EPiGRAM

Exascale ProGRAmming Models

Towards Exascale Programming Models

HPC 2014

Cetraro

Erwin Laure, Stefano Markidis, KTH

Exascale Programming Models

- With the evolution of HPC architecture towards excascale, new approaches for programming these machines need to be found - EPiGRAM focuses on exploring programming models for the exascale era.

- Intense discussion whether existing models can be improved to exascale or whether disruptive changes are needed.

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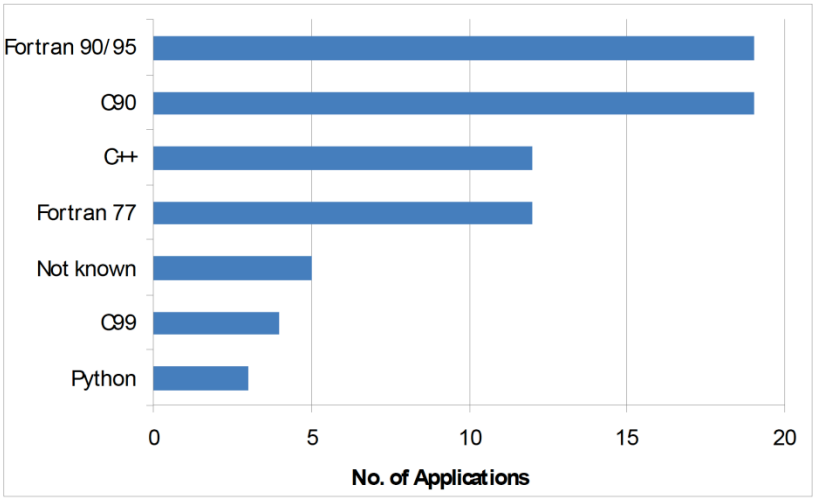
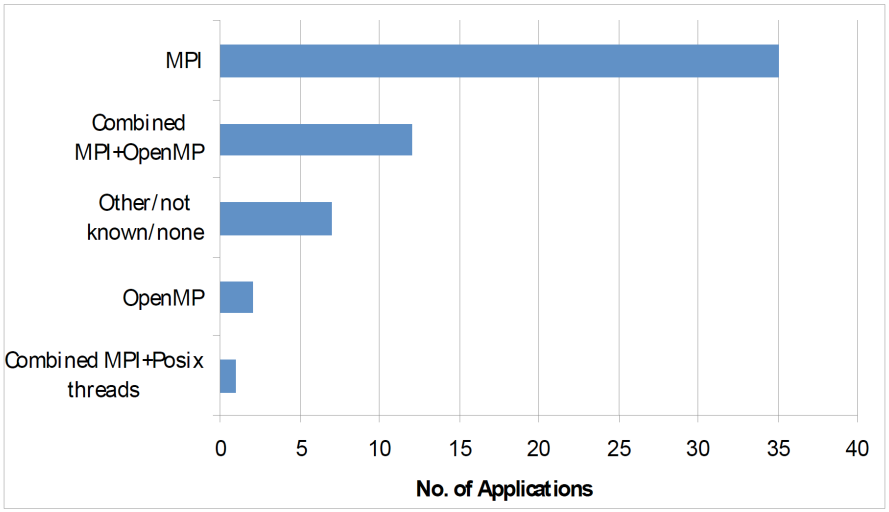
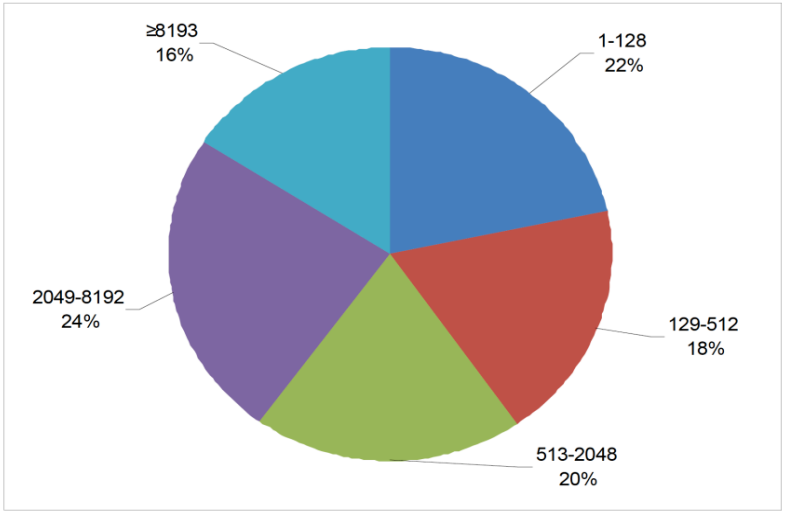
What is used today?







Figures from a study of the 57 leading applications used in Europe by the PRACE Project

PRACE

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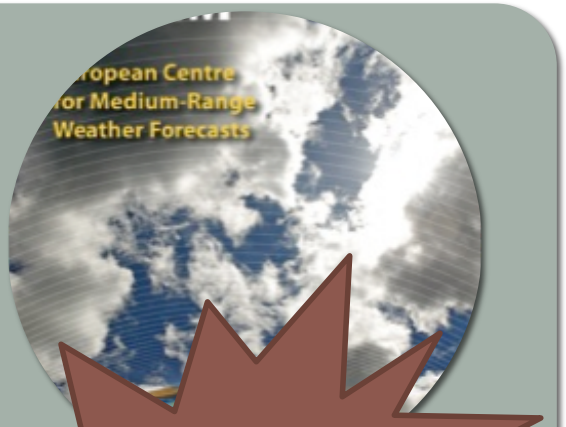
CRESTA experiences



