Task-Based Programming at Scale: Challenges and New Approaches

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15.12.2022

INNOVATIVE COMPUTING LABORATORY

THE UNIVERSITY OF TENNESSEE KNOXVILLE

Who am I?

- 2005–2012: Dipl-Inf. TU Dresden, ZIH
- 2012–2013: Oak Ridge National Laboratory
- 2013–2016: ZIH, EE-HPC
- 2016–2020: Dr.-Ing., Stuttgart University, HLRS
- Since 2020: University of Tennessee, Knoxville
  Innovative Computing Laboratory

What is ICL?

- Head: **Hartwig Anzt** (frmly Jack)
- Linear Algebra ([Sca]LAPACK, heFFTe, SLATE, Mixed precision computation, …)
- Performance Analysis Tools
  - PAPI
- **Distributed Computing**

Distributed Computing Group (DISCO)

- Message Passing Interface
  - MPI Forum members
  - Open MPI: P2P & collective operations, datatypes, RMA
  - Fault Tolerance: User-Level Fault Mitigation (ULFM)
- Distributed Tasking:
  - PaRSEC: distributed task-based runtime system
  - DPLASMA: task-based replacement for ScaLAPACK

Task-Based Programming

Traditional MPI programs

- **Sequential** control flow
- Easier to write, harder to scale
- Limited latency hiding potential

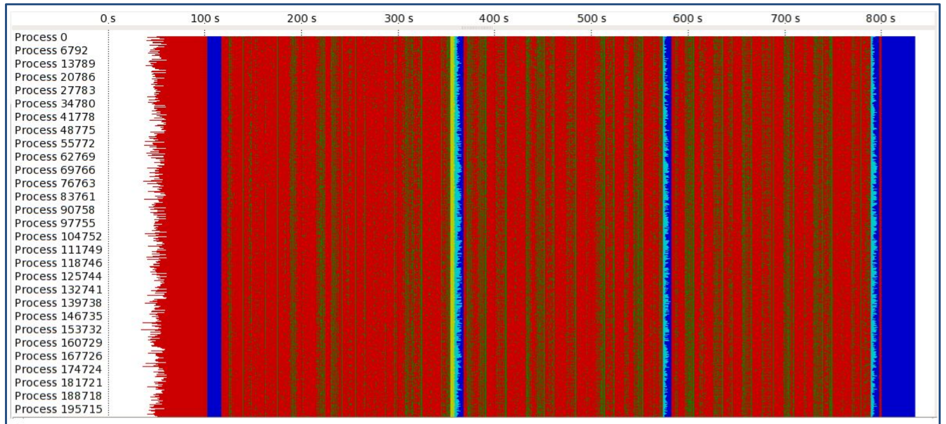
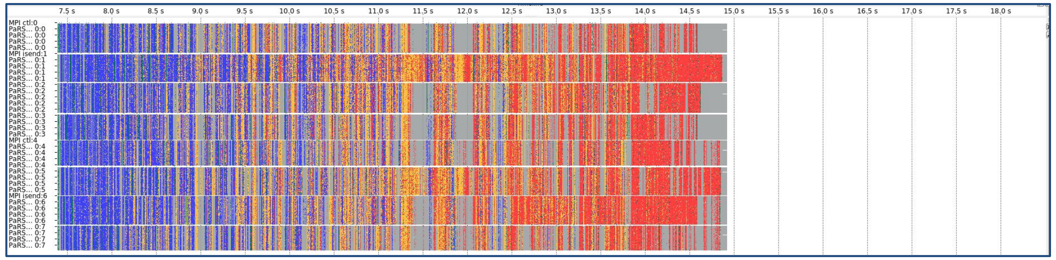


Figure 10: Screenshot of Vampir visualizing a trace of the S3D application using 200,448 cores on JaguarPF. User functions are shown in green, MPI operations in red, and activities of the measurement environment in yellow (file open), light blue (trace I/O) and dark blue (synchronization).

Task-based programs

- Oversubscription of work
- Scheduler-managed control flow
  - Harder to reason about
- Significant **latency hiding** potential



Levels of Task-Based Programming

Shared Memory

- All tasks local
- Communication between threads on the same process
- OpenMP, OmpSs, CUDA graphs
- Coupling with distributed models like MPI

```
#pragma omp parallel master
  for (step in 0:NUM_STEPS) {
    for (field in 0:NUM_LOCAL_FIELDS)
#pragma omp task depend(inout: data[field], in: data[field-1])
      compute_field_in_step(data, field, step);
  }
```

Distributed Memory

- Data-flow across process boundaries
- Distributed scheduling decisions
- **PaRSEC**, HPX, UPC++, Legion, StarPU, **TTG**, **DASH**, …
- Different models for different types of applications

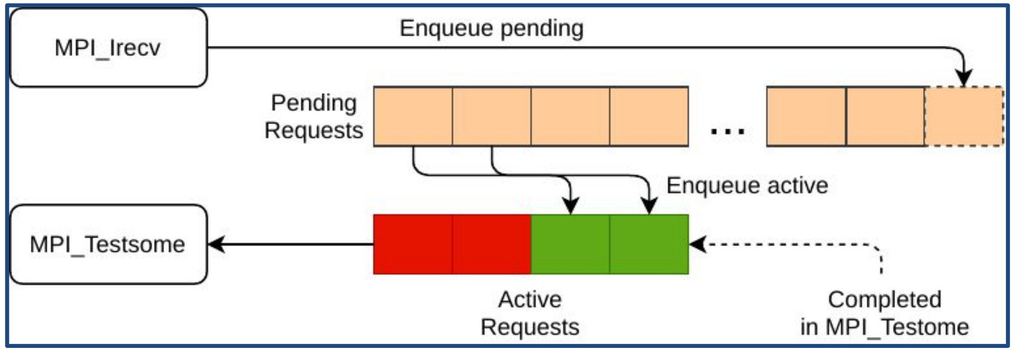
```
for (step in 0:NUM_STEPS) {
  for (field in 0:NUM_GLOBAL_FIELDS)
    insert_task(
      &compute_field_in_step, data, field, step,
      INOUT(data[field]), IN(data[field-1]));
}
```

Part One

Coupling asynchronous programming models with MPI

Nonblocking MPI Operations

- MPI provides nonblocking P2P, Collective, RMA, I/O



MPI_Irecv

Enqueue pending

Pending Requests

…

Enqueue active

MPI_Testsome

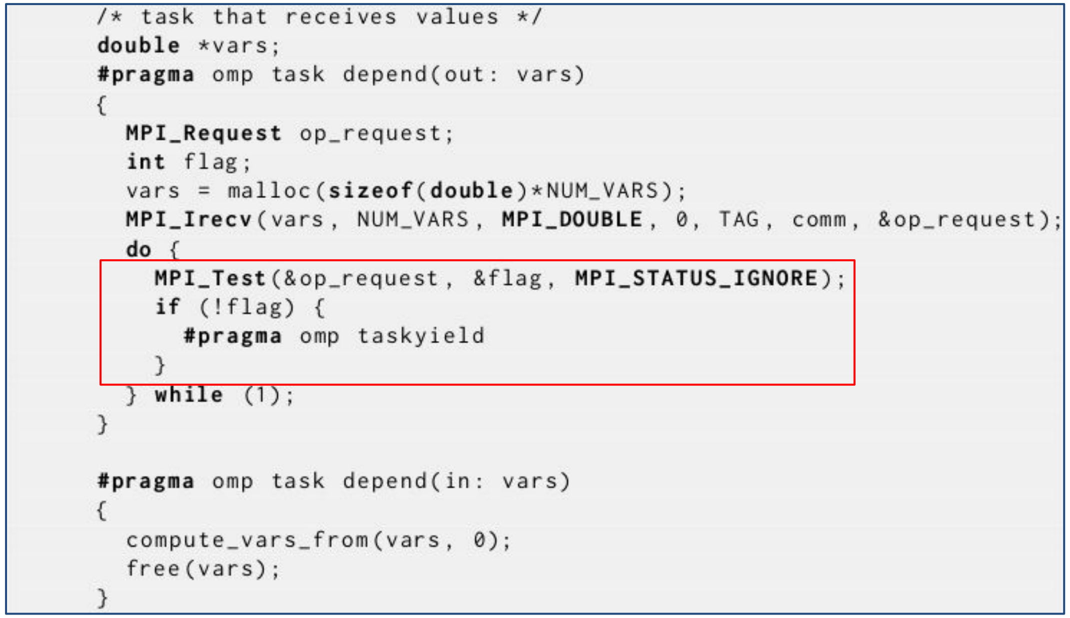
Active Requests

Completed in MPI_Testome

- Completion detection through polling only
  - MPI_Test, MPI_Wait and friends
- Applications manage requests
  - Challenging and error-prone in asynchronous/irregular applications
- Prior proposals are **not portable**
  - ULT integration with MPI (Qthreads, Argobots)
  - TAMPI

Motivation: Communicating OpenMP Tasks

- Polling is insufficient
- Not all yields are created equal



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/* task that receives values */
double *vars;
#pragma omp task depend(out: vars)
{
  MPI_Request op_request;
  int flag;
  vars = malloc(sizeof(double)*NUM_VARS);
  MPI_Irecv(vars, NUM_VARS, MPI_DOUBLE, 0, TAG, comm, &op_request);
  do {
    MPI_Test(&op_request, &flag, MPI_STATUS_IGNORE);
    if (!flag) {
      #pragma omp taskyield
    }
  } while (1);
}

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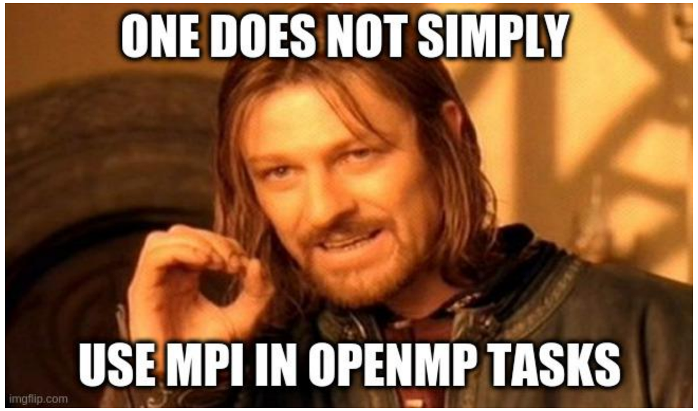

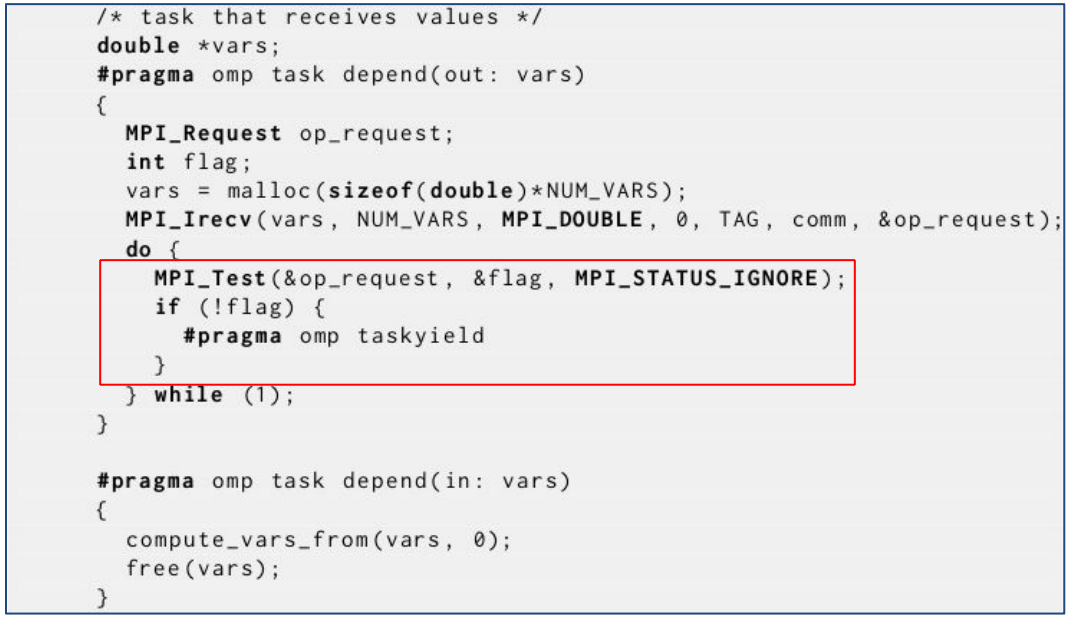

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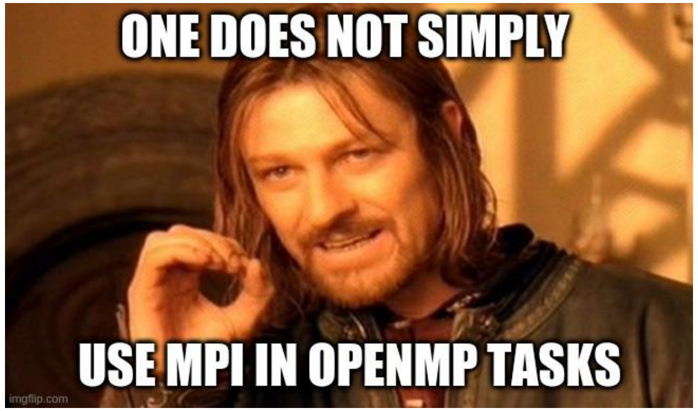
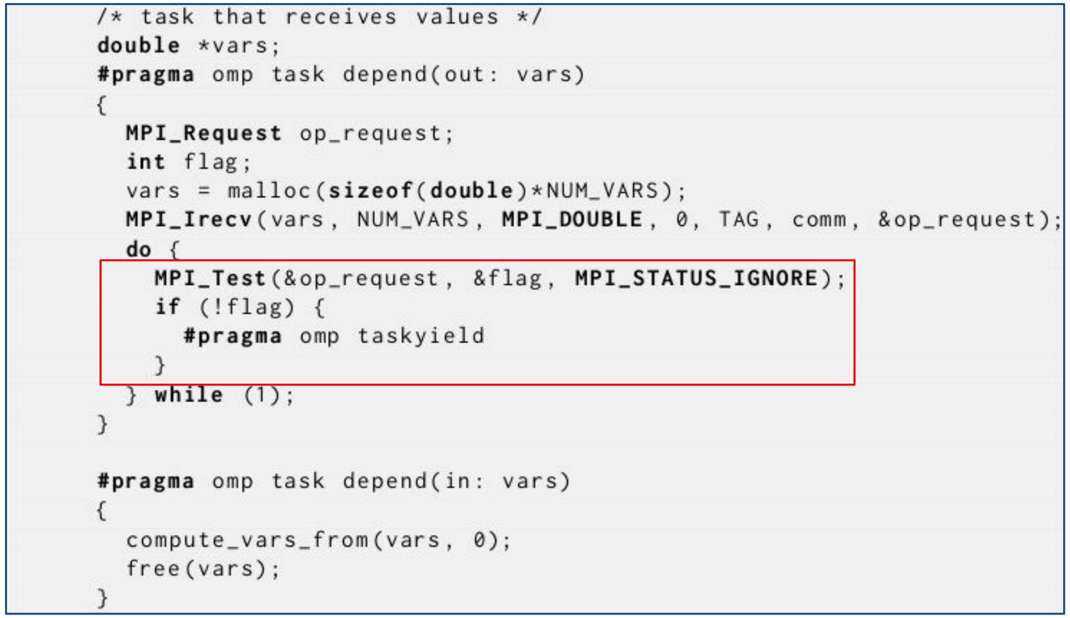
  - Central polling infrastructure
- Alternative 2:
  - **Return request to MPI**, for good





