PhD Thesis Proposal

A Hybrid Model for Reducing the Cost of Communication in Large-Scale Applications

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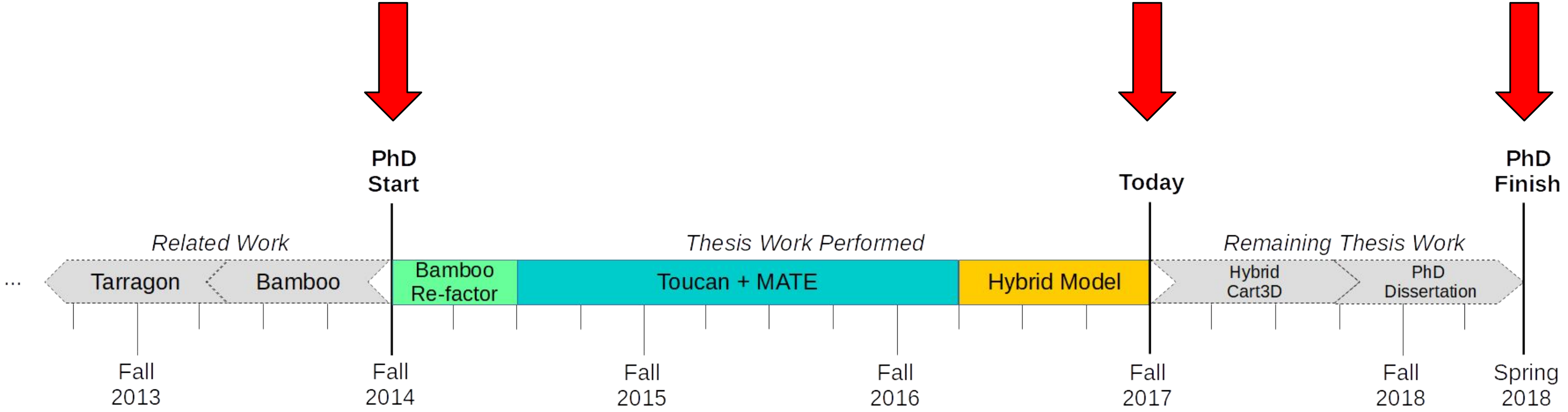
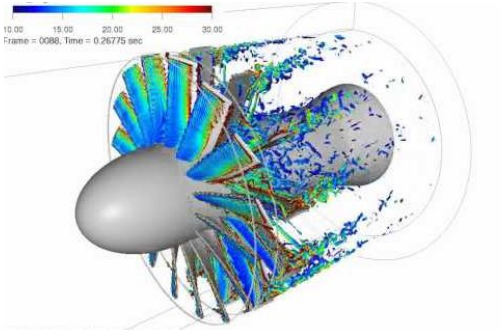
PhD Thesis Timeline

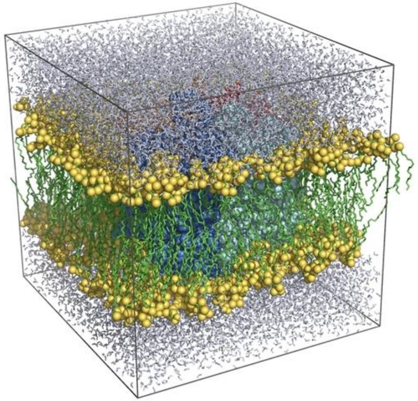


High-Performance Computing

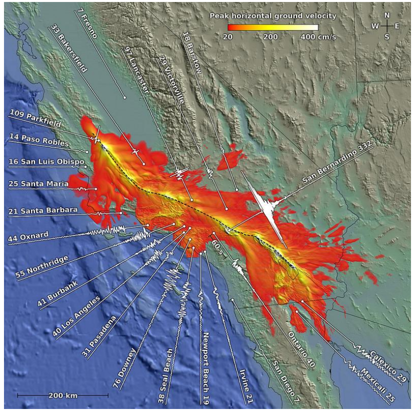
HPC is an essential tool in developments in science and technology.



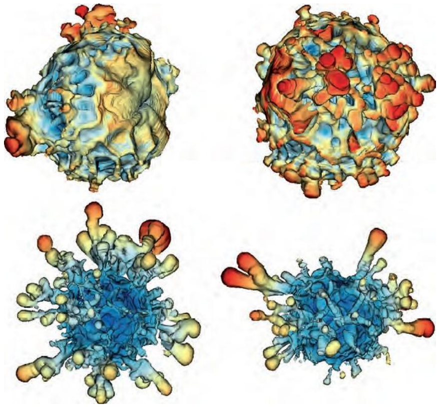
Aerospace Engineering



Computational Biology



Natural Disaster & Climate Modeling



Astrophysics

High-Performance Computing

Relies on the power of Supercomputers
(Hardware + Interconnect)

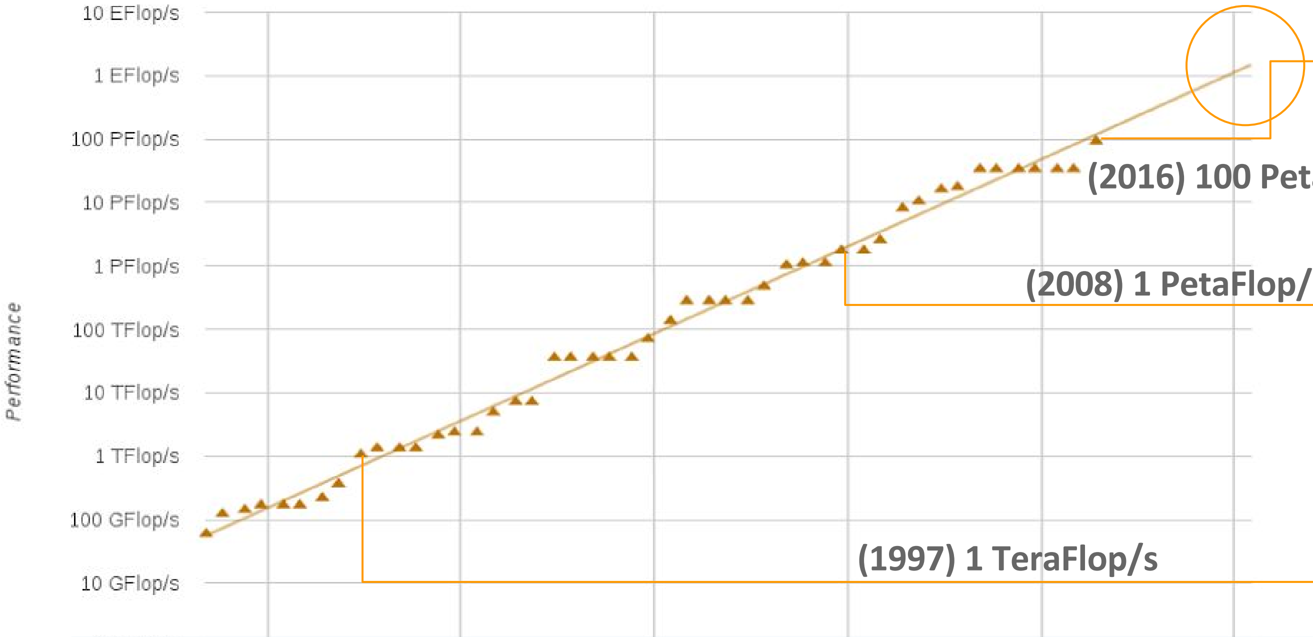
That's me @ Berkeley Lab

Requires a
Parallel Programming Framework

- Parallel Programming Models
- Communication Libraries
- Runtime Systems
- Threading Libraries
- Compilers / Translators

Evolution of Supercomputers

Source: *Top500.org*



(2020?) 1 ExaFlop/s

(2016) 100 PetaFlop/s

(2008) 1 PetaFlop/s

(1997) 1 TeraFlop/s

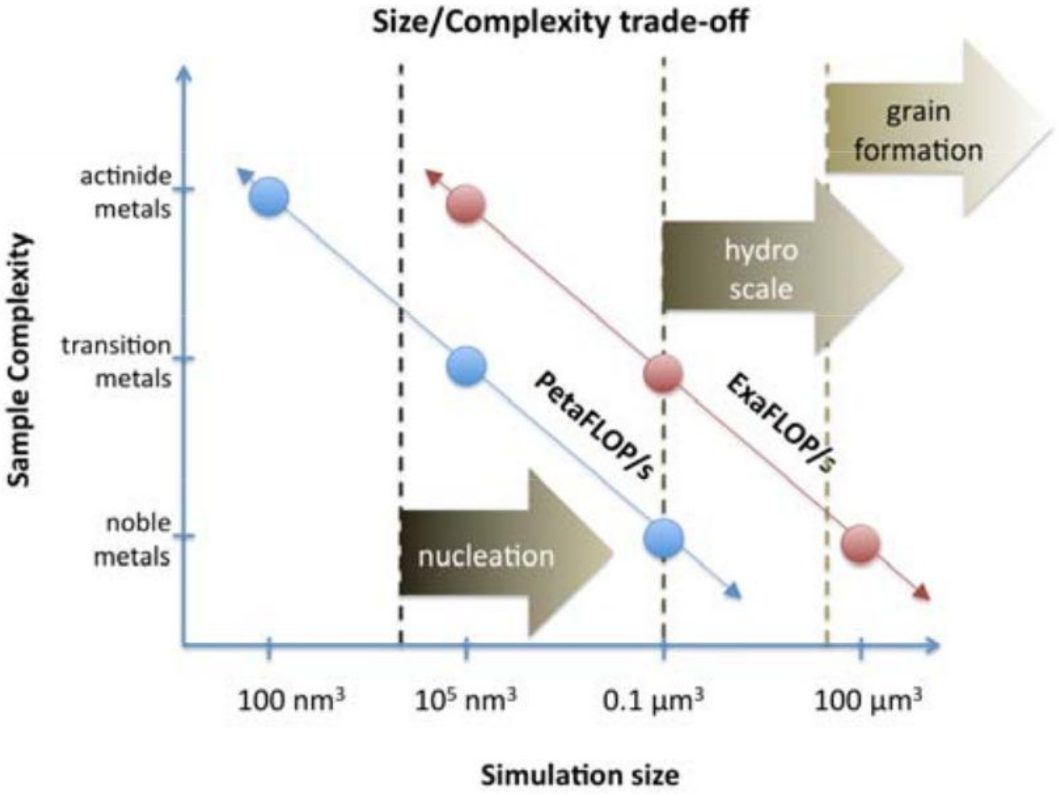
Sunway TaihuLight (NSC, China)

IBM Roadrunner (Los Alamos Lab, US)

“The mission and science opportunities in going to exascale are compelling”

“The opportunities and challenges of exascale computing”. S. Ashby et al. In: Summary Report of the US DOE ASC. 2010

Example: Design of advanced materials.



Challenges of Exascale Computing

3 Main Challenges[1]:

- Reduce Energy Consumption (From 200MW estimated to 20MW[2]).
- Ensure Reliability and Fault-Tolerance.
- Exploit Massive Parallelism.
    - Provide an adaptive response to load imbalance.
    - Develop multi-core and memory hierarchy-aware algorithms.
    - **Reduce the cost of communication.** ⇦

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[1] **"The opportunities and challenges of exascale computing",** S. Ashby et al, Summary Report of the US DOE ASCR, 2010

[2] **"Algorithmic Challenges of Exascale Computing",** K. Yelick, Presentation, Lawrence Berkeley National Laboratory 2012

Thesis Motivation (1/3)

Communication cost comprises a significant part of large-scale application running time[1].

(Moreover, communication overheads are continuing to grow towards the ***Exascale***.)

For this reason...

