Using Coroutines to Support Accelerators in TTG

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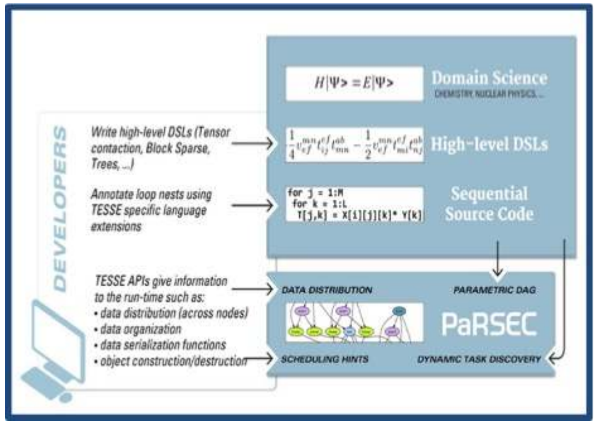
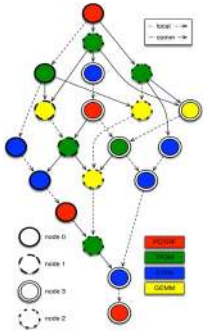
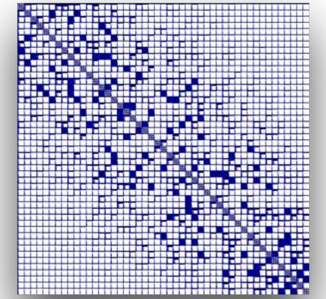
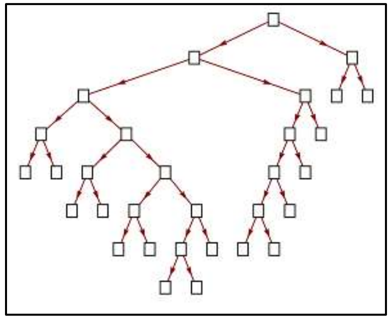


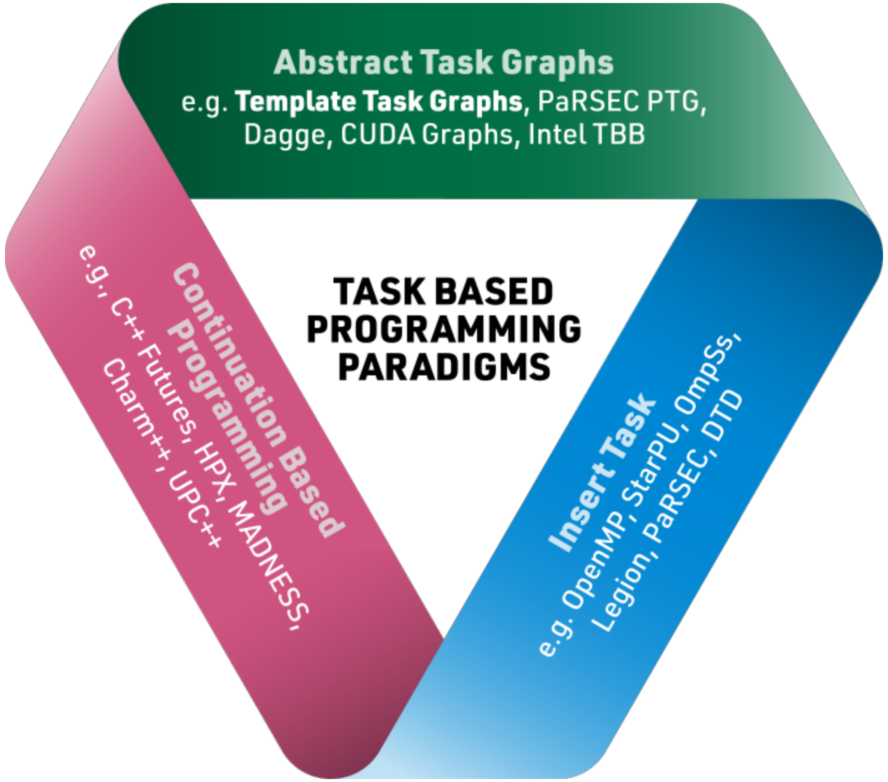

dense linear algebra


block-rank sparse algebra for quantum chemistry/physics


adaptive spectral-element calculus Multi-Resolution Analysis

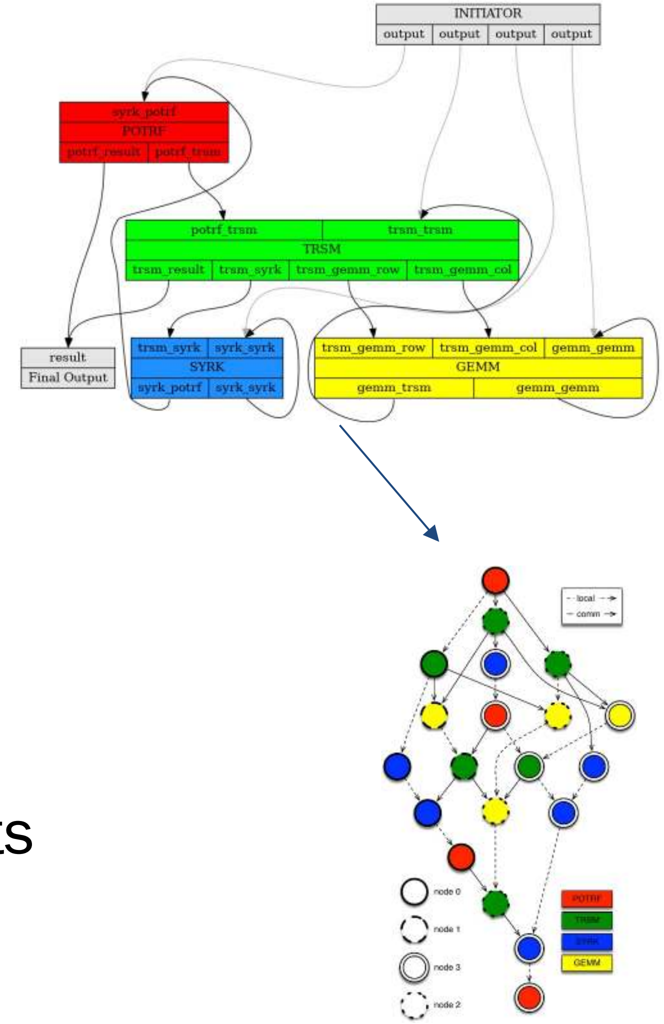
Task Systems

- Insert Task:
  - OpenMP, StarPU, PaRSEC DTD
  - Orchestration through dependencies on memory locations
- Continuations:
  - Futures representing results of tasks
  - Callbacks as reaction to the completion of tasks
- Abstract task graphs:
  - CUDA Graphs, C++ sender/receiver, PaRSEC, TTG
  - A priori description of task-graph instantiated during execution



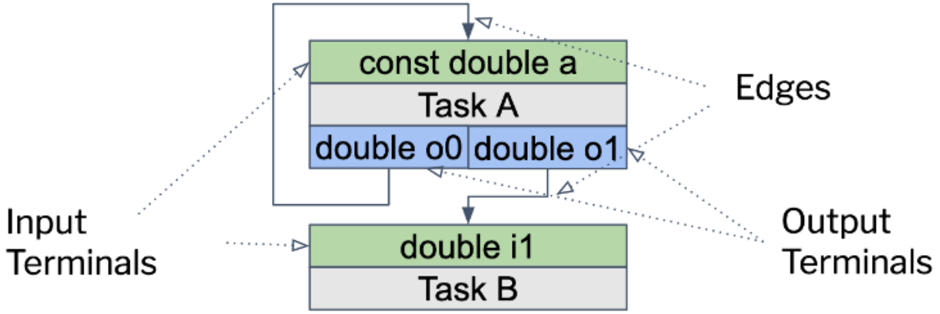
TTG: Overview

- Distributed Data Flow as Abstract Task Graph
  - May contain cycles
  - Nodes: template tasks
  - Edges: possible data flow between tasks
- Template Task Graph unrolled during execution
  - Tasks identified through (hashable) IDs (keys)
  - Data flows along edges as Pair {TaskID, Data}
- Data-dependent task discovery
  - Data may flow along different edges depending on results
- Scalable distributed task discovery



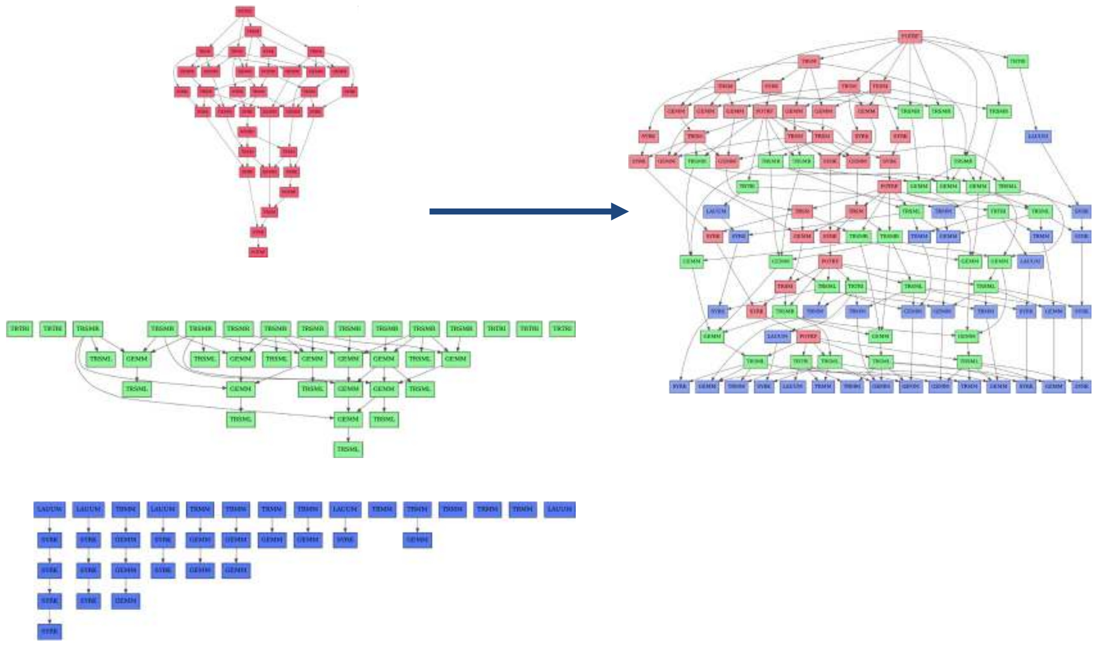
TTG: Tasks, Terminals, and Edges

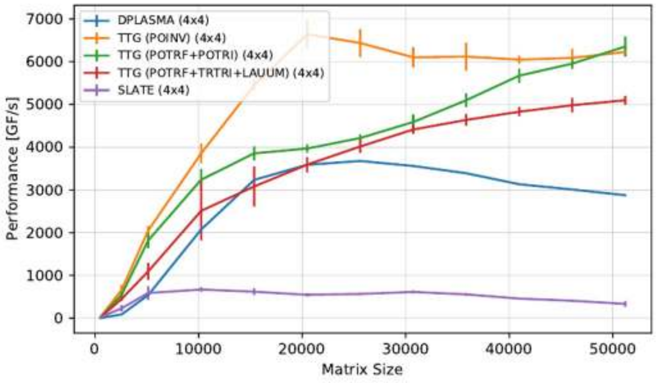
- Tasks: task with set number of inputs and outputs
  - Instantiated when first discovered
  - Executed once all inputs are available
- Terminals: inputs and outputs of a task, hidden from user code
- Edges: connects output terminals to input terminals
  - Data flows along edges
  - All possible paths between template tasks expressed through edges
  - Represent sets of data