CAF to overlap communication with computation

IFS

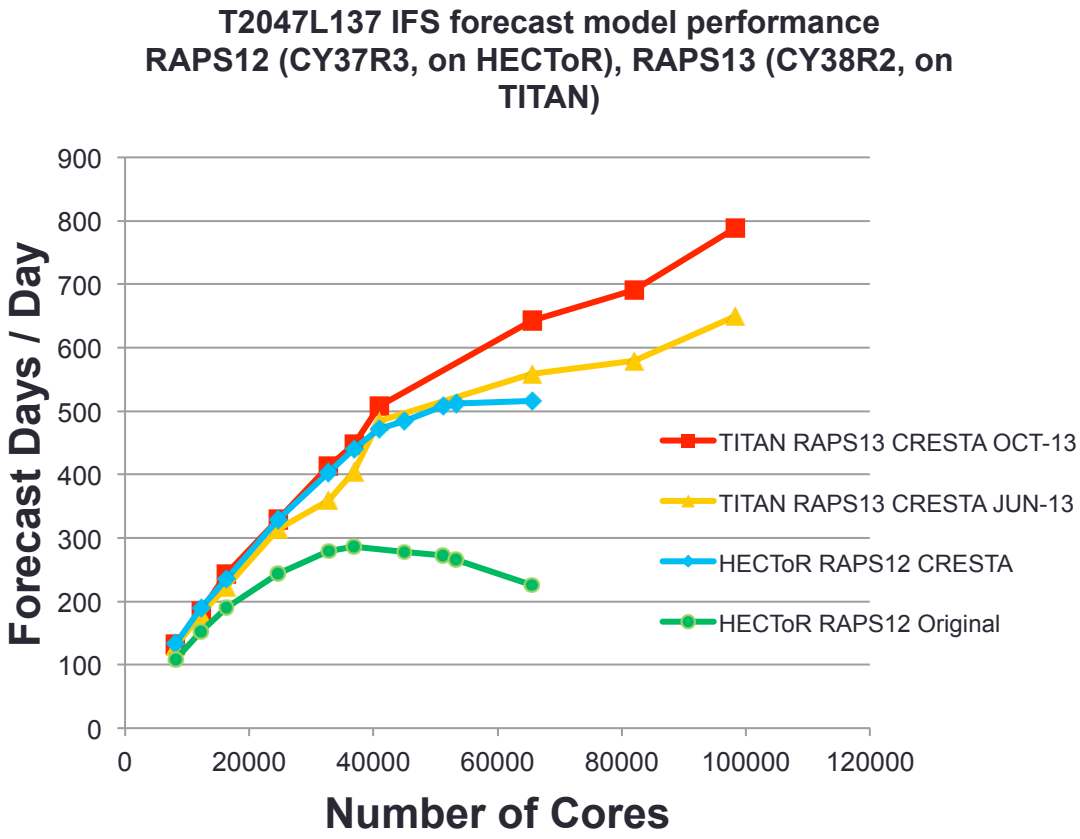
Ti eather

f e lives

Simu g e trajectory of hurric ne Sandy

Acceleration
Task-graph based parallelization
New communication models

CRESTA



EPiGRAM believes in the incremental approach and that the most promising parallel programming environments can be scaled to exascale:

Message Passing and PGAS

A Window of Opportunity

- MPI 3.0 is a major step forward but still not ready for exascale
- By extending and improving GPI to exascale we will consolidate the role of GPI and establish it as the European PGAS approach.
- EPiGRAM can complement the European CRESTA, DEEP, and Mont-Blanc exascale projects.
  - by exploring additional innovative PGAS approaches that go well beyond those considered in the current CRESTA project
  - by investigating efficient MP mechanisms that might useful for hybrid Cluster-Booster architecture in DEEP
  - by studying and analyzing one-sided communication approaches for diverse memory spaces such as the one in hybrid ARM-GPU systems in Mont-Blanc.

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Key Objectives of the Project

- Address the **scalability** (performance and memory consumption) problem for MP and PGAS models.
- Propose **GPI as the European PGAS** approach to exascale.
- Design an **hybrid MP-PGAS** programming model that combines the best features of the two approaches.
- Contribute to **standardization** efforts
- Prepare two **applications** to exascale by redesigning and implementing their communications kernels.

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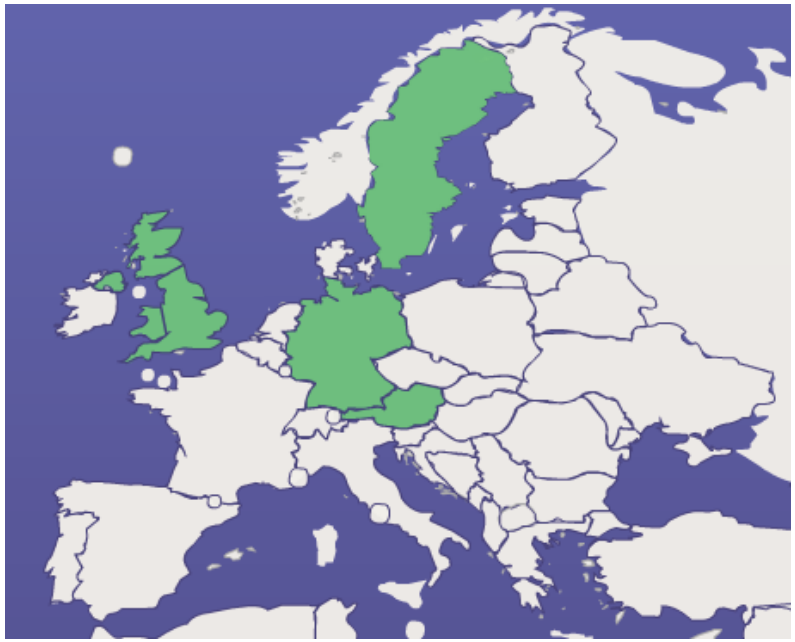
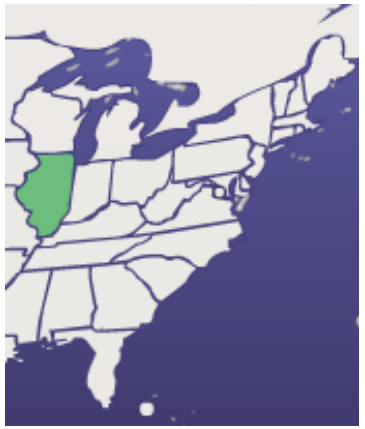
Key Players and Their Main Focus