① “[...] There is a need to investigate algorithms that reduce communication to a minimum.”[2]

[2] **“The opportunities and challenges of exascale computing",** S. Ashby et al, Summary Report of the US DOE ASCR, 2010

[1] **“Communication Avoiding and Overlapping for Numerical Linear Algebra",** E. Georganas et al, SC12, 2012

Traditional Parallel Programmin

- **Based on shared memory.**
- **Limited to a single node.**

Models	Variants	Languages/Interfaces
Threading Model	Kernel Threads	POSIX Threads, OpenMP
Message Passing Model	Flat MPI	MPI
	Fine-Grained MPI	FP-MPI, TMPI, AzequiaMPI
	MPI+X	MPI+OpenMP, MPI+PThreads, MPI+MPI
Dataflow Models	Concurrent Collections	Habanero CnC, DAGuE
	Statement-Level D	
	Task-Level Dataflow	Tarragon, SMPSs

- **Based on Message Passing.**
- **Enables inter-node communication.**

Adapted and Simplified from: **"Analysis of Parallel Programming Models for Exascale Computing",** S. Martin, CSE Research Exam 2016

Anatomy of a naive MPI Application

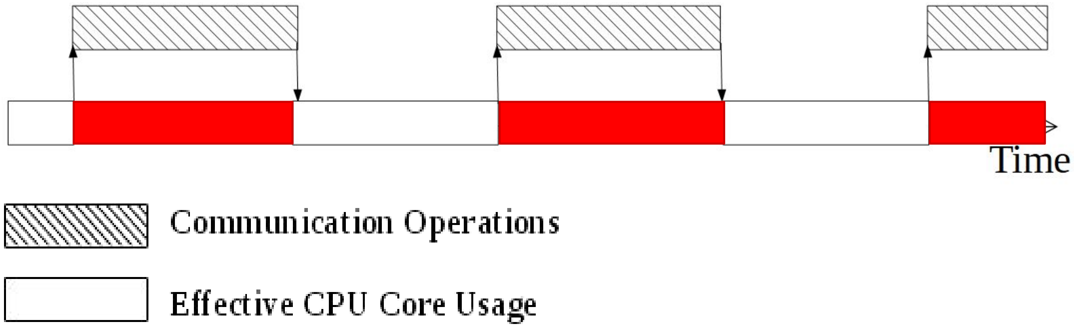
Main Loop

```
For (iterations)
 {
  … Receive Requests…
  … Send Requests…
  -- Wait for Requests --
  … Compute …
 }
```

Communication Phase

Computation Phase

Core Usage Timeline:



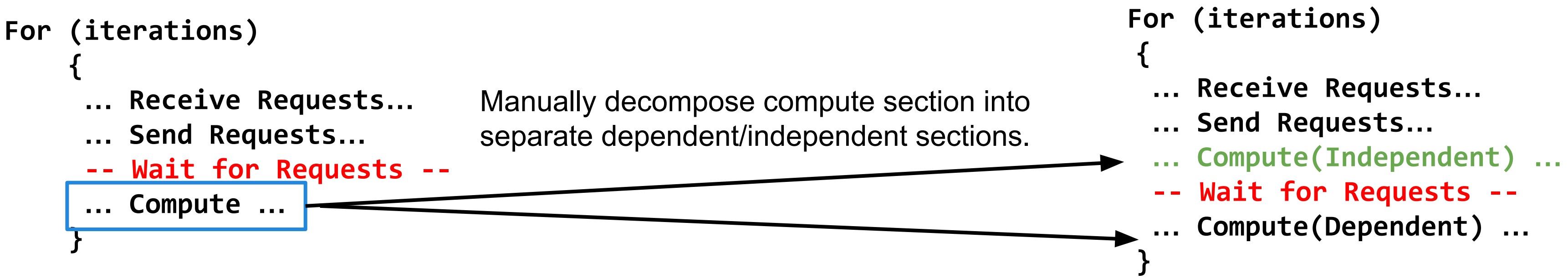
- **Problem:** Naive MPI applications suffer from the full cost of communication.
- **Coping strategies:**
  - Hiding Strategy: Overlap communication with computation[1,2].
  - Avoiding Strategy: Performing less and/or more efficient communication[3].

[1] **"A Programming Model for Block-Structured Scientific Calculations on SMP Clusters ",** Ph. D. Dissertation, '98

[2] **"Latency Hiding and Performance Tuning with Graph-Based Execution",** P. Cicotti and S. Baden. In DFM'11

[3] **"Communication-optimal parallel 2.5D matrix multiplication and LU factorization algorithms",** E. Solomonik and J. Demmel. In EuroPar'01

Manual Optimization for Overlap



```
For (iterations)
    {
     … Receive Requests…
     … Send Requests…
     -- Wait for Requests --
     … Compute …
    }
```

Manually decompose compute section into separate dependent/independent sections.

```
For (iterations)
{
  … Receive Requests…
  … Send Requests…
  … Compute(Independent) …
  -- Wait for Requests --
  … Compute(Dependent) …
}
```

Shortfalls of re-factoring MPI applications manually:

- Embeds policy decisions into the application code.
- They may require non-trivial algorithmic changes.
- Transformations are hard to maintain (architecture-dependent).
- For some large applications, these transformations are unviable.

Thesis Motivation (2/3)

Communication cost comprises a significant part of large-scale application running time[1].

(Moreover, communication overheads are continuing to grow towards the ***Exascale***.)

For this reason...

① "[...] There is a need to investigate algorithms that reduce communication to a minimum."[2]

However...

② Manual re-factoring of legacy MPI applications can be impractical.

[2] **"The opportunities and challenges of exascale computing",** S. Ashby et al, Summary Report of the US DOE ASCR, 2010

[1] **"Communication Avoiding and Overlapping for Numerical Linear Algebra",** E. Georganas et al, SC12, 2012

Alternative Parallel Programming Models

Models		rfaces
Threading Model	Ker	MP
Message Passing Model	Flat MPI	MPI
	Fine-Grained MPI	FP-M
	MPI+X	MPI+ MPI+MPI
Dataflow Models	Concurrent Collections	Habanero-CnC, DAGuE
	Stat	
	Tas	MPSs

- **Simple, intuitive, easy to use.**
- **Most widely used. Plenty of Legacy code.**
- **Hard to optimize for hiding communication cost.**

Is automatic conversion possible?

- **Data-dependency flow of execution.**
- **(Arguably) Less intuitive.**
- **Better suited to design communication-tolerant applications**

Adapted and Simplified from: **"Analysis of Parallel Programming Models for Exascale Computing",** S. Martin, CSE Research Exam 2016

Automatic Translation

Alternative approach to manual re-factoring:

- Use translation-based tools to achieve communication/computation overlap[1,2].
- Idea first proposed by the authors of the **Bamboo Model**[3].
- Convert a traditional MPI program into a dataflow-model program automatically.
- The semantics of the source code remain unaltered.

[1] **"Perilla: Metadata-based Optimizations of an Asynchronous Runtime for Adaptive Mesh Refinement"**, T. Nguyen et al. In: SC'16

[2] **"Petal Tool for Analyzing and Transforming Legacy MPI Applications"**, H Ahmed et al. In: LCPC '15

[3] **"Bamboo - Translating MPI applications to a latency-tolerant, data-driven form"** Nguyen et al. In SC'12

Thesis Motivation (3/3)

Communication cost comprises a significant part of large-scale application running time[1].

(Moreover, communication overheads are continuing to grow towards the ***Exascale***.)

For this reason...

① “[...] There is a need to investigate algorithms that reduce communication to a minimum.”[2]

However...

② Manual re-factoring of legacy MPI applications is impractical.

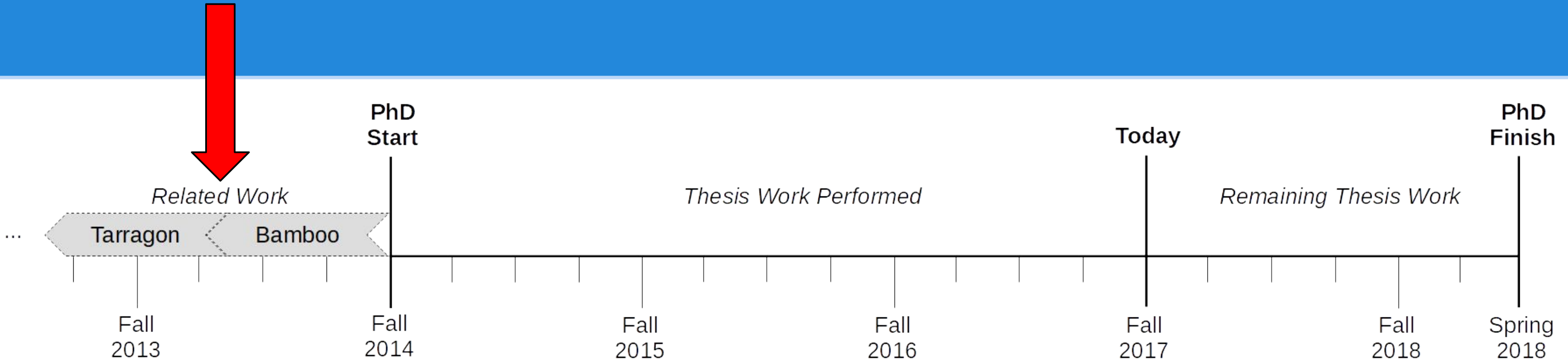
Therefore...

③ Automatic translation can help towards communication-efficient Exascale computing.

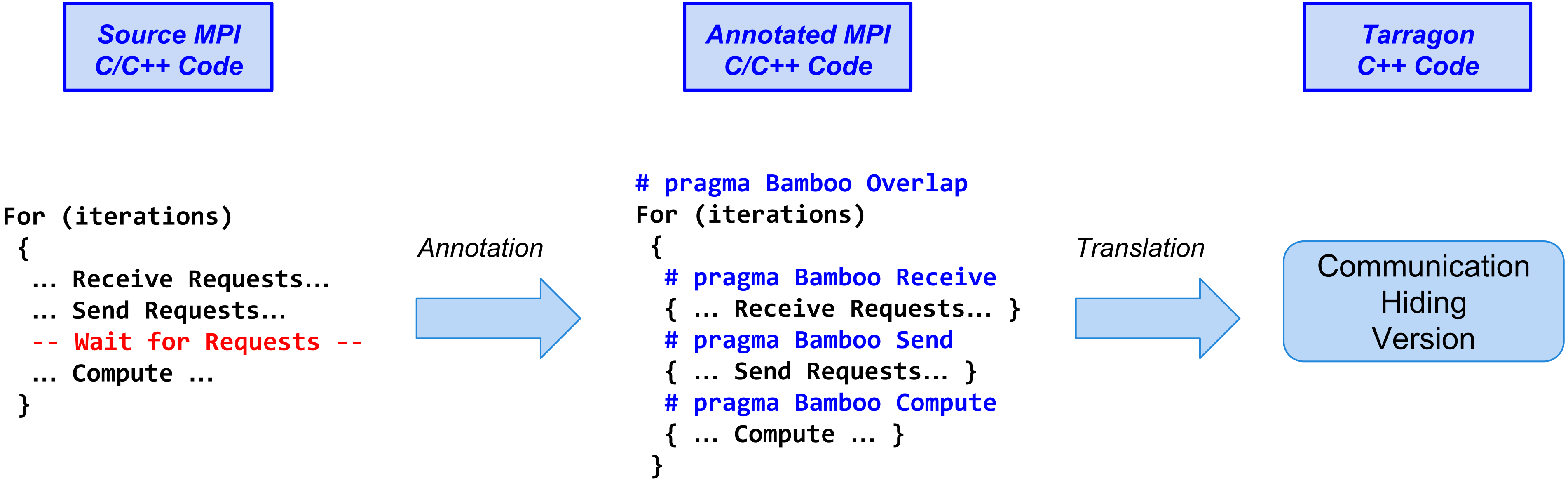
[2] **“The opportunities and challenges of exascale computing",** S. Ashby et al, Summary Report of the US DOE ASCR, 2010

[1] **“Communication Avoiding and Overlapping for Numerical Linear Algebra",** E. Georganas et al, SC12, 2012

Related Work



Bamboo Model



Source MPI C/C++ Code

```
For (iterations)
 {
  … Receive Requests…
  … Send Requests…
  -- Wait for Requests --
  … Compute …
 }
```

Annotation

Annotated MPI C/C++ Code

```
# pragma Bamboo Overlap
For (iterations)
 {
  # pragma Bamboo Receive
  { … Receive Requests… }
  # pragma Bamboo Send
  { … Send Requests… }
  # pragma Bamboo Compute
  { … Compute … }
 }
```

Translation

Tarragon C++ Code

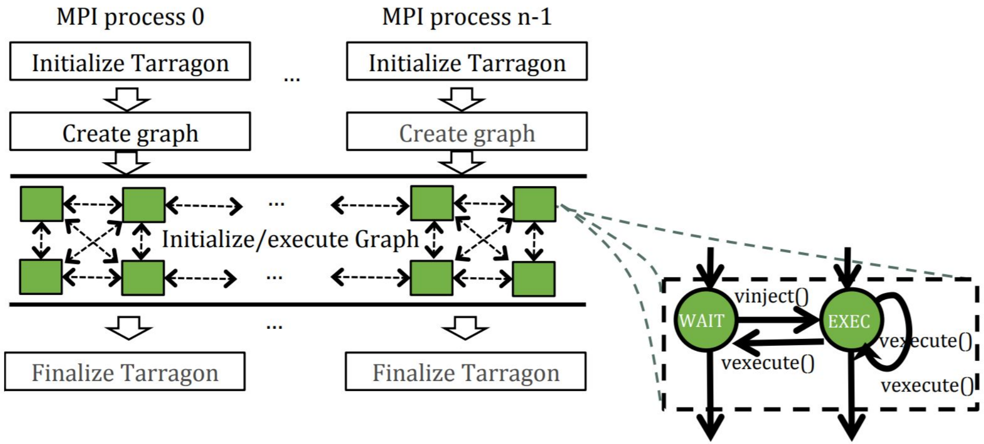
Communication Hiding Version

Tarragon Model

A Bamboo-Translated code runs as a Tarragon[1] program.