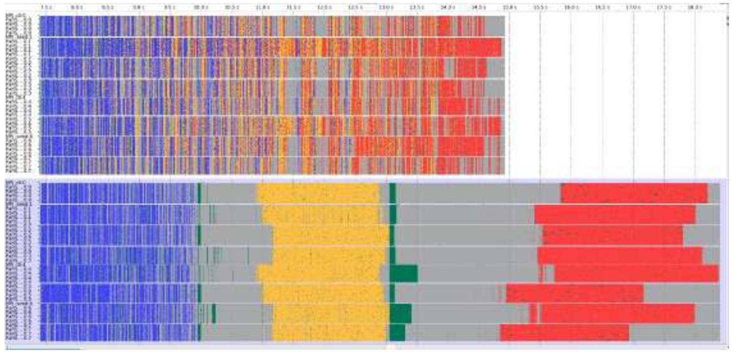
Task Graph Composition: POINV

- Edges enable composition of black-box task-graphs
- POINV = POTRF ⊕ TRTRI ⊕ LAUUM
- Benefits esp for small tiles



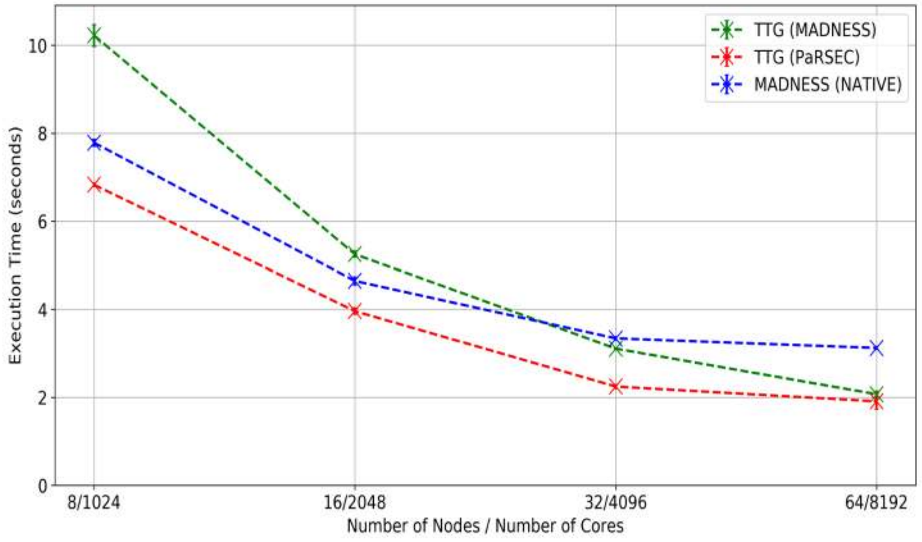


(a) Tile size 128.



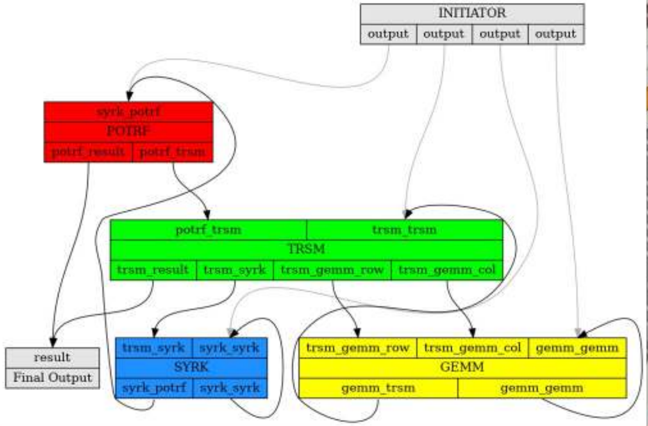
Target Applications: Multi-Resolution Analysis

- Order-10 multiwavelet representation of 3-D Gaussian functions, originally implemented in MADNESS
  - Hawk: 400 Functions, 8x16 threads per node



TTG Execution Model (General)

- SPMD: all processes execute the same program in main thread
- ttg::World: query number of processes and local rank
  - Split processes between multiple worlds (i.e., communicators)
- Single or multiple entry points into the DAG
  - Process(es) kick off computation by feeding data into the task graph
  - Executing process controlled through mapper function
- Worker threads non-preemptively execute tasks
- Fence to wait for execution to complete
- Multiple task-graphs can be active concurrently



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TTG: Small Example

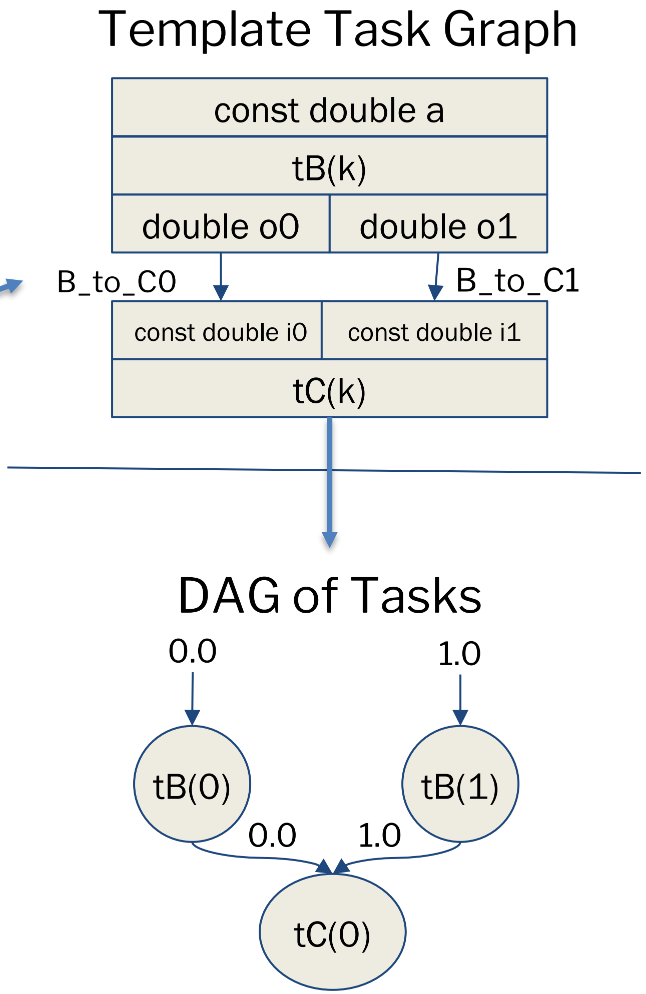
```
ttg::Edge<int, double> to_B("to_B");
ttg::Edge<int, double> B_to_C0("B_to_C0");
ttg::Edge<int, double> B_to_C1("B_to_C1");

auto tb = ttg::make_tt([](const int &k, const double &a) {
    // Task tB(k) received value a for input 0
    if(0 == k) ttg::send<0>(0, a);
    if(1 == k) ttg::send<1>(0, a);
  },
  ttg::edges(to_B),
  ttg::edges(B_to_C0, B_to_C1));

auto tc = ttg::make_tt([](const int &k, const double &i0, const double &i1)
  {
    // Task tC(k) received two inputs: i0 and i1
  },
  ttg::edges(B_to_C0, B_to_C1),
  ttg::edges());

ttg::make_graph_executable(tb);
if(tb->get_world().rank() == 0) {
  tb->invoke(0, 0.0);
  tb->invoke(1, 1.0);
}
ttg::execute();
ttg::fence();
```

Input edges

Output edges

Input edges

Kick off tasks

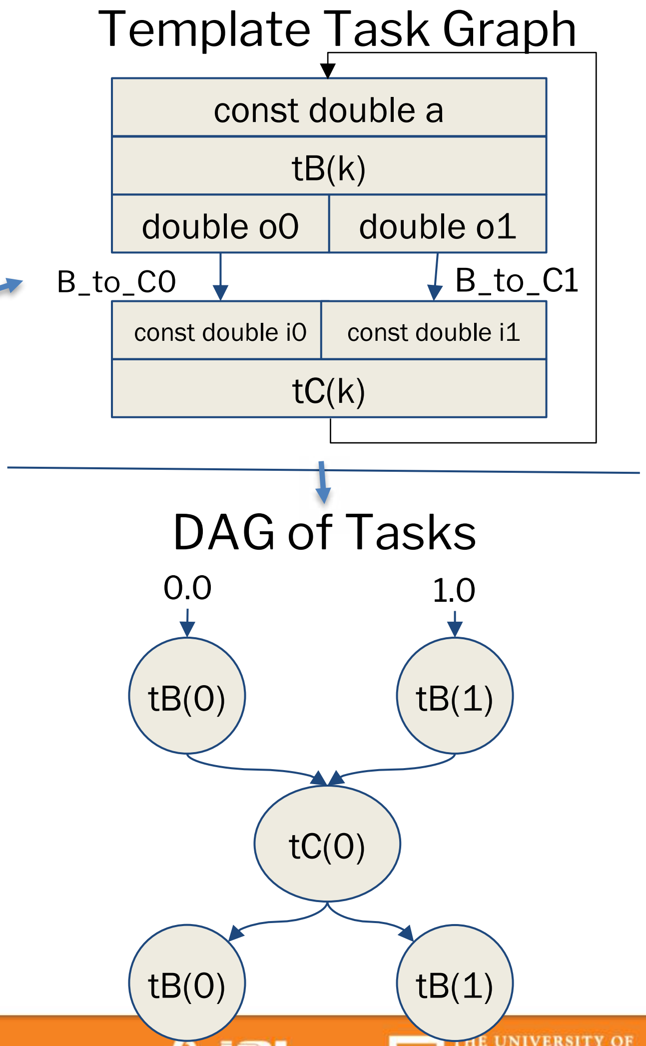


Simplifications work in progress

TTG: Small Example / Cycle

```
ttg::Edge<int, double> to_B("to_B");
ttg::Edge<int, double> B_to_C0("B_to_C0");
ttg::Edge<int, double> B_to_C1("B_to_C1");
ttg::Edge<int, double> C_to_B(”C_to_B");

auto tb = ttg::make_tt([](const int &k, const double &a) {
    // Task tB(k) received value a for input 0
    if(0 == k) ttg::send<0>(0, a);
    if(1 == k) ttg::send<1>(0, a);
  },
  ttg::edges(ttg::fuse(to_B, C_to_B),
  ttg::edges(B_to_C0, B_to_C1));

auto tc = ttg::make_tt([](const int &k, const double &i0, const double &i1)
  {
    if (need_recursion(i0, i1)) {
      ttg::send<0>(0, i0); // send i0 back to task B
      ttg::send<0>(1, i1); // send i1 back to task B
    }
  },
  ttg::edges(B_to_C0, B_to_C1),
  ttg::edges(C_to_B));

ttg::make_graph_executable(tb);
if(tb->get_world().rank() == 0) {
  tb->invoke(0, 0.0);
  tb->invoke(1, 1.0);
}
ttg::execute();
ttg::fence();
```