- **KTH**: management (WP1), applications (WP6)
- **TUW**: exascale MP (WP2)
- **FRAUNHOFER**: exascale PGAS (WP3)
- **CRAY UK**: programming models for diverse memory spaces (WP3)
- **EPCC**: PGAS-based MPI (WP4)

- External Contributor: **UNIVERSITY OF ILLINOIS**: exascale MP (WP2)





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Exascale Message Passing

1. Dealing with limited and slower memory:
   - in-depth analysis of MPI **derived datatype** mechanism for saving copy-operations;
   - analysis of MPI **collective interface** specification with suggestions for improvement
2. Collective communication at scale:
   - proposal for specification of homogeneous stencils, towards improved (homogeneous, regular) sparse collectives
3. Other issues to be addressed:
   - collective communication in sparse networks
   - Multi-threaded MPI
   - MPI with other models (threads, PGAS, extended message-passing models)

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MPI derived datatype mechanism

MPI derived datatype mechanism (functionality for defining application-specific, structured, units of communication) enables

Zero-copy implementation:

- No explicit pack/unpack and other process local data reorganization.
- All necessary (process local) data movement implicit by communication operations.

Higher-level, descriptive advantages, can lead to genuine performance improvements

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Implementing a Classic: Zero-copy all-to-all communication with MPI derived datatypes

Jesper Larsson Träff, Antoine Rougier, Sascha Hunold
traff@par.tuwien.ac.at
Vienna University of Technology (TU Wien)
Faculty of Informatics
Institute for Information Systems
Research Group Parallel Computing

Case study: Zero-copy implementation of a classic, log-round alltoall algorithm

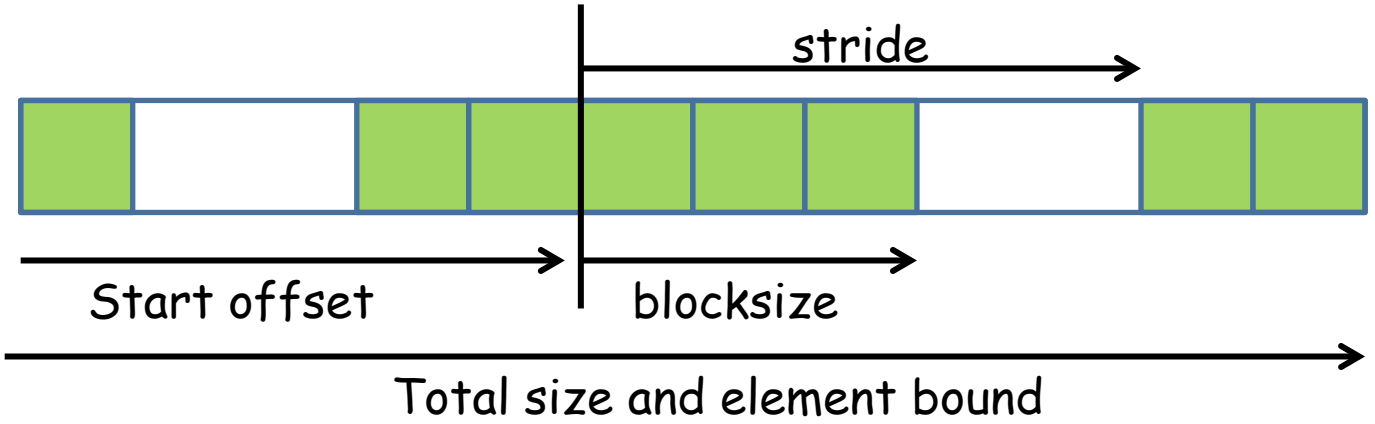
J. Bruck, Ching-Tien Ho, S. Kipnis, E. Upfal, D. Weathersby: Efficient Algorithms for All-to-All Communications in Multiport Message-Passing Systems. IEEE Trans. Parallel Distrib. Syst. 8(11): 1143-1156 (1997)

Standard formulation:
Step 1: process-local rotate of data elements
Step 2: log rounds of communication, roughly p/2 (non-contiguous) elements grouped together and send/received per round
Step 3: process-local reverse and rotate of elements

We propose:
- Algorithmic change to get rid of Step 3
- Using per-element double-buffering and datatypes to achieve zero-copy implementation