[1] **"Latency Hiding and Performance Tuning with Graph-Based Execution"** P. Cicotti and S. Baden. In DFM'11

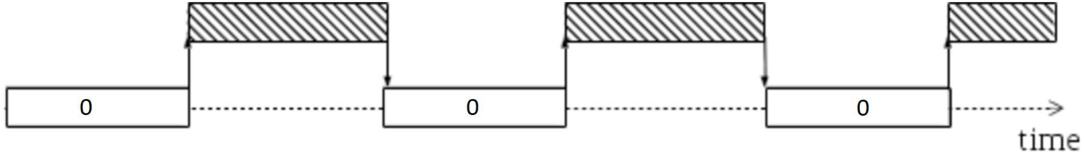
- Tarragon is a parallel programming model for communication-tolerant algorithms.
- Bamboo converts each original MPI process into a **set** (>1) of Tarragon tasks.
- Tarragon tasks are not assigned resources until data dependencies are satisfied.
- Communication cost is hidden by executing ready tasks while others are communicating.



Source: **"Bamboo: Automatic Translation of MPI Source into a Latency-Tolerant Form"** T. Nguyen. PhD Thesis '14.

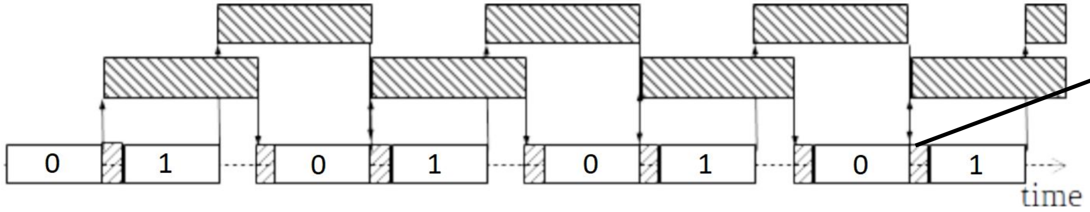
Core Usage Timeline

Untranslated MPI Code



No overlap

Translated Code
2 Tasks / MPI Process



Additional Comm
D-Cache Flushing
Context Switch Cost

Comm/Comp Overlap. Better core usage.

Observation: The optimal task number is dependent on both the application and the system.

Bamboo’s Limitations

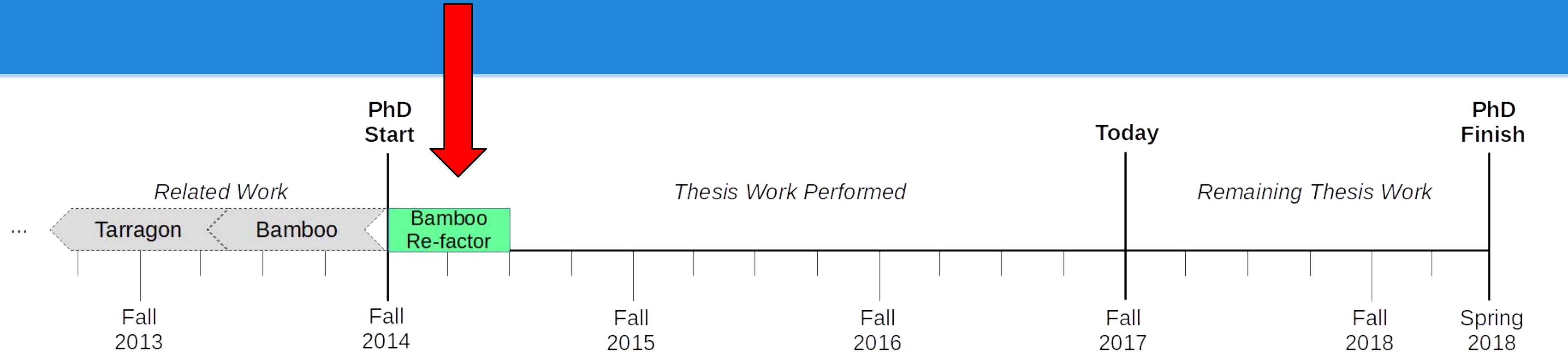
Bamboo demonstrated automatic translation can be used to the cost of communication, however:

- **Bamboo and Tarragon were not co-designed.**
    - Bamboo’s translation logic was constrained to the Tarragon runtime system’s design.

- **Static Scheduling Problem**
    - Tarragon provides a single execution entry point per task (*Tarragon_Execute*).
    - Bamboo needs embed static scheduling logic into the translated code.
        - Code Bloating: **15x** increase. Difficult to debug.
        - **No support for recursive code.** Incompatible with some production applications.

- **Handling MPI⇔Tarragon Communication**
    - A description of the communication graph layout is required by Tarragon.
        - This is a problem domain-specific setting.
    - All communication needs to be annotated (even initialization/finalization).
    - Buffering and header wrapping is required to translate Tarragon to MPI messages.
        - This requires additional CPU overhead (memcpy) and memory bandwidth.

Refactoring Bamboo/Tarragon



Refactoring Bamboo/Tarragon

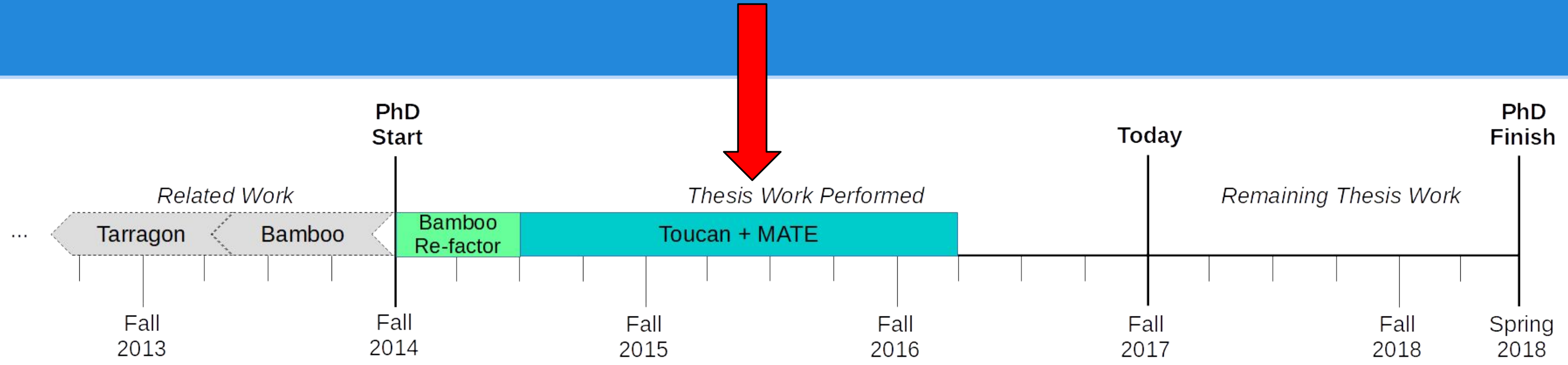
Goal: Refactor Bamboo and Tarragon simultaneously to address their limitations.

- **Milestone 1: Learn how Bamboo & Tarragon operate**
  1. Examine translated codes.
  2. Examine the source code of Bamboo (15k LoC) and Tarragon (16k LoC).

- **Milestone 2:** Transfer scheduling/communication functionality from Bamboo to Tarragon.

- **Bittersweet results:**
  - Reduced code bloating by a factor of ~3x.
  - Recursion remained a problem due to Tarragon’s single entry point mechanism.
    - Further re-factoring was impractical due to Bamboo and Tarragon’s complexity.
    - Could not get Tarragon to run efficiently in new architectures, but:
  - **Gained the how-to for building both a Translator and a Runtime System.**

Toucan/MATE


PhD Start
Today
PhD Finish
Related Work
Thesis Work Performed
Remaining Thesis Work
…
Tarragon
Bamboo
Bamboo Re-factor
Toucan + MATE
Fall 2013
Fall 2014
Fall 2015
Fall 2016
Fall 2017
Fall 2018
Spring 2018

New Project

New Goal: Co-Design a new translator and a new runtime system simultaneously.

- **Design a new Translator**
    - Minimal intervention: no static scheduling embedded in the code.
        - Negligible Code Bloating.
        - Debuggable code.
    - Minimal annotation requirements
        - No problem domain-specific annotations.
        - Annotated/non-annotated communication can co-exist.

- **Co-Designed with a new Runtime-System**
    - Supports multiple entry points.
    - Manages all MPI message handling.
    - Supports Recursive Execution.

Introducing **Toucan/MATE**

- **Toucan: an improved MPI Translator**
    - Built using the ROSE Compiler Framework (LLNL).
    - Uses a reduced set of Bamboo’s annotations (4 directives)

Toucan

- **MATE Runtime System**
    - Uses lightweight threads (Coroutines) instead of static scheduling.
    - Coroutines can exit/re-entry a function at any given point.
    - Creates and schedules the dependency graph dynamically.

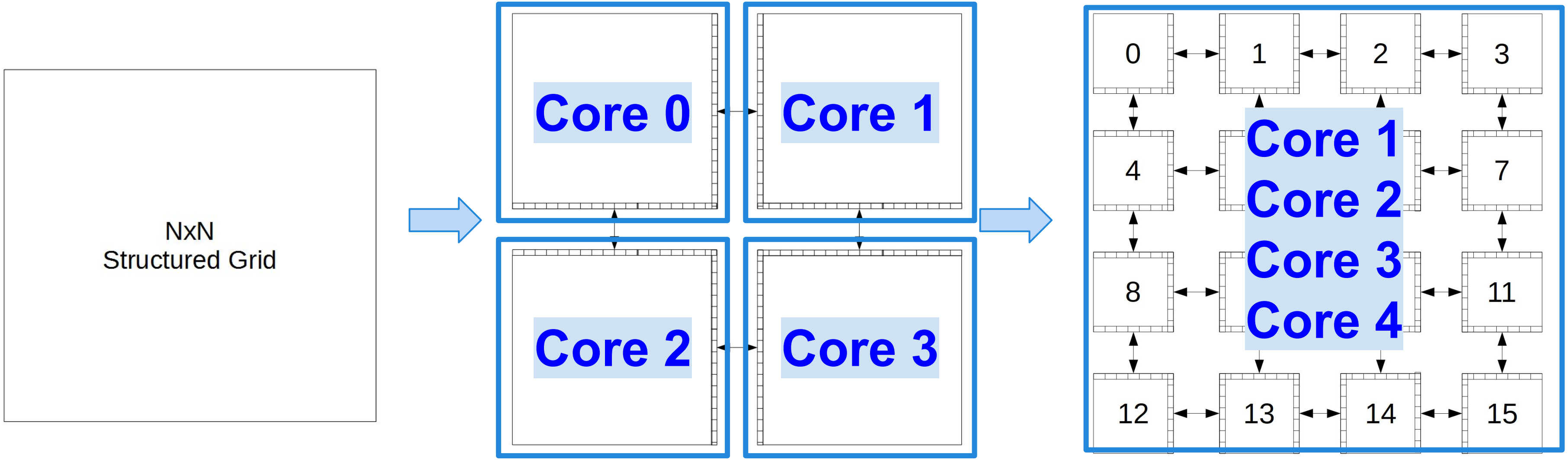
MATE

(Pronounced ‘Mah-tay’)

- **Toucan/MATE rely on two mechanisms:**
    1. Oversubscription of processor cores.
    2. Code region-aware scheduling.

Core Oversubscription in Toucan/MATE

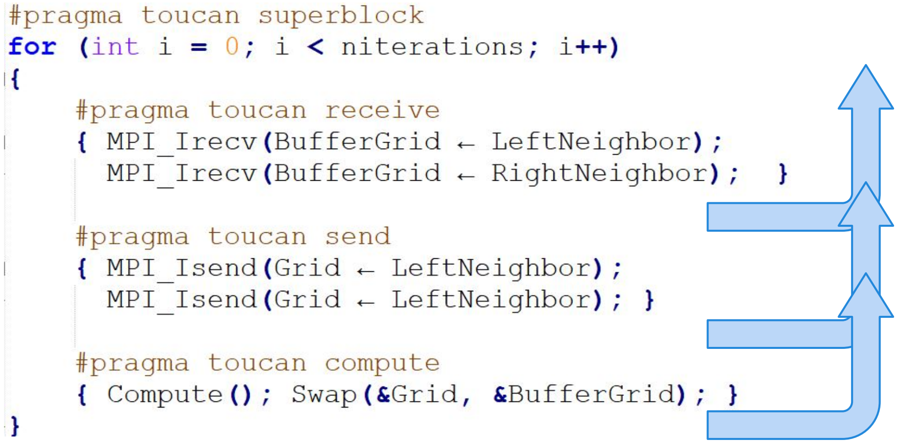
Split the problem domain into more partitions than useful cores in the system.