Fused Edges



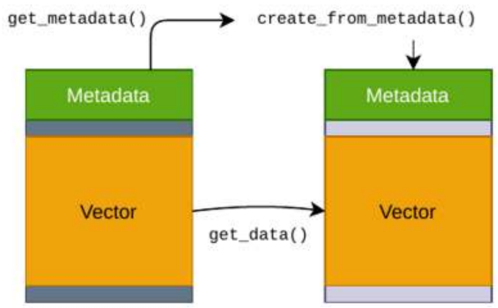
Task IDs and Process Mapping

- Tasks identified by hashable objects
  - Typically pairs, tuples, small structs
- Default mapping: round-robin
- Application may provide custom mapping of task IDs to processes
- Similar mechanism for task priorities

```
struct Key {
  int i, j;
  std::size_t hash() {
    return (i<<32) + j;
  }
};

Matrix A = ...; // matrix instance
auto tt = ttg::make_tt(...);
tt->set_procmap(
  [&](const Key& key){
    // map {i, j} coords to owner of tile
    return A.process_of({key.i, key.j});
  });

tt->set_priomap(
  [&](const Key& key){
    // generate priority for task {i, j}
    return priority_of(key.i, key.j);
  });
```

TTG Memory Model (General)

- TTG manages transfers between processes
  - No explicit receives
  - Only send/broadcast to successor tasks, addressed by keys
- All data flowing along edges must be
  - Serializable (MADNESS/Boost/trivially copyable); or
  - Zero-copyable (Split Metadata API)
- Immutable objects shared between tasks
  - C++ const and move semantics
- Mutable data copied unless moved



Const and Move Semantics

- Runtime tracks and reuses object copies wherever possible
- Const input parameters allow objects shared between tasks
- Move semantics signal that mutable objects are not mutated anymore
- Non-const inputs may require additional copies (except for single-use inputs)

```
// Sending mutable data
[](const int &k, T&& a) {
    mutate(a);              // updates a
    ttg::send<0>(k+1, a); // creates a new copy
    reset(a);               // a is mutated again
    ttg::send<1>(k+1, a); // create yet another copy
}

// Moving input data
[](const int &k, T&& a) {
    mutate(a); // update a
    ttg::send<0>(k+1, std::move(a)); // no new copy
}

// Forwarding const input data
[](const int &k, const T& a) {
    ttg::send<0>(k-1, a); // no new copy
    ttg::send<0>(k,   a); // no new copy
    ttg::send<0>(k+1, a); // no new copy
}

// Sending stack-based data
[](const int &k) {
    T a = new_obj(k);
    ttg::send<0>(k-1, std::move(a)); // potential copy
}
```

Send and Broadcast

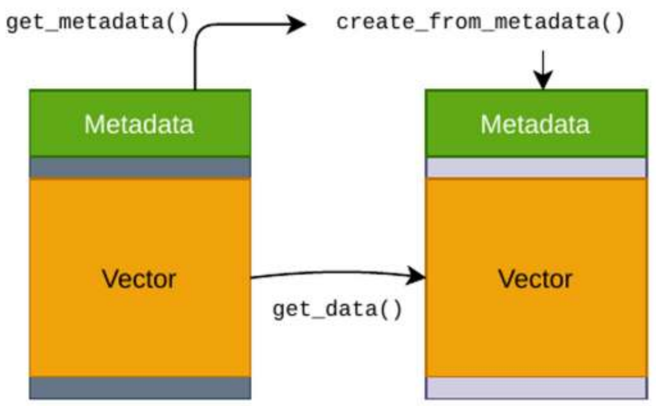
- Broadcasts provide single-statement data transfers to multiple successor tasks
- May send on one or more output terminals (i.e., along multipe edges)

```
// Sending mutable data to one successor
[](const int &k, T&& a) {
    mutate(a);            // updates a
    ttg::send<0>(k+1, std::move(a));
}

// Sending mutable data to multiple successors
[](const int &k, T&& a) {
    mutate(a);
    std::vector<int> broadcast_keys;
    for (int i = 0; i < num_successor; ++i) {
      broadcast_keys.push_back(k+i);
    }
    ttg::broadcast<0>(broadcast_keys, std::move(a));
}

// Sending mutable data to multiple successors on
different output terminals
[](const int &k, T&& a) {
    mutate(a);
    std::vector<int> broadcast0_keys;
    std::array<int, 3> broadcast1_keys = {k+1, k+2, k+3};
    for (int i = 0; i < num_successor; ++i) {
      broadcast0_keys.push_back(k+i);
    }
    ttg::broadcast<0,1>(broadcast0_keys,
                        broadcast1_keys,
                        std::move(a));
}
```

Zero-copy Data Movement

- Used for transfers between processes to avoid serialization

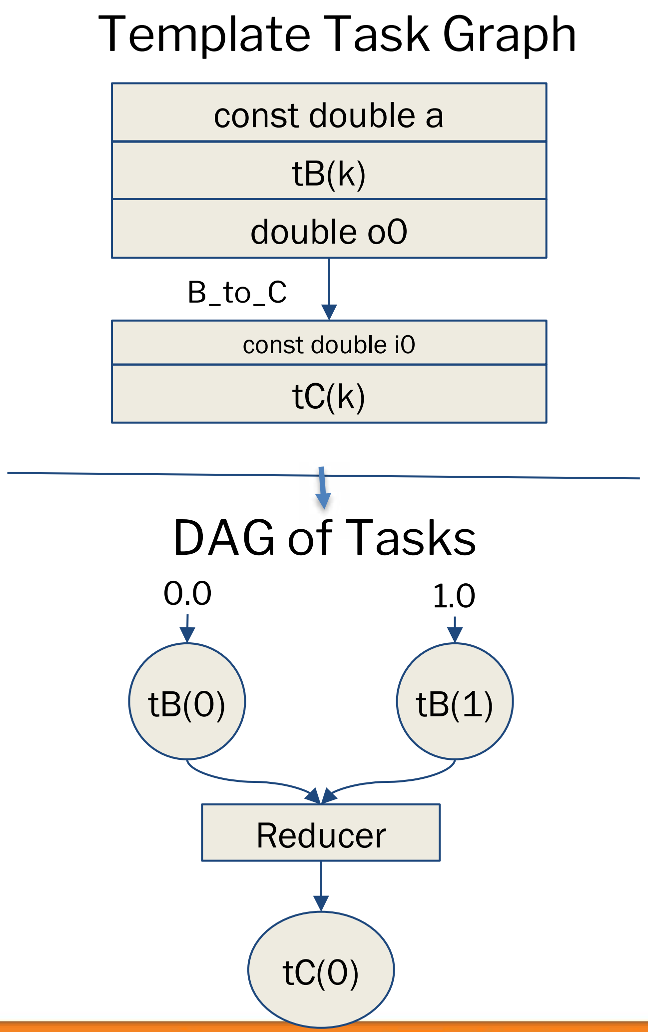
```
struct Tile {
  std::size_t m, n, lda;
  std::vector<double> data;
  struct metadata {
    std::size_t m, n, lda;
  };
  ... // ctors, dtors, accessors
};

template<typename T>
struct ttg::SplitMetadataDescriptor<Tile<T>> {
 // provide metadata
  auto get_metadata(const Tile<T>& t) {
    return Tile<T>::metadata{t.m(), tile.n(), tile.lda()};
  }
 // provide payload to be transferred
  auto get_data(Tile<T>& t) {
    return std::array<ttg::iovec, 1>{{t.size(), t.data()}};
  }
  // create an empty tile from metadata
  auto create_from_metadata(const typename Tile<T>::metadata& md) {
    return Tile<T>{md.m, md.n, md.lda};
  }
};
```



Reduction Terminals

- So far: one parameter per input
- Tasks may have a large number of inputs that can be reduced to a single value

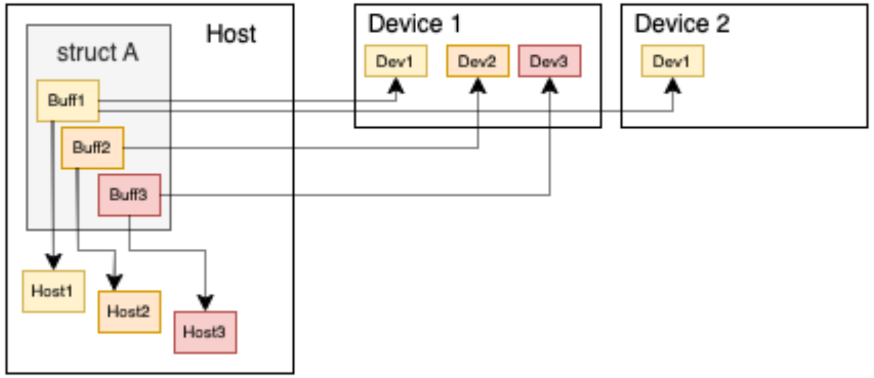
```
ttg::Edge<int, double> to_B("to_B");
ttg::Edge<int, double> B_to_C("B_to_C");

auto tb = ttg::make_tt([](const int &k, const double &a) {
    // Task tB(k) received value a for input 0
    ttg::send<0>(0, a);
  },
  ttg::edges(to_B),
  ttg::edges(B_to_C));

auto tc = ttg::make_tt([](const int &k, const double &i)
  {
    // Task tC(k) received sum of inputs: i
  },
  ttg::edges(B_to_C), ttg::edges());

// set reducer on input terminal 0: lhs = lhs ⊕ rhs
tc->template set_input_reducer<0>(
  [](double& lhs, const double& rhs){
    lhs += rhs;
  }, 2);
```



TTG Memory Model (Device)

- TTG manages device memory
- Host memory serves as backup for transparent eviction
  - Memory oversubscription supported by default
- Transparent data movement between devices and host
  - Automatic migration from device to host tasks
- ttg::Buffer: owning/non-owning host memory mirror

