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### **TORSTEN HOEFLER**

Systems @ ETH zurich

### **Theory and practice in HPC:**

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# Modeling, Programming, and Networking



Lugano 26-28 June 2017

CLIMATE & WEATHER SOLID EARTH LIFE SCIENCE CHEMISTRY & MATERIALS PHYSICS COMPUTER SCIENCE & MATHEMATICS ENGINEERING EMERGING DOMAINS POISSON & ECONTROL



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Attendees

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Technische Universität Chemnitz, Saxony, Germany





JITSU COMPUTERS

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# High **Performance** Cluster Computing







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### HPC is used to solve complex problems!

# Treat performance-centric programming and system design like physical systems

Image credit: Serena Donnin, Sarah Rauscher, Ivo Kabashow





### **Scientific Performance Engineering**



State States





### **Part I: Observe**





# Observe the state of the art in performance measurement

Stratified random sample of three top HPC conferences for four years

HPDC, PPoPP, SC (years: 2011, 2012, 2013, 2014)10 random papers from each (10-50% of population)120 total papers, 20% (25) did not report performance (were excluded)



enough information to allow scientists to understand the experiment, draw own conclusions, assess their certainty, and possibly generalize results.

TH. Belli: Scientific Be	enchmarking of Parallel Computing Sys	tems. IEE	E/ACM SC15						







### **Example: Simple ping-pong latency benchmark**







Did you assume

normality?

### **Dealing with variation**

The 99.9% confidence interval is 1.765us to 1.775us



Ugs, the data is not normal at all. The <u>nonparametric</u> 99.9% CI is much wider: 1.6us to 1.9us!

TH, Belli: Scientific Benchmarking of Parallel Computing Systems, IEEE/ACM SC15



NORMAL DISTRIBUTION

Can we test for normality?







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# Scientific benchmarking of parallel computing systems

ACM/IEEE Supercomputing 2015 (SC15)

### Scientific Benchmarking of Parallel Computing Systems

Twelve ways to tell the masses when reporting performance results

Torsten Hoefler Dept. of Computer Science ETH Zurich Zurich, Switzerland htor@inf.ethz.ch

#### ABSTRACT

Measuring and reporting performance of parallel computers constitutes the basis for scientific advancement of high-performance computing (HPC). Most scientific reports show performance improvements of new techniques and are thus obliged to ensure reproducibility or at least interpretability. Our investigation of a stratified sample of 120 papers across three top conferences in the field shows that the state of the practice is lacking. For example, it is often unclear if reported improvements are deterministic or observed by chance. In addition to distilling best practices from existing work, we propose statistically sound analysis and reporting techniques and simple guidelines for experimental design in parallel computing and codify them in a portable benchmarking library. We Roberto Belli Dept. of Computer Science ETH Zurich Zurich, Switzerland bellir@inf.ethz.ch

Reproducing experiments is one of the main principles of the scientific method. It is well known that the performance of a computer program depends on the application, the input, the compiler, the runtime environment, the machine, and the measurement methodology [20, 43]. If a single one of these aspects of *experimental design* is not appropriately motivated and described, presented results can hardly be reproduced and may even be misleading or incorrect.

The complexity and uniqueness of many supercomputers makes reproducibility a hard task. For example, it is practically impossible to recreate most hero-runs that utilize the world's largest machines because these machines are often unique and their software configurations changes regularly. We introduce the notion of *interpretability*, which is weaker than reproducibility. We call an ex-



erpret the by lines if alid.





# Simplifying Measuring and Reporting: LibSciBench

```
#include <mpi.h>
#include <liblsb.h>
#include <stdlib.h>
#define N 1024
#define RUNS 10
int main(int argc,_char *argv[]){
    int i, j, rank, buffer[N];
    MPI_Init(&argc, &argv);
    LSB_Init("test_bcast", 0);
    MPI Comm rank(MPI COMM WORLD, &rank);
    /* Output the info (i.e., rank, runs) in the results file */
    LSB_Set_Rparam_int("rank", rank);
    LSB Set Rparam int("runs", RUNS);
    for (sz=1; sz<=N; sz*=2){</pre>
      for (j=0; j<RUNS; j++){</pre>
        /* Reset the counters */
        LSB_Res();
        /* Perform the operation */
        MPI_Bcast(buffer, sz, MPI_INT, 0, MPI_COMM_WORLD);
        /* Register the j-th measurement of size sz */
        LSB_Rec(sz);
    LSB Finalize();
    MPI Finalize();
    return 0:
```

- Simple MPI-like C/C+ interface
- High-resolution timers
- Flexible data collection
- Controlled by environment variables
- Tested up to 512k ranks
- Parallel timer synchronization
- R scripts for data analysis and visualization







### We have the (statistically sound) data, now what?



The 99% confidence interval is within 1% of the reported median.

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We have the (statistically sound) data, now what?



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### Part II: Model







**Burnham, Anderson:** "A model is a simplification or approximation of reality and hence will not reflect all of reality. ... Box noted that "all models are wrong, but some are useful." While a model can never be "truth," a model might be ranked from very useful, to useful, to somewhat useful to, finally, essentially useless."

This is generally true for all kinds of modeling. We focus on **performance modeling** in the following!







## **Requirements modeling I: Six-step performance modeling**







### **Requirements modeling II: Automated best-fit modeling**

- Manual kernel selection and hