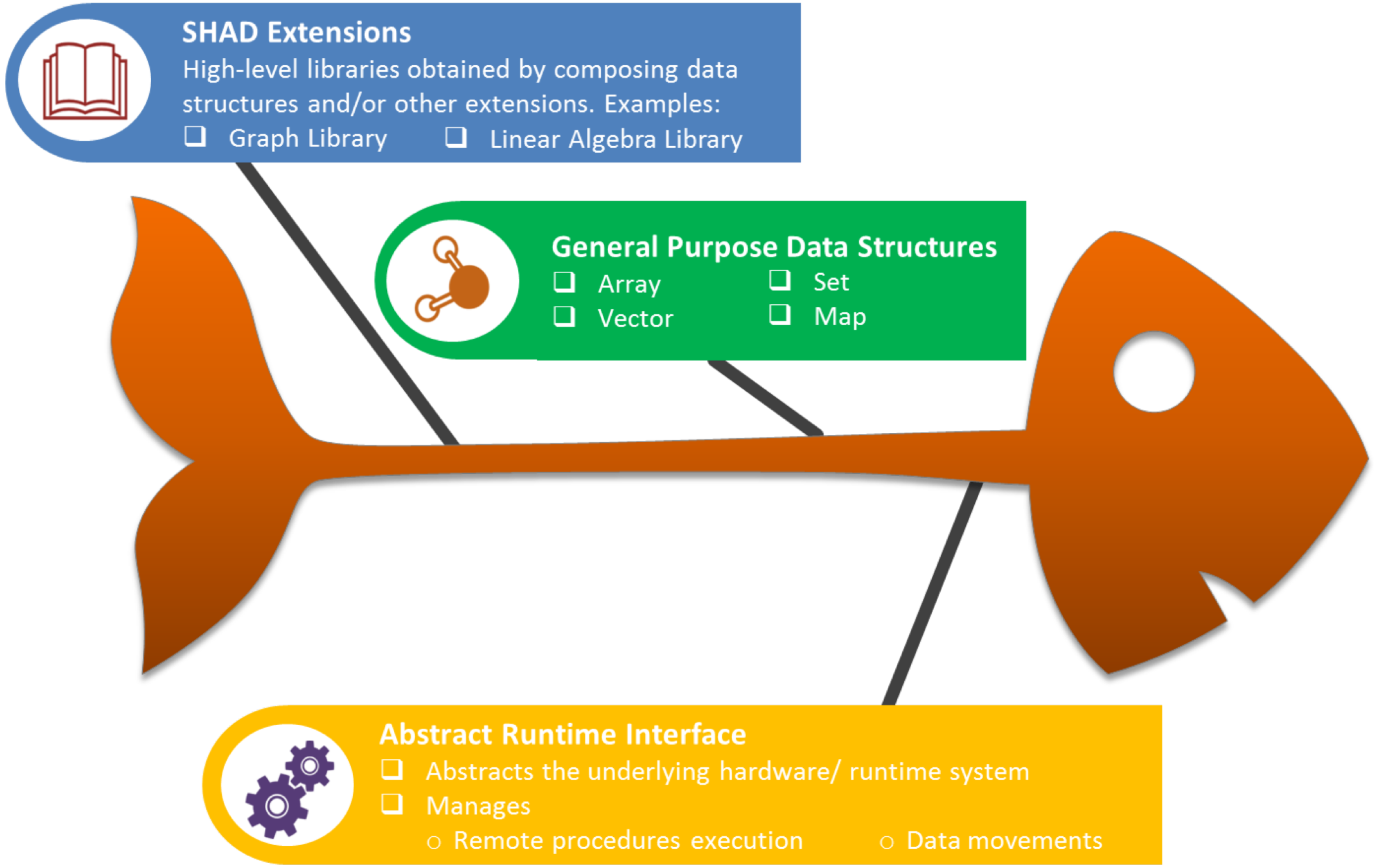
~5 Billions
options/sec

~585x speedup
vs plain STL

How did we get there?

Let’s take a closer look

SHAD Design Overview



SHAD Extensions

High-level libraries obtained by composing data structures and/or other extensions. Examples:

- □ Graph Library
- □ Linear Algebra Library

General Purpose Data Structures

- □ Array
- □ Vector
- □ Set
- □ Map

Abstract Runtime Interface

- □ Abstracts the underlying hardware/ runtime system
- □ Manages
  - ○ Remote procedures execution
  - ○ Data movements

Abstract Runtime Interface: main concepts

Machine Abstraction

- Locality
  - Entity in which memory is directly accessible
  - Examples: node in a cluster, core, NUMA domain
- Task
  - Basic unit of computation
  - Can be executed on any locality
  - Can be asynchronous
- “*Handles*”
  - Identifiers for spawning activities
  - Used to check for task completion
  - Multiple tasks may be associated to the same handle -> task groups

