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The UPC++ Library for Exascale and Data Intensive Computing

http://upcxx.lbl.gov

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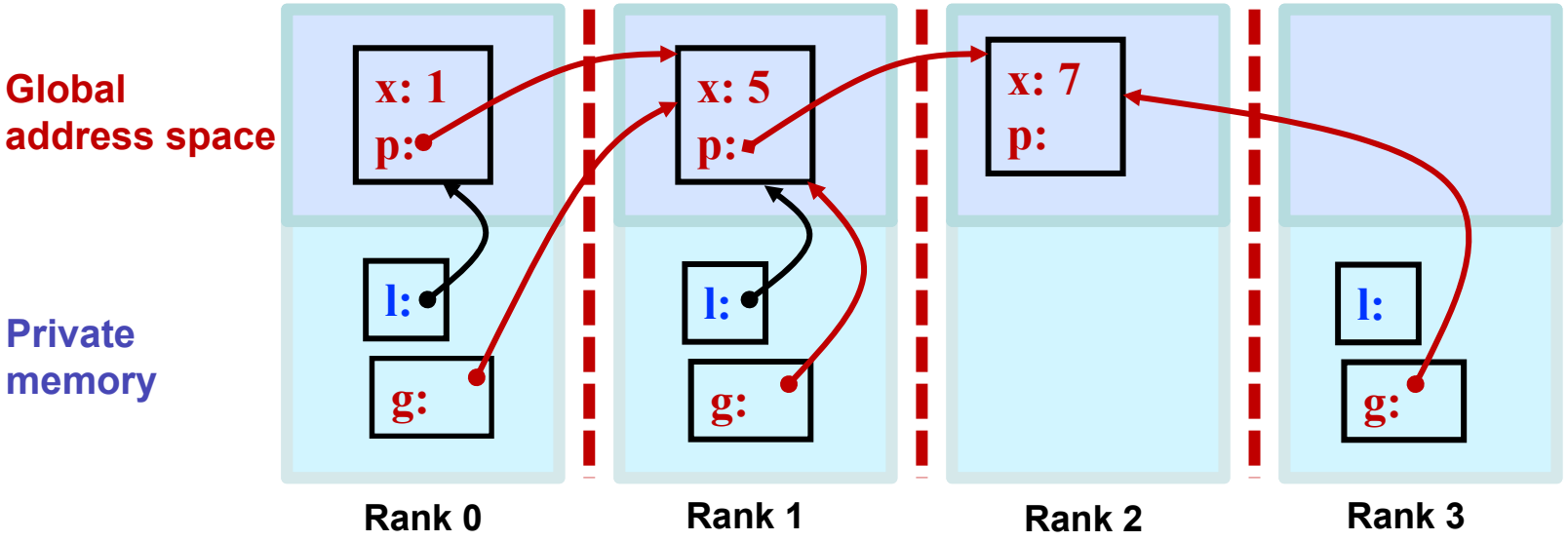
UPC++: a C++ PGAS Library [iPDPS19]

- Global Address Space (P**GAS**)
  - A portion of the physically distributed address space is visible to all processes. Now generalized to handle GPU memory
- Partitioned (**P**GAS)
  - *Global pointers* to shared memory segments have an *affinity* to a particular rank
  - Explicitly managed by the programmer to optimize for locality



What does UPC++ offer?

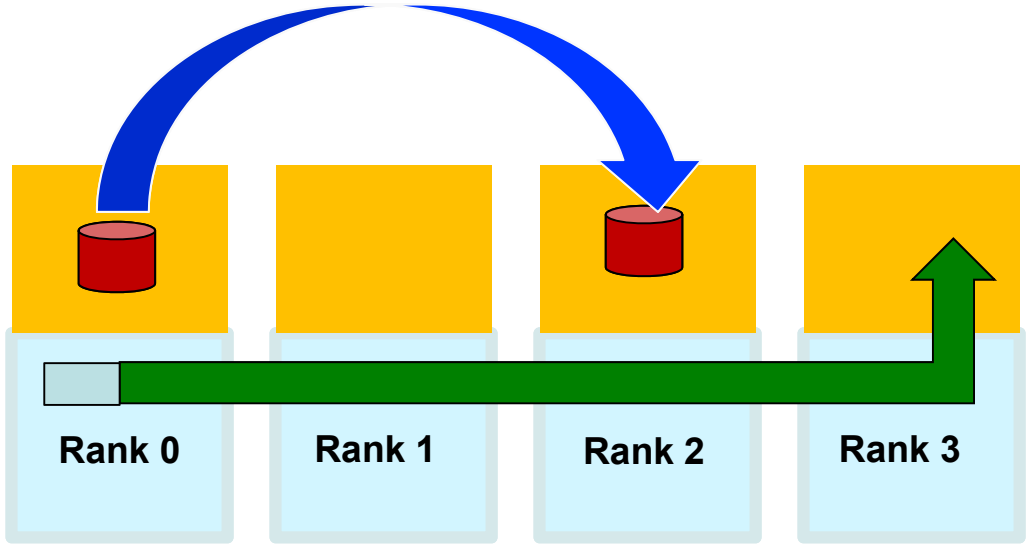
- Asynchronous behavior based on futures/promises
  - RMA: Low overhead, zero-copy 1 sided communication. Get/put to a remote location in another address space
  - RPC: Remote Procedure Call: invoke a function remotely A higher level of abstraction, though at a cost
- Design principles encourage performant program design
  - All communication is explicit (unlike UPC)
  - All communication is asynchronous: futures and promises
  - Scalability

Remote procedure call (RPC)

Global address space (Shared segments)