Typical MPI Decomposition
1 Subdomain per Core

Toucan’s Overdecomposed Grid
4 Subdomains per Core
(Single Task Pool per Node)

Code Regions



```
#pragma toucan superblock
for (int i = 0; i < niterations; i++)
{
    #pragma toucan receive
    { MPI_Irecv(BufferGrid ← LeftNeighbor);
      MPI_Irecv(BufferGrid ← RightNeighbor);   }

    #pragma toucan send
    { MPI_Isend(Grid ← LeftNeighbor);
      MPI_Isend(Grid ← LeftNeighbor); }

    #pragma toucan compute
    { Compute(); Swap(&Grid, &BufferGrid); }
}
```

Toucan defines 3 code region types:
(Compute, Send, Receive)

Loop is divided into 3 separate steps.

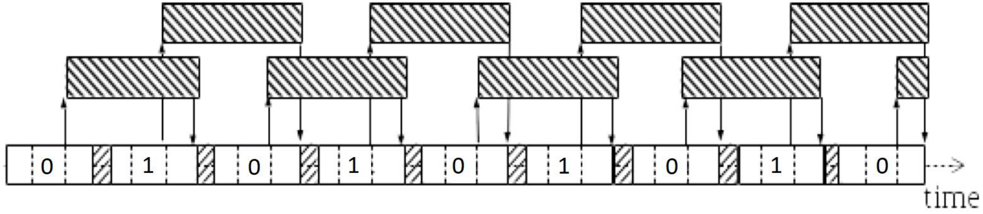
Coroutine yields to MATE Scheduler (instead of OS)

Dependency Graph defined implicitly:

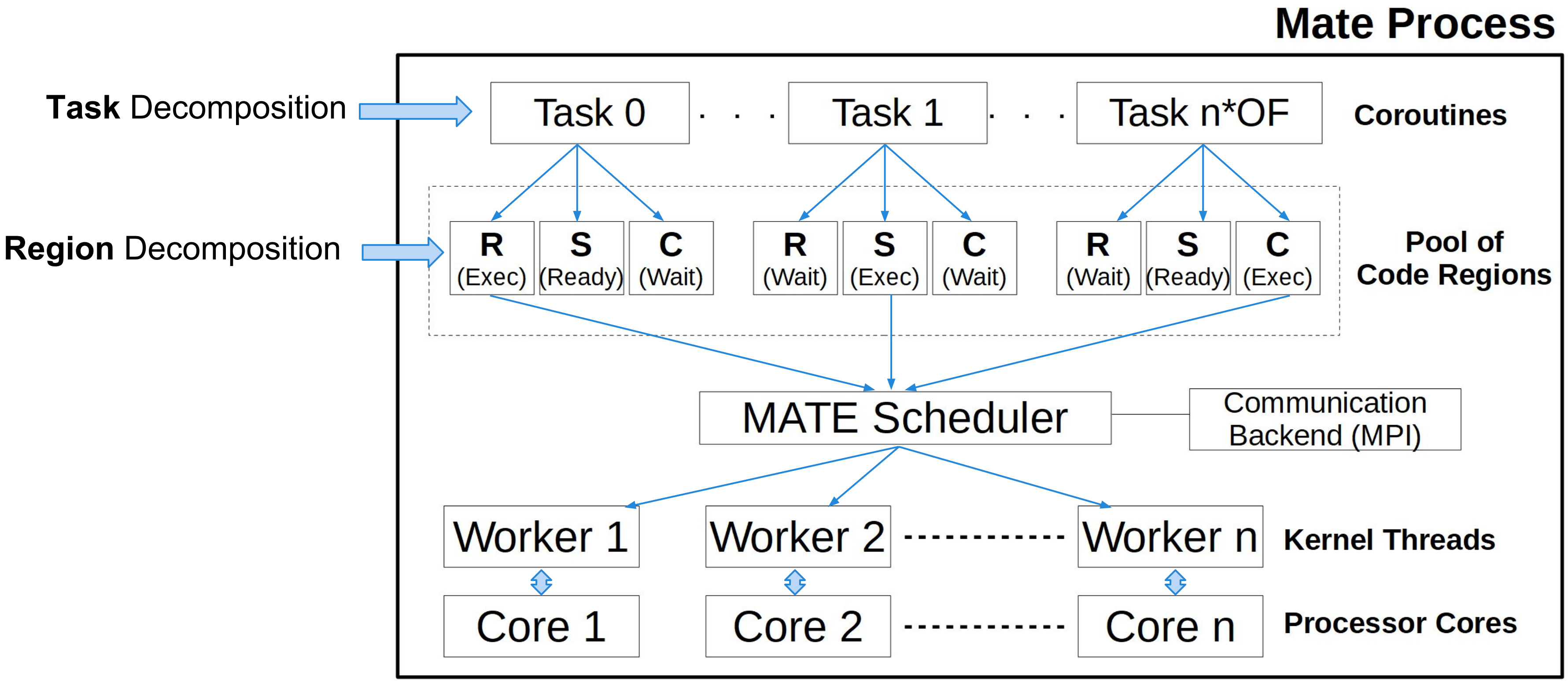
- Compute depends only on receive
- Receive depends on compute*
- Send depends on compute* and send*

***From previous iteration**

Timeline at Steady State:

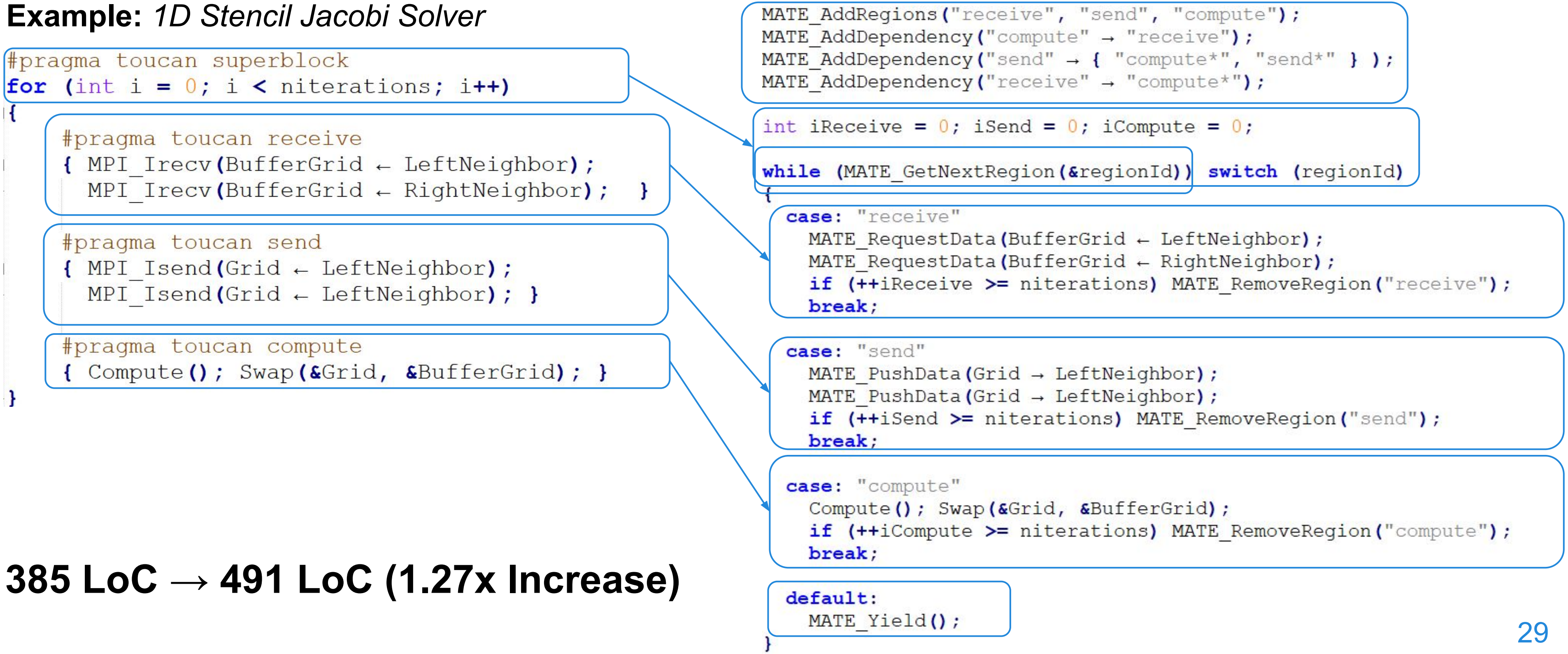


Runtime System (MATE/Toucan)



Toucan Translation Process

Example: *1D Stencil Jacobi Solver*



```
#pragma toucan superblock
for (int i = 0; i < niterations; i++)
{
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    { MPI_Isend(Grid ← LeftNeighbor);
      MPI_Isend(Grid ← LeftNeighbor); }

    #pragma toucan compute
    { Compute(); Swap(&Grid, &BufferGrid); }
}
```
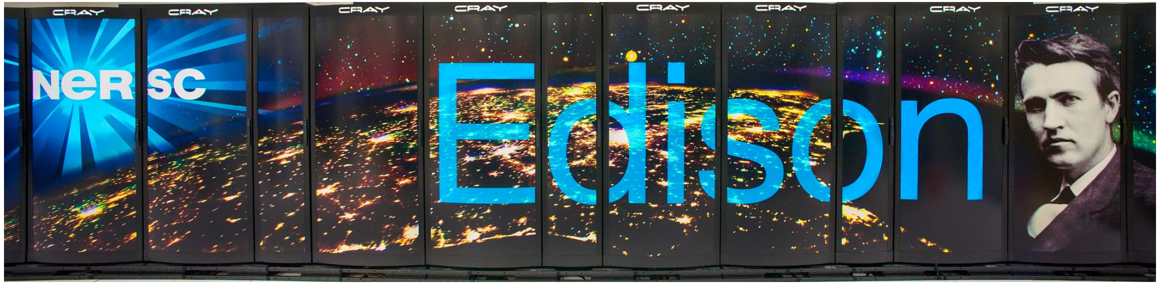

```
MATE_AddRegions("receive", "send", "compute");
MATE_AddDependency("compute" → "receive");
MATE_AddDependency("send" → { "compute*", "send*" } );
MATE_AddDependency("receive" → "compute*");

int iReceive = 0; iSend = 0; iCompute = 0;

while (MATE_GetNextRegion(&regionId)) switch (regionId)
{
  case: "receive"
    MATE_RequestData(BufferGrid ← LeftNeighbor);
    MATE_RequestData(BufferGrid ← RightNeighbor);
    if (++iReceive >= niterations) MATE_RemoveRegion("receive");
    break;

  case: "send"
    MATE_PushData(Grid → LeftNeighbor);
    MATE_PushData(Grid → LeftNeighbor);
    if (++iSend >= niterations) MATE_RemoveRegion("send");
    break;

  case: "compute"
    Compute(); Swap(&Grid, &BufferGrid);
    if (++iCompute >= niterations) MATE_RemoveRegion("compute");
    break;

  default:
    MATE_Yield();
}
```

385 LoC → 491 LoC (1.27x Increase)

Hardware Testbed: Edison @ NERSC

NERSC Edison Supercomputer:
5586 Computing Nodes



Processor: 2x12-core Intel "Ivy Bridge" @2.4Ghz

Memory: 64 Gb DDR3 Total per Node

Software:

- Cray-MPICH v7.4.1
- Intel icc compiler 15.0.1 (-O3)
- Intel MKL Library (for *dgemm)*

Test Cases

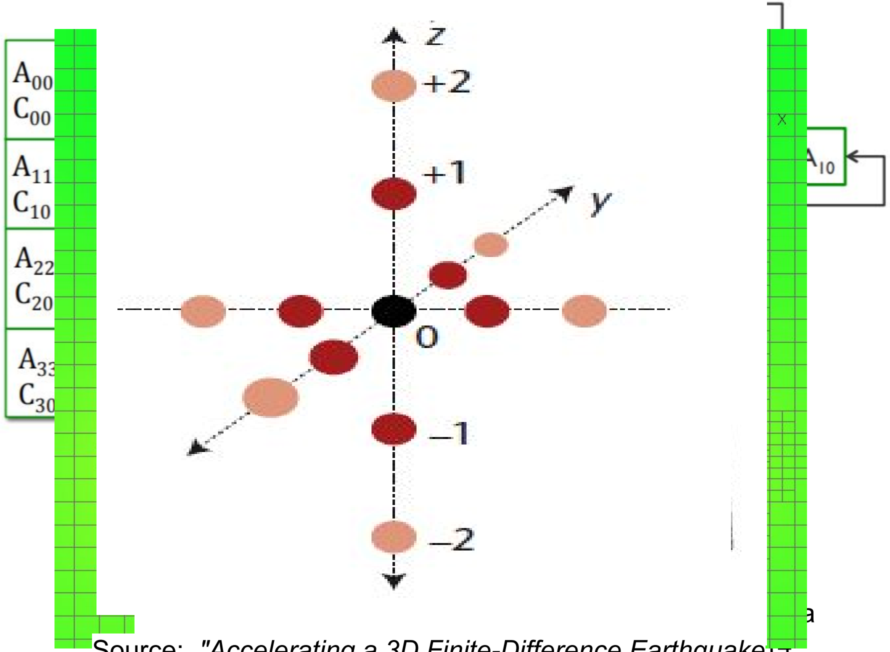
We used 4 examples from 3 common scientific application motifs[1]:

Cannon 2D (Dense Linear Algebra)
Computes the matrix product of two matrices.