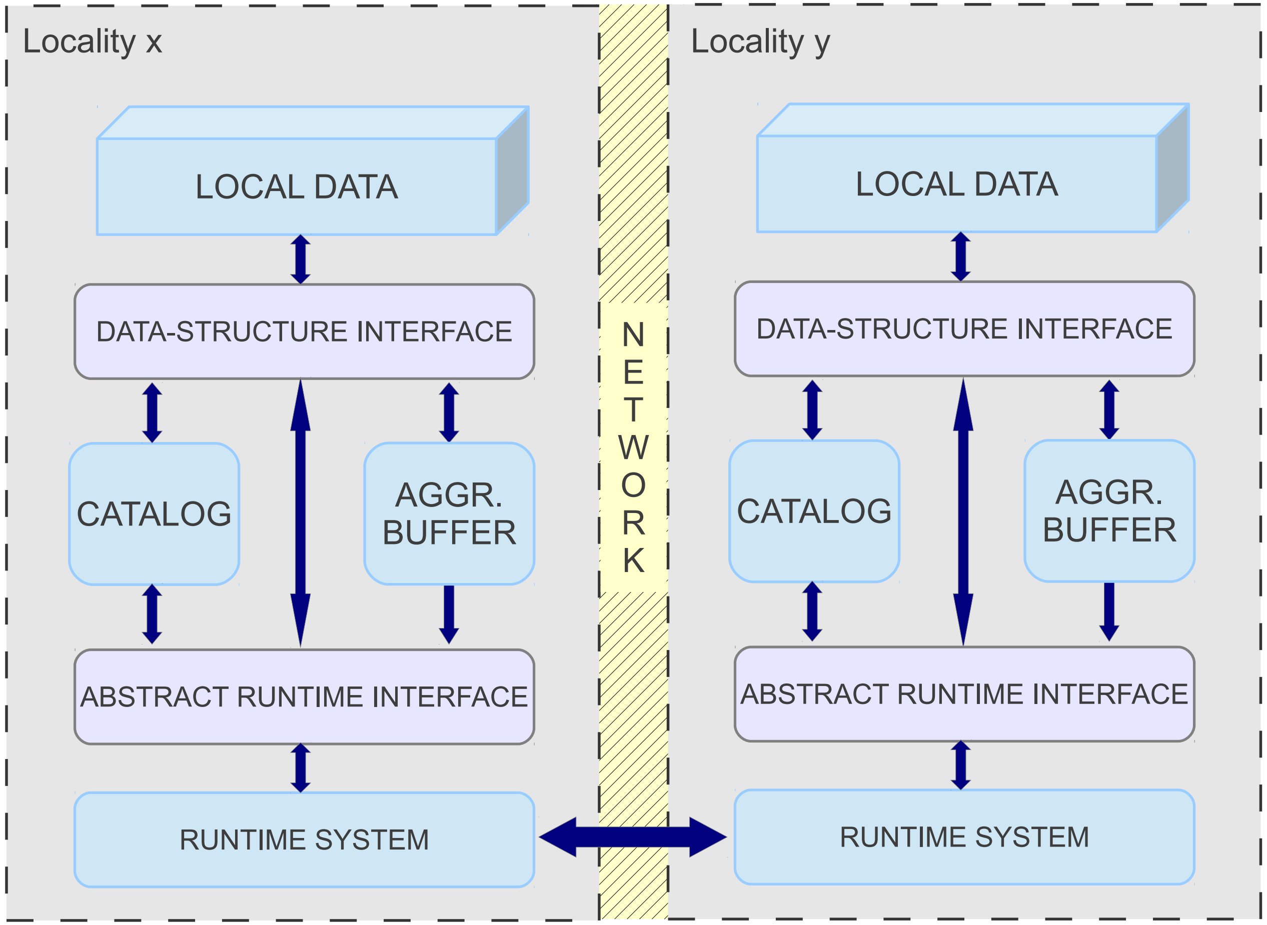
Abstract Runtime Interface Mappings

- Plain C++
  - Fast prototyping
- PNNL’s Global Memory and Threading (GMT) library
  - Targets commodity clusters
  - Available at **https://github.com/pnnl/gmt**
- Intel’ Threading Building Blocks (TBB)
  - Targets shared memory systems
    - … these may include your laptop ☺
- PNNL’s ARTS
  - Under development under the HIVE DARPA project
  - Available at **https://github.com/pnnl/ARTS**
  - SHAD-mapping not yet available on the repo
- Other mappings coming soon!