Circular vector: derived, derived datatype

Useful derived datatype, not in MPI



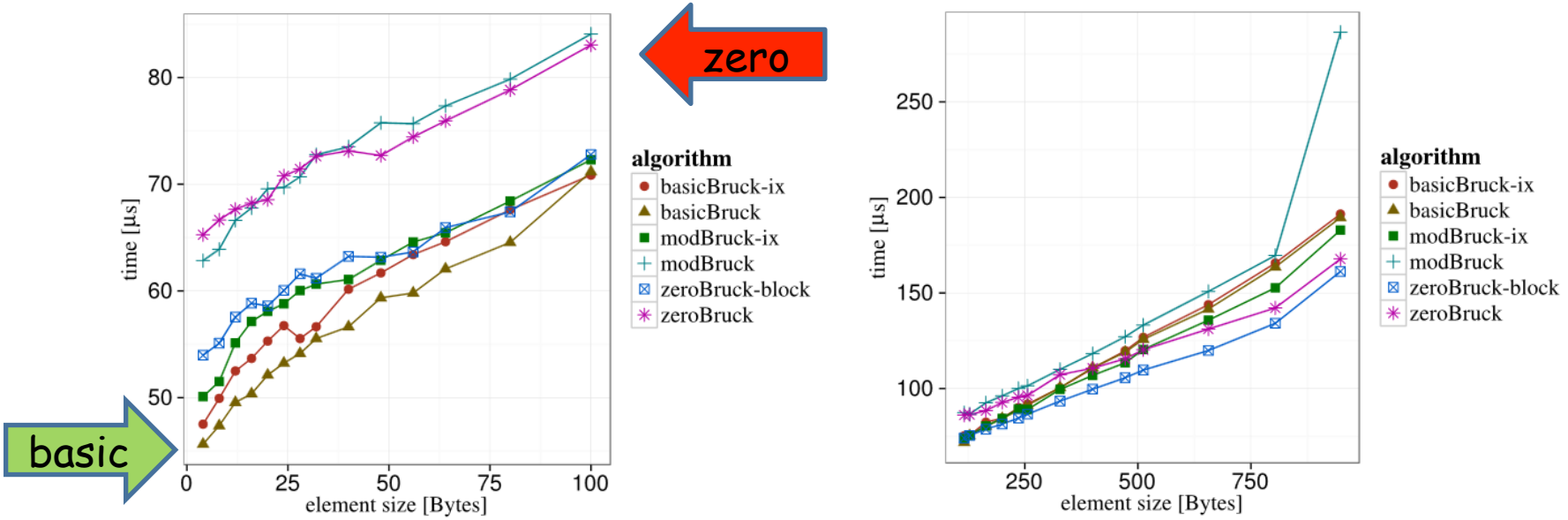
Can also be implemented using existing MPI constructors (struct of vector and contig); but quite tedious, with high overhead, and possibly more efficiently handled as native type

The Zero-copy implementation

```
for (k=1; k<p; k<<1) { // communication round
  for (j=k; j<p; j++) {
    // analyze bits of j
    ..
    b++; // number of blocks to send/receive
  }
  MPI_Type_create_struct(b,…,&sendblocktype);
  MPI_Type_create_struct(b,…,&recvblocktype);
  MPI_Type_commit(&sendblocktype);
  MPI_Type_commit(&recvblocktype);

  MPI_Sendrecv(MPI_BOTTOM,1,sendblocktype,
               MPI_BOTTOM,1,recvblocktype,…);
  MPI_Type_free(&sendblocktype);
  MPI_Type_free(&recvblocktype);
}
```

Jupiter, 36x1 MPI processes (small problems)



- BasicBruck: Bounded vector better than indexed-block
- ModBruck: Circular vector expensive

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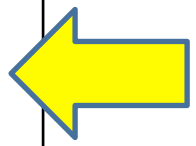


Per round overhead

Proposal, not in MPI: persistent collective operation

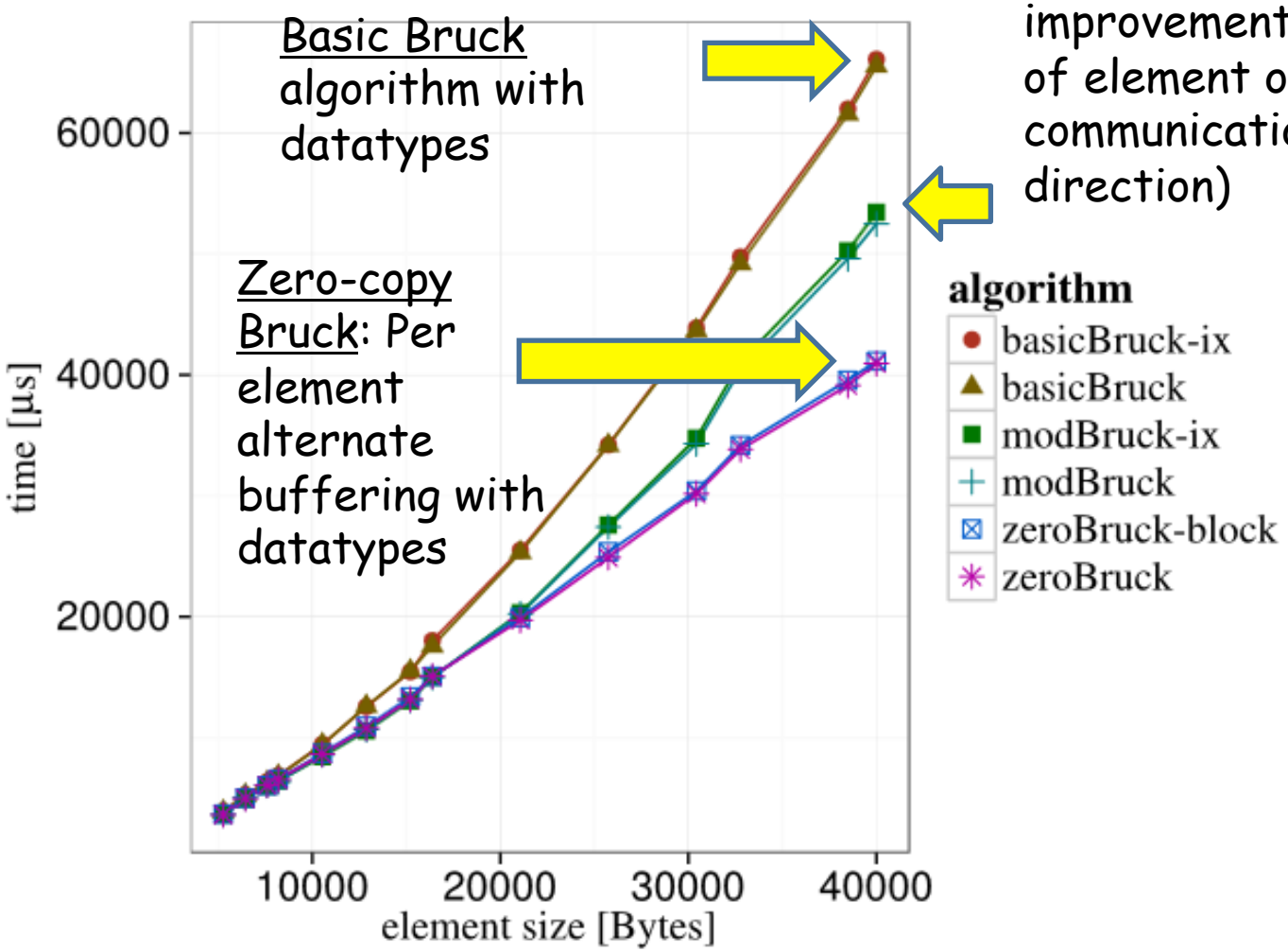
```
MPI_Alltoall_init(sendbuf,sendcount,sendtype,

recvbuf,recvcount,recvtype,comm,  &req);
```