LULESH 2.0 (Unstructured Grid)
Solves the Sedov blast problem. Developed at LLNL.

Cart3D (Unstructured Grid)
Multigrid solver of Euler equations. Relies on recursive code.

Jacobi 3D (Structured Grid)
Solves the Poisson equation for 3D PDEs.



Source: *"Accelerating a 3D Finite-Difference Earthquake Simulation with a C-to-CUDA Translator"*, Cai et al.

Source: Lawrence Livermore National Laboratory

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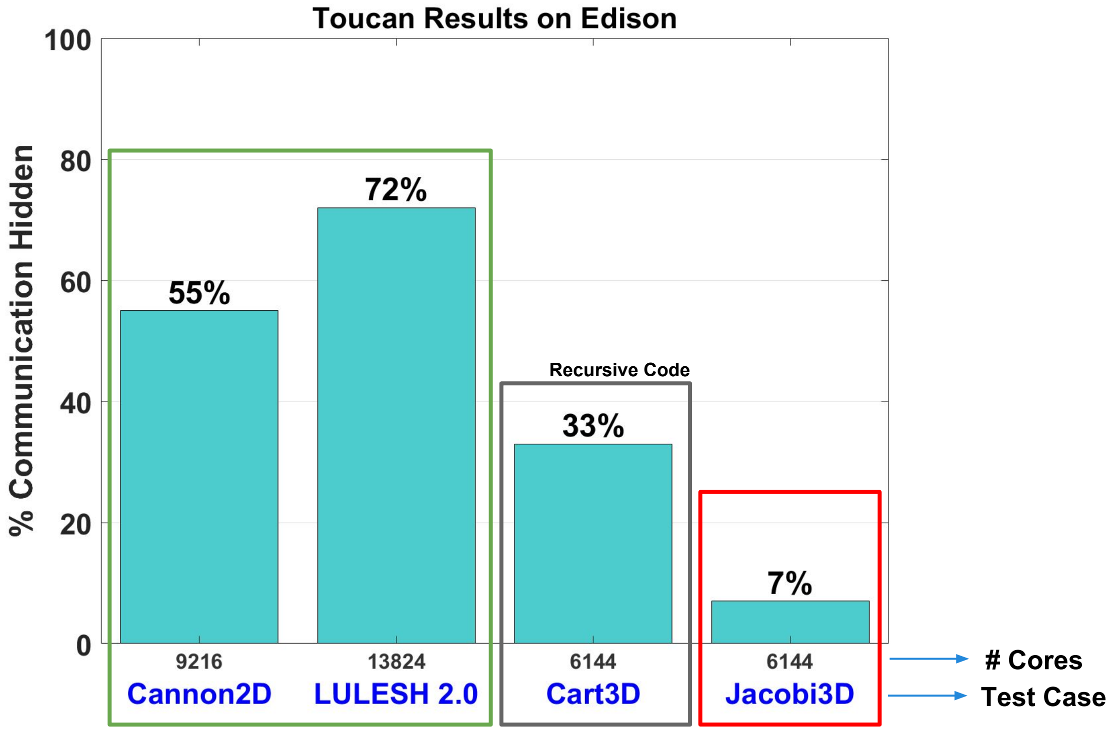
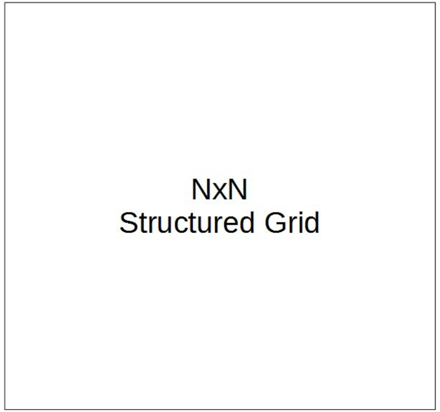
[1] **"Defining Software Requirements for Scientific Computing",** P. Colella, LBL 2016

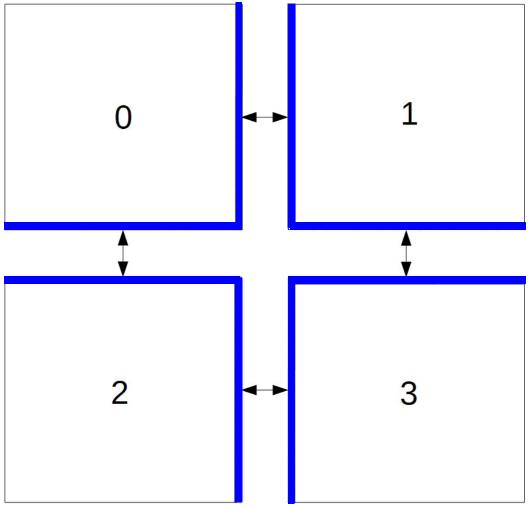
Results @ Edison



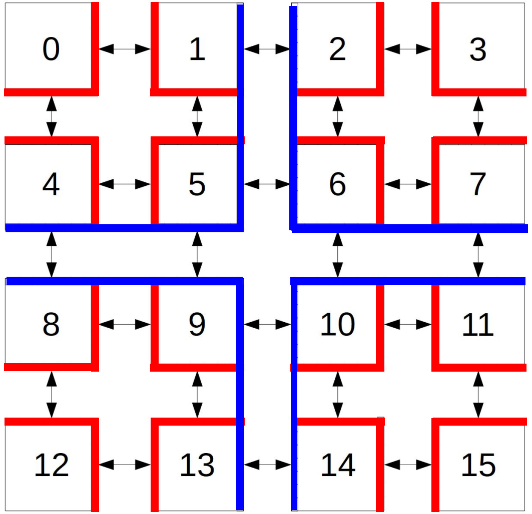
"Toucan - A Translator for Communication Tolerant MPI Applications." S. Martin, M. J. Berger, S. Baden. In IPDPS'17

Toucan Model Limitation





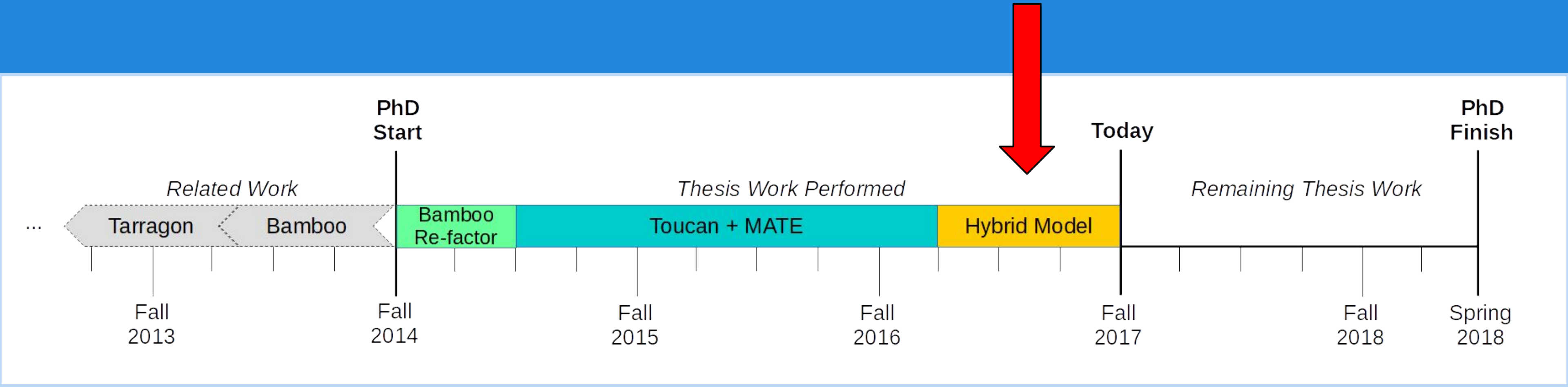
Typical MPI Decomposition
1 Subdomain / Core



Overdecomposed Grid
4 Subdomains / Core

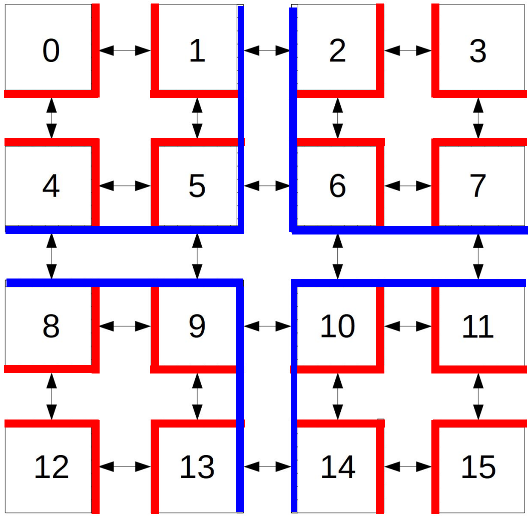
Observation: Overdecomposition requires additional ***internal*** communication.

Hybrid Model

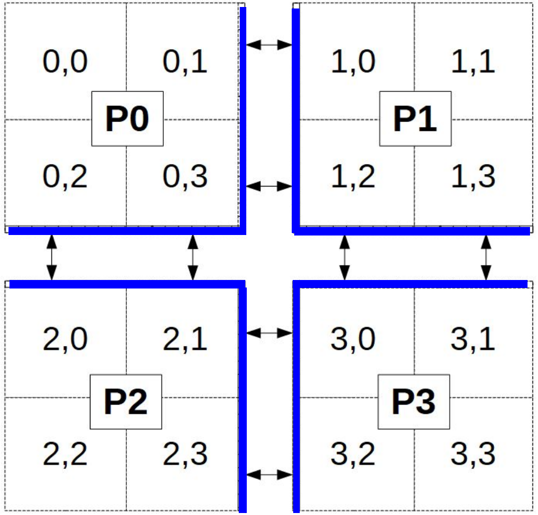


MATE Hybrid Model

- **New Model:** Workload decomposed twice. (1) Process-wide and (2) Within Shared Domain



Toucan Model
4 Subdomains / Core

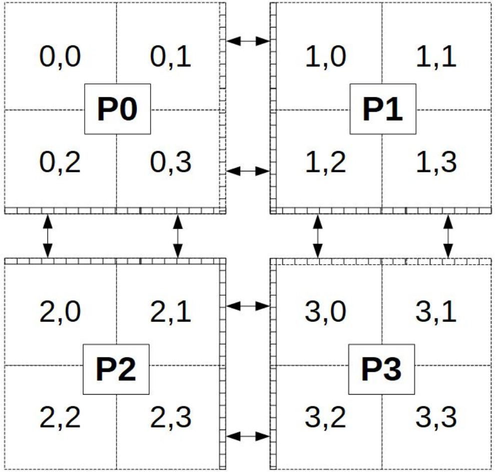


Hybrid Model - 2-Level Decomposition
4 Subdomains / Core

Observation: Hybrid model only requires synchronization for tasks sharing the same subdomain.