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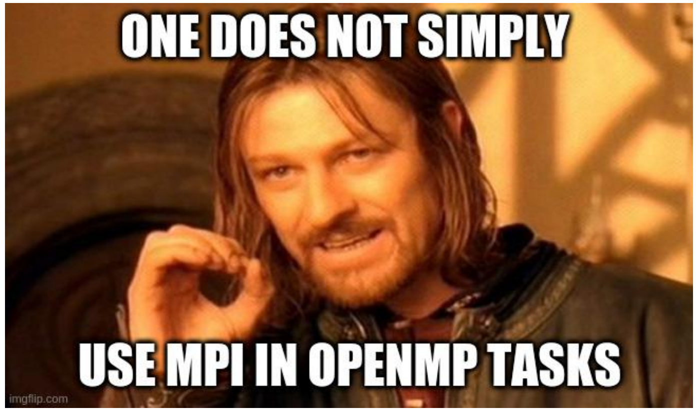

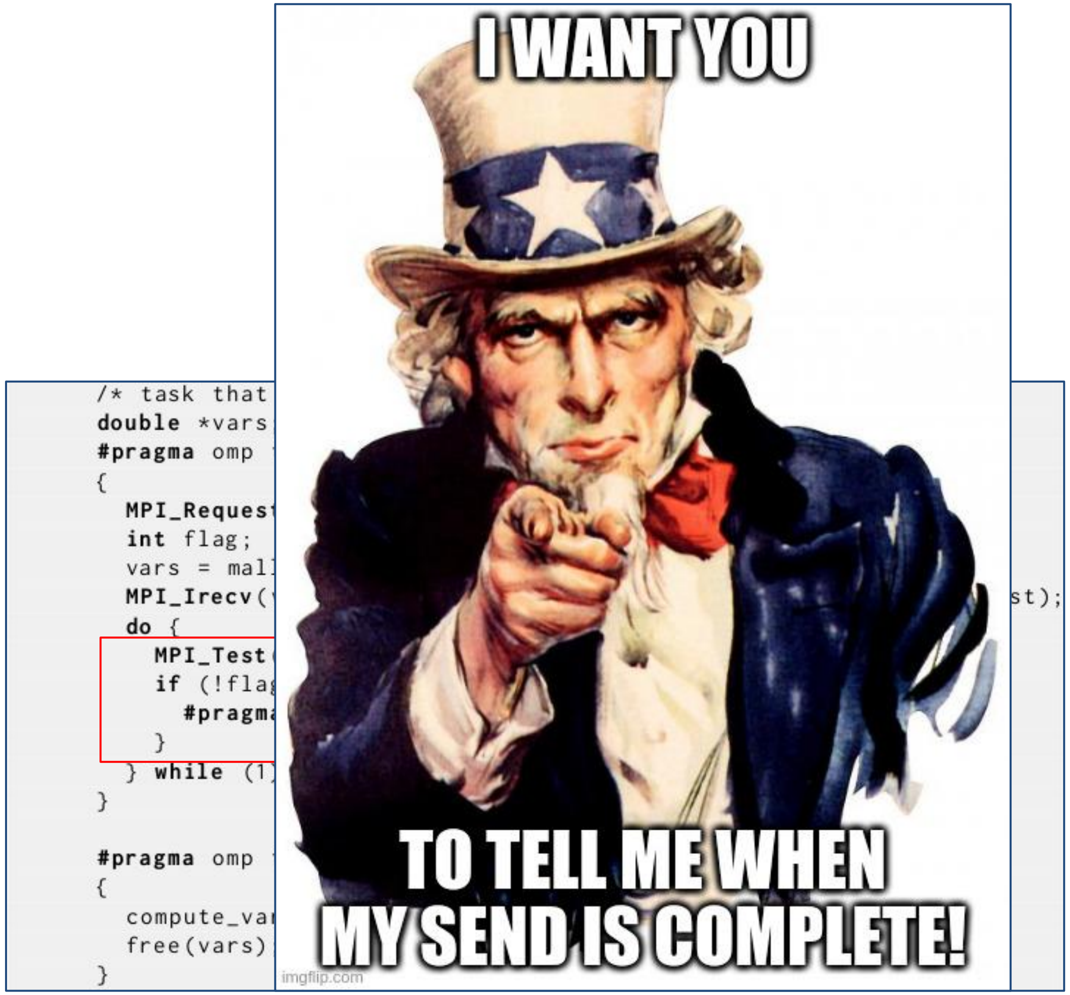

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/* task that
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{
  MPI_Request
  int flag;
  vars = mal
  MPI_Irecv(
                                               st);
  do {
    MPI_Test
    if (!flag
      #pragma
    }
  } while (1
}

#pragma omp
{
  compute_va
  free(vars)
}
```

The Hollywood Principle

- Requests are created and free’d by MPI
- Applications receive, store, and test requests
- **Observations**:
  - Requests are only a control device
  - Applications care about **completion of operations**

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    - Return requests to MPI
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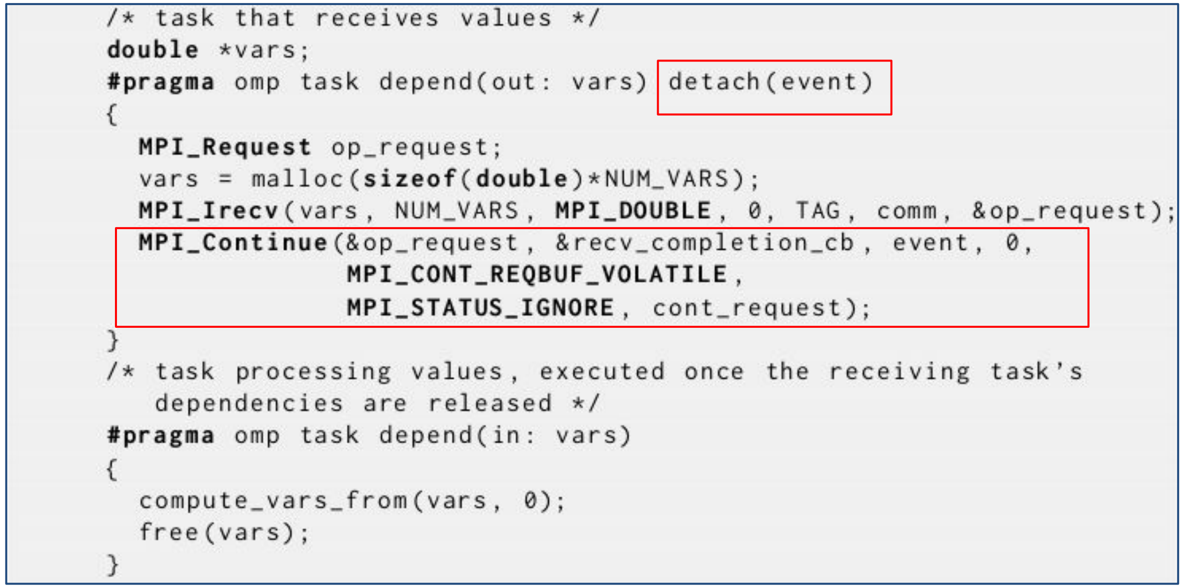
Don't call us, we'll call you back.

Introducing: MPI Continuations

- Continuations are *attached* to one or more operations
- MPI takes back request ownership*
- Invokes callback once the operation is complete
- **Inputs**:
  - Flags
  - Callback function pointer
  - User-data pointer
  - Status (optional)
  - *Continuation request*



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/* task that receives values */
double *vars;
#pragma omp task depend(out: vars) detach(event)
{
  MPI_Request op_request;
  vars = malloc(sizeof(double)*NUM_VARS);
  MPI_Irecv(vars, NUM_VARS, MPI_DOUBLE, 0, TAG, comm, &op_request);
  MPI_Continue(&op_request, &recv_completion_cb, event, 0,
               MPI_CONT_REQBUF_VOLATILE,
               MPI_STATUS_IGNORE, cont_request);
}
/* task processing values, executed once the receiving task's
   dependencies are released */
#pragma omp task depend(in: vars)
{
  compute_vars_from(vars, 0);
  free(vars);
}
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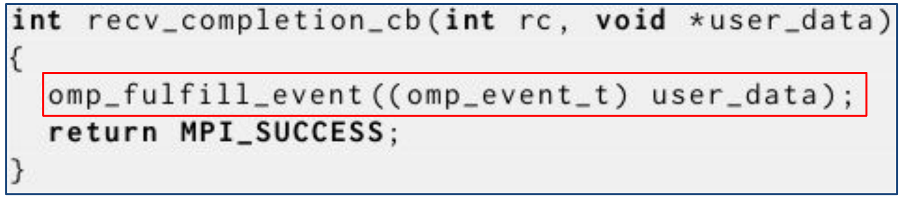