One sided communication

Private memory



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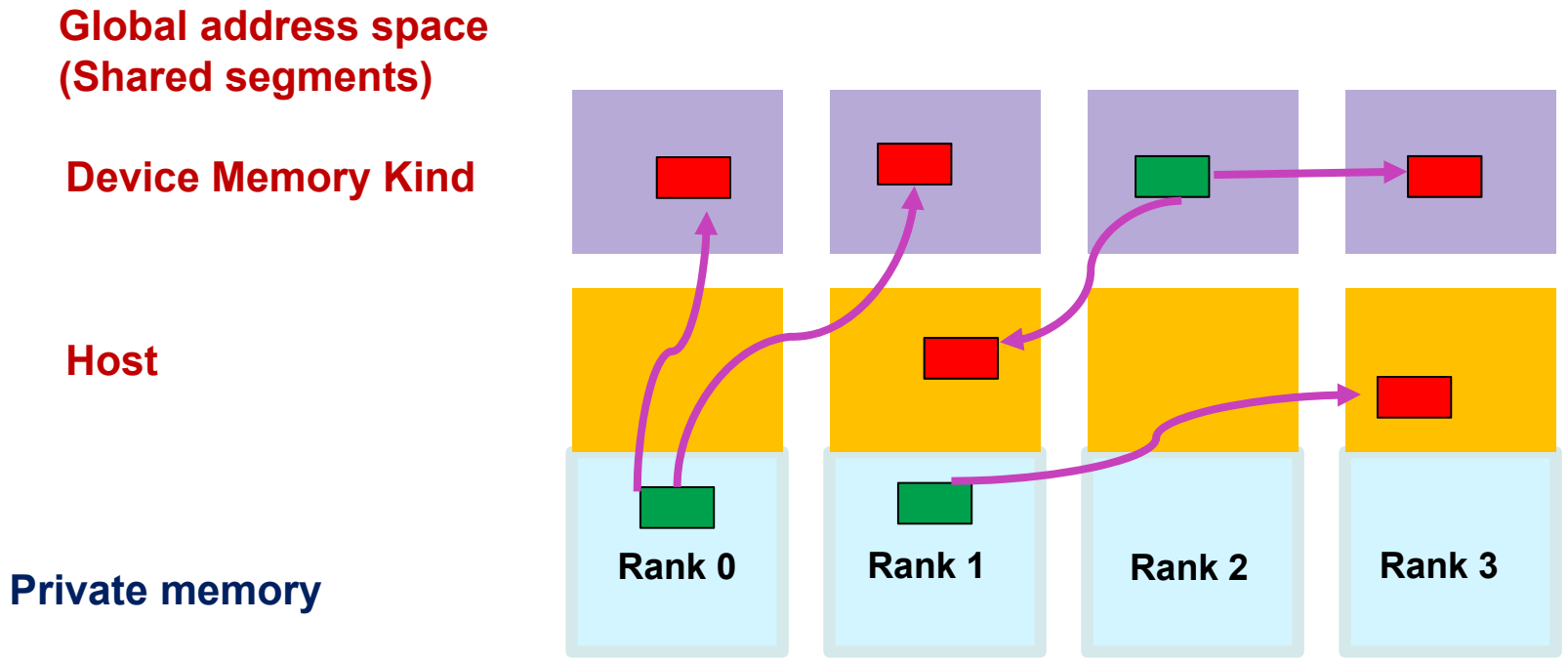
Memory Kinds

- UPC++ now supports memory kinds, which provides a uniform RMA interface for moving data between DRAM and GPU memory (or between GPU memories) transparently
- Avoids the need for different access methods

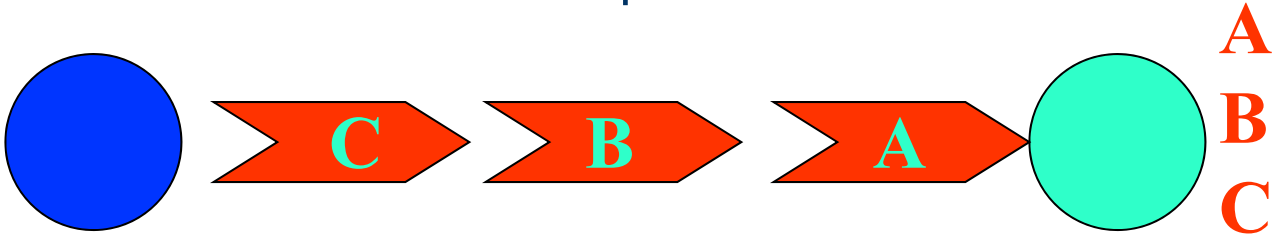


Why is PGAS attractive?

- The overheads are low
  Multithreading can't speed up overhead
- Memory per core is dropping, requiring reduced communication granularity
- Irregular applications exacerbate granularity problem
- Software managed memories are becoming more common, with different access methods.
  We need a unified method for accessing them
- Current and future HPC networks use one-sided transfers at their lowest level and the PGAS model matches this hardware with very little overhead

Where does message passing overhead come from?

- Matching sends to receives
  - Messages have an associated context that needs to be matched to handle incoming messages correctly
  - Data movement and synchronization are coupled
- Ordering guarantees are not semantically matched to the hardware
- UPC++ avoids these factors that increase the overhead
  - No matching overhead between source and target
  - Executes fewer instructions to perform a transfer



How does UPC++ deliver the PGAS model?