Programming with Hybrid Model

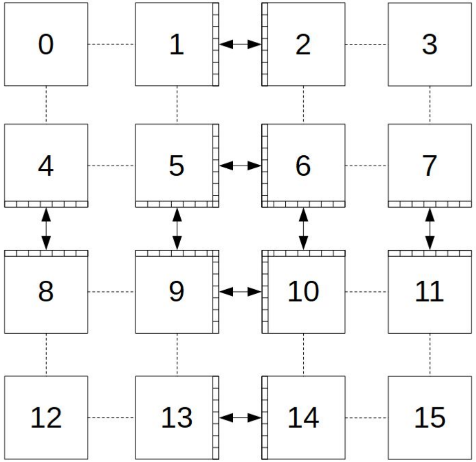
- Hybrid Model requires manual changes in the workload distribution part of the application.
- Two possible approaches:



Decompose by Process, Decompose by Subrank

Pros:
- Single shared malloc
- Contiguous Access

Cons:
- Requires two decompositions
- Cache blocking sensitive

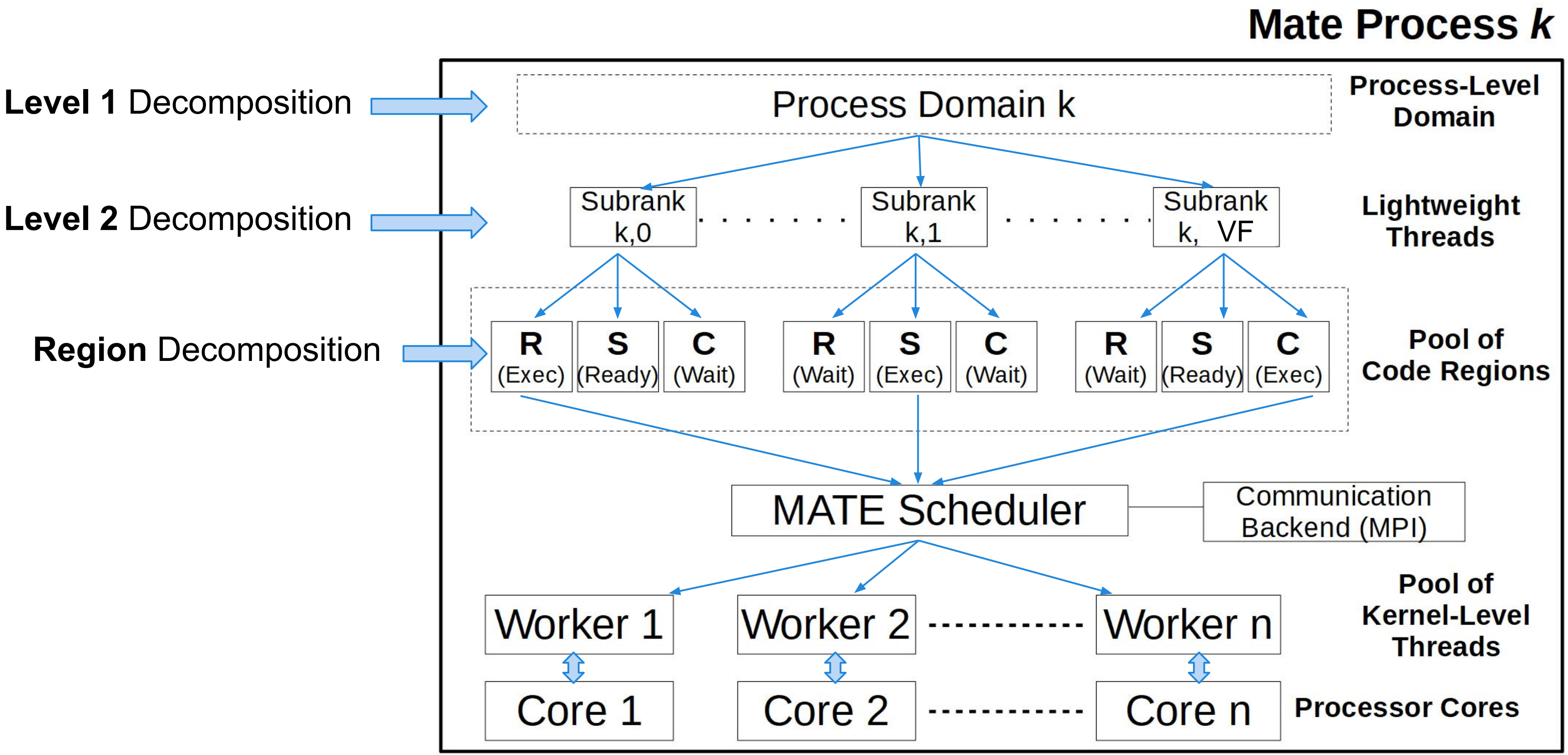


Decompose by Subrank, Local Pointer Access

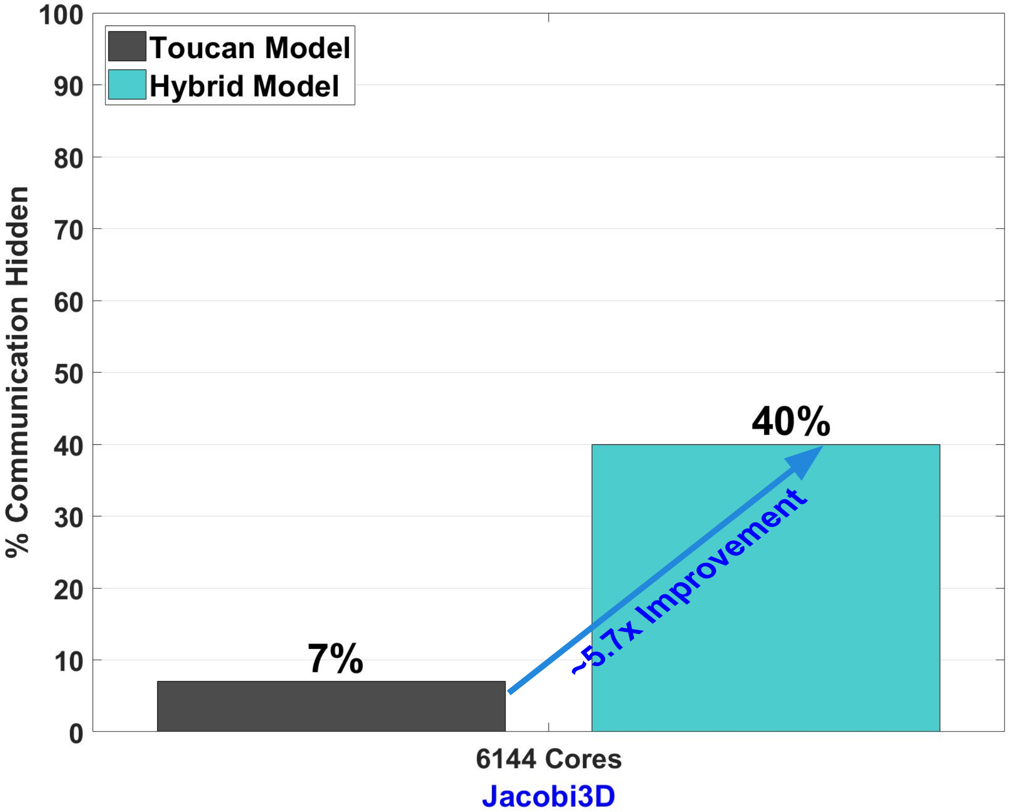
Pros:
- Re-uses original decomp.
- Cache efficient

Cons:
- Requires pointer passing
- Non-contiguous access

Runtime System (MATE/Hybrid)



Results @ Edison



Testbed Transition

(2017) Having shown promise with the Hybrid model, we decided to shift to a newer platform:

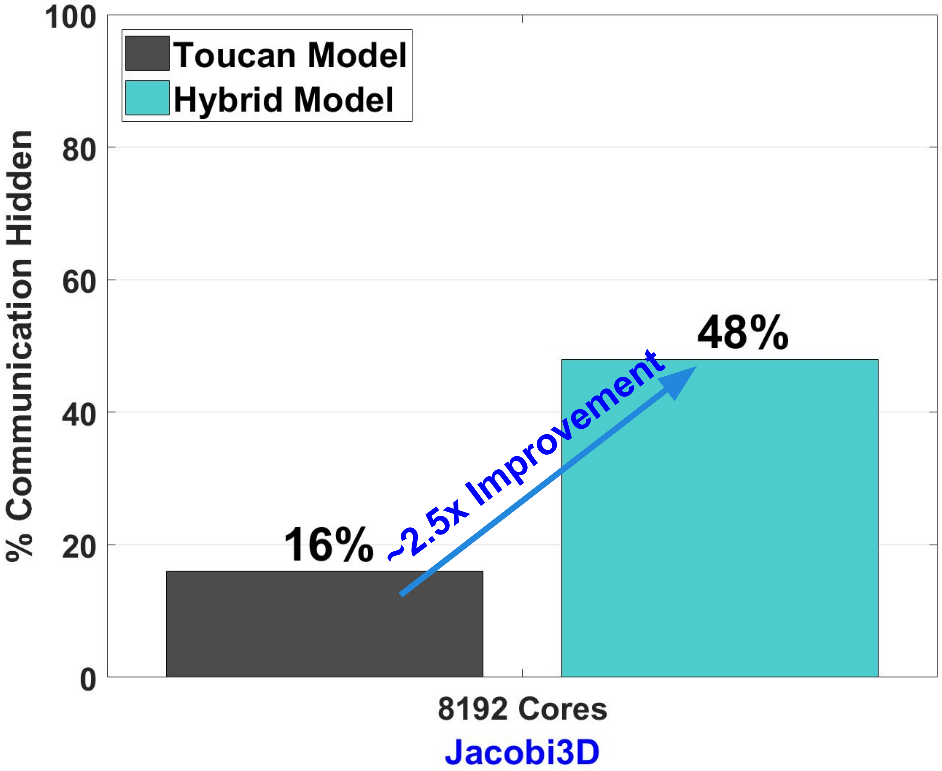
NERSC Edison Supercomputer:
Operational since 2013

NERSC Cori KNL Supercomputer:
Operational since 2017

Node Configuration:
- 2x12-core Intel "Ivy Bridge" @2.4Ghz
- 460 Gflops/node

Node Configuration:
- 68-core Intel “Knights Landing” @1.4Ghz
- 3000 GFlops/node

Results @ Cori KNL

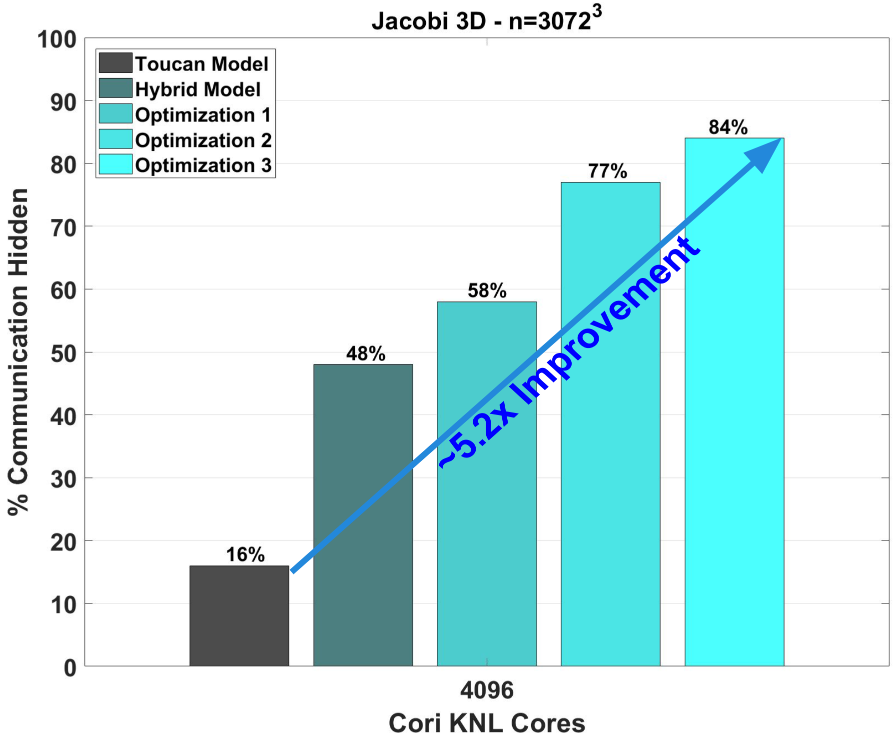


Progression Roadmap (2017)

Progression since Winter 2017.