```
int recv_completion_cb(int rc, void *user_data)
{
  omp_fulfill_event((omp_event_t) user_data);
  return MPI_SUCCESS;
}
```

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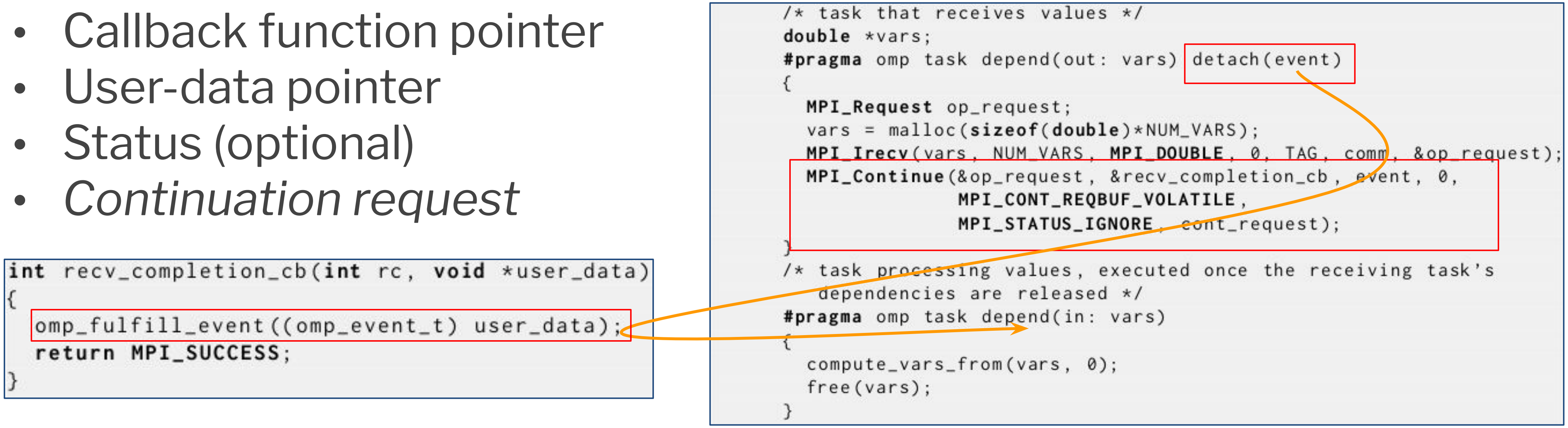

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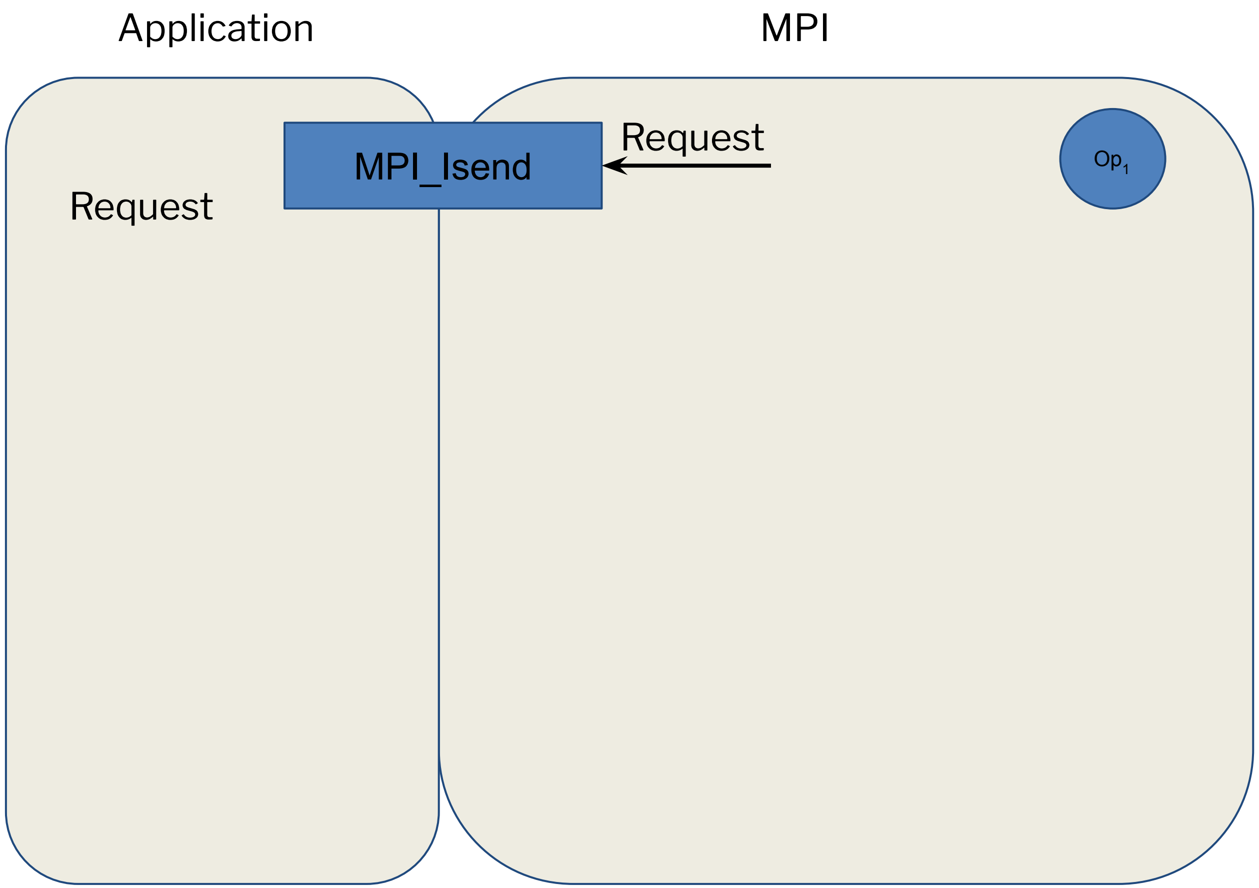
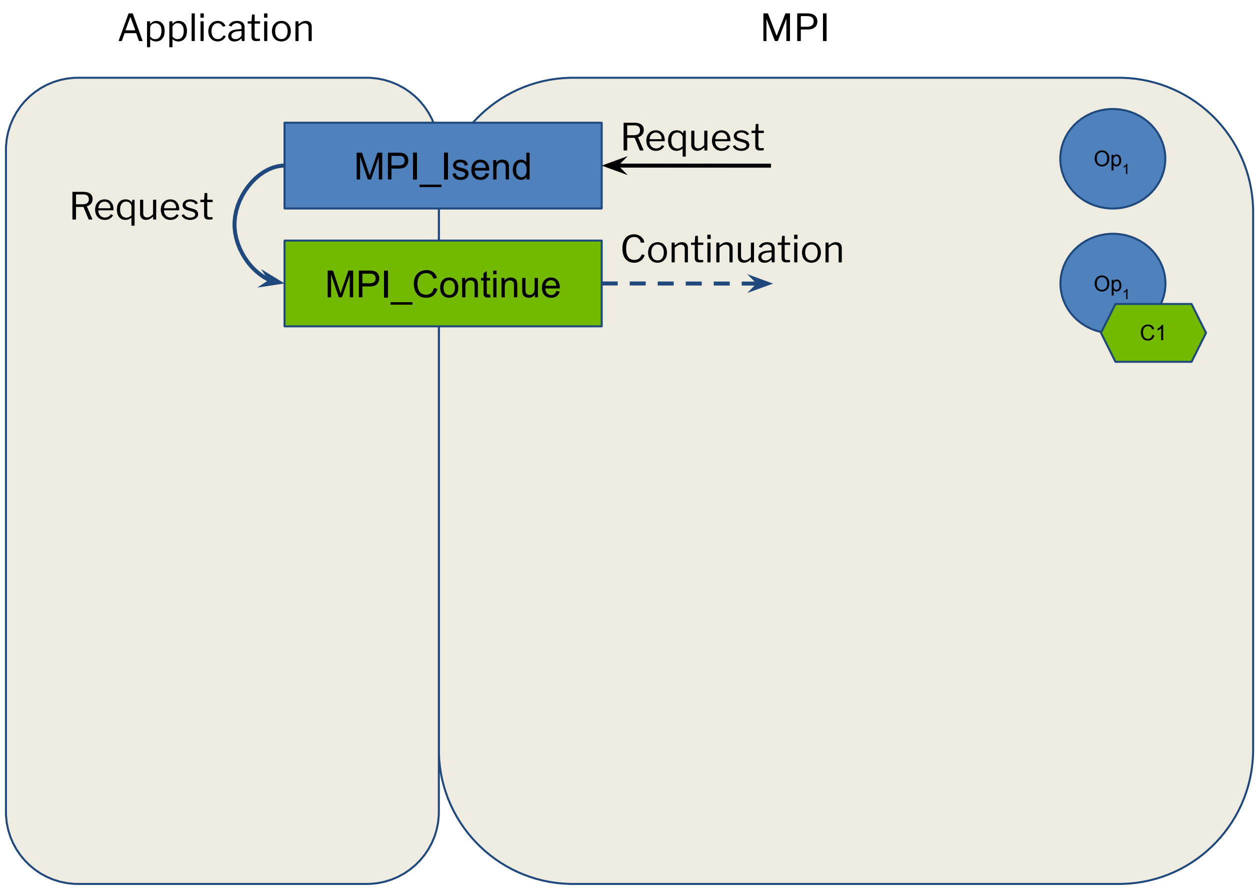
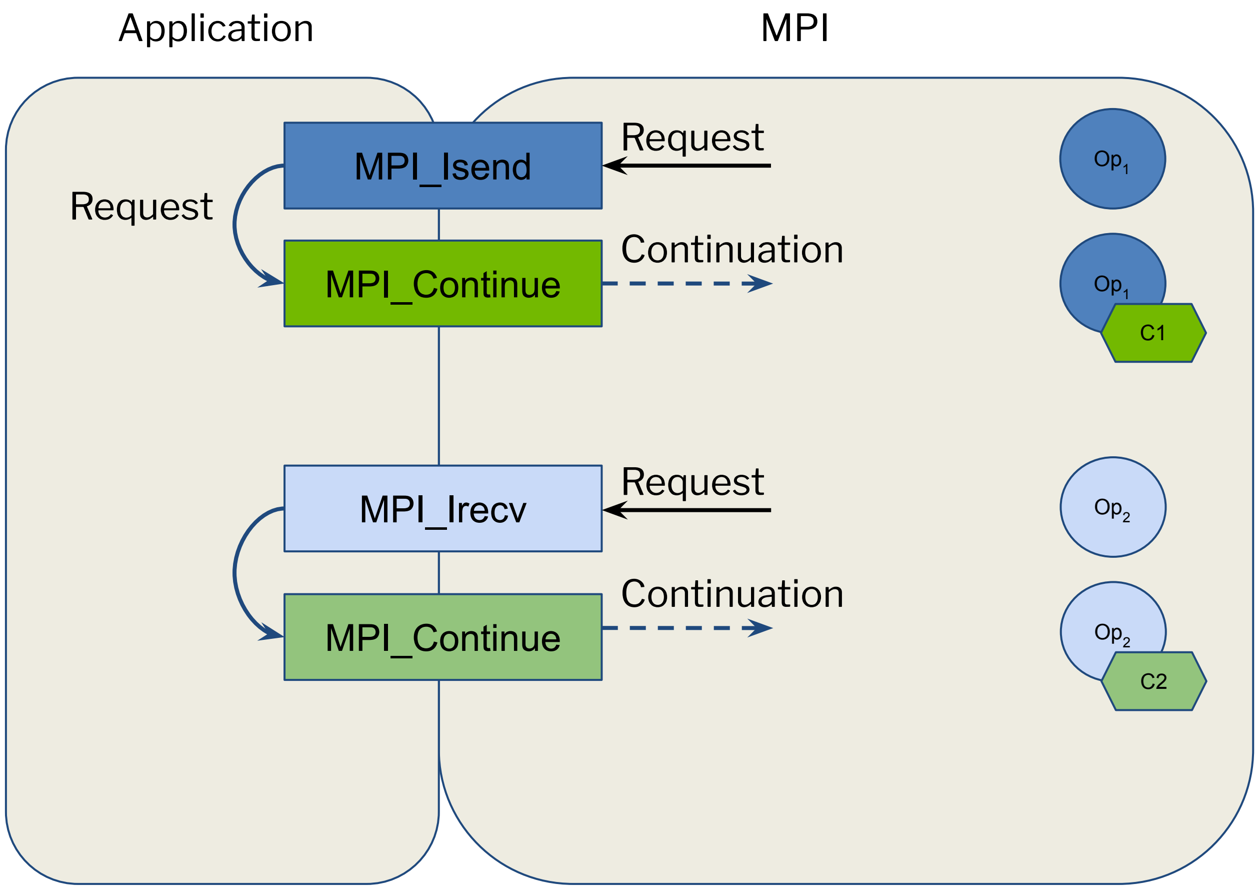
Continuations Control Flow



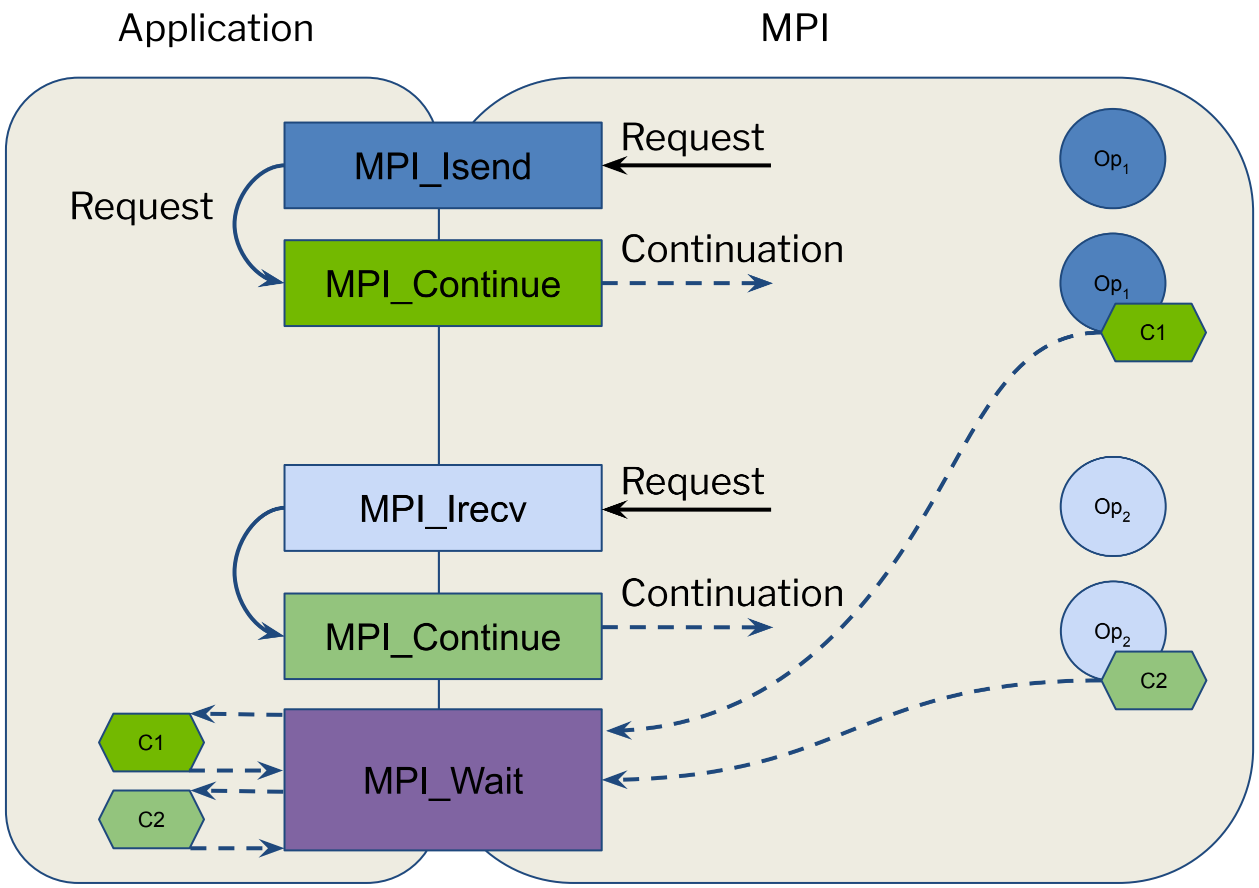
Continuations Control Flow



Continuations Control Flow

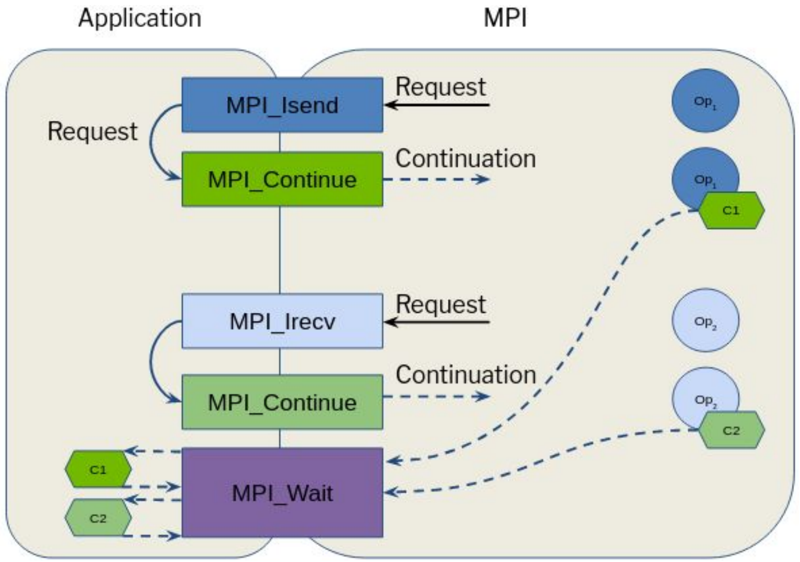


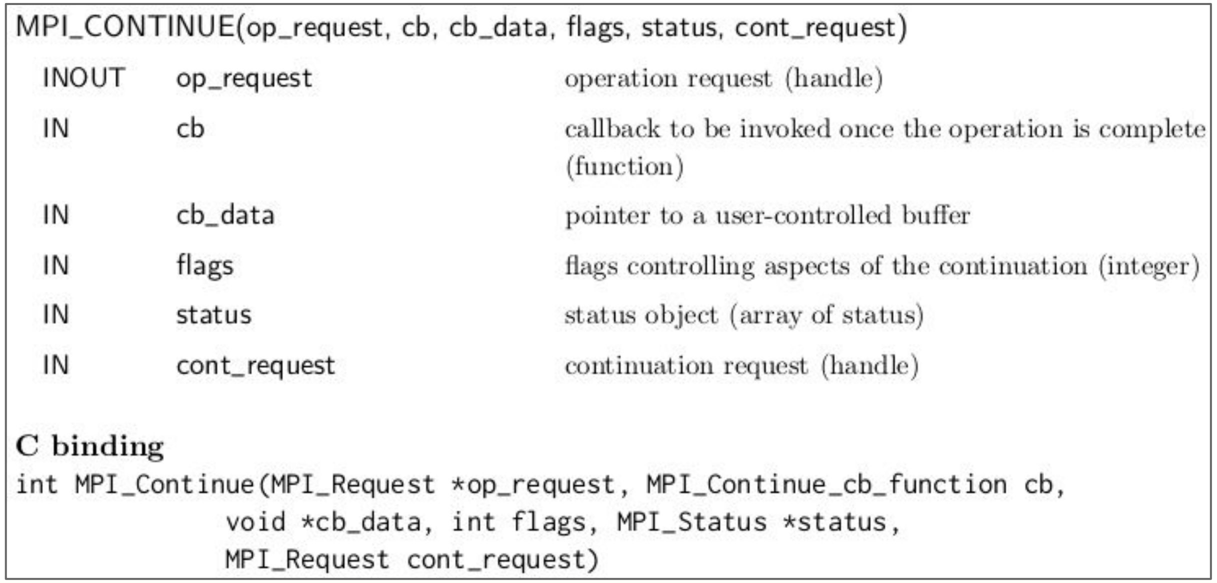
Continuations Control Flow



Attaching a Continuation: MPI_Continue

- *Attaches* a continuation to **one** operation
- Flags control behavior
- Status filled before callback is invoked




MPI_CONTINUE(op_request, cb, cb_data, flags, status, cont_request)

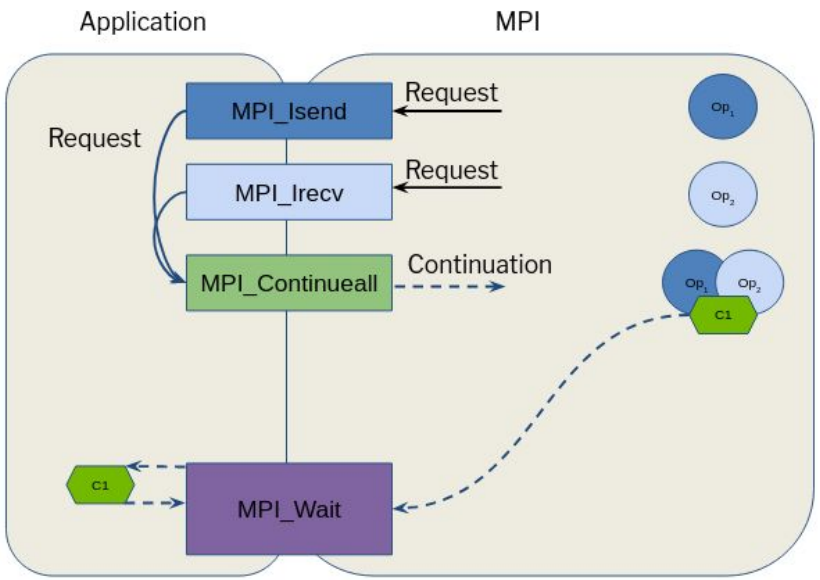
INOUT	op_request	operation request (handle)
IN	cb	callback to be invoked once the operation is complete (function)
IN	cb_data	pointer to a user-controlled buffer
IN	flags	flags controlling aspects of the continuation (integer)
IN	status	status object (array of status)
IN	cont_request	continuation request (handle)

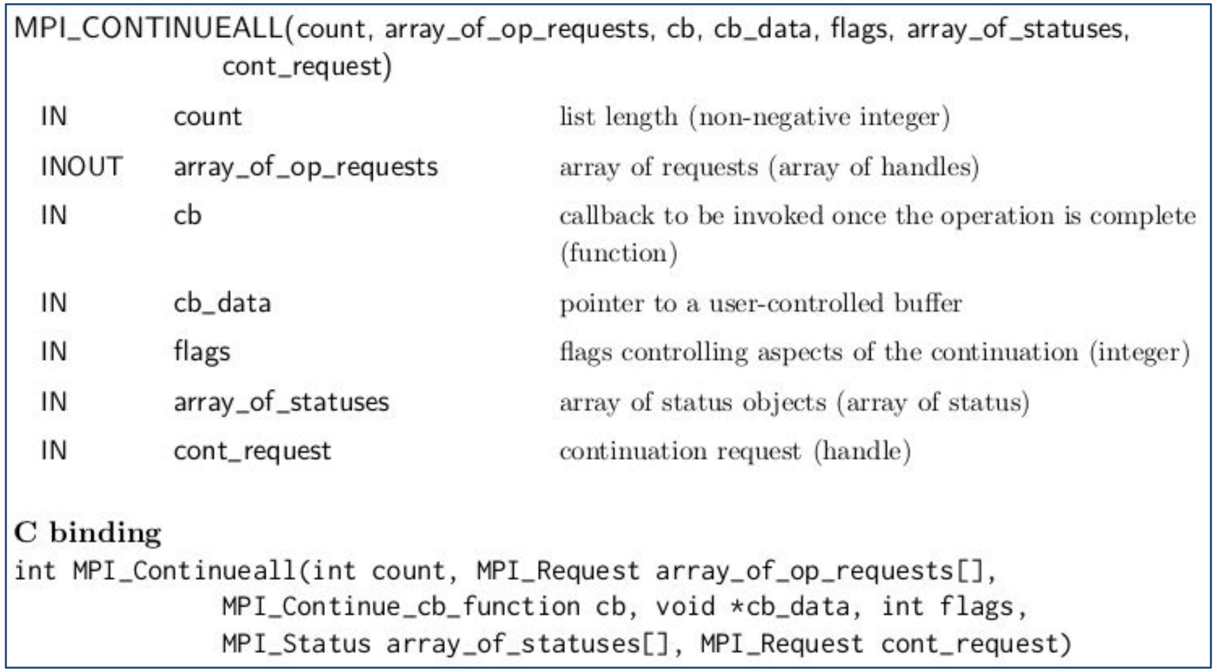
C binding