- A “Compiler-Free” approach
  - Need only a standard C++ compiler, leverage C++ standards
  - UPC++ is a C++ template library

- Relies on GASNet-EX for low overhead communication
  - Efficiently utilizes the network, whatever that network may be, including any special purpose offload support

- Designed to allow interoperation with existing programming systems
  - 1-to-1 mapping between MPI and UPC++ ranks
  - OpenMP and CUDA can be mixed with UPC++ in the same way as MPI+X

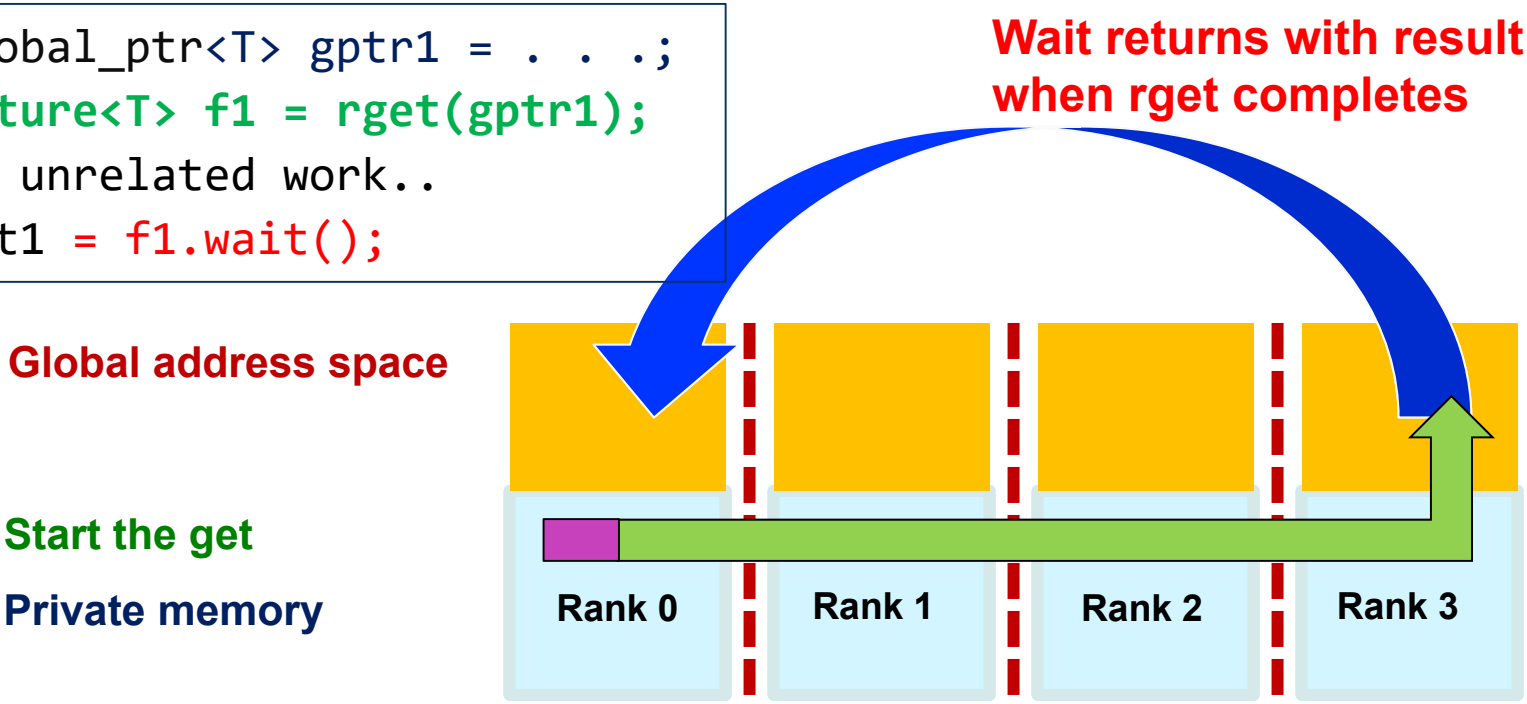
A simple example of asynchronous execution

By default, all communication ops are split-phased

- Initiate operation
- Wait for completion

  A future holds a value and a state: ready/not ready

```
global_ptr<T> gptr1 = . . .;
future<T> f1 = rget(gptr1);
// unrelated work..
T t1 = f1.wait();
```