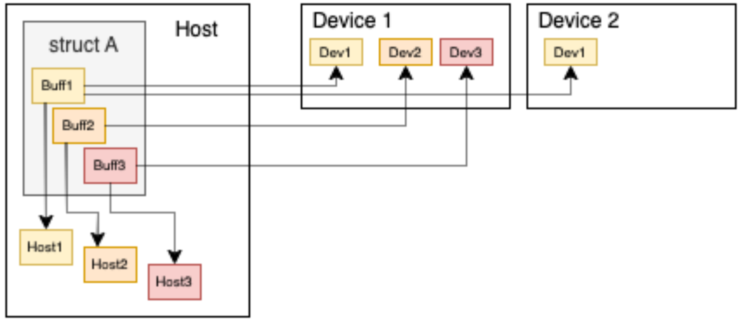
TTG Device integration still experimental



Buffers: Device memory containers

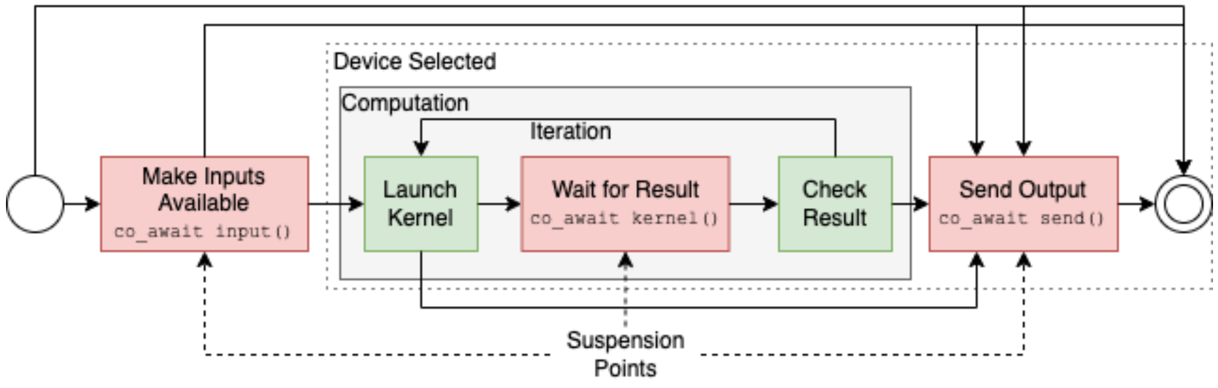
- Owns host memory, unless user-provided
- Tracks last device task location
- Enables transparent migration of data between devices and host
- Allows partial mapping of complex data structures to devices
  - Some tasks may not require all object data on the device

```
template<typename T>
struct Tile {
  ttg::Buffer<T> buf;
  size_t m, n, lda;
  Tile(size_t m, size_t n, size_t lda)
  : buf(m*n) // buffer owns host memory
  { }
  Tile(T *ptr, size_t m, size_t n, size_t lda)
  : buf(ptr, m*n) // buffer does not own host memory
  { }
  // other constructors and accessors
};
```



TTG Execution Model (Device)

1. Tasks declare input data (ttg::Buffer, scratch data)
2. TTG runtime assigns a device and execution stream based on inputs and device load
   - One management thread per device (PaRSEC)
3. Tasks submit kernels and H2D transfers into stream and suspend
4. Runtime returns once execution completed
5. Task may:
   - Submit more kernels; or
   - Send out results to successors



TTG Device Tasks

- "co_await input()" selects device
- "co_await kernel()" accepts buffers/scratch to return to host
- Task may submit and wait for multiple kernels
- Sending outputs is last step of task

```
template<typename T>
struct Tile {
  ttg::Buffer<T> buf;
  size_t m, n, lda;
  Tile(size_t m, size_t n, size_t lda)
  : buf(m*n) // buffer owns host memory
  { }
  Tile(T *ptr, size_t m, size_t n, size_t lda)
  : buf(ptr, m*n) // buffer does not own host memory
  { }
  // other constructors and accessors
};
```

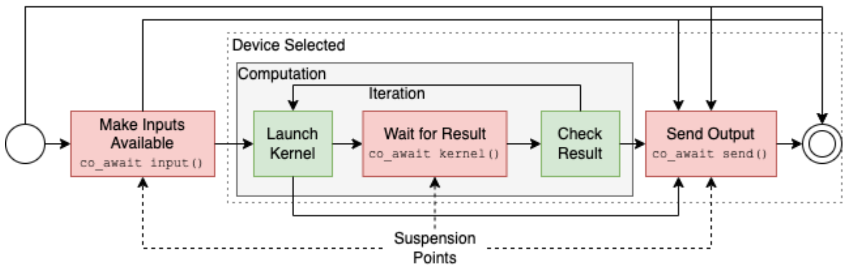
```
using Key = std::pair<int, int>; // tile position in matrix

auto tb = ttg::make_tt([](const Key& k, Tile&& a)
          -> ttg::device::task {
    co_await ttg::device::input(A.buf); // make A available
    submit_kernel(a);
    co_await ttg::device::kernel(); // optional if no result required
    co_return ttg::device::send<0>(k, std::move(a));
  }, ...);
```

Make inputs available

Submit work

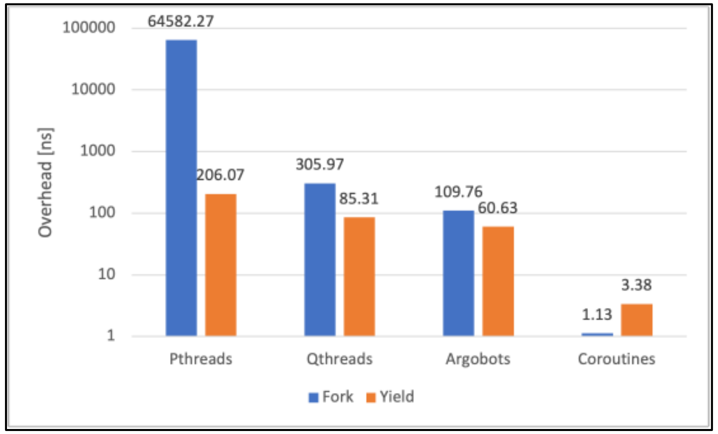
Wait for kernel to execute (optional)

Send Output

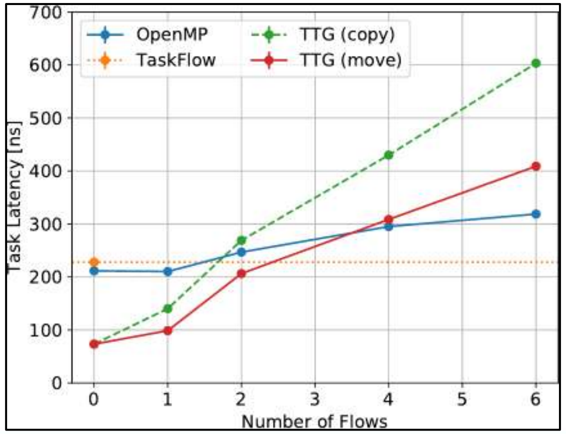


Why Coroutines?

- TTG provides low-overhead task execution
- Device tasks:
  - Kernel submission
  - Successor discovery
- Fibers/ULTs provide flexibility, at a cost
- Compiler-assisted suspension ~ function call
- Avoids code fragmentation



Task Overhead



Coroutines vs Continuations

- Continuation-passing causes to code fragmentation
- Worse yet: careful handling of task-local state

```
using Key = std::pair<int, int>; // tile position in matrix

auto tb = ttg::make_tt([](const Key& k, Tile&& a) {
    ttg::device::input(A.buf)
      .then(
        [](double *ptr){ return submit_kernel(ptr); }
      ).then(
        [&](){ ttg::send<0>(k, std::move(a)); }
      )
    );
  }, ...);
```

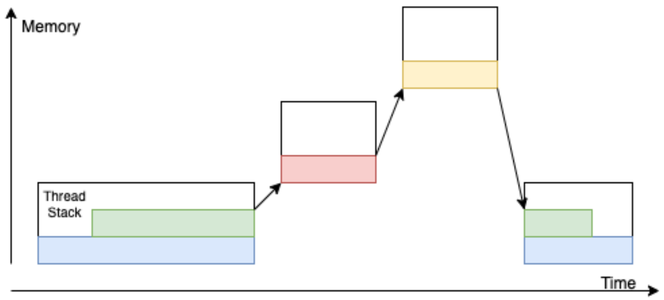
Reduced code fragmentation

```
using Key = std::pair<int, int>; // tile position in matrix

auto tb = ttg::make_tt([](const Key& k, Tile&& a)
          -> ttg::device::task {
    co_await ttg::device::input(A.buf); // make A available
    submit_kernel(a);
    co_await ttg::device::kernel(); // optional if no result required
    co_return ttg::device::send<0>(k, std::move(a));
  }, ...);
```

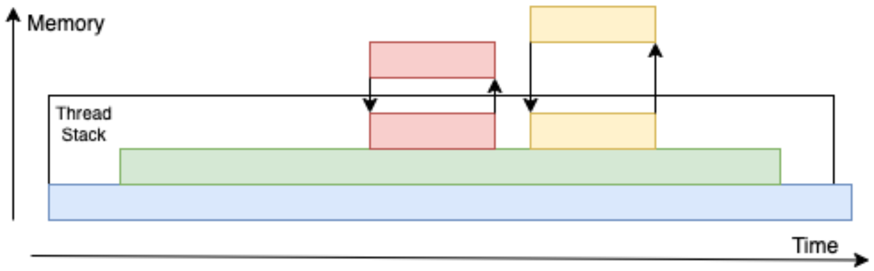
Coroutines vs Fibers/ULTs

- Fibers switch the stack of the executing thread
- Require allocation of stacks, likely unused
- Coroutines only allocate state saved between invocations and act like function calls