precomputes all datatypes, creates communication schedule (log p round loop), and

```
MPI_Start(&req);
```

initiates and completes next alltoall operation (with given parameters)

Analogous to persistent point-to-point operations (in MPI)



Note: Also for small problems, where the algorithm is competitive, we have a statistically significant improvement

Other zero-copy investigations

1. Hierarchical alltoall algorithms – use new MPI 3.0 functionality, competitive performance, complex reorderings by datatypes and MPI_Alltoallw. We identify a lack of functionality in MPI_Gather/Scatter interfaces

2. Hierarchical gather/scatter/allgather algorithms: we conclusively show that zero-copy implementations are not possible. A change of interface specification is elaborated on (perhaps for discussion with MPI Forum?), a collection of new datatype constructors discussed

3. Datatype normalization: Complexity issues have never been formally studied. We show that the problem can be solved optimally in polynomial time when only vector and index-block constructors are allowed

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Exascale PGAS

- Objectives:
  - To investigate current limitations of traditional PGAS.
  - To propose concrete solutions to current PGAS limitations.
  - To increase scalability of collective operations and synchronization in GPI.
  - To support fault-tolerance in GPI.
  - Exploitation of diverse and hierarchical memory spaces in PGAS.

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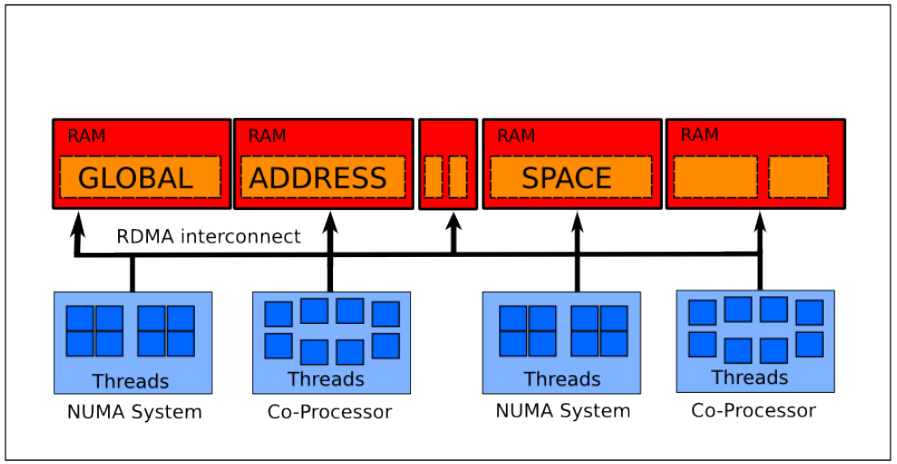
Global Address Space API: GPI
Intranode communication API

- **GPI: G**lobal Address Space A**PI**
- RDMA over IB, RoCE, Cray
- Low Latency & Wire-speed
- C/C++, Fortan
- Thread safe
    - Intel Xeon Phi, GPUs
- MPI Interoperability



- **Asynchronous communication between segments, one-sided, non-blocking**
- **Zero-copy, no CPU cycles for communication**
- **Support for fault tolerance by a timeout mechanism**
- **(Sparse) collectives with time based blocking**
- **fast remote notification**

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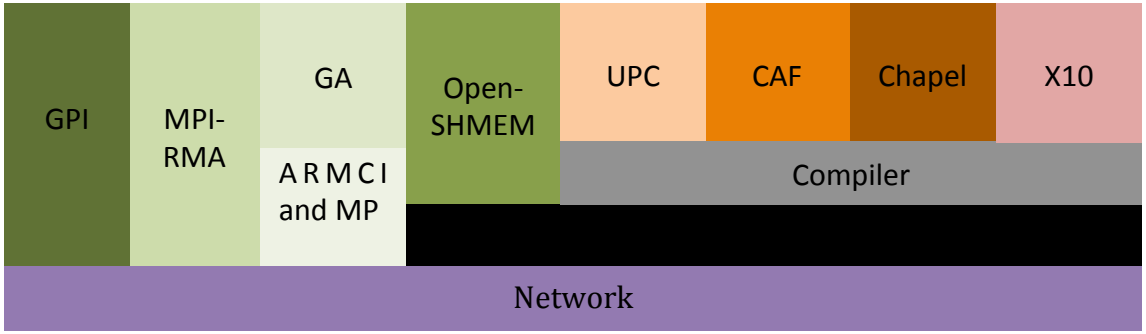
Overview over the relevant PGAS software stack