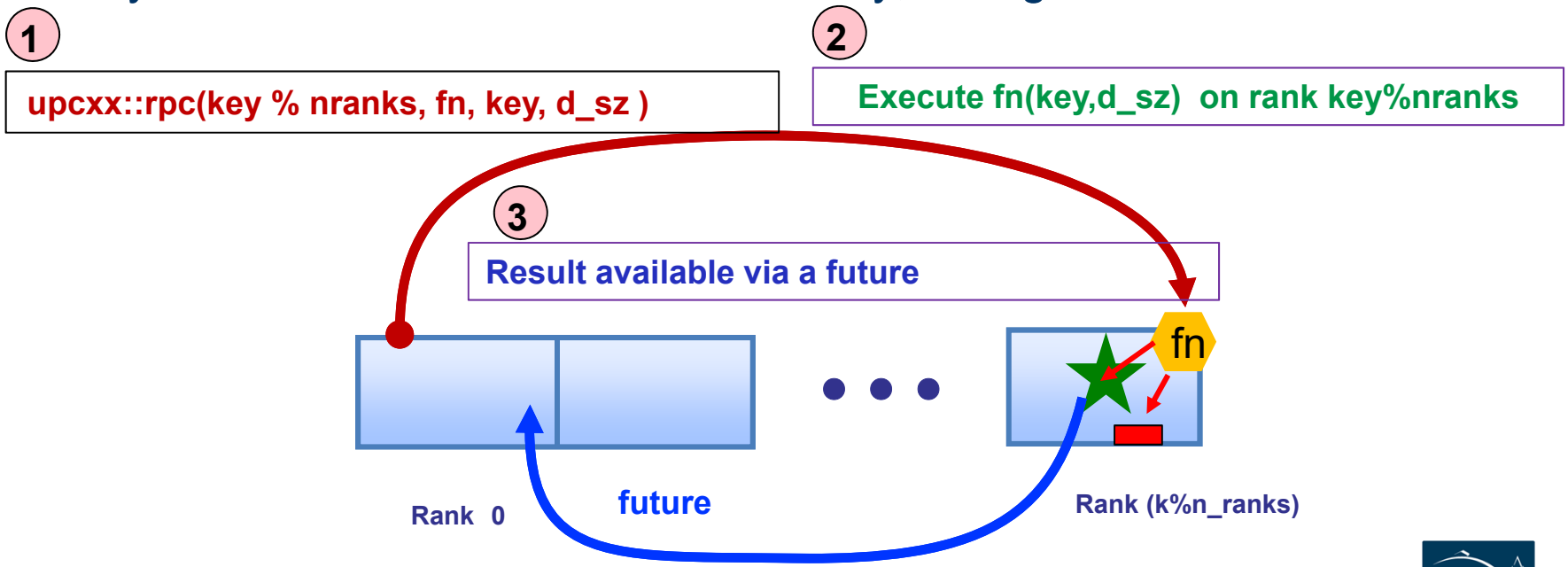


Simple example of remote procedure call

Execute a function on another rank, sending arguments and returning an optional result

1. Injects the RPC to the *target rank* key % nranks
2. Executes fn(key, d_sz) on target rank at some future time determined at the target
3. Result becomes available to the caller via the future

Many invocations can run simultaneously, hiding data movement



Composing asynchronous operations

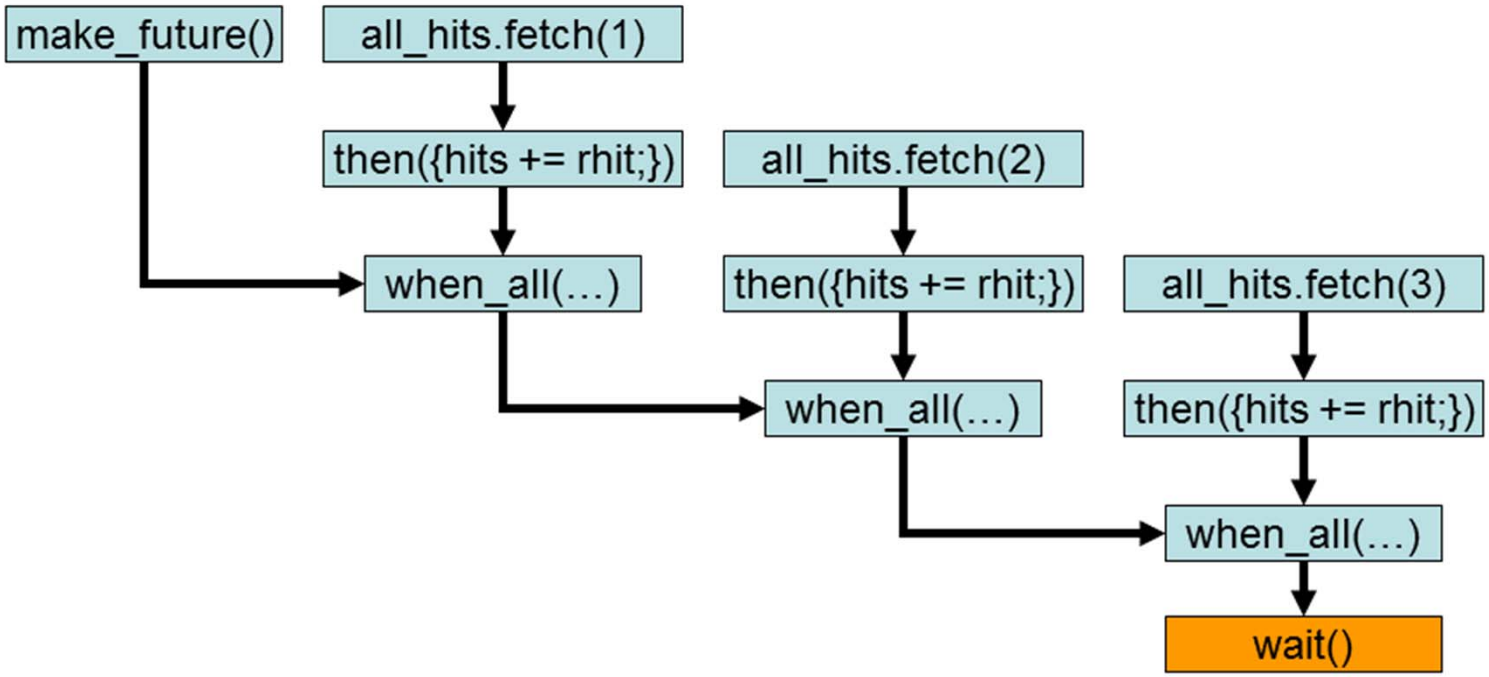
- Rput, rget and rpc return a future
- We can build a DAG of futures, synchronize on the whole rather than on the individual operations
  - Attach a callback: **`.then(Foo)`**
  - **`Foo`** is the completion handler, a function or λ
    - runs locally when the **`rget`** completes
    - receives arguments containing result associated with the future

```
double Foo(int x){ return sqrt(2*x); }

global_ptr<int> gptr1;
// …  gptr1 initialized
future<int>    f1 = rget(gptr1);
future<double> f2 = f1.then(Foo);
// DO SOMETHING ELSE
double y = f2.wait();
```

Conjoining futures

- We can join futures using when_all()
- (Example taken from *UPC++ Programmer's Guide*)



Road Map

An application

Memory Kinds (GPU Memory)

Inside UPC++

Distributed data structures

UPC++ in Context

Application: *De Novo* Genome Assembly

Construct a genome (chromosome) from a pool of short fragments, called *reads*, produced by sequencers

Analogy: shred many copies of a book, and reconstruct the book by examining the pieces