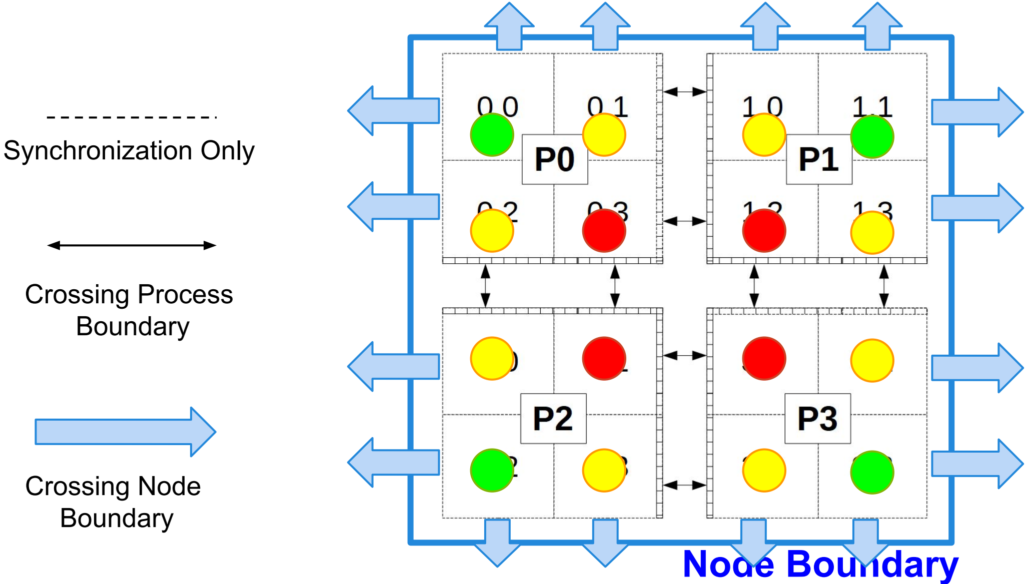
Starting from Toucan **(16%)** until today **(84%)**.

Each bar represents an improvement.



Optimization 1: Subrank Prioritization

- **Fact:** Not all subranks incur the same communication cost.
- **Idea[1]:** Prioritize subranks with higher communication cost to execute first.
- **Effect:** Initialize costly communication first.



Adaptive Algorithm in MATE:

🟢 Higher Priority (mostly Node Boundary)

🟡 Medium Priority (Mixed Boundaries)

🔴 Low Priority (Inner Tasks)

[1] **"Performance tradeoffs in multi-tier formulation of a finite difference method"** S. B. Baden and D. Shalit. In: ICCS 2001.

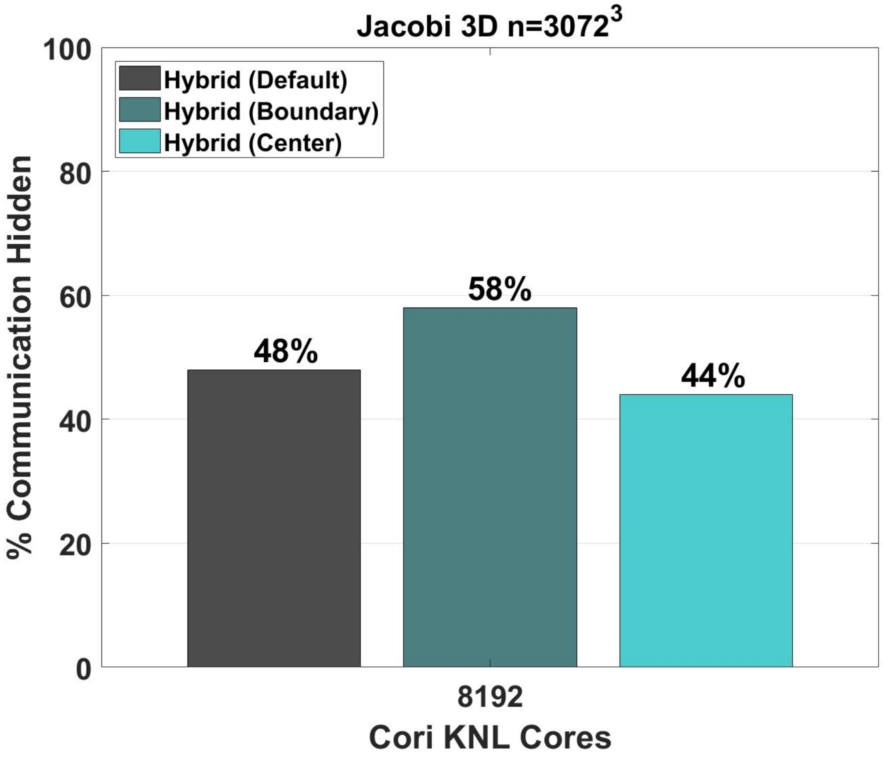
Results: Prioritization

Comparing 3 Variants:

Hybrid (Default)
No priority scheme.

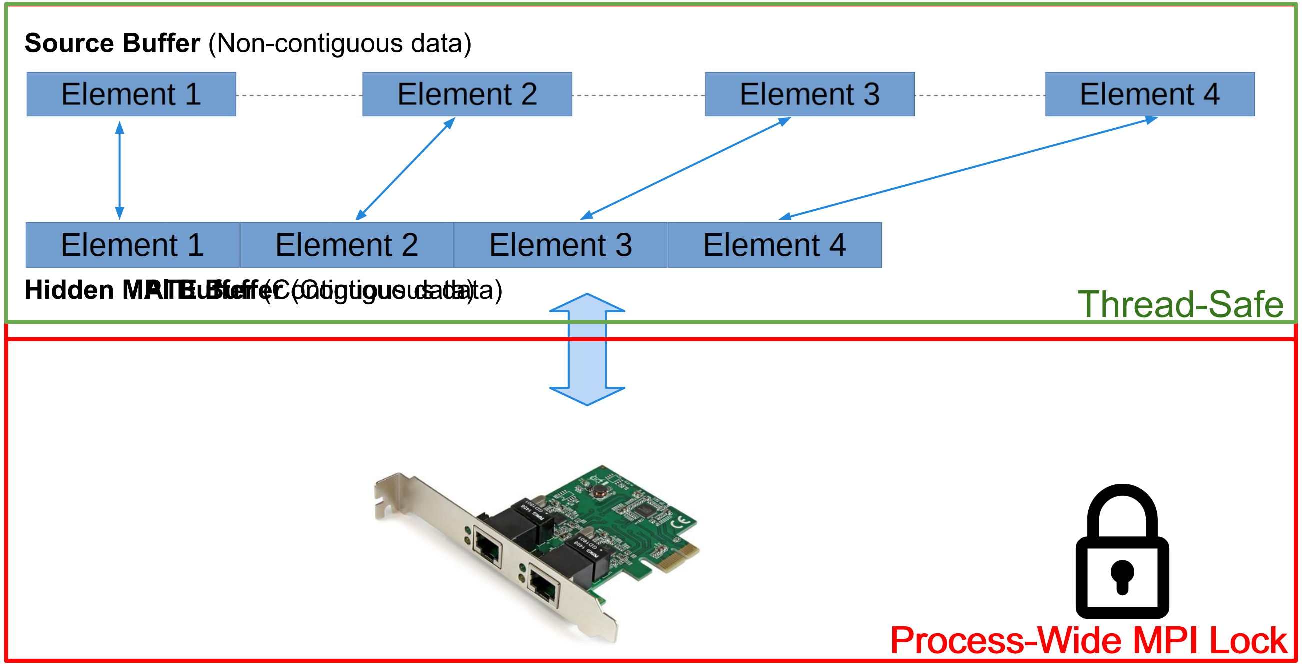
Hybrid (Boundary)
+Priority to Boundary Subranks

Hybrid (Center)
-Priority to Boundary Subranks



Optimization (2/3): Thread Concurrency

- Non-Contiguous buffers in MPI need to be packed before communicating.
- MPI implements a process-wide lock, which limits communication concurrency.
- **Solution:** Have MATE perform automatic thread-safe packing before calling MPI.



Source Buffer (Non-contiguous data)

Element 1 | Element 2 | Element 3 | Element 4

Element 1 | Element 2 | Element 3 | Element 4

Hidden MATE Buffer (Contiguous data)

Hidden MPI Buffer (Contiguous data)

Thread-Safe

Process-Wide MPI Lock

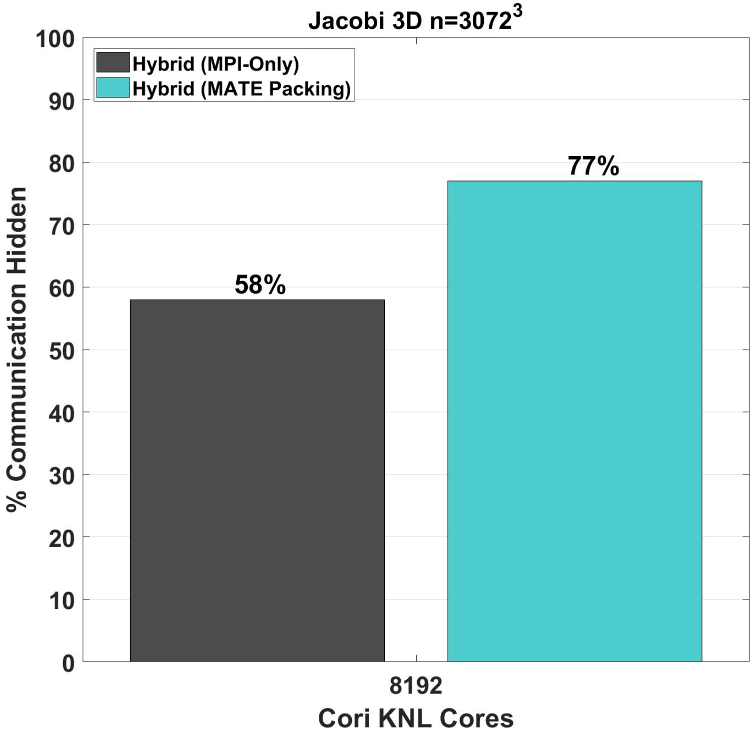
MATE Workers

Results: MPI vs. Mate Packing

Comparing 2 Variants:

Hybrid
MPI-Only

Hybrid
Mate Packing + MPI

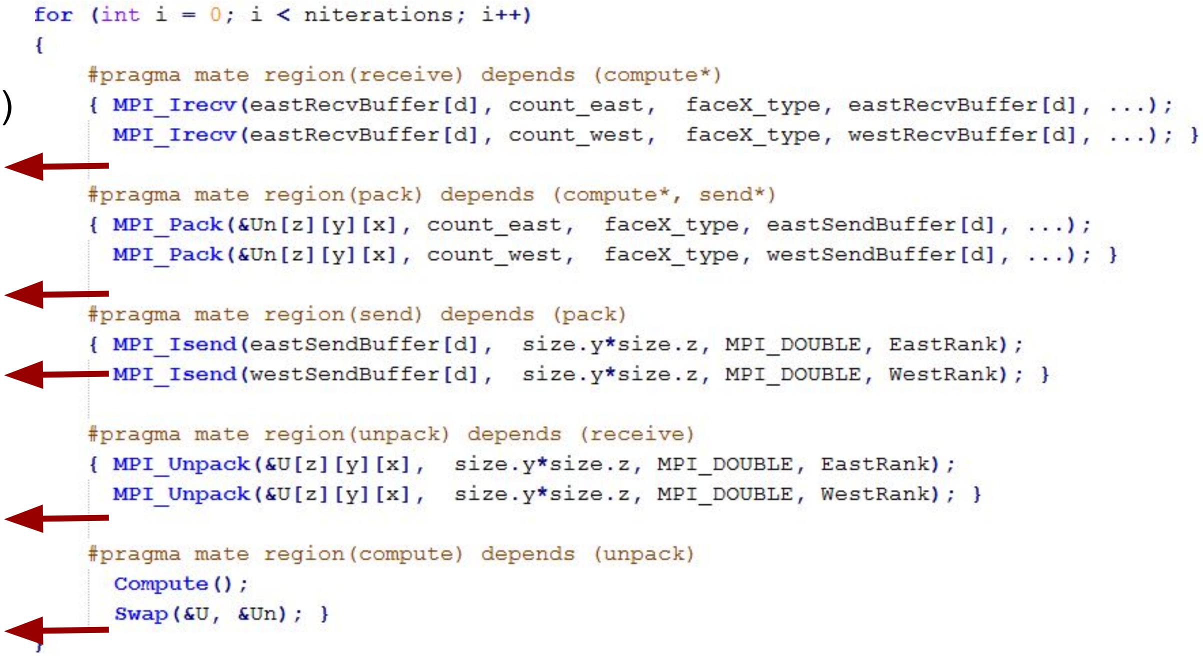


Optimization (3/3): Explicit Graph in MATE

5 pragma annotations:
(Compute, Pack, Send, Receive, Unpack)