PGAS approaches can be roughly divided into:

- Languages:
  - UPC which extends the C language, CAF which extends Fortran, Chapel and X10 as standalone languages)
  - Easy to switch to, however a lot of pressure on the compiler

- APIs (GPI, GA, ARMCI, OpenShmem):
  - Explicitly implement the communication between the nodes
  - To be used by application developers (like GPI) or by tool developers (like ARMCI)

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Gap Analysis for Exascale

Heterogeneous hardware	fine
Data Types	fine
Fault Tolerance	Will become more important at Exascale, minimal requirements need to be checked
Migration Paths from MPI to PGAS	**MPI end-points** proposal will help future interoperability to map PGAS with MPI processing elements
Isolation of Libraries	Resources shared between main application and a library make isolation difficult
Locality	Topology information needs to be incorporated in PGAS approaches to quantify a distance to data

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PGAS-based MPI

- Objectives:
  - Implement and evaluate efficient message passing libraries on top of RDMA operations
  - Implement and evaluate collective operations on top of RDMA operations
  - Prototype implementation of MPI endpoints proposal
  - Develop recommendations for MPI to allow efficient implementation on top of RDMA
  - Develop recommendations for RDMA hardware

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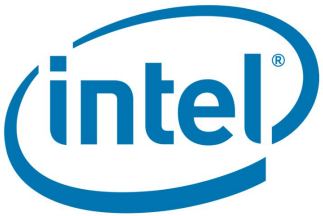
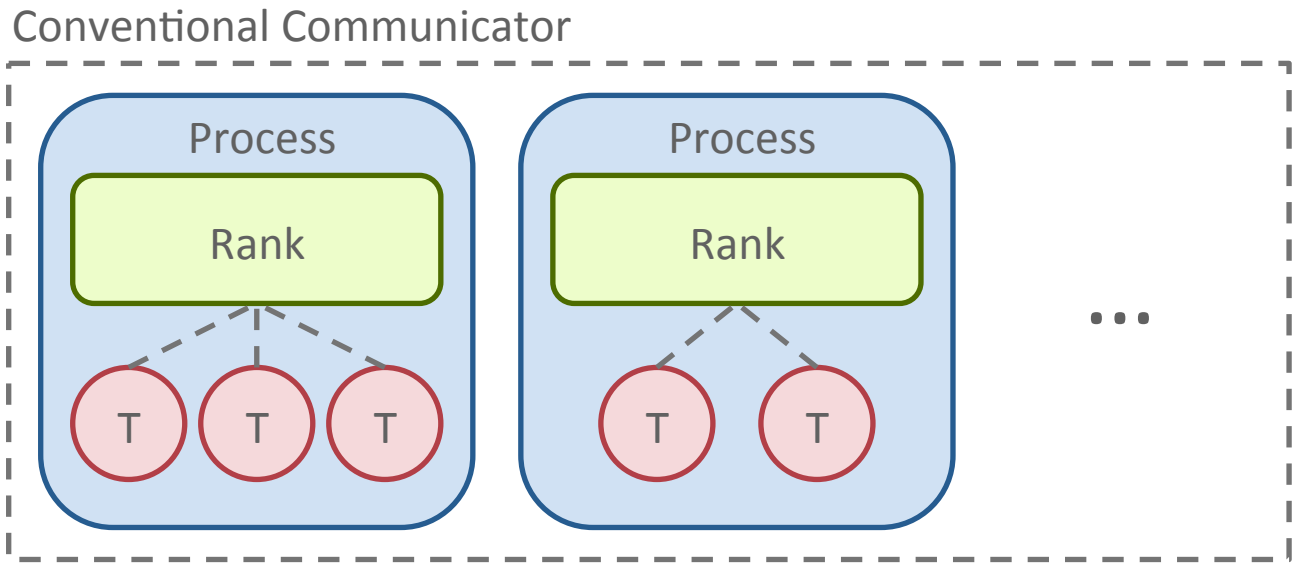
Enabling MPI Interoperability Through Flexible Communication Endpoints

James Dinan, Pavan Balaji, David Goodell,
Douglas Miller, Marc Snir, and Rajeev Thakur



Mapping of Ranks to Processes in MPI



- MPI provides a 1-to-1 mapping of ranks to processes
- This was good in the past, but usage models have evolved
  - Programmers use many-to-one mapping of threads to processes
    - E.g. Hybrid parallel programming with OpenMP/threads
  - Other programming models also use many-to-one mapping
    - Interoperability is a key objective, e.g. with Charm++, etc…