```
int MPI_Continue(MPI_Request *op_request, MPI_Continue_cb_function cb,
              void *cb_data, int flags, MPI_Status *status,
              MPI_Request cont_request)
```

Attaching a Continuation: MPI_Continueall

- *Attaches* a continuation to **multiple** operations
- Flags control behavior
- Status filled before callback is invoked




MPI_CONTINUEALL(count, array_of_op_requests, cb, cb_data, flags, array_of_statuses, cont_request)

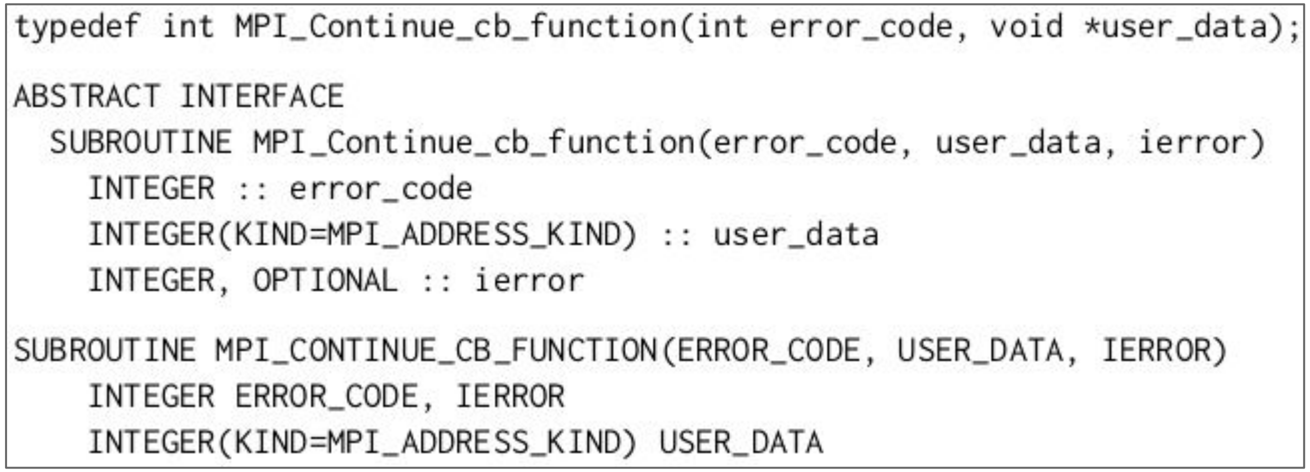
IN	count	list length (non-negative integer)
INOUT	array_of_op_requests	array of requests (array of handles)
IN	cb	callback to be invoked once the operation is complete (function)
IN	cb_data	pointer to a user-controlled buffer
IN	flags	flags controlling aspects of the continuation (integer)
IN	array_of_statuses	array of status objects (array of status)
IN	cont_request	continuation request (handle)

C binding

```
int MPI_Continueall(int count, MPI_Request array_of_op_requests[],
              MPI_Continue_cb_function cb, void *cb_data, int flags,
              MPI_Status array_of_statuses[], MPI_Request cont_request)
```

Callback Functions

- **Inputs**:
  - Error code: MPI_SUCCESS (or error if operation failed)
  - User-data provided during creation
- **Returns**:
  - Error code: MPI_SUCCESS or error code
- May call MPI procedures
  - Blocking procedures discouraged



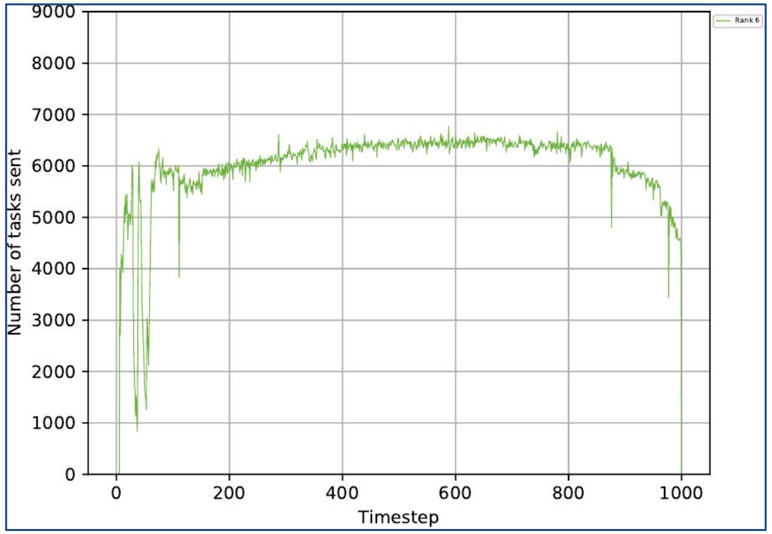
```
typedef int MPI_Continue_cb_function(int error_code, void *user_data);

ABSTRACT INTERFACE
  SUBROUTINE MPI_Continue_cb_function(error_code, user_data, ierror)
    INTEGER :: error_code
    INTEGER(KIND=MPI_ADDRESS_KIND) :: user_data
    INTEGER, OPTIONAL :: ierror