Complications: shreds of other books may be intermixed, can also contain errors

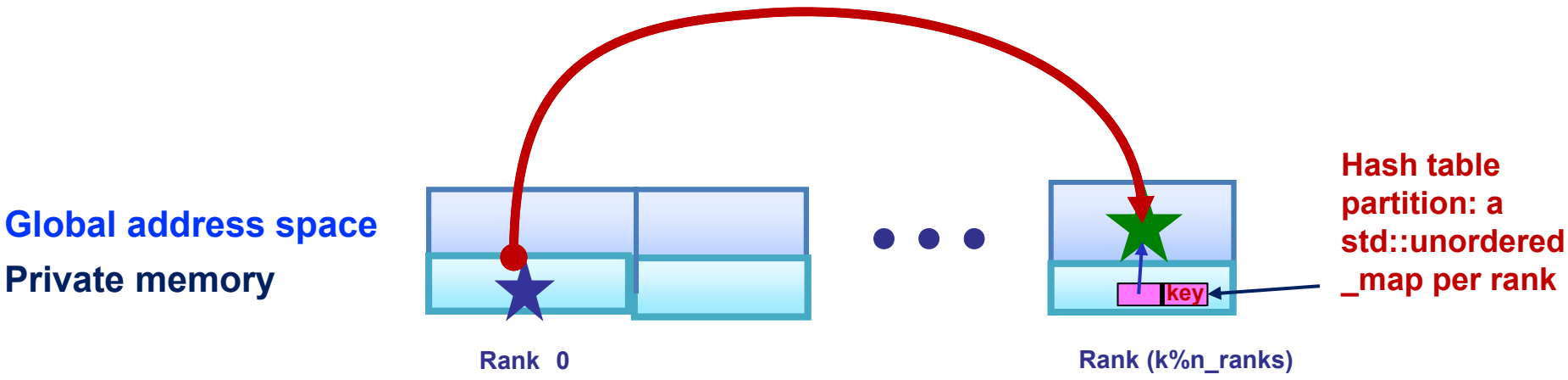
Chop the reads into fixed-length fragments (k-mers)

K-mers form a De Bruijn graph, traverse the graph to construct longer sequences

Graph is stored in a *distributed hash table*

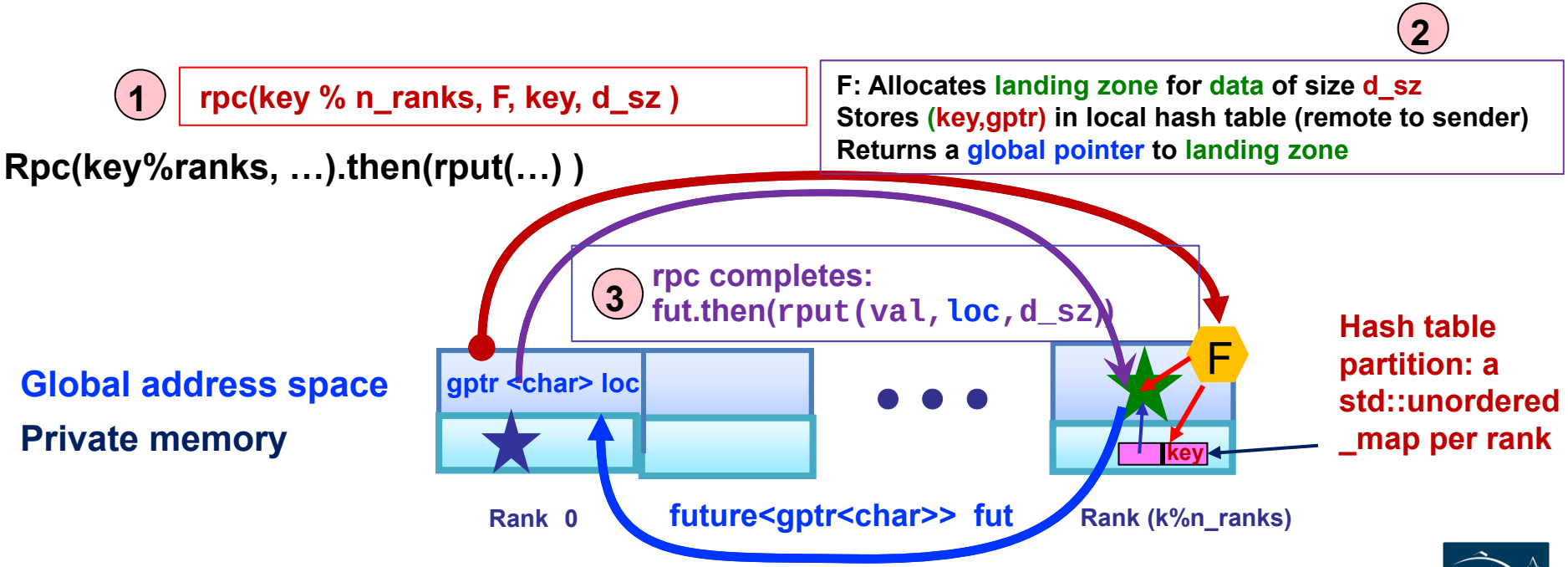
Distributed hash table implementation

- **Used in de-novo Genome Assembly**
- **This example motivates Remote Procedure Call (RPC)**
- **RPC** simplifies the distributed hash table design
- Store value in a distributed hash table, at a remote location



Distributed hash table implementation

- Store value in a distributed hash table, at a remote location
- RPC inserts the key @ target and obtains a landing zone pointer
- Once the RPC completes, an attached callback (.then) uses rput to store the associated data
- We use futures to build a small chain of dependent operations
- The returned future represents the whole operation



The hash table code

- We use lambda for the RPC function in this example
- RPC inserts key meta data at the target, & allocates the landing zone
  - Leverage implicit synchronization of rpc execution
- Once the RPC completes, the callback (.then()) that was attached to the RPC uses a zero copy rput to store the associated data
  - Exploits the power of rput for high performance RMA where available