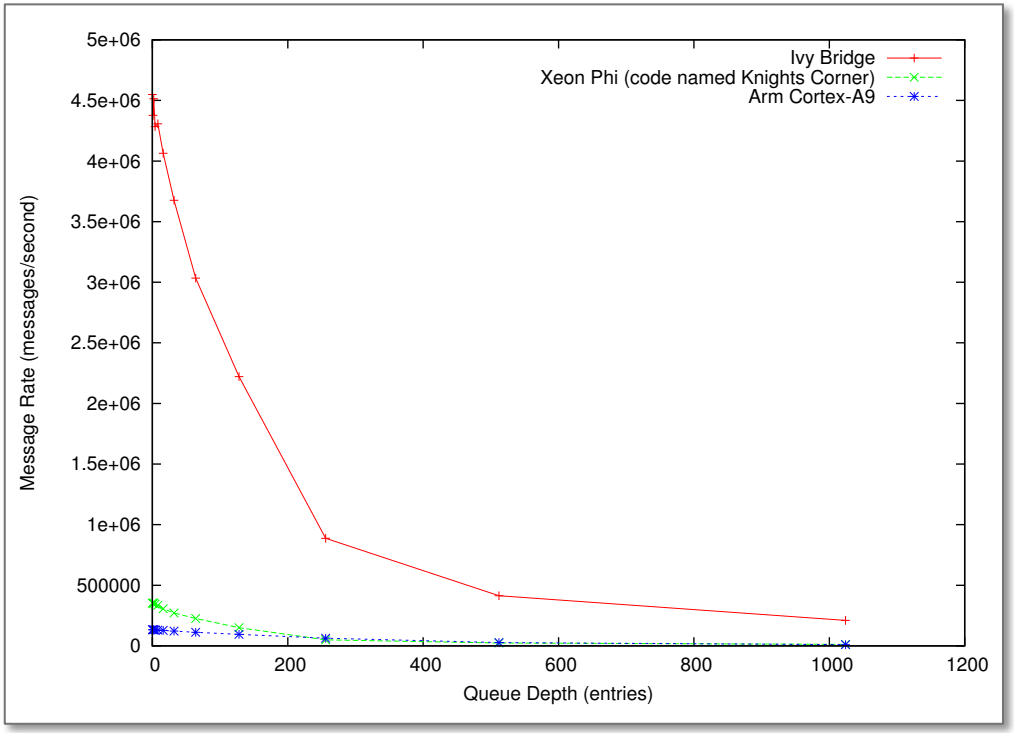
Current Approaches to Hybrid MPI+Threads

- MPI message matching space: `<communicator, sender, tag>`
- Two approaches to using THREAD_MULTIPLE

1. Match specific thread using the tag:
   - Partition the tag space to address individual threads
   - Limitations:
     - Collectives – Multiple threads at a process can't participate concurrently
     - Wildcards – Multiple threads concurrently requires care

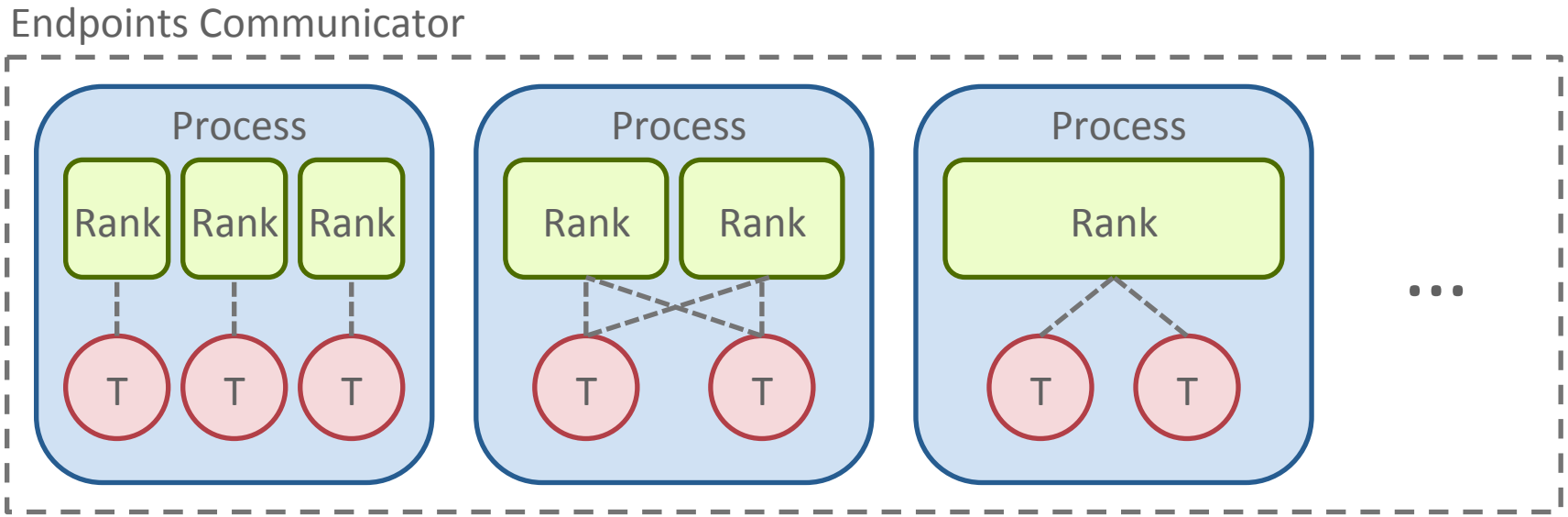
2. Match specific thread using the communicator:
   - Split threads across different communicators (e.g. Dup and assign)
   - Can use wildcards and collectives
   - However, limits connectivity of threads with each other

Impact of Light Cores and Threads on Message Rate



- Shamelessly stolen from Brian Barrett, et al. [EuroMPI '13]
- Threads sharing a rank increase posted receive queue depth (x-axis)
- Solution: More ranks!
  - Adding more MPI processes fragments the node
  - Can't do shared memory programming across the whole node

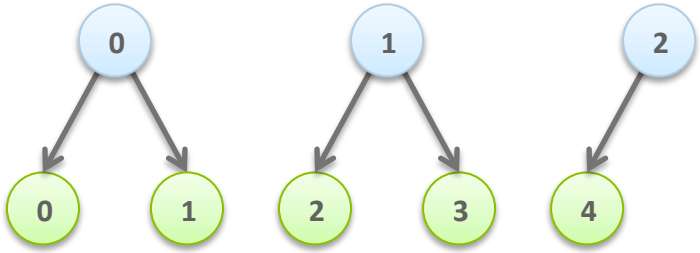
Endpoints: Flexible Mapping of Ranks to Processes