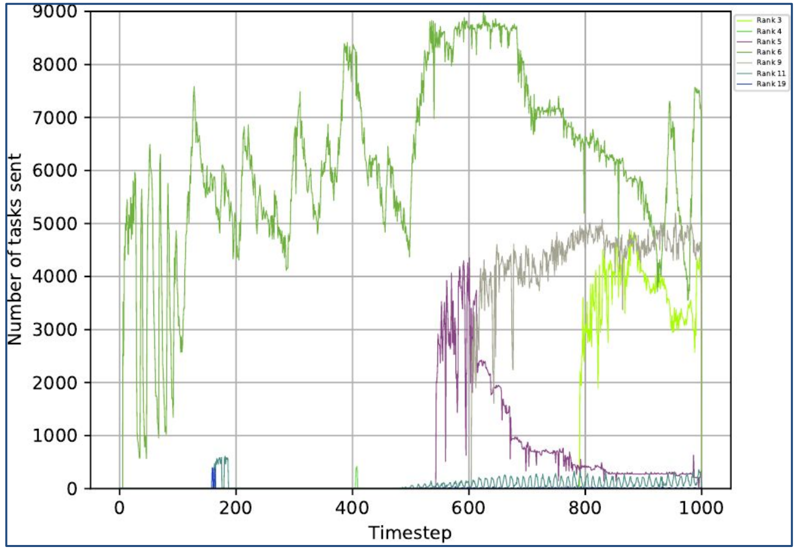
SUBROUTINE MPI_CONTINUE_CB_FUNCTION(ERROR_CODE, USER_DATA, IERROR)
    INTEGER ERROR_CODE, IERROR
    INTEGER(KIND=MPI_ADDRESS_KIND) USER_DATA
```

Evaluation: ExaHype

- Compressible Navier Stokes equations for cloud simulation
- Dynamic load balancing via task migration
- Continuations simplified request handling, leading to 25% higher offload rates and improved balancing



Reference implementation

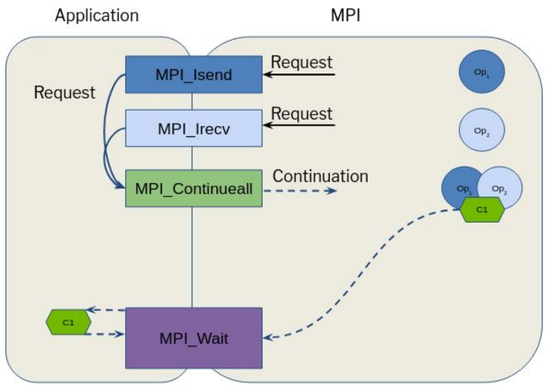


Using MPI Continuations

Joseph Schuchart, Philipp Samfass, Christoph Niethammer, José Gracia, George Bosilca, Callback-based completion notification using MPI Continuations, Parallel Computing, 2021

Part One: Summary

- MPI must better support asynchronous programming models
- Requests are merely a device
- Callbacks are **flexible** and allow for **fast reaction** to state changes
- Fine-grain control over execution behavior



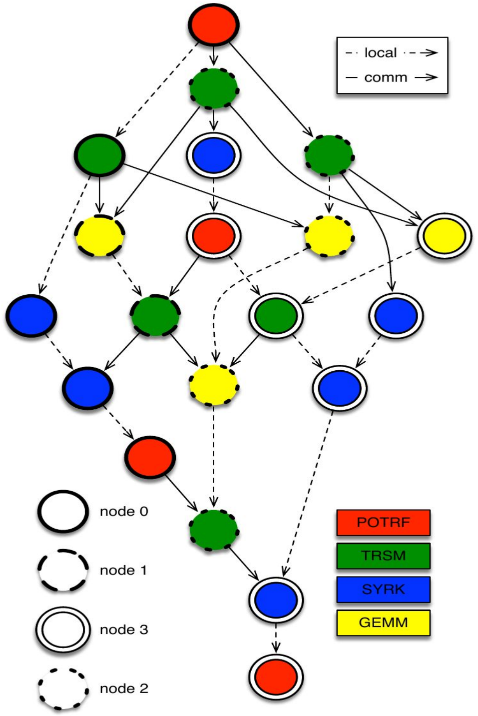
Part Two

A new task model for distributed memory task programming

Why distributed task models?

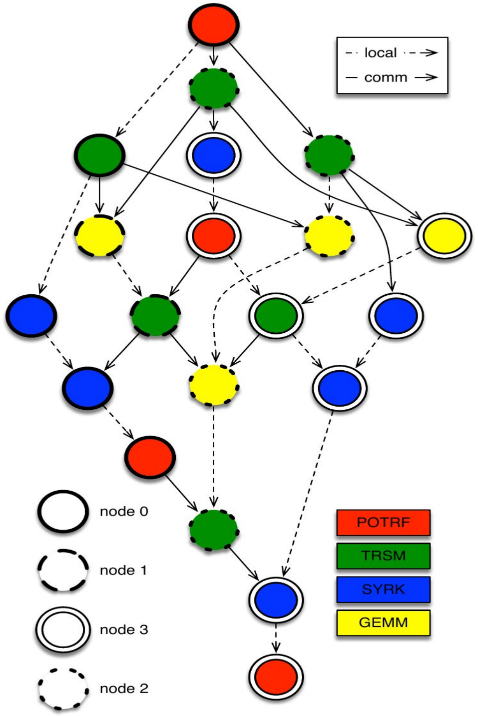
- Shared memory tasking models have serious limitations
  - Local-only scheduling decisions
  - Communication managed by user
  - Separation problematic

- Distributed Models provide
  - Managed communication
  - Global view scheduling decisions
  - Minimal synchronization



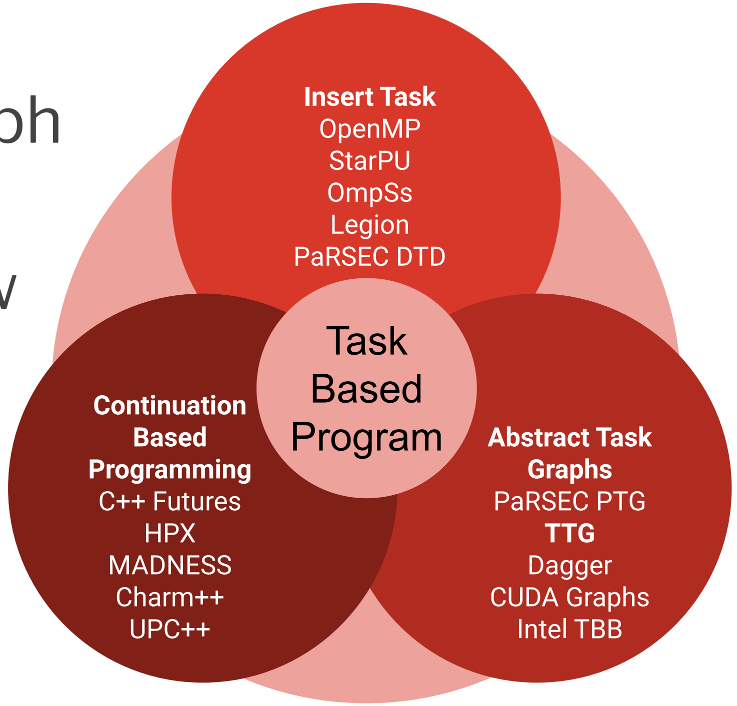
Distributed Task Graph Requirements

1. Task graph discovery (DAGs of tasks)
2. Data flow (moving data between processes)
3. Task Execution (along the critical path)



Distributed Task Graph Discovery

- **Insert task**:
  - Sequential discovery of global task graph on all processes
  - **Limited scalability**
- **Continuation-based** programming:
  - Explicit spawning of activities at places
  - **Handle for each data** flowing through the graph
- **Abstract Task Graphs**
  - Compact representation of *potential* data flow
  - **Scoped discovery** of tasks



Insert Task
OpenMP
StarPU
OmpSs
Legion
PaRSEC DTD

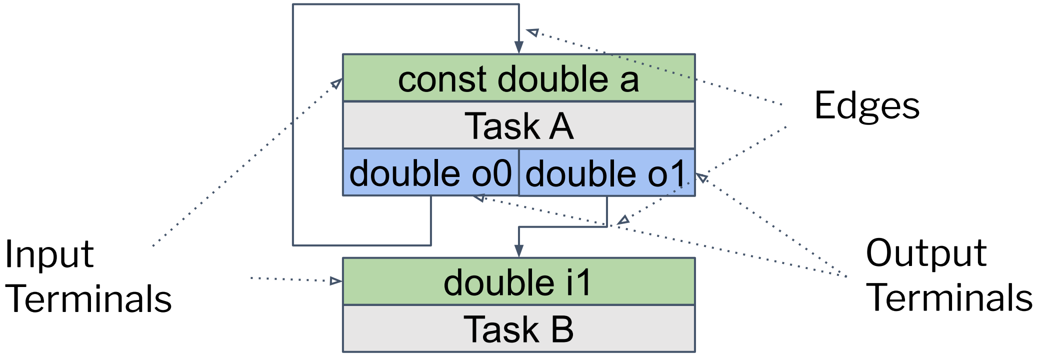
Task
Based
Program

Continuation Based Programming
C++ Futures
HPX
MADNESS
Charm++
UPC++

Abstract Task Graphs
PaRSEC PTG
TTG
Dagger
CUDA Graphs
Intel TBB

TTG: Template Task Graphs

- Abstract task graph unfolds into DAG during execution
    - **Template Tasks**: instantiated at execution
    - **Terminals**: input/output points
    - **Edges**: connecting input/output terminals
- Data-dependent selection of successors



J. Schuchart, P. Nookala, M. Javanmard, T. Herault, E. Valeev, G. Bosilca, R. Harrison. Generalized Flow-Graph Programming Using Template Task-Graphs: Initial Implementation and Assessment. IPDPS 2021.

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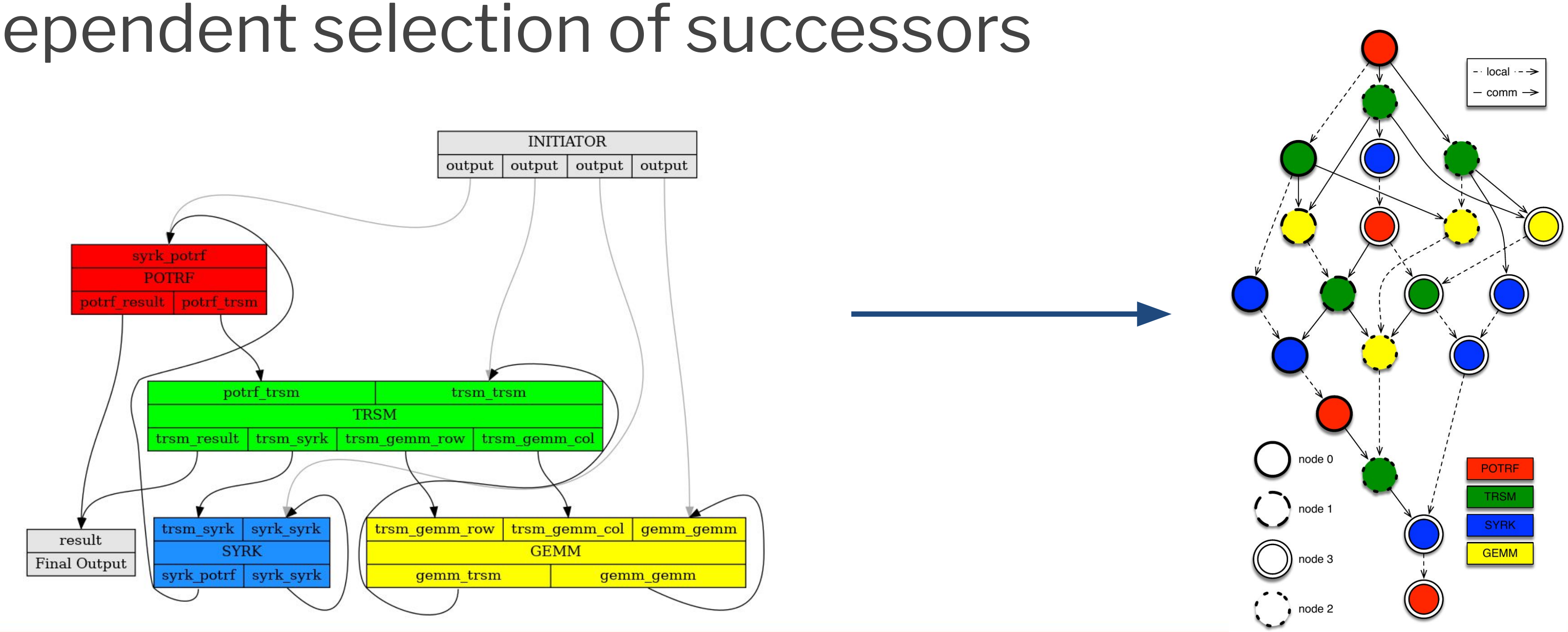

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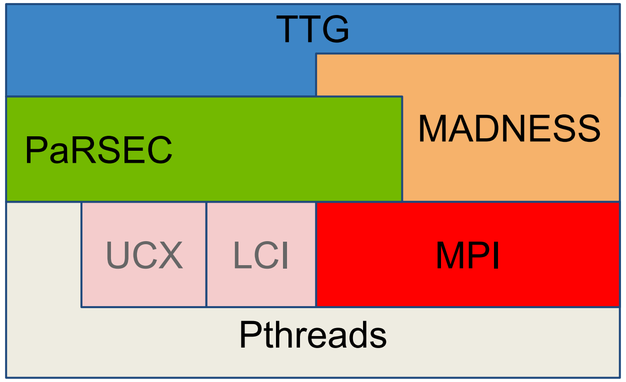
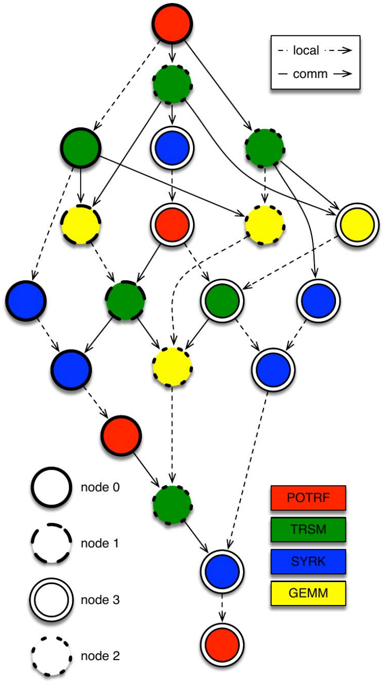
Data Moves through the Graph

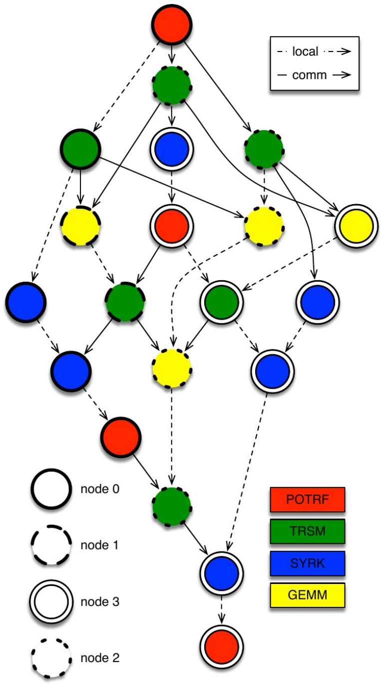
- Tasks send data to successors
  - Become eligible for execution once all input terminals received value
  - Unaware of predecessors
- Scalable distributed task discovery
- Flexible backend implementation
  - Available: PaRSEC, MADNESS
  - MPI main communication backend

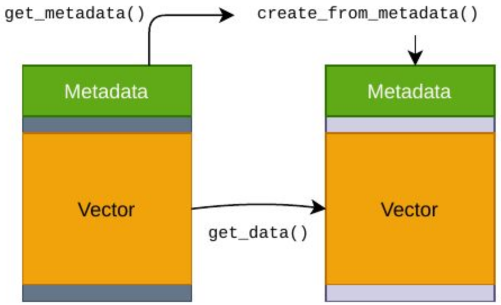




Data Movement

- Data traverses through unfolding task graph
- Goal: minimize number of data copies
  - Utilize C++ `move` and `const` semantics
  - Avoid copying data if we know its is immutable
- Zero-copy transfer mechanism
  - Serialize meta-data, copy payload directly



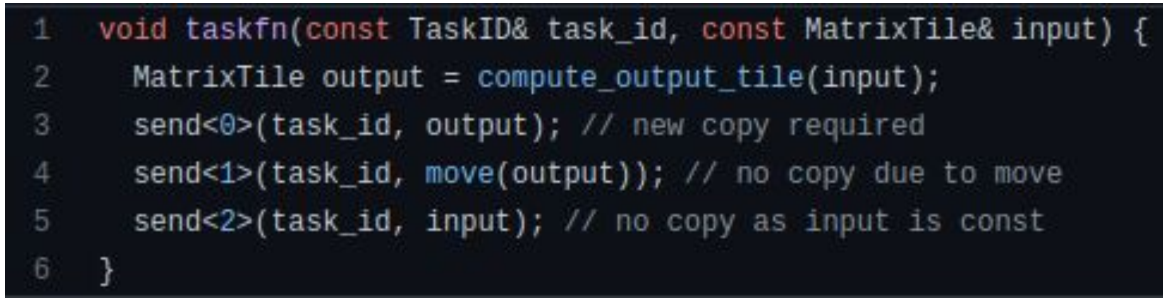


```
template<>
struct SplitMetadataDescriptor<MatrixTile> {

  auto get_metadata(const MatrixTile& t) {
    return t.metadata();
  }

  auto get_data(MatrixTile& t) {
    return std::array<iovec, 1>({t.size(),
                                 t.data()});
  }

  auto create_from_metadata(metadata_t& meta) {
    return MatrixTile(meta);
  }
};
```