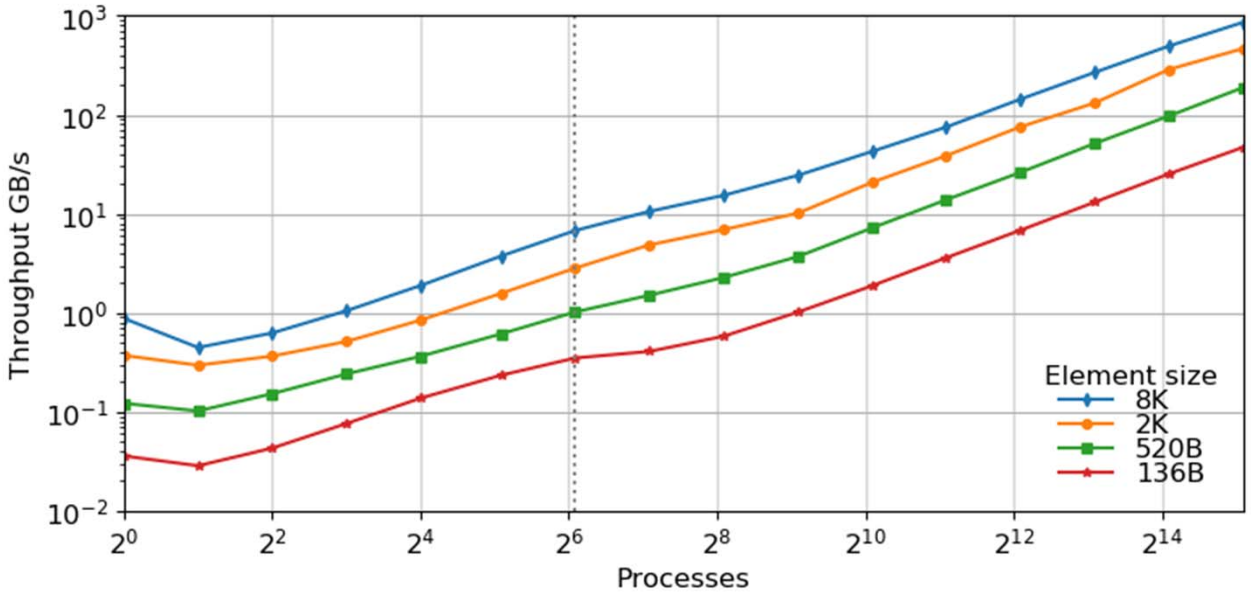
λ function

λ for callback

```
// C++ global variables correspond to rank-local state
std::unordered_map<uint64_t, global_ptr<char> > local_map;
// insert a key-value pair and return a future
future<> dht_insert(uint64_t key, char *val, size_t d_sz) {
   auto f1 = rpc(key % rank_n(),  // RPC obtains location for the data
             [](uint64_t key, size_t d_sz) -> global_ptr<char> {
                global_ptr<char> gptr = new_array<char>(d_sz);
                local_map[key] = gptr;              // insert in local map
                return gptr;
             }, key, d_sz);
   return f1.then( // callback executes when RPC completes
      [val,d_sz](global_ptr<char> loc) -> future<> { // λ: RMA put
                return rput(val, loc, d_sz); }
   );
}
```

Benefits of UPC++: distributed hash table

- Randomly distributed keys
- Excellent weak scaling up to 32K cores
- RPC leads to simplified and more efficient design
  - Key insertion and storage allocation handled at target
  - Without RPC, complex updates would require explicit synchronization and the need to use global storage, e.g. OpenSHMEM and MPI one-sided



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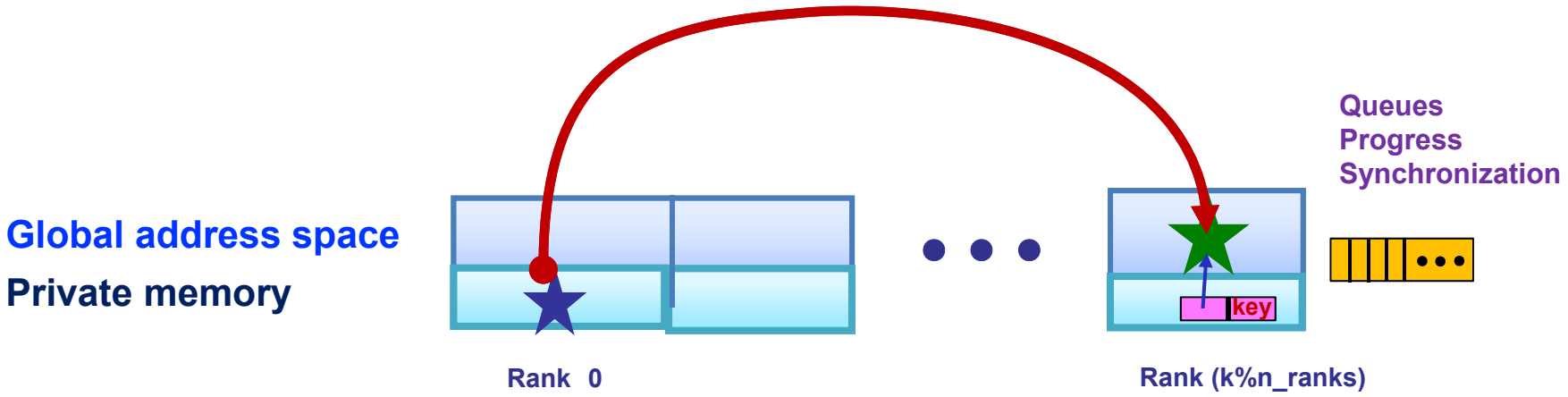
The productivity benefit of RPC