Fibers



Coroutines



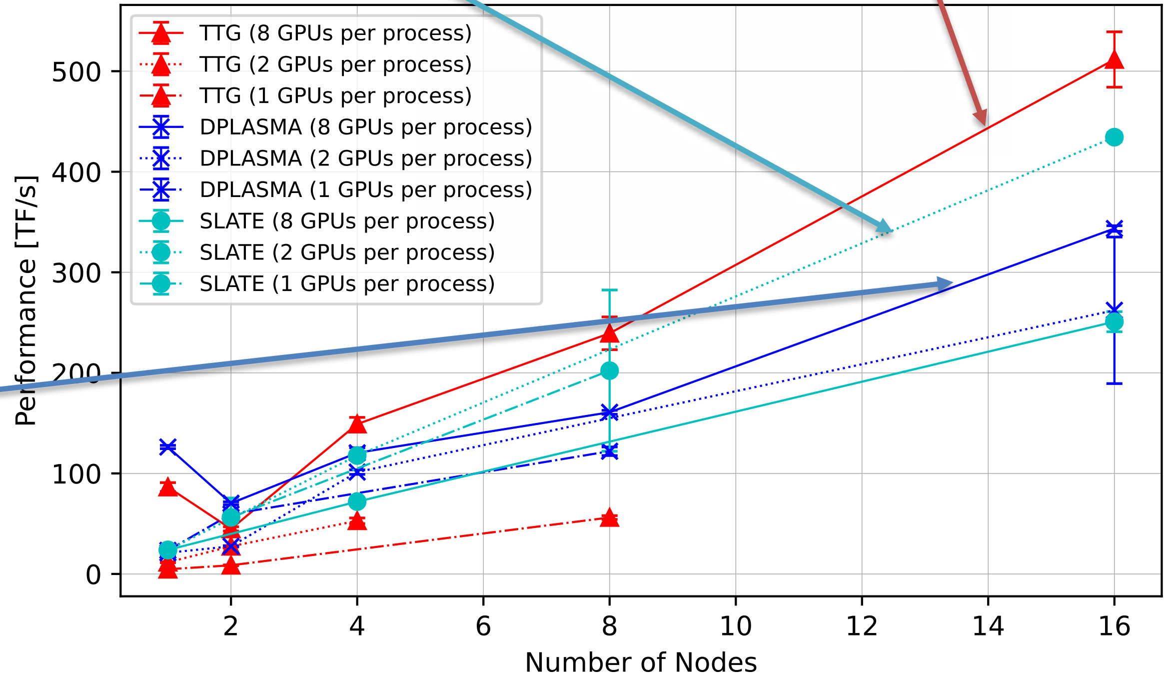
Preliminary Result: Dense GEMM

- Frontier: 8x MI250X per node
- Weak scaling: 32x32 1k tiles per GPU

SLATE: 2 GPUs per process

TTG: 8 GPUs per process

DPLASMA: 8 GPUs per process

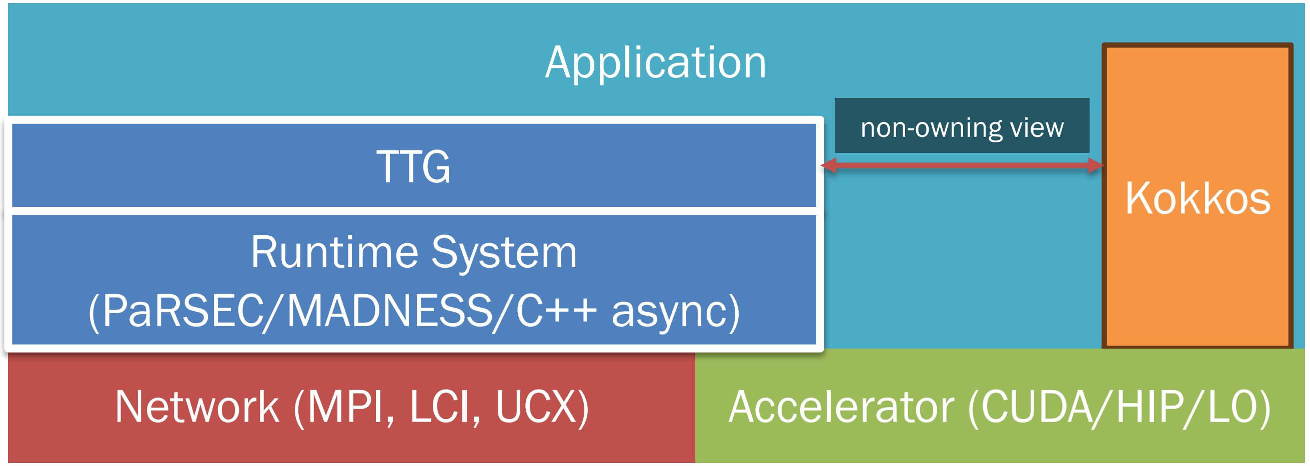


TTG shows good scaling but results are incomplete…

Kokkos and TTG

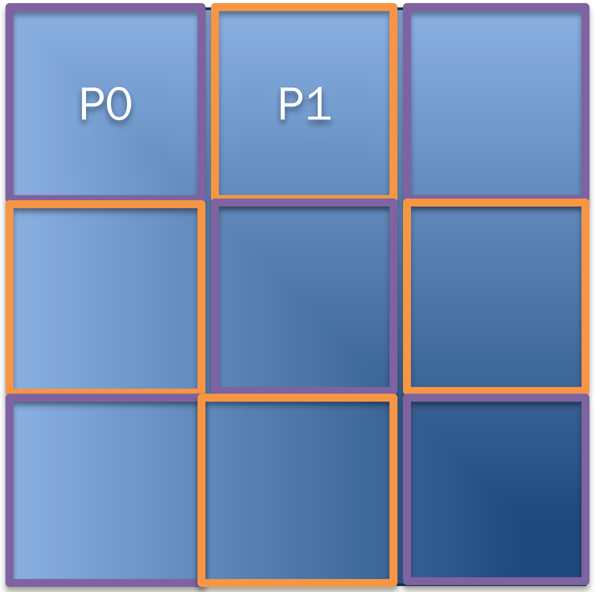
- TTG: distributed data-flow programming
  - No interest in providing task-level concurrency
- Integration point: non-owning Kokkos::View & execution environments
  - TTG manages device memory (ttg::buffer) and distributed execution
  - Kokkos provides accelerator programming infrastructure

Open challenge: Multi-GPU support in Kokkos



TTG and Kokkos: PLGSY

- PLGSY: generation of symmetric diagonally dominant matrix
  - Independent of process grid and tile size
- Position of tile: encoded in task ID
- Not an official BLAS function
  - Part of (D)PLASMA
- Initialization of tiles fed into task graph



Kokkos PLGSY Kernel

```
TiledMatrix<T> matrix; // provides

using Key = std::pair<int, int>; // tile position in matrix

void CORE_plgsy(const Key& key, T* tile, int m, int n, int lda, T bump) {
  using layout_type = Kokkos::LayoutStride;
  auto layout = layout_type(m, lda, n, 1);
  auto view = Kokkos::View<T**, layout_type>(tile, layout);
  auto es = Kokkos::Cuda(ttg::device::current_stream());
  if ( m0 == n0 ) { // diagonal
    Kokkos::parallel_for("diagonal",
      Kokkos::MDRangePolicy<Kokkos::Cuda, Kokkos::Rank<2>>(es, {0, 0}, {n, m}),
      KOKKOS_LAMBDA(int row, int col) {
        view(row, col) = gen(m, n, lda, key); // generate value for element
        if (row == col) { // bump diagonal element
          view(row, col) += bump;
        }
      });
   } else if (...) {
    ...
}

auto tb = ttg::make_tt([](const Key& k, Tile&& tile)
          -> ttg::device::task {


    co_await ttg::device::to_device(tile.buf); // make tile available
    auto ptr = tile.buf.current_device_ptr(); // memory on assigned device
    CORE_plgsy(key, ptr, tile.m(), tile.n(), tile.n(), ...);



    co_return ttg::device::send<0>(k, std::move(A));
  }, ...);
```

- Stride Layout
- CUDA w/ explicit stream
- MDRange
- Make tile memory available
- Submit Kokkos kernel
- Send to successor

Kokkos PLGSY Kernel w/ Norm

- Useful for debugging

```
TiledMatrix<T> matrix; // provides

using Key = std::pair<int, int>; // tile position in matrix

void CORE_plgsy(const Key& key, T* tile, int m, int n, int lda, T bump) {
  using layout_type = Kokkos::LayoutStride;
  auto layout = layout_type(m, lda, n, 1);
  auto view = Kokkos::View<T**, layout_type>(tile, layout);
  auto es = Kokkos::Cuda(ttg::device::current_stream());
  if ( m0 == n0 ) { // diagonal
    Kokkos::parallel_for("diagonal",
      Kokkos::MDRangePolicy<Kokkos::Cuda, Kokkos::Rank<2>>(es, {0, 0}, {n, m}),
      KOKKOS_LAMBDA(int row, int col) {
        view(row, col) = gen(m, n, lda, key); // generate value for element
        if (row == col) { // bump diagonal element
          view(row, col) += bump;
        }
      });
  } else if (m0 > n0) {
    ...
}

auto tb = ttg::make_tt([](const Key& k, Tile&& tile)
          -> ttg::device::task { // make lambda a coroutine
    T norm;
    auto scratch = ttg::make_scratch(&norm);
    co_await ttg::device::to_device(tile.buf, scratch); // make tile available
    auto ptr = tile.buf.current_device_ptr(); // memory on assigned device
    CORE_plgsy(key, ptr, tile.m(), tile.n(), tile.n(), ...);
    compute_norm(ptr, scratch.device_ptr());
    co_await ttg::device::wait_kernel(scratch); // optional if no result required
    tile.set_norm(norm);
    co_return ttg::device::send<0>(k, std::move(A));
  }, ...);
```

Scratch valid for task lifetime

Calls *blas*nrm2

Waits for norm transfer

Summary

- TTG provides scalable task discovery through abstract task graphs
- Coroutines simplify data and kernel management on the device
- Early results on GPUs promising

- Future Work:
  - Aggregation and pull terminals
  - Expanded use of coroutines (e.g., task ID generator in broadcasts)
  - Device-first memory allocation (on-demand host allocation)
  - Batched kernel tasks
  - Applications (SPMM, MRA, MADNESS/TA integration, ?)

Part 2: (Results of) Using Co-routines to Support Accelerators in TTG

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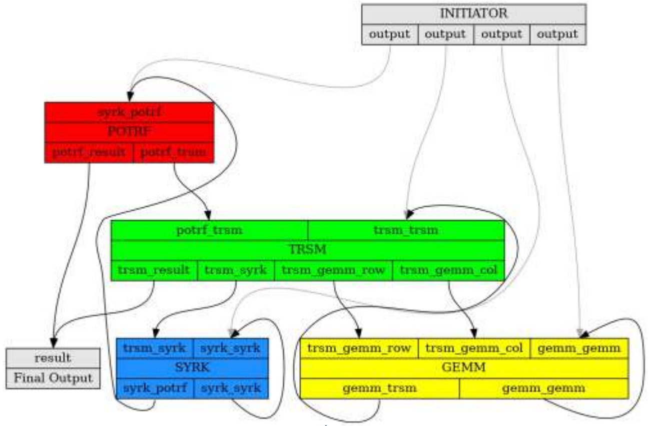
Stony Brook University (IACS)