```
void taskfn(const TaskID& task_id, const MatrixTile& input) {
  MatrixTile output = compute_output_tile(input);
  send<0>(task_id, output); // new copy required
  send<1>(task_id, move(output)); // no copy due to move
  send<2>(task_id, input); // no copy as input is const
}
```

TTG Task Functions

- Function object invoked once all inputs are satisfied.
- Key is optional (for task templates with single task instance)

```
[=](const keyT &k) {
  ttg::print(“This is task B(“ , k, “)”);
}
```

control flow (= flow of “void” data)

```
[=](const keyT &k, const T& val) {
  ttg::print(“This is task B(“ , k, “, “ val, “)”);
}
```

immutable data

```
[=](const keyT &k, T&& val) {
  ttg::print(“This is task B(“ , k, “, “ val, “)”);
}
```

mutable data

```
[=](const keyT &k, auto& val) {
  ttg::print(“This is task B(“ , k, “, “ val, “)”);
}
```

immutable generic data

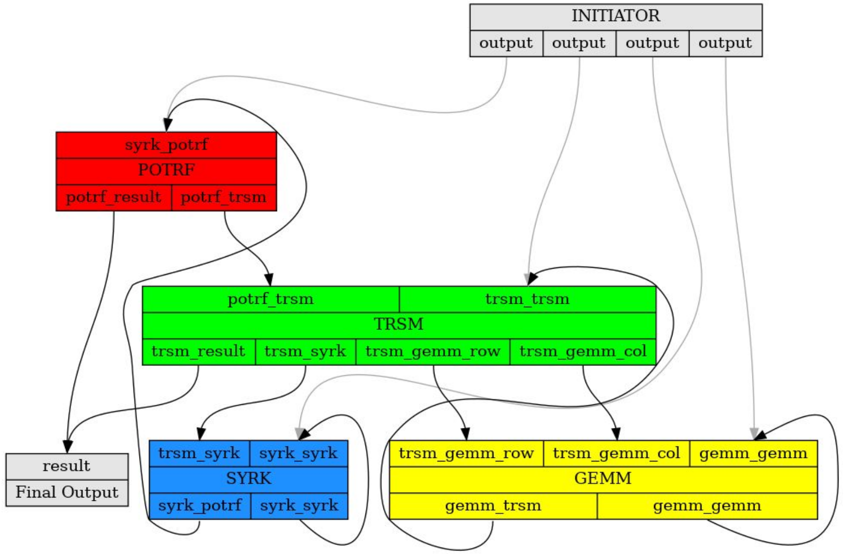
```
[=](const keyT &k, auto&& val) {
  ttg::print(“This is task B(“ , k, “, “ val, “)”);
}
```

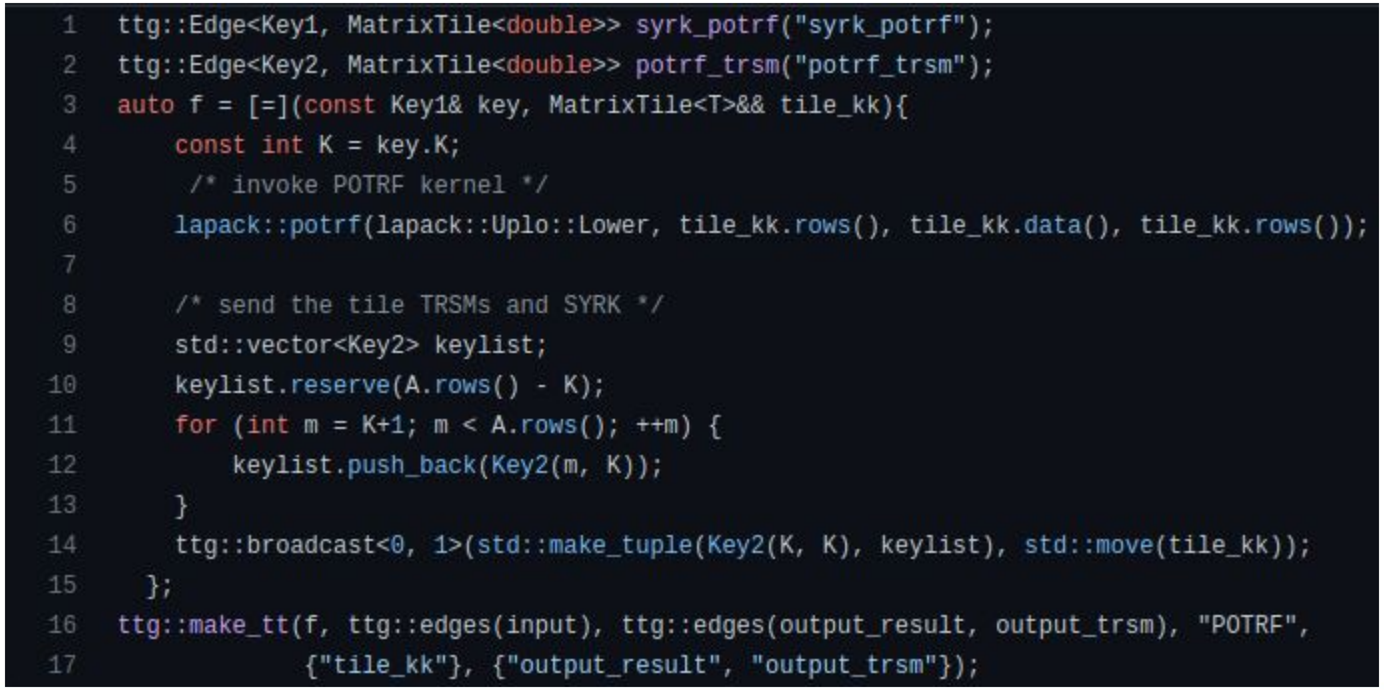
mutable generic data

We need C++ introspection!

Example: Data Movement

- Data is sent or broadcast through the graph
- POTRF kernel:
  - Invoke kernel
  - Populate successor keys
  - Broadcast keys and data





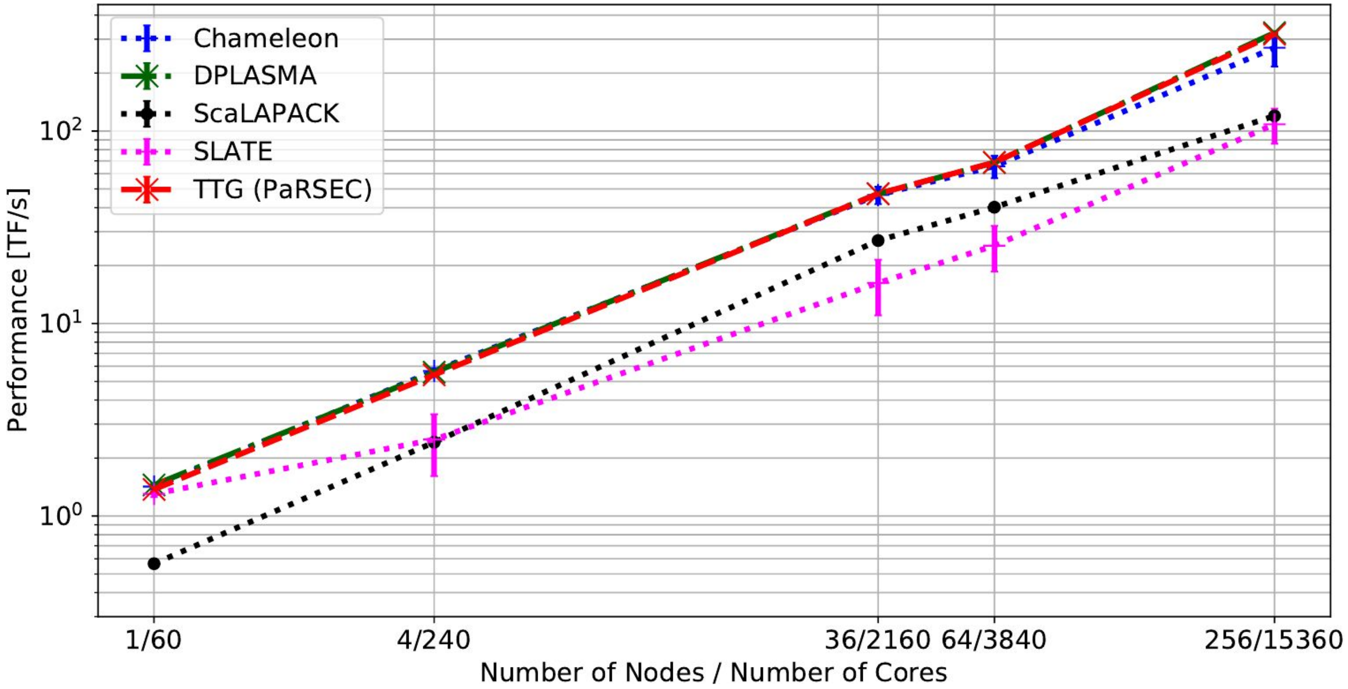
```
ttg::Edge<Key1, MatrixTile<double>> syrk_potrf("syrk_potrf");
ttg::Edge<Key2, MatrixTile<double>> potrf_trsm("potrf_trsm");
auto f = [=](const Key1& key, MatrixTile<T>&& tile_kk){
    const int K = key.K;
     /* invoke POTRF kernel */
    lapack::potrf(lapack::Uplo::Lower, tile_kk.rows(), tile_kk.data(), tile_kk.rows());