- More natural to express hash table insertion with RPC than with one sided communication or message passing
- RPC encapsulates argument passing, queue management and progress, factoring them out of the application code
- More generally, RPC simplifies the coding in updating complicated distributed data structures



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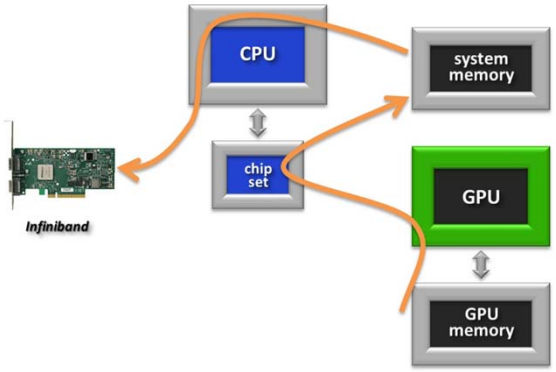
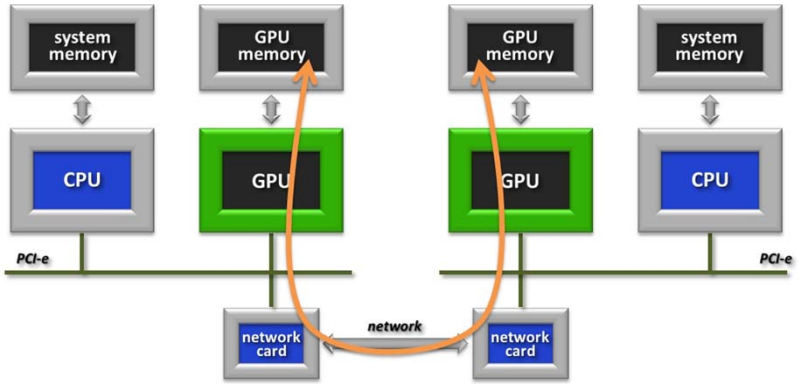
Memory kinds

In heterogeneous systems, we can have regions of memory requiring different access methods or performance properties (e.g. HBM, NVRAM)

Programming models can hide (or not hide) details

- MPI + CUDA (minimum of 2 additional copies)
- CUDA aware MPI (may or may not avoid 2 additional copies)



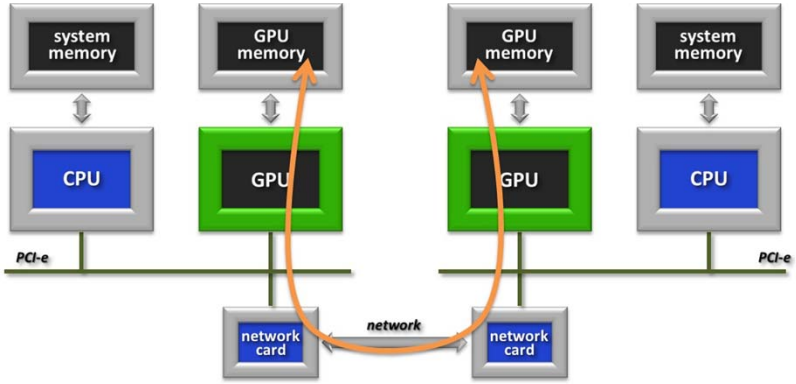


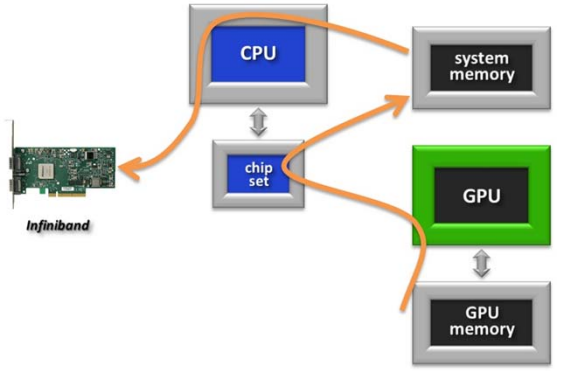
Figures courtesy Cheng, Grossman, and McKercher. *Professional Cuda C Programming*. John Wiley & Sons, 2014.

Memory kinds

UPCxx adds GPU memory kinds support (v2019.3.0)

- RMA transfers handled transparently between DRAM and Device Memory using global pointers
- Current implementation uses the extra copy model under the hood - so the user doesn't see the copying
- Future implementations (FY20) will use hardware support for direct communication





Figures courtesy Cheng, Grossman, and McKercher. *Professional Cuda C Programming*. John Wiley & Sons, 2014.

The API

We are required to construct an allocator for GPU memory with a specified segment size

Global pointers can refer to host or device storage

A single copy( ) method moves the data

```
auto gpu_device = cuda_device( 0 ); // Open device 0
// Construct and allocator with a 256 MB GPU segment
size_t segsize = 256*1024*1024;
auto gpu_alloc = device_allocator<cuda_device>(gpu_device, segsize);

// Use the allocator allocate an array of 1024 doubles on GPU
global_ptr<double,memory_kind::cuda_device> gpu_array =
gpu_alloc.allocate<double>(1024);

// Allocate an array of 1024 doubles on host
global_ptr<double> host_array = new_array<double>(1024);
// Transfer data from host buffer to device buffer
copy(host_array, gpu_array, 1024).wait();
```