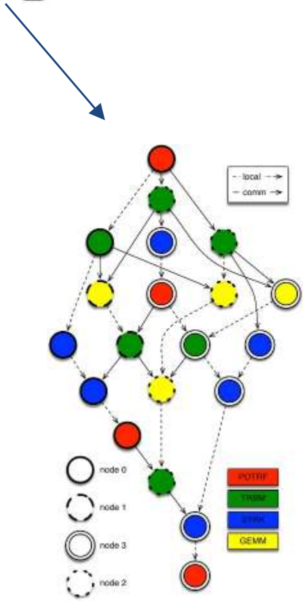
HiHAT Monthly Review
January 16, 2024

Recap

TTG: Overview

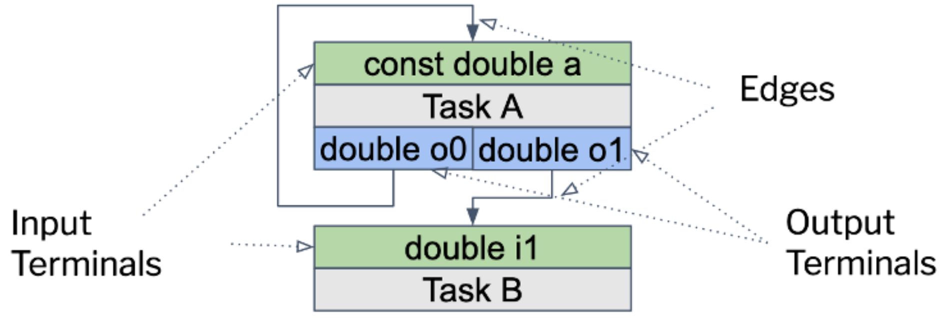
- Distributed Data Flow as Abstract Task Graph
  - May contain cycles
  - Nodes: template tasks
  - Edges: possible data flow between tasks
- Template Task Graph unrolled during execution
  - Tasks identified through (hashable) IDs (keys)
  - Data flows along edges as Pair {TaskID, Data}
- Data-dependent task discovery
  - Data may flow along different edges depending on results
- Scalable distributed task discovery





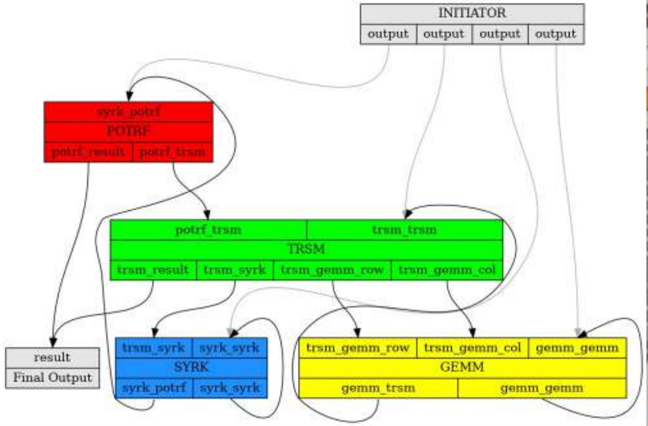
TTG: Tasks, Terminals, and Edges

- Tasks: task with set number of inputs and outputs
  - Instantiated when first discovered
  - Executed once all inputs are available
- Terminals: inputs and outputs of a task, hidden from user code
- Edges: connects output terminals to input terminals
  - Data flows along edges
  - All possible paths between template tasks expressed through edges
  - Represent sets of data



TTG Execution Model (General)

- SPMD: all processes execute the same program in main thread
- ttg::World: query number of processes and local rank
  - Split processes between multiple worlds (i.e., communicators)
- Single or multiple entry points into the DAG
  - Process(es) kick off computation by feeding data into the task graph
  - Executing process controlled through mapper function
- Worker threads non-preemptively execute tasks
- Fence to wait for execution to complete
- Multiple task-graphs can be active concurrently



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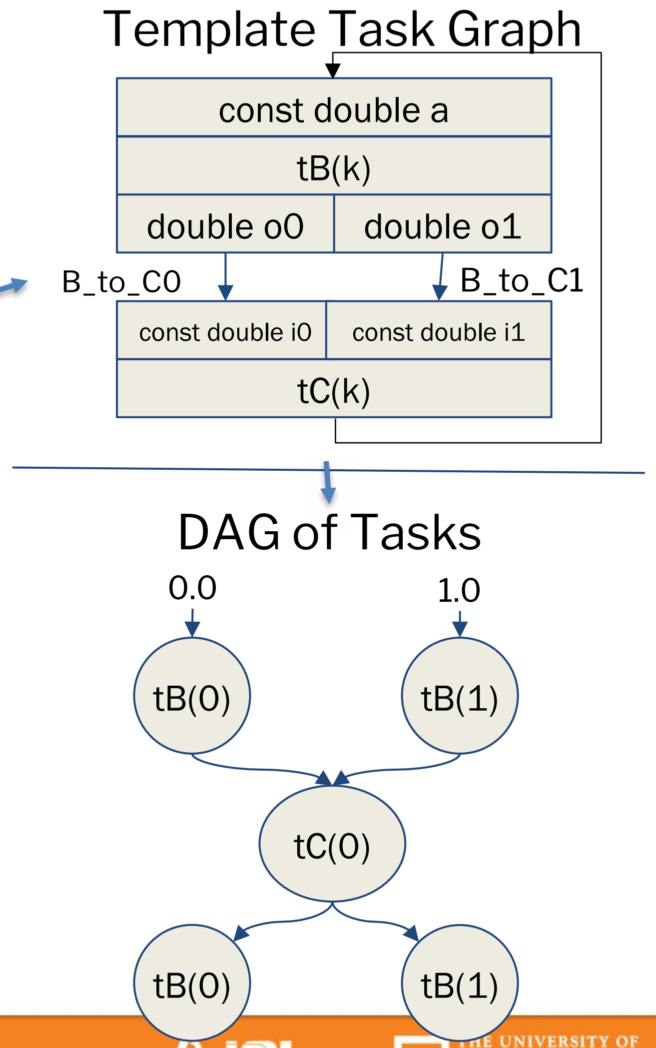
Simplifications work in progress

TG: Small Example / Cycle

```
ttg::Edge<int, double> to_B("to_B");
ttg::Edge<int, double> B_to_C0("B_to_C0");
ttg::Edge<int, double> B_to_C1("B_to_C1");
ttg::Edge<int, double> C_to_B(”C_to_B");

auto tb = ttg::make_tt([](const int &k, const double &a) {
    // Task tB(k) received value a for input 0
    if(0 == k) ttg::send<0>(0, a);
    if(1 == k) ttg::send<1>(0, a);
  },
  ttg::edges(ttg::fuse(to_B, C_to_B),
  ttg::edges(B_to_C0, B_to_C1));

auto tc = ttg::make_tt([](const int &k, const double &i0, const double &i1)
  {
    if (need_recursion(i0, i1)) {
      ttg::send<0>(0, i0); // send i0 back to task B
      ttg::send<0>(1, i1); // send i1 back to task B
    }
  },
  ttg::edges(B_to_C0, B_to_C1),
  ttg::edges(C_to_B));

ttg::make_graph_executable(tb);
if(tb->get_world().rank() == 0) {
  tb->invoke(0, 0.0);
  tb->invoke(1, 1.0);
}
ttg::execute();
ttg::fence();
```

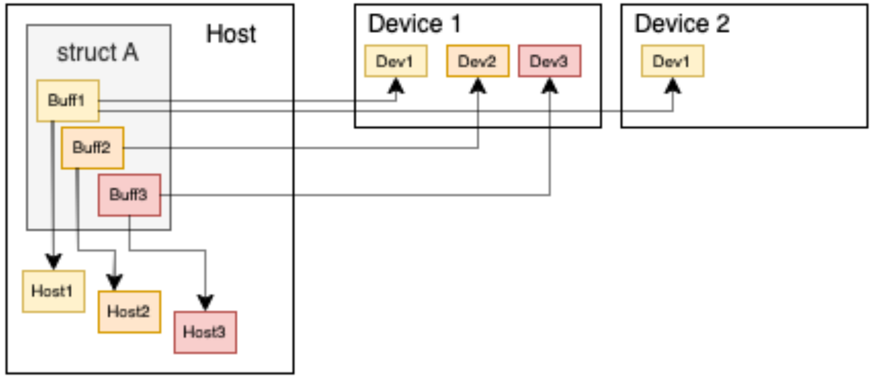
Fused Edges



TTG Memory Model (Device)

- TTG manages device memory
- Host memory serves as backup for transparent eviction
  - Memory oversubscription supported by default
- Transparent data movement between devices and host
  - Automatic migration from device to host tasks
- ttg::Buffer: owning/non-owning host memory mirror

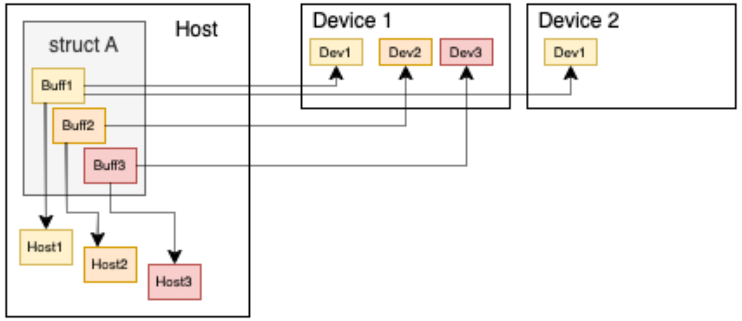
TTG Device integration still experimental



Buffers: Device memory containers

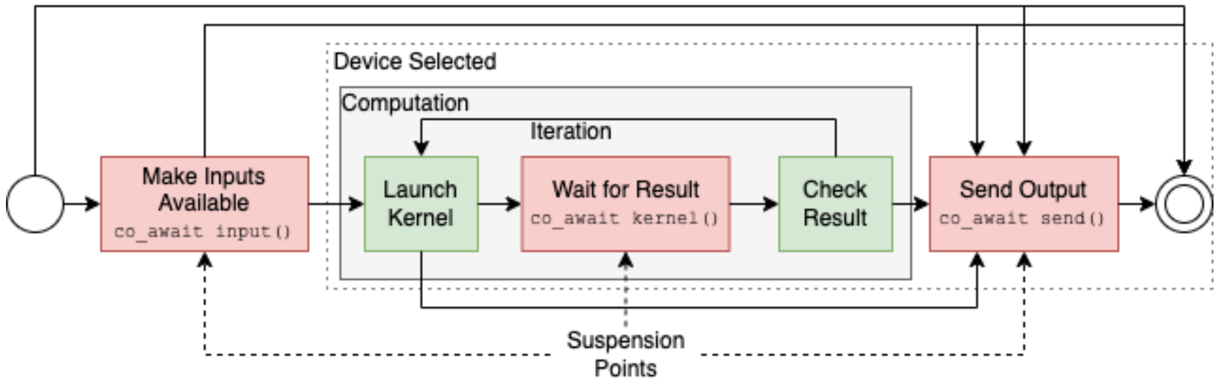
- Owns host memory, unless user-provided
- Tracks last device task location
- Enables transparent migration of data between devices and host
- Allows partial mapping of complex data structures to devices
  - Some tasks may not require all object data on the device

```
template<typename T>
struct Tile {
  ttg::Buffer<T> buf;
  size_t m, n, lda;
  Tile(size_t m, size_t n, size_t lda)
  : buf(m*n) // buffer owns host memory
  { }
  Tile(T *ptr, size_t m, size_t n, size_t lda)
  : buf(ptr, m*n) // buffer does not own host memory
  { }
  // other constructors and accessors
};
```