- Provide a many-to-one mapping of ranks to processes
  - Allows threads to act as first-class participants in MPI operations
  - Improve programmability of MPI + node-level and MPI + system-level models
  - Potential for improving performance of hybrid MPI + X
- A rank represents a communication “endpoint”
  - Set of resources that supports the independent execution of MPI communications
- Note: Figure demonstrates many usages, some may impact performance

Putting It All Together: Proposed Interface

```
int MPI_Comm_create_endpoints(
        MPI_Comm parent_comm,
        int my_num_ep,
        MPI_Info info,
        MPI_Comm *out_comm_hdls[])
```



- Each rank in *parent_comm* gets *my_num_ep* ranks in *out_comm*
  - *My_num_ep* can be different at each process
  - Rank order: process 0's ranks, process 1's ranks, etc.
- Output is an array of communicator handles
  - i^{th} handle corresponds to i^{th} endpoint create by parent process
  - To use that endpoint, use the corresponding handle

Usage Models are Many…

- Intranode parallel programming with MPI
  - Spawn endpoints off MPI_COMM_SELF
- Allow true thread multiple, with each thread addressable
  - Spawn endpoints off MPI_COMM_WORLD
- Obtain better performance
  - Partition threads into groups and assign a rank to each group
  - Performance benefits without partitioning shared memory programming model
- Interoperability
  - Examples: OpenMP and UPC

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- Context id allocation algorithm
  - Multiple instantiations of the algorithm with identical answer
  - influence the implementations in both MPICH and OpenMPI
- Alpha prototype implementation in McMPI
- Beta prototype implementation in T3DMPI
- Participation in the Hybrid working group

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Applications

- Objectives:
  - Use of the exascale MP, PGAS and PGAS-based MPI software in two real-world applications: Nek5000, iPIC3D
  - Analyze the performance of newly developed communication kernels in Nek5000 and iPIC3D
  - Provide feed-back and guidance to the development of exascale programming models

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EPiGRAM Applications

- Two real-world application with exascale needs:
  - Nek5000 (https://nek5000.mcs.anl.gov/):
    - CFD code for simulation of nuclear reactors and fluid turbulence
    - F77 (95%) C (5%) and MPI
    - Regular communication pattern involving neighbor processes
  - iPIC3D (https://github.com/CmPA/iPic3D/):
    - Particle code for simulation of interaction of solar wind with Earth's magnetosphere (space weather)
    - C++ and MPI
    - Regular communication pattern involving neighbor processes
- Initial work:
  - Identifying possible improvement in MPI communication kernels
    - Use of non-blocking CG and GMRes linear solvers. This requires redesign of solvers.
    - Use of sparse-collective to replace neighbor communication (might have improvement of message scheduling).
  - Porting applications to GPI
    - Identify interoperability issues between MPI and GPI.
    - Performance improvement with GPI One-sided.

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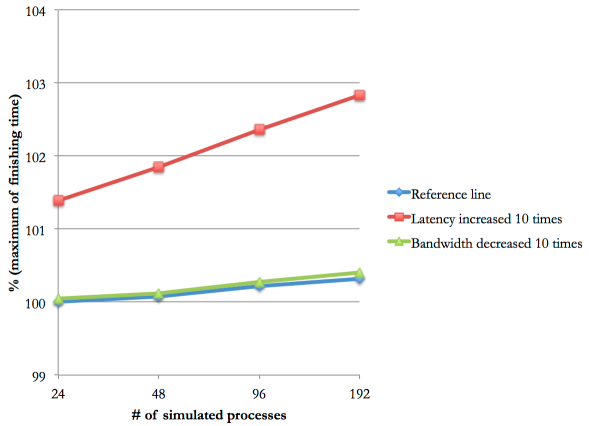
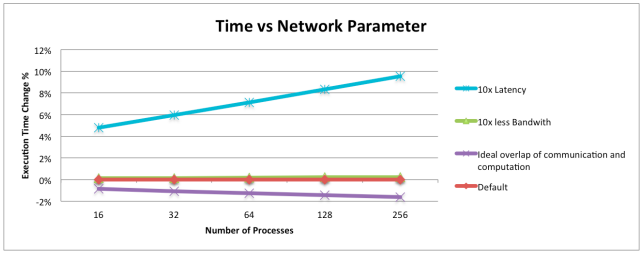
Thinking Exascale

- We use the LogGOPSim simulator (1), based on the LOGGops model, to:
  - Simulate the EPiGRAM applications on million nodes.
  - Assess the dependency of communication kernel performance on network bandwidth and latency.
  - Assess the importance of noise on applications communication kernel
- We consider additional data-driven applications with irregular application patterns and : Graph500 (Graph construction + Breadth-first search), mpiBLAST (nucleotide or proteing alignment search)





(1) Hoefler, Torsten, Timo Schneider, and Andrew Lumsdaine. "LogGOPSim: simulating large-scale applications in the LogGOPS model." In Proceedings of the 19th ACM International Symposium on High Performance Distributed Computing, pp. 597-604. ACM, 2010.

Summary

- MPI and PGAS will likely be important programming models on exascale systems
- Scalability and performance issues need to be resolved
- EPiGRAM tackles some of the important issues (collectives, data types, interoperability)

EPiGRAM

ExaMPI Workshop @ SC14

- Explore potential and issues of MPI for the exascale era
- Keynotes and invited talks from world-leading experts
- Explore hybrid systems
  - Booster, GPU, MIC, PGAS

- http://www.epigram-project.eu/exampi14/

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