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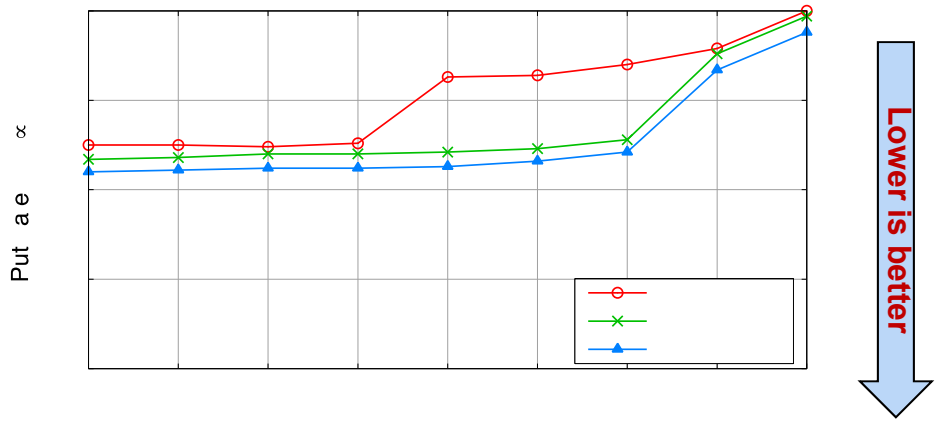
UPC++ in Context

A look under the hood of UPC++

- Relies on GASNet-EX to provide low overhead communication
  - Efficiently utilizes the network, whatever that network may be, including any special purpose support - low overheads
  - Get/put map directly onto the network hardware's global address support, when available
- RPC uses an active message (AM) to enqueue the function handle remotely.
  - Any return result is also transmitted via an AM
- RPCs can only make progress inside a call to a UPC++ method (Also a distinguished progress() method)
  - Thus, RPCs are serialized at the target, and this attribute can be used to avoid explicit synchronization

Performance of UPC++ - Latency

- Ping pong microbenchmark using blocking RMA
  - ~20% latency improvement from 16 to 256 bytes
  - Lines never cross at long message sizes not shown
- UPC++ rput, GASNet-Ex *testsmall* and publicly available MPI/IMB-RMA benchmark suite
  - Long sequence of blocking operations:
    issue put, wait for remote completion, repeat…
  - Latency = average time



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Toward distributed data structures

- Other models (UPC, CAF, OpenSHMEM) implement shared arrays via a symmetric heap
  - Scalable and portable implementation is difficult
  - Requires globally collective allocation that does not compose with subset teams
- UPC++ doesn't have a symmetric heap: heap allocation is not collective
- Initially, each rank only knows the locations of shared objects that it allocated
- How does a rank learn the locations of shared objects allocated by other ranks?

Distributed objects in UPC++

- How does a rank learn the locations of shared objects allocated by other ranks?
- UPC++ provides the *distributed object* (like co-arrays)
  - Globally unique name for each distributed object
  - Each entry holds a rank-specific value
  - Retrieve a remote value using a rank ID
  - Can be used to build a scalable, globally visible directory
- Distributed objects can be used to build shared distributed arrays, among other data structures
- UPC++ does not prescribe solutions, rather it provides building blocks for constructing them

Distributed 1D Arrays over UPC++

- Design is a work in progress
  - Likely similar to UPC pure-blocked shared array
  - Will support dynamic length and block size
  - Will be built over distributed objects, so it will have a scalable representation and support subset teams
- Exposes the cost of moving distributed data across the network. Compare with UPC, which supports off rank subscripting, but at a cost

```
dist_array<double> array(N, some_team);
// fetch ith element of array
future<global_ptr<double>> fut1 = array.pointer_to(i);
future<double> fut2 = fut1.then(rget);
// ... other work
double val = fut2.wait();
```

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UPC++ in context

- Only existing library with PGAS support that also offers RPC (X10, Chapel and Habanero are languages)
- OpenSHMEM is considering adding RPC
- Besides DASH, only model that support subset teams
- UPC++ supports distributed objects, a generalization of distributed arrays
  - Can construct an object over a subset team
  - Avoids a symmetric heap, which is not scalable
  - Distributed arrays: UPC, OpenSHMEM, DASH, X10, Chapel, co-array C++ via co-arrays

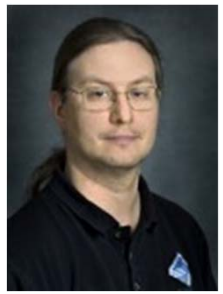
Persistent storage

- Idea: let's provide a unified global address space that spans storage and memories
- We map objects on disk into the shared segment
- Copy operators works with global pointers
- But not all persistent data can live in memory simultaneously, so we have to manage let the run time cache the data (custom paging)
- A useful operation is remote method invocation, which can leverage hardware offload support to carry out some filtering in the device controller:
  "find me all the data that meets a certain property"

Summary

- UPC++ provides future and continuation-based completion handling; RPC; one-sided communication
  - Embraces communication networks that use one-sided transfers at their lowest level: low overhead reduces the cost of fine-grained communication
  - Combines explicit locality control with shared memory
  - Overlap communication via asynchronous execution
- Productivity
  - Develop incrementally, enhance code selectively
  - Interoperates with MPI, OpenMP and CUDA
- More advanced constructs (not discussed)
  - Remote atomics, Distributed objects, teams and collectives
  - Promises, personas (end points), generalized completion
  - Serialization, non-contiguous transfers

The Pagoda Team

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Code and documentation at http://upcxx.lbl.gov

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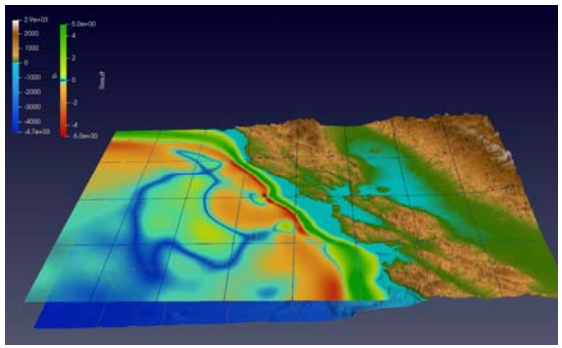

Figure courtesy Alexander Pöppl