TTG Execution Model (Device)

1. Tasks declare input data (ttg::Buffer, scratch data)
2. TTG runtime assigns a device and execution stream based on inputs and device load
   - One management thread per device (PaRSEC)
3. Tasks submit kernels and H2D transfers into stream and suspend
4. Runtime returns once execution completed
5. Task may:
   - Submit more kernels; or
   - Send out results to successors



TTG Device Tasks

- “co_await select()” selects device
- “co_await kernel()” waits for kernel and potential transfers back to host
- Task may submit and wait for multiple kernels
- Sending outputs is last step of task

```
template<typename T>
struct Tile {
  ttg::Buffer<T> buf;
  size_t m, n, lda;
  Tile(size_t m, size_t n, size_t lda)
  : buf(m*n) // buffer owns host memory
  { }
  Tile(T *ptr, size_t m, size_t n, size_t lda)
  : buf(ptr, m*n) // buffer does not own host memory
  { }
  // other constructors and accessors
};
```

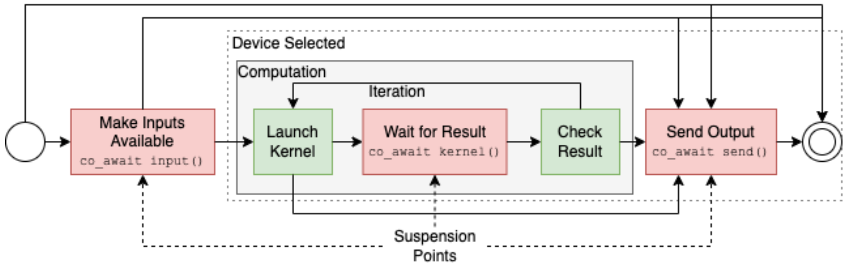
```
using Key = std::pair<int, int>; // tile position in matrix

auto tb = ttg::make_tt([](const Key& k, Tile&& a)
          -> ttg::device::task {
    co_await ttg::device::select(A.buf); // make A available
    submit_kernel(a);
    co_await ttg::device::kernel(); // optional if no result required
    co_return ttg::device::send<0>(k, std::move(a));
  }, ...);
```

Select device based on inputs

Submit work

Wait for kernel to execute (optional)

Send Output



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Since the last meeting…

- Reworked part of PaRSEC's GPU integration
- Improved transparent handling of device copies
- Alas, issues running on Frontier beyond handful of nodes…

- Tool integration: generation of Perfetto traces

- Block sparse matrix multiplication

GPU Binding: POTRF

- Transparent multi-device scheduling
- Automatic load-balancing is great but not perfect
- Provide a hint to runtime which device to use
- Schedule tiles on row to same device

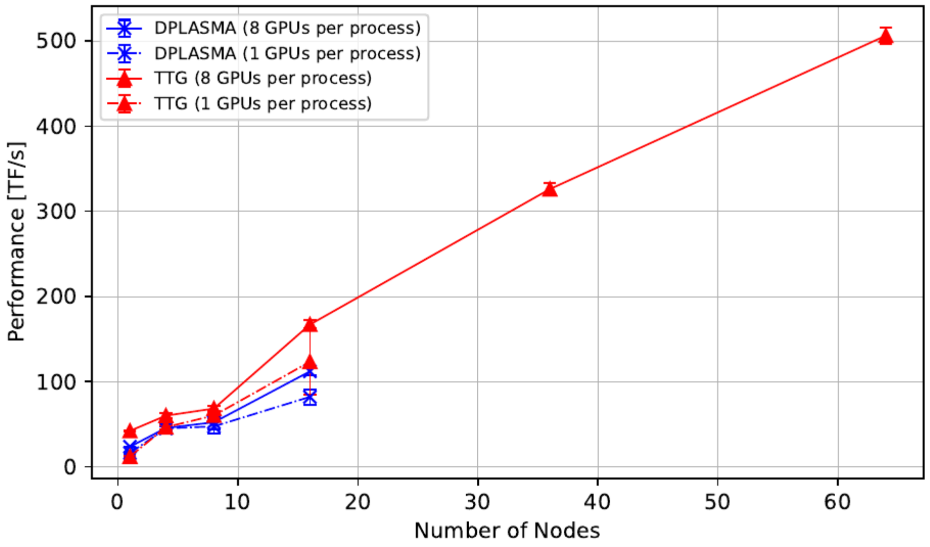
```
using Key = std::pair<int, int>; // tile position in matrix

auto tb = ttg::make_tt([](const Key& k, Tile&& a)
          -> ttg::device::task {
    co_await ttg::device::input(A.buf); // make A available
    submit_kernel(a);
    co_await ttg::device::kernel(); // optional if no result required
    co_return ttg::device::send<0>(k, std::move(a));
  }, ...);
tb->set_devicehint([](const Key& k){
    return (key[0] / A.P()) % ttg::device::num_devices();
  });
```

POTRF on Frontier

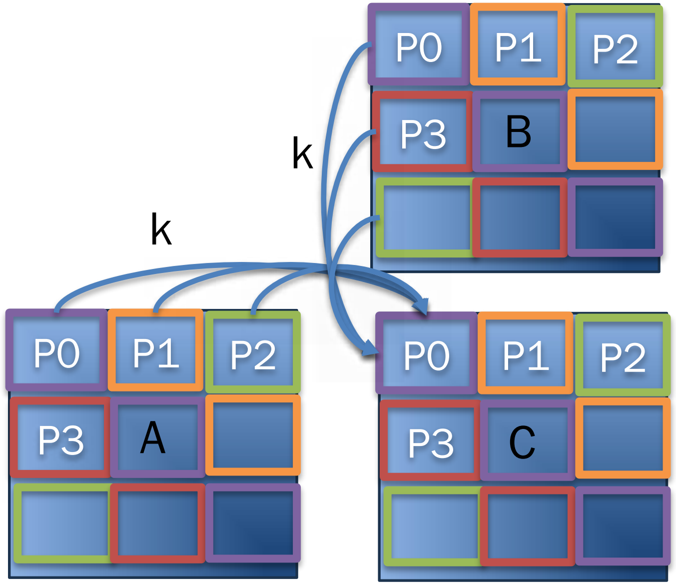
- Significant performance improvement over DPLASMA
- Issues running PaRSEC at scale on Frontier

64k / node, 2k tiles, DP



Towards BSpMM in TTG

- Input tiles flow A/B owners to C owner
- Challenge: throttling tile exchange in dataflow system
- Manual control flow (void Edges) error-prone and complex



Throttling Data Exchange Through Constraints

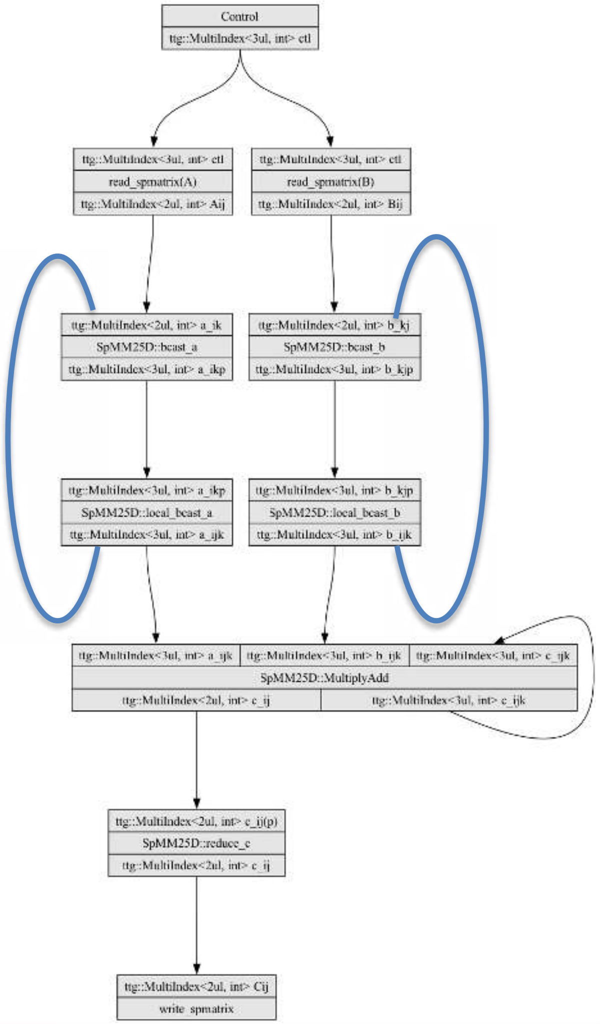
- Constrain tile broadcasts based on previous k iterations
- Attach a `SequencedKeysConstraint` to the broadcast and release from GEMM
- Blocks [k+1…K] broadcasts until prior [0…k] broadcasts completed
- Mapper: key → sequence ID (here: k)
- **Auto release**: automatically release on prior k
- **Manual release:**
  GEMM releases k+1 bcasts once all GEMM of k are done

```
struct Key{ int m, n, k; }; // tile position in matrix
auto constraint = ttg::make_shared_constraint<ttg::SequencedKeysConstraint<Key>>();

auto bcast_a = make_A_broadcast(...);
auto bcast_b = make_B_broadcast(...);
bcast_a->add_constraint(constraint, [](const Key<2>& key){ return key.k; });
bcast_b->add_constraint(constraint, [](const Key<2>& key){ return key.k; });
```