Explicit Dependency Graph

5 Task Exit Points.



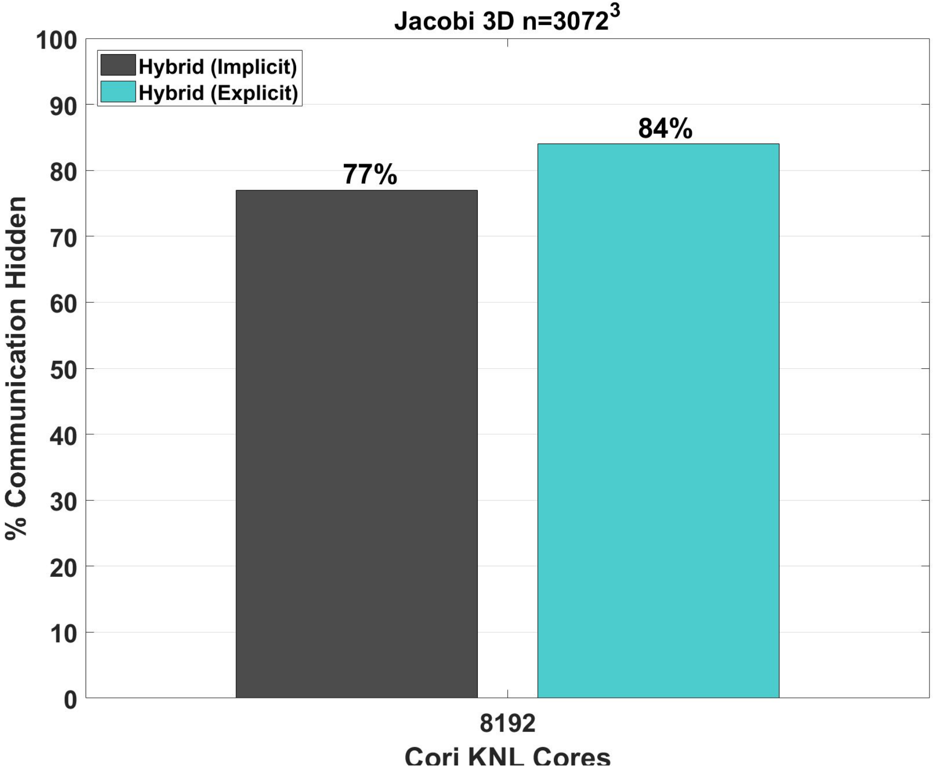
```
for (int i = 0; i < niterations; i++)
{
    #pragma mate region(receive) depends (compute*)
    { MPI_Irecv(eastRecvBuffer[d], count_east,  faceX_type, eastRecvBuffer[d], ...);
      MPI_Irecv(eastRecvBuffer[d], count_west,  faceX_type, westRecvBuffer[d], ...); }

    #pragma mate region(pack) depends (compute*, send*)
    { MPI_Pack(&Un[z][y][x], count_east,  faceX_type, eastSendBuffer[d], ...);
      MPI_Pack(&Un[z][y][x], count_west,  faceX_type, westSendBuffer[d], ...); }

    #pragma mate region(send) depends (pack)
    { MPI_Isend(eastSendBuffer[d],  size.y*size.z, MPI_DOUBLE, EastRank);
      MPI_Isend(westSendBuffer[d],  size.y*size.z, MPI_DOUBLE, WestRank); }

    #pragma mate region(unpack) depends (receive)
    { MPI_Unpack(&U[z][y][x],  size.y*size.z, MPI_DOUBLE, EastRank);
      MPI_Unpack(&U[z][y][x],  size.y*size.z, MPI_DOUBLE, WestRank); }

    #pragma mate region(compute) depends (unpack)
    { Compute();
      Swap(&U, &Un); }
}
```

Results: Dependency Graph Variants

Comparing 3 Variants:

Hybrid (Implicit)
Toucan Model

Hybrid (Explicit)
+Pack/Unpack Regions



Hybrid Model Conclusions

- **The Hybrid Model exceeds the efficiency of the Toucan Model.**
  - Hides communication by oversubscribing cores (like Toucan) but,
  - It does not require additional communication.

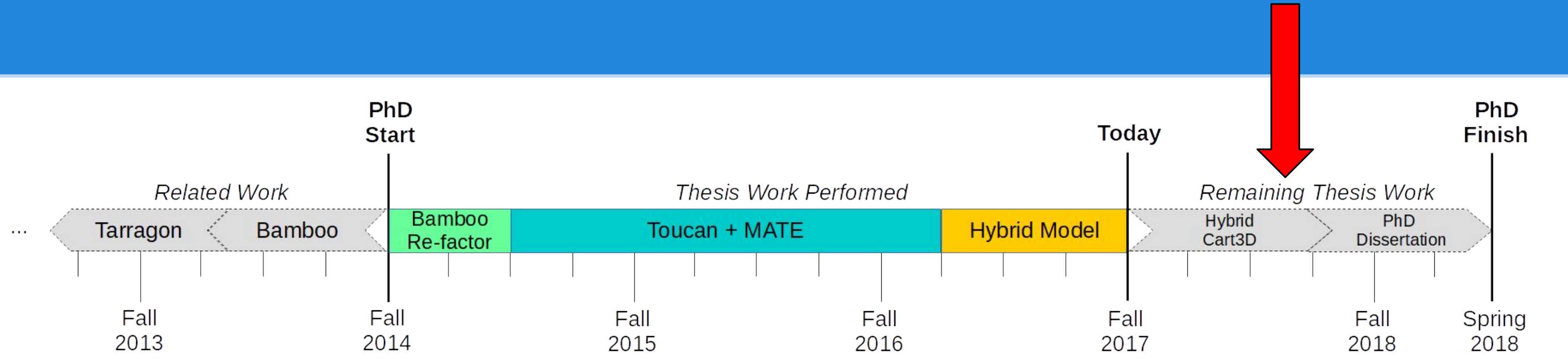
- **Subrank prioritization can have a substantial impact on performance.**
  - MATE can assign priorities adaptively during execution.

- **Thread concurrency is still an important issue to be solved.**
  - Packing can be performed concurrently, but MPI still locks comm ops.
  - Solution: Use a different communication layer? (GasNET / UPC++)

- **It is possible to refine dependency graphs explicitly.**

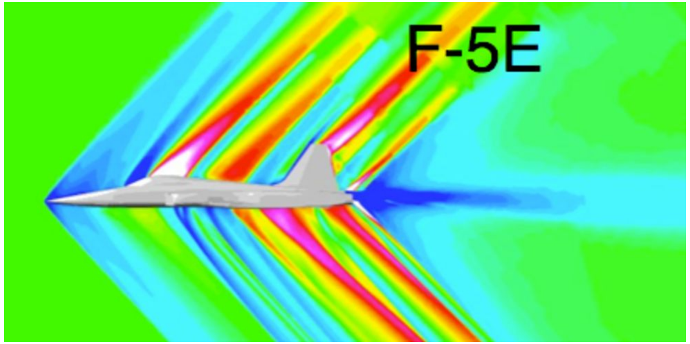
- **Limitation: Require some manual changes to the workload distribution logic.**
  - Possible topic for another thesis: make translation fully automatic.

Remaining Work

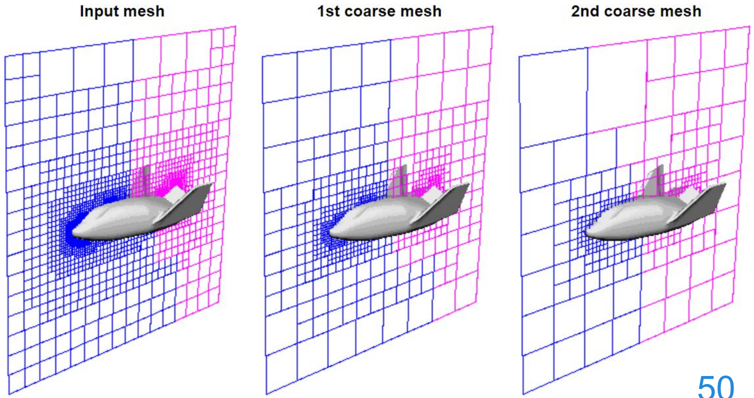


Cart3D in Depth

Cart3D is a high-fidelity analysis package for aerodynamic design.



- Production code developed by NASA Ames and NYU Courant Institute of Mathematics.
- Has hundreds of users.
- Uses a multigrid with irregular meshes.
- Complex Code: 38k Lines of Code + Recursion.
- Non-trivial communication:
  - Irregular (asymmetric) communication.
  - Non-contiguous data types.
  - 4 communication regions in the main loop.



Source: https://www.nas.nasa.gov/publications/software/docs/cart3d/

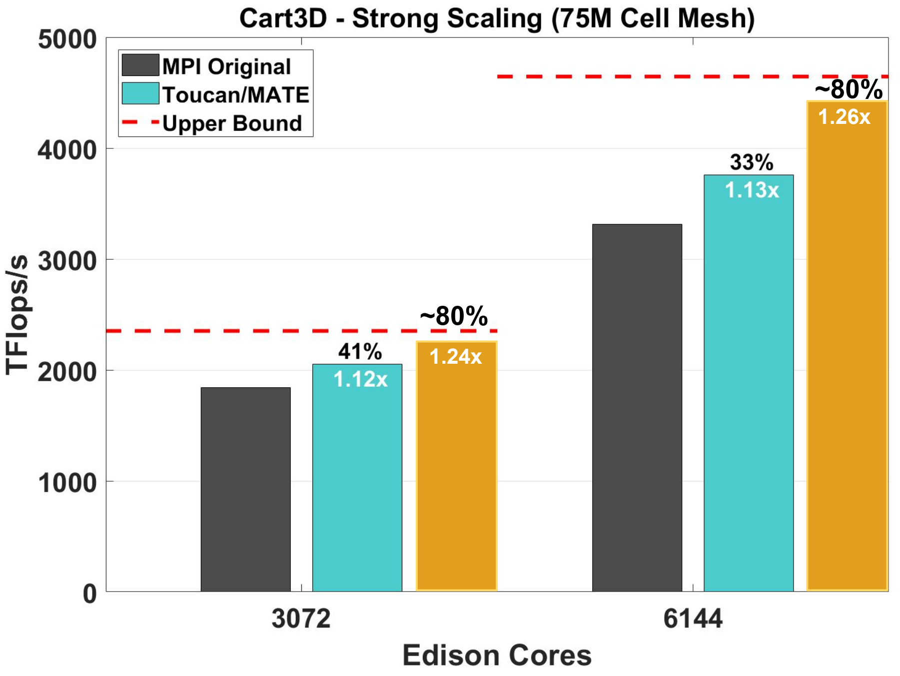
Why is Cart3D Important?

Cart3D is an ideal test case:

- Demonstrates that translation can improve the performance of a production code at scale.
- We are working with developers at NYU / NASA.
- We have shown that Toucan can hide **33 to 41%** of communication cost at scale in our Edison experiments (256 nodes).

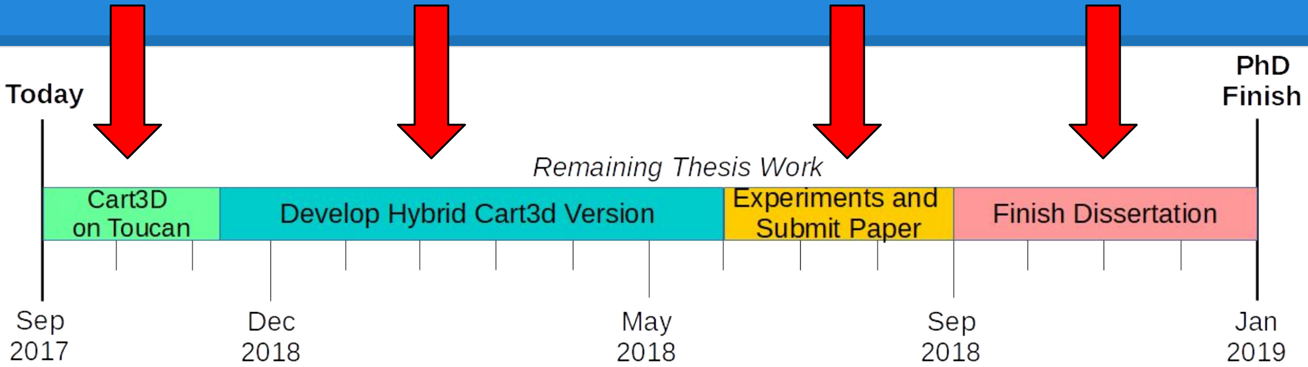
Hybrid Model can outperform Cart3D on Toucan:

- Cart3D on Toucan suffers from added communication.
- We expect to achieve similar improvements as with Jacobi3D (**~80%** of communication hidden)



“Toucan - A Translator for Communication Tolerant MPI Applications.”
S. Martin, M. J. Berger, S. Baden. In IPDPS’17

Next Milestones



- Apply Toucan to the latest version of Cart3D. **(1~2 Months)**
- Develop the Hybrid Model variant of Cart3D. This requires manual restructuring of Cart3D. **(6~7 Months)**
    - Run experiments at scale (>1024 Nodes) for Cart3D and other test cases.
    - Use parallel profiling tools (HPC Toolkit) to examine the low-level effects of our models. **(2~3 Months)**
    - Write and submit a paper to a main HPC conference (*e.g.* SC, IPDPS, EuroPar)
- Write and defend PhD Dissertation **(~3 Months)**
- Total: **~13-15 Months**

Questions?