    /* send the tile TRSMs and SYRK */
    std::vector<Key2> keylist;
    keylist.reserve(A.rows() - K);
    for (int m = K+1; m < A.rows(); ++m) {
        keylist.push_back(Key2(m, K));
    }
    ttg::broadcast<0, 1>(std::make_tuple(Key2(K, K), keylist), std::move(tile_kk));
  };
ttg::make_tt(f, ttg::edges(input), ttg::edges(output_result, output_trsm), "POTRF",
             {"tile_kk"}, {"output_result", "output_trsm"});
```

Cholesky Factorization: Weak Scaling

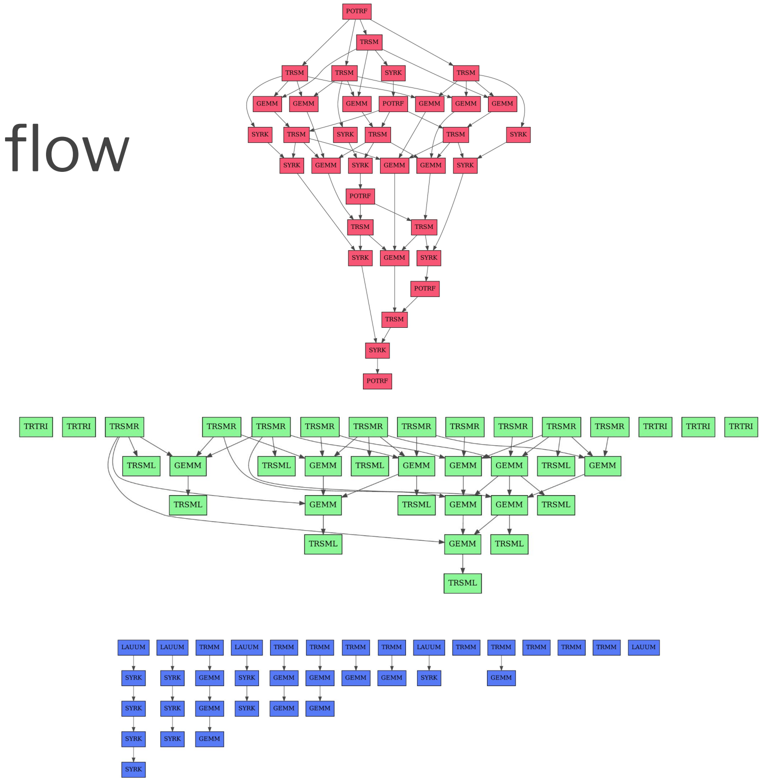
- Hawk, 1 – 256 nodes
- Matrix: 30k per node, tiles size 512

Performance of TTG matches DPLASMA

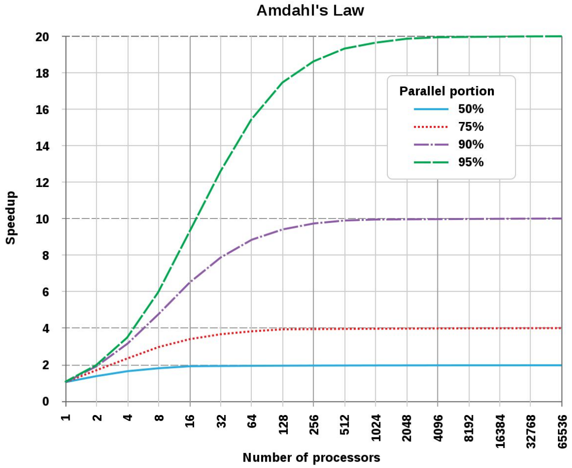


Task Graph Composition

- Assume N consecutive functions implemented using the same task programming model
    - N forks and joins without composition
    - Write-back to data structures instead of direct flow
    - Gene Amdahl says that’s bad



https://upload.wikimedia.org/wikipedia/commons/1/1a/Gene_Amdahl_on_a_classic_grey_Ferguson_tractor_at_Amdahl.JPG



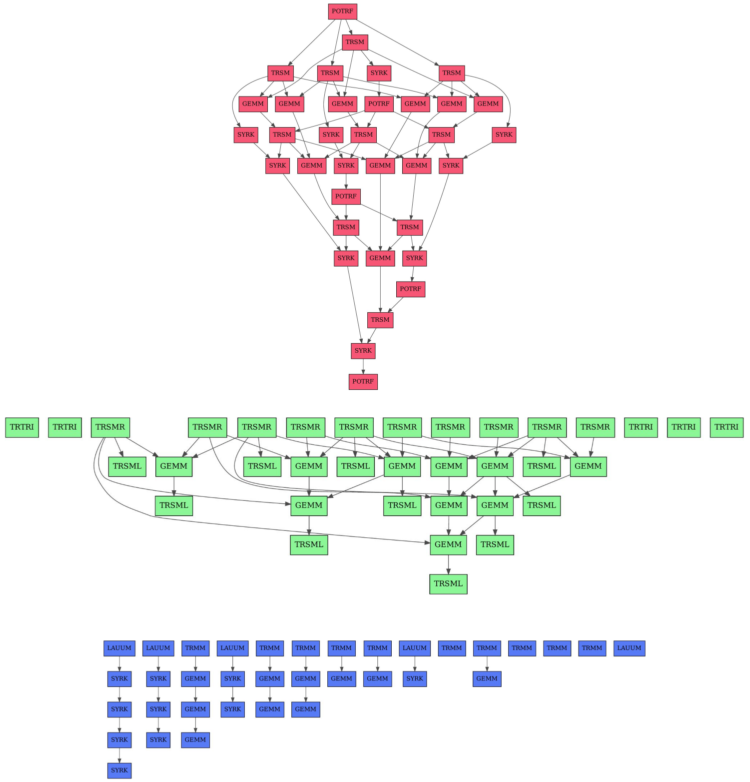
https://en.wikipedia.org/wiki/Amdahl%27s_law#/media/File:AmdahlsLaw.svg

Example: Cholesky Matrix Inversion

- Cholesky Factorization (POTRF) followed by matrix inversion
  - Given A, compute A^{-1}
  - A: Hermitian positive-definite matrix

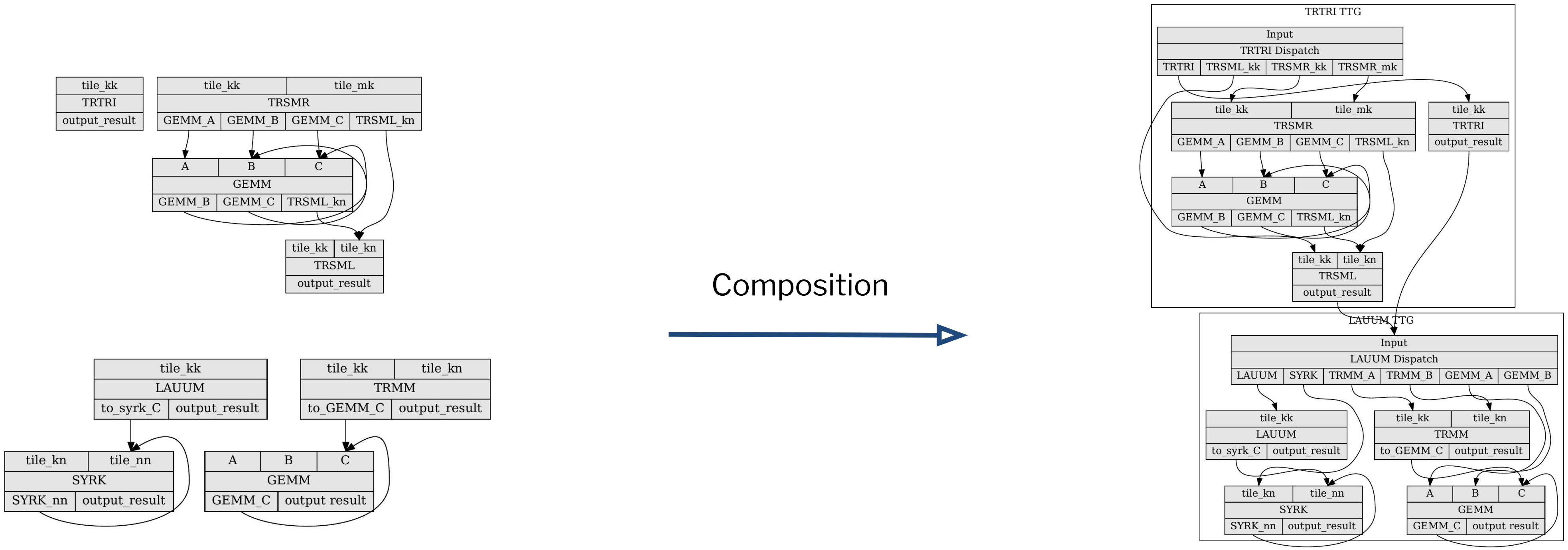
- Inversion: Given L from POTRF
  - Compute L^{-1} from L (TRTRI)
  - Compute $A^{-1} = (L^{-1})^T L^{-1}$ (LAUUM)
  - POTRI = TRTRI ⊕ LAUUM

- POINV = POTRF ⊕ POTRI
  = POTRF ⊕ TRTRI ⊕ LAUUM

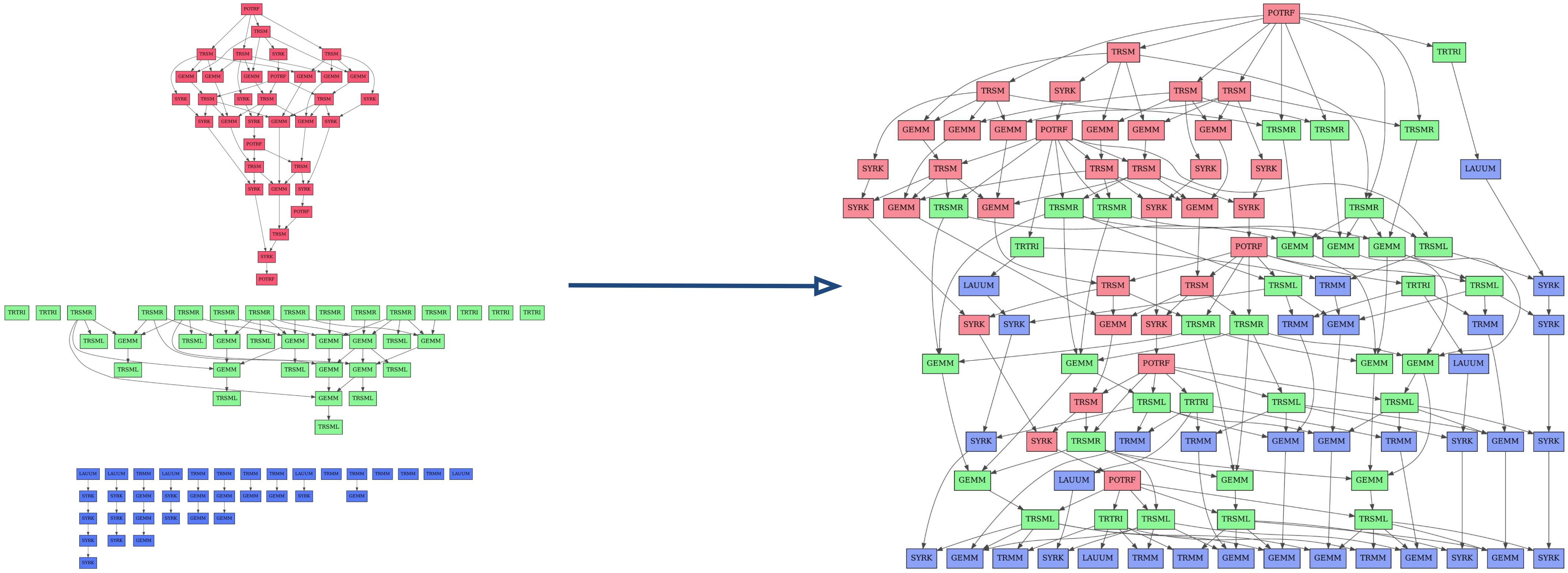


Connecting Graphs: Edges as Composition Devices

- Use Edges to connect algorithm graphs
  - Algorithms as black bloxes
  - Data flows in through Edge, comes out through Edge

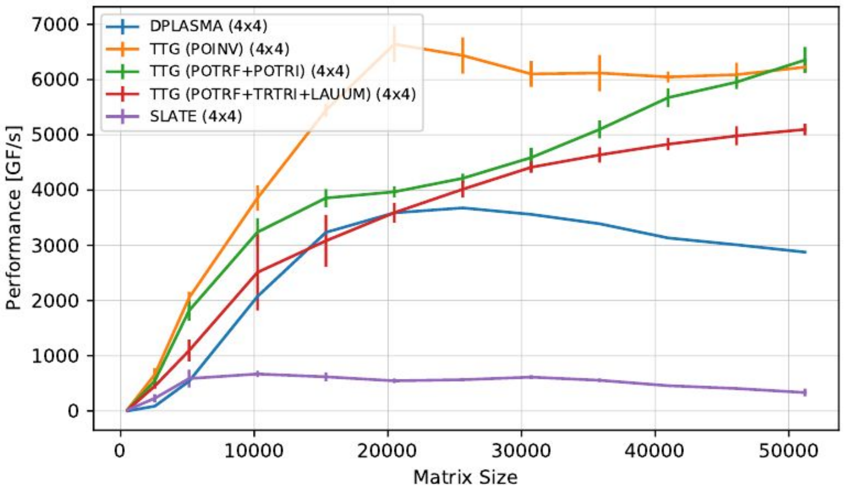


Task Graph Composition at Work

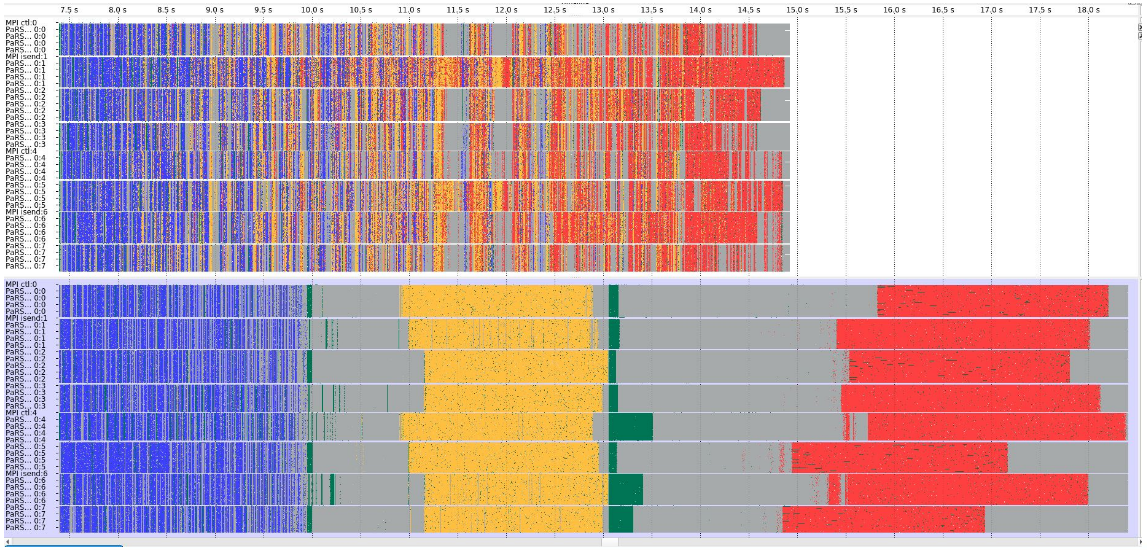


POINV Composition

- 16 nodes on Hawk, 64 threads each
- Full composition beneficial for small tile sizes
  - Fine-grain composition helps hide communication latency
  - Beats both DPLASMA (based on PaRSEC PTG) and SLATE



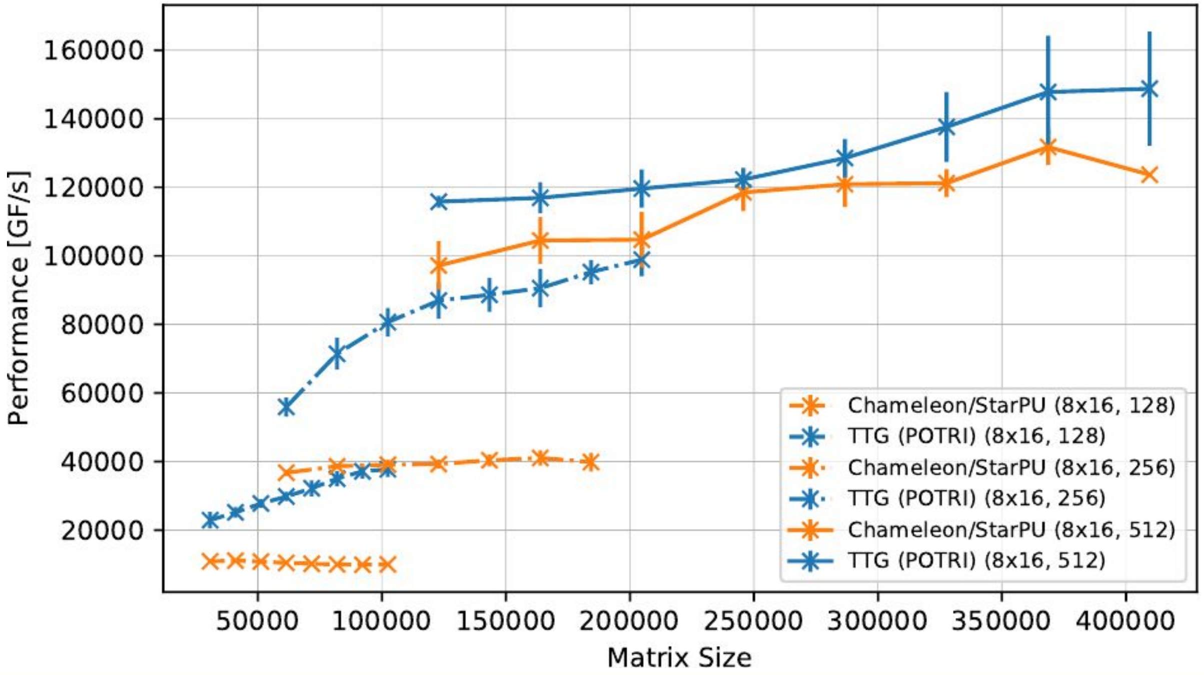
(a) Tile size 128.



T. Herault, J. Schuchart, G. Bosilca, E. Valeev. Composition of Algorithmic Building Blocks in Template Task Graphs. PAW-ATM 2022.

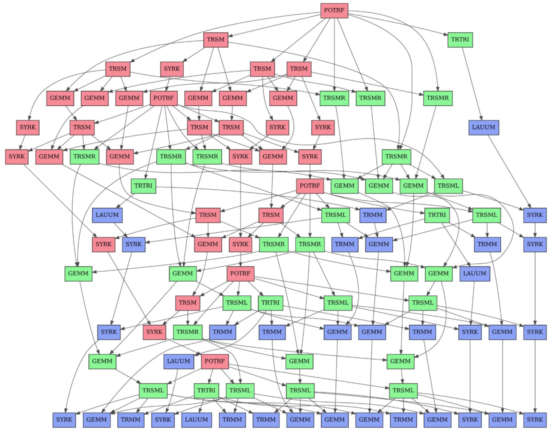
POTRI: Comparison with Chameleon

- 128 nodes on Hawk
- Chameleon (v1.1.0, using StarPU 1.3.9)
- POTRI : TRTRI ⊕ LAUUM
- TTG performance benefits
  - Depth-first execution
  - Parallel distributed task discovery



Part 2: Summary

- Global task discovery limits scalability
- Template Task Graphs provide
    - **Scoped task discovery**, with C++ semantics