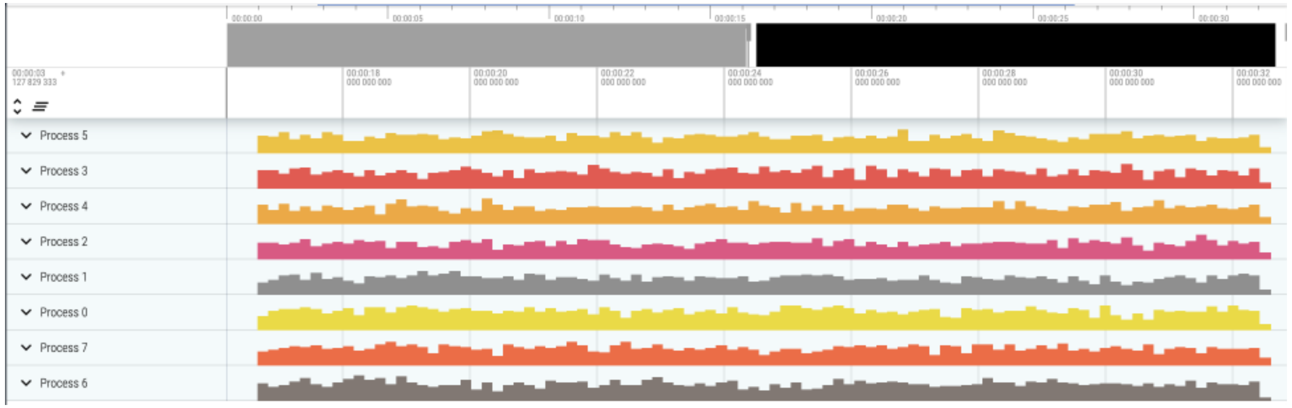
Automatic Constraint Release

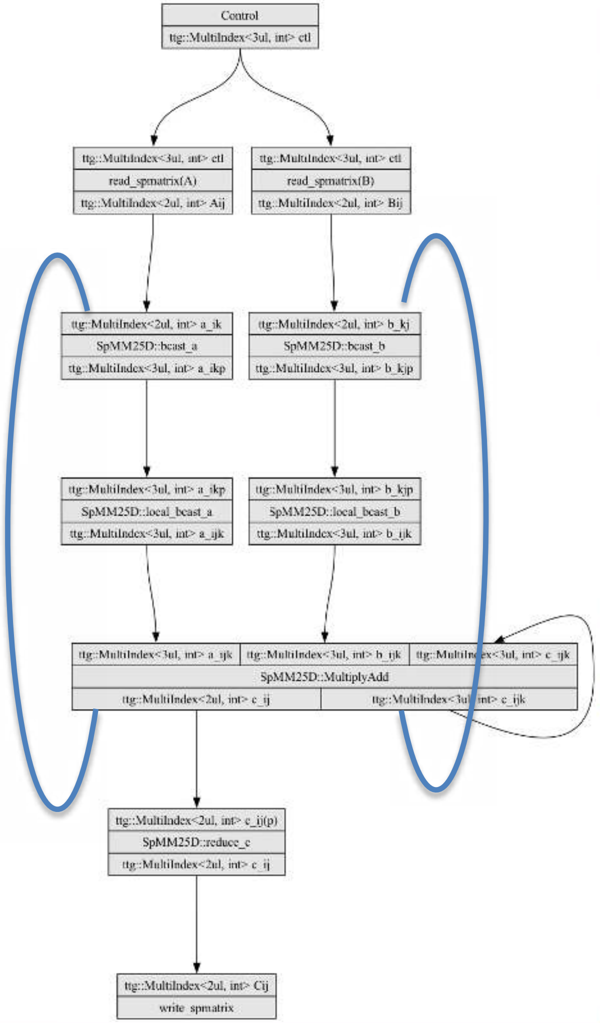
- Inserts local control to replace explicit control flow edges
- Global broadcasts implicitly depend on local broadcasts
- Still risk of flooding due to slower consumer



Manual Constraint Release

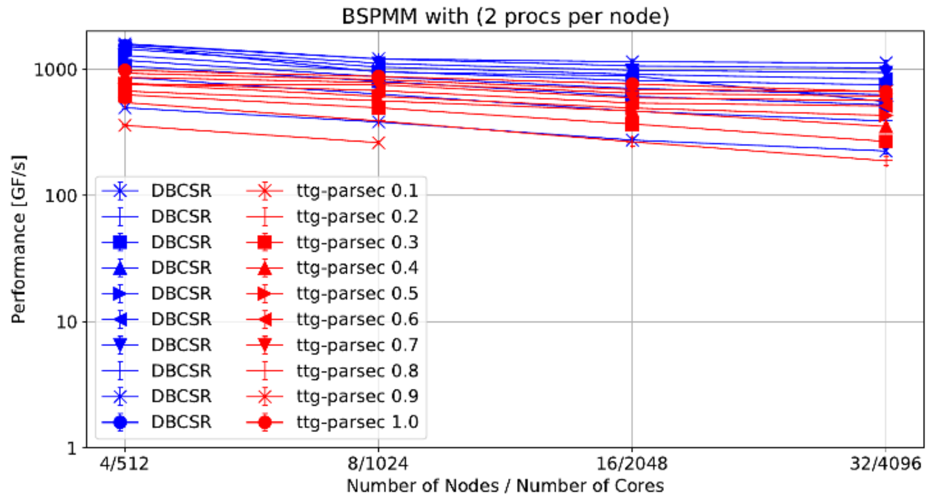
- Inserts local control to replace explicit control flow edges
- Global broadcasts released by previous k GEMM
  - Window of k to execute at a time
  - Overlap of broadcasts and GEMM
  - Counting broadcasts/GEMM for each k





BSpMM Results

- Performance on Hawk (2x64C AMD EPYC)
  - 64k matrix, 128 elements per tile
- Higher density yields better performance
- Performance not yet competitive with DBCSR



Also in the works…

- Coroutine-based key generators (for LA implementations)
- Improved memory allocation
  - Avoid host-side backup allocations
  - Integrate with application allocators
- Device to device communication
  - Source device enabled today (if MPI allows)
  - Target device will need restructuring of GPU/Comm backends

MADNESS Integration

- Implementation of Multi-Resolution Analysis with GPU support

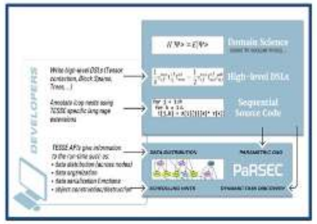

George Bosilca

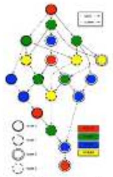

Thomas Herault

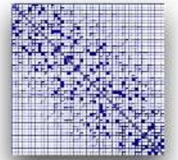

Joseph Schuchart

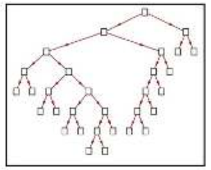

Eduard Valeev

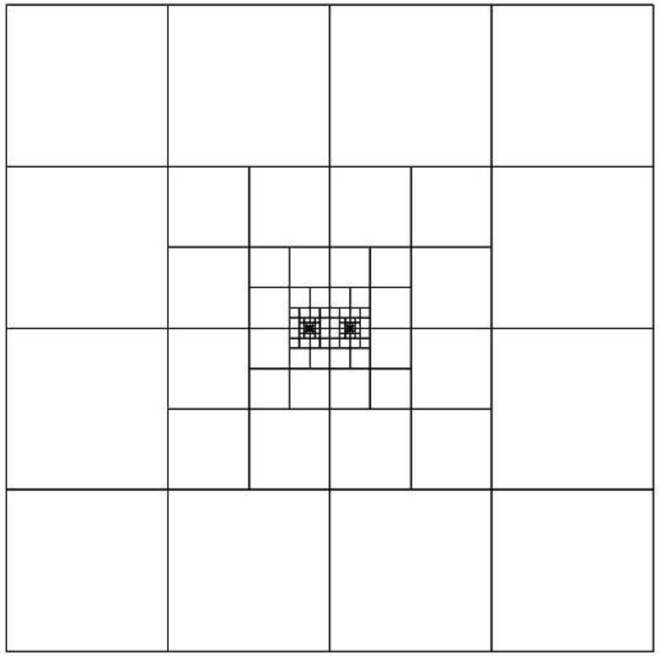

Robert Harrison




dense linear algebra


block-rank sparse algebra for quantum chemistry/physics


adaptive spectral-element calculus Multi-Resolution Analysis



- Slice thru grid used to represent the nuclear potential for H_2 using k=7 to a precision of 10^{-5}.
- Automatically adapts – it does not know a priori where the nuclei are.
- Nuclei at dyadic points on level 5 – refinement stops at level 8
- If were at non-dyadic points refinement continues (to level ??) but the precision is still guaranteed.
- In future will unevenly subdivide boxes to force nuclei to dyadic points.

Who we are

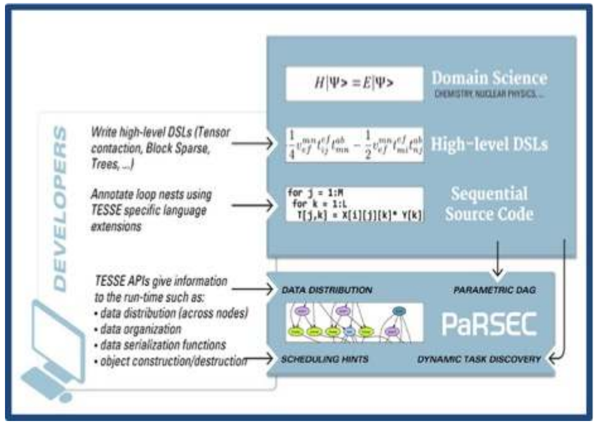
George Bosilca

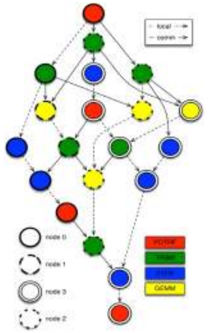
Thomas Herault

Joseph Schuchart

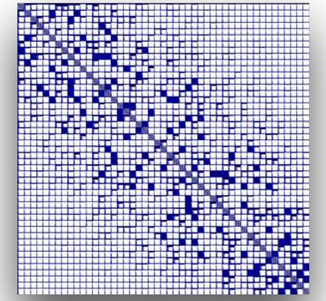
Eduard Valeev

Robert Harrison

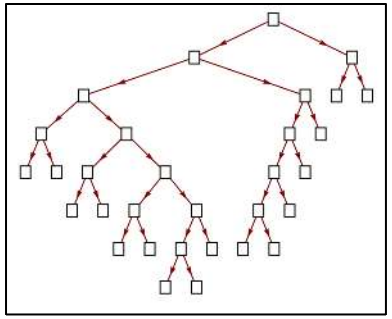




dense linear algebra



block-rank sparse algebra for quantum chemistry/physics



adaptive spectral-element calculus Multi-Resolution Analysis

Acknowledgements

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Resources

- ECP Tutorial: https://www.exascaleproject.org/event/ttg-2022/
- Paper:
  - J. Schuchart *et al.*, "Generalized Flow-Graph Programming Using Template Task-Graphs: Initial Implementation and Assessment," *2022 IEEE International Parallel and Distributed Processing Symposium (IPDPS).*
  - J. Schuchart, P. Nookala, T. Herault, E. F. Valeev and G. Bosilca, "Pushing the Boundaries of Small Tasks: Scalable Low-Overhead Data-Flow Programming in TTG," *2022 IEEE International Conference on Cluster Computing (CLUSTER)*.
  - T. Herault, J. Schuchart, E. F. Valeev and G. Bosilca, "Composition of Algorithmic Building Blocks in Template Task Graphs," *2022 IEEE/ACM Parallel Applications Workshop: Alternatives To MPI+X (PAW-ATM)*.
- Github: https://github.com/TESSEorg/ttg/

This research was supported partly by NSF awards #1931347 and #1931384, and by the Exascale Computing Project (17-SC-20-SC), a collaborative effort of the U.S. Department of Energy Office of Science and the National Nuclear Security Administration. We gratefully acknowledge the provision of computational resources by the High-Performance Computing Center (HLRS) at the University of Stuttgart, Germany.