General Purpose Algorithms and Data-structures

- Include: array, vector, unordered set and map
- They "look like" STL, but they
  - Can be distributed on several localities
    - High capacity (TB+ scale data)
  - Are thread safe
  - Can be modified and accessed in parallel
    - High performance
  - Automatically manage synchronization and data-movements

Data-structures design template



SHAD extensions

- Higher-level or domain specific libraries
- Built on top of the General Purpose library
- Can be composed, to obtain application-specific libraries
  - High flexibility
  - *Evolving* framework

- Examples of SHAD extensions
  - Attributed Graph Lib (Prototype Available)
  - Linear Algebra Lib (Ongoing Work)
  - Machine Learning Lib (Future Work)

STL Interfaces

From STL *inspired* to STL compliant

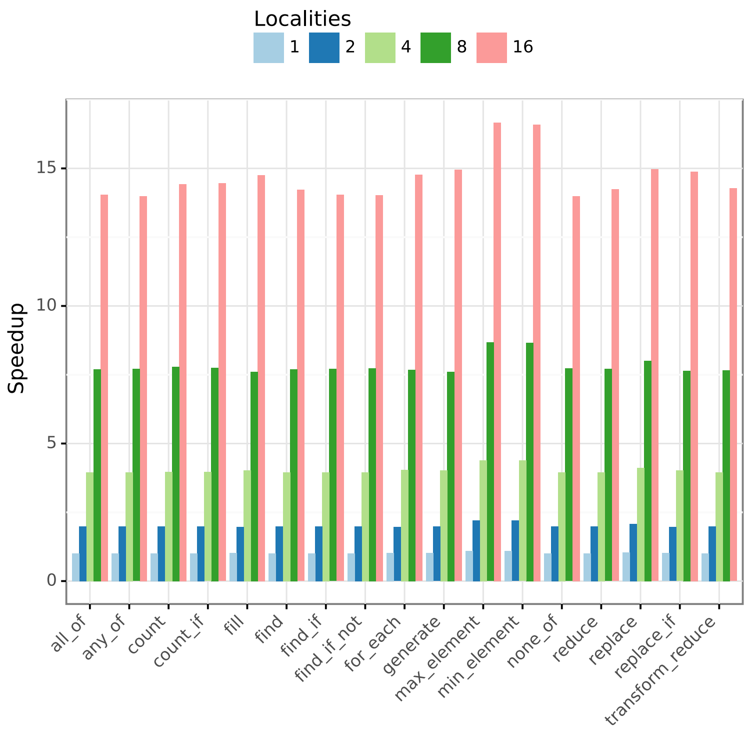
- Semantics, concepts and syntax analogous to STL’s APIs
  - Iterators, ranges, algorithms

- All STL’s algorithms can be executed on SHAD’s data structures
  - But you shouldn’t do that
    - Severe performance penalties due to sync remote memory operations

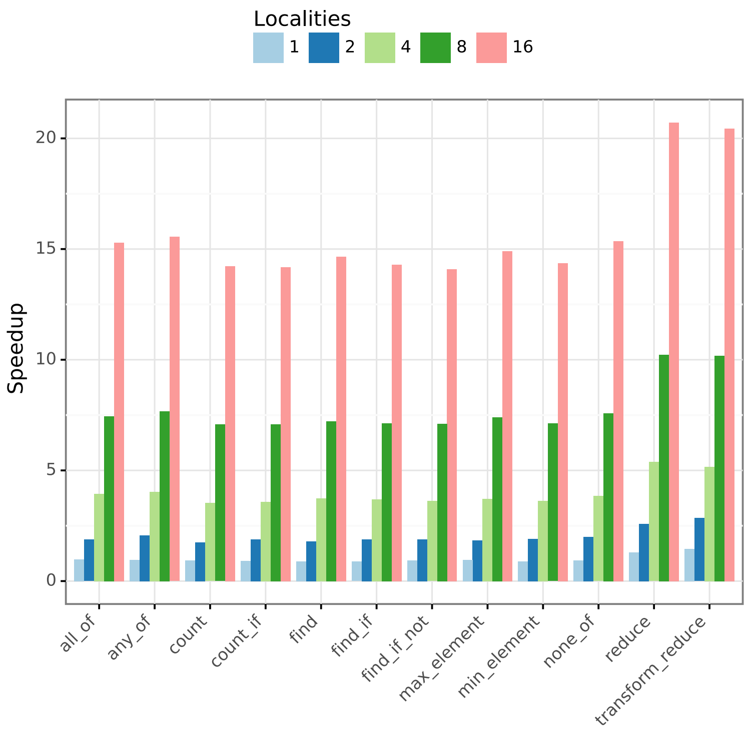
- Additional execution policies for performance
  - distributed_sequential
    - Algorithms with sequential semantics (e.g. left –folding)
  - distributed_parallel
    - Analougus to std::par

Preliminary results

array



unordered_set



- Commodity cluster equipped with Xeon E5-2680 v2 CPUs @ 2.8 GHz
- distributed_parallel policy
- 1 Billion elements of size_t type

And what if I don’t like C++?

SHADEs: The SHAD Exploration System

- Client-server Architecture, inspired by Arkouda
  - Client/server communications via ZMQ library
- Jupyter Notebook / Python frontend, SHAD backend
- Front-end commands are mapped to SHAD functions
- Multiple clients can connect to the same backend at the same time
- Clients can connect to multiple backends
- Debutted on Github!
  - https://github.com/pnnl/SHADEs

SHAD

https://github.com/pnnl/SHAD

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