    - Without the baggage of futures
- Edges represent *sets of values* and simplify composition
- Future work includes
    - Integrated device support (using C++ coroutines)
    - Porting of MADNESS/TiledArray on top of TTG

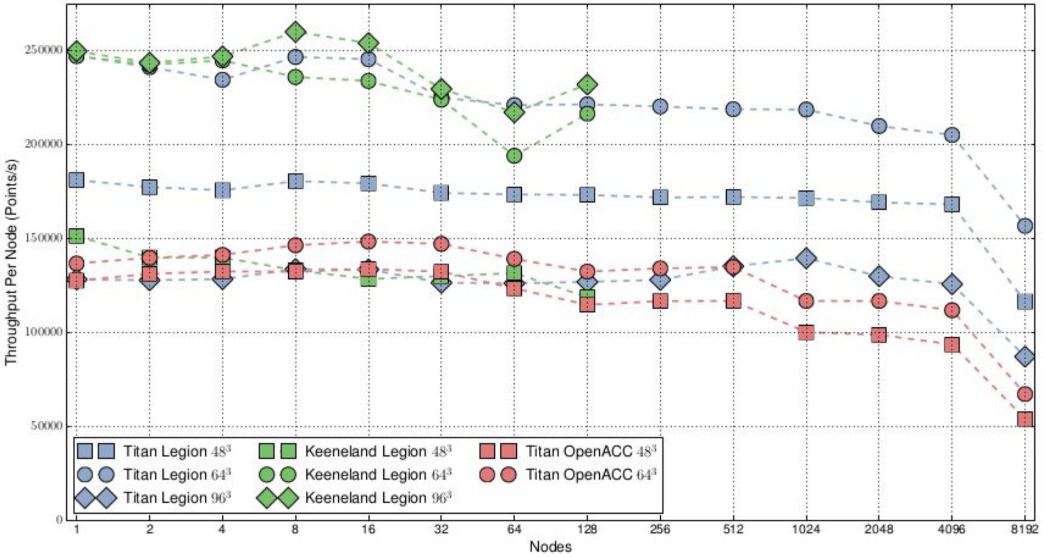


Part Three

Why are asynchronous models so hard to use?

Challenges and Benefits of Tasks

- S3D using MPI vs Legion



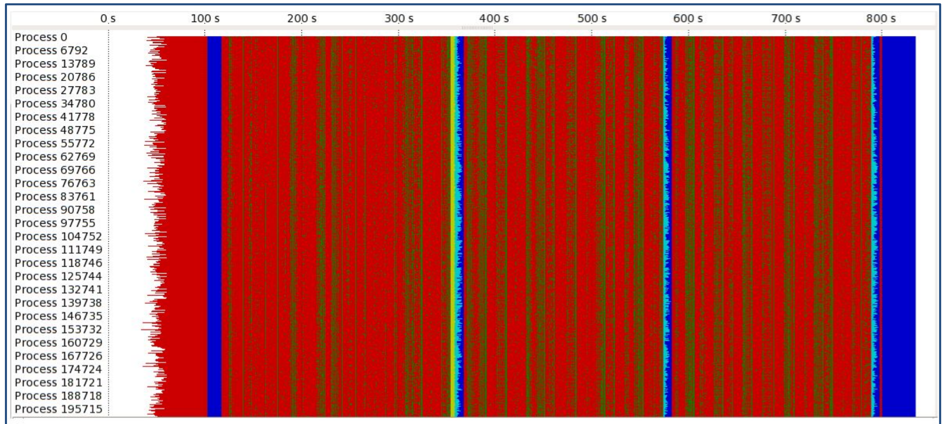
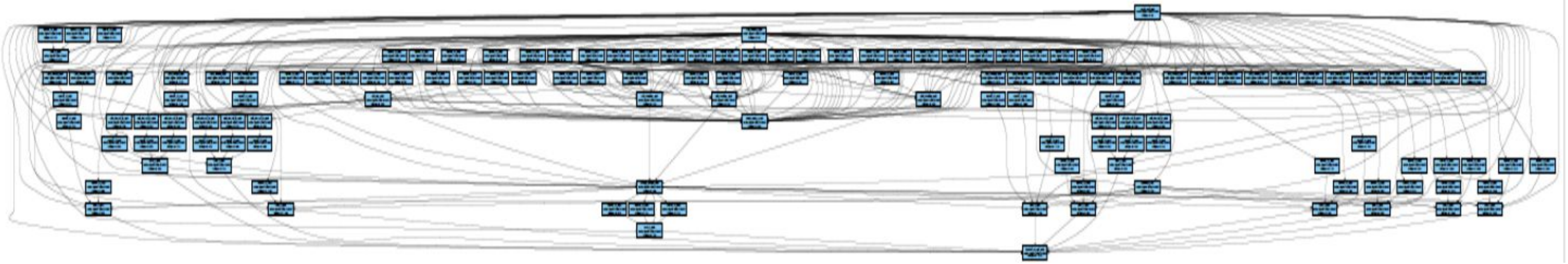


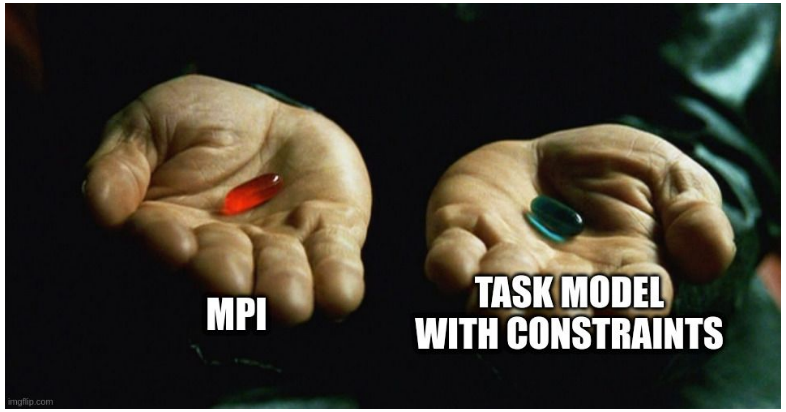
Figure 10: Screenshot of Vampir visualizing a trace of the S3D application using 200,448 cores on JaguarPF. User functions are shown in green, MPI operations in red, and activities of the measurement environment in yellow (file open), light blue (trace I/O) and dark blue (synchronization).



https://hpc.pnl.gov/conf/wolfhpc/2015/talks/aiken.pdf

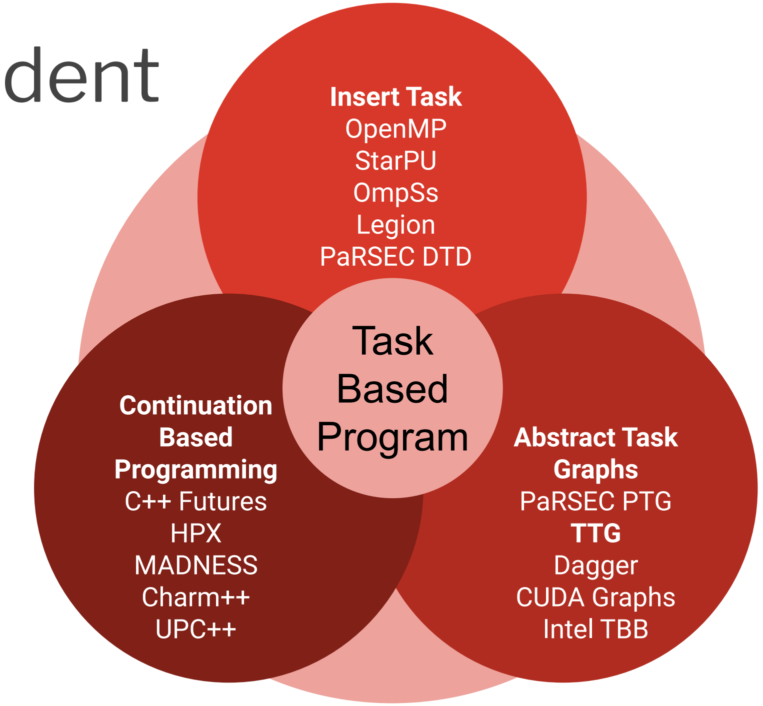
Challenges of Programming in Tasks

- Porting existing applications to new programming models is a significant investment (>1PY)
- Higher level abstractions → more constraints:
  - Less flexible than MPI
  - Likely to run into (non-MPI) barriers at some point
- Clear separation of concerns with MPI/OpenMP
- Flag-ship task applications vs broad acceptance?
  - Octotiger (HPX)
  - S3D (Legion)
  - ExaGeoStat (PaRSEC)



A Plethora of Models

- Which is the right model for my application?
- How long will that model be supported?
- How much flexibility do I need?
- How many constraints can I accept?
- Can I maintain the code once the PhD student is gone?



Insert Task
OpenMP
StarPU
OmpSs
Legion
PaRSEC DTD

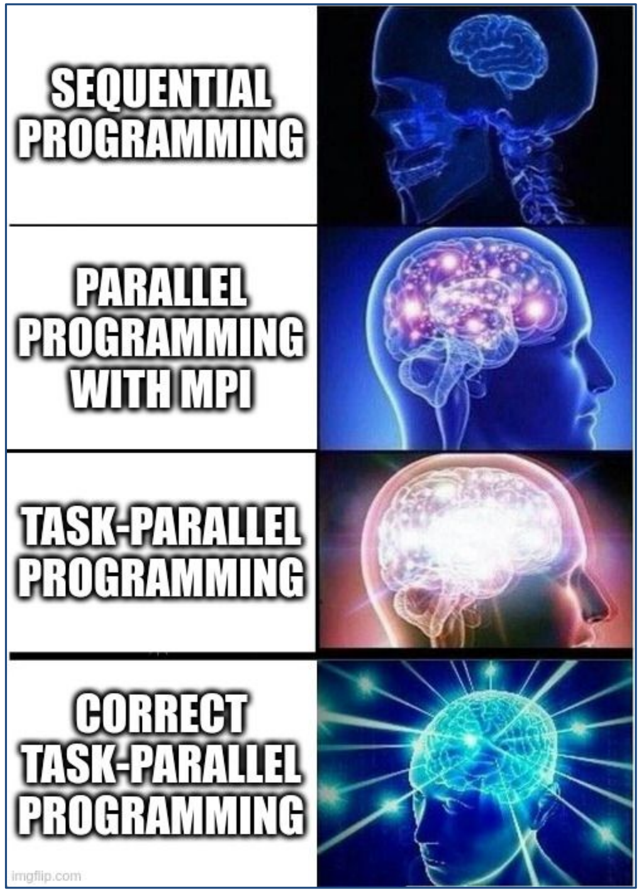
Task Based Program

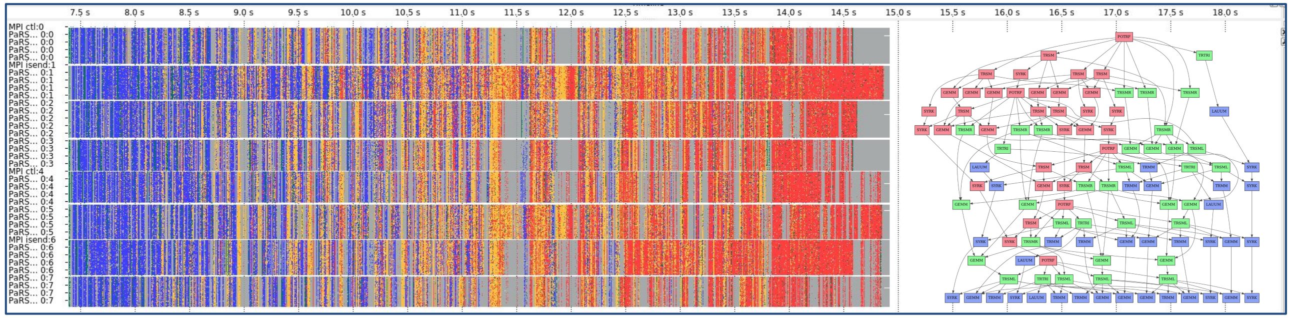
Continuation Based Programming
C++ Futures
HPX
MADNESS
Charm++
UPC++

Abstract Task Graphs
PaRSEC PTG
TTG
Dagger
CUDA Graphs
Intel TBB

The Complexity of Models

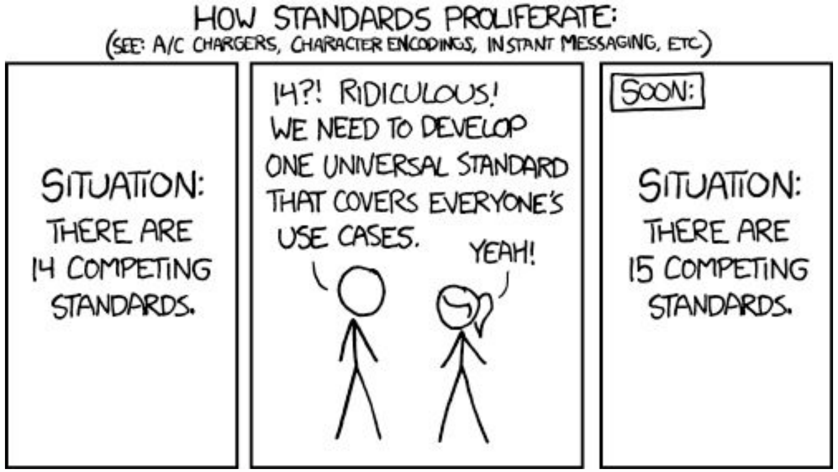
- Are developers able to grasp the complexity of fully asynchronous programming?
    - Just a matter of teaching?
- We typically think sequentially
    - Task-based programming like juggling
- We need better tools for debugging & performance analysis





Conclusions

- Task-based programming comes with significant benefits and challenges
- We need better **support from MPI** to support async models
- Better **tool support** for application & runtime developers
- There is (likely) no single model to rule all applications
- But: Can we establish interoperability between models?
  - Past efforts had limited success



A Shameless Plug

- ICL is hiring
  - PhD students
  - PostDocs
  - Visitors (3-12 months)
- Talk to me if you're interested :)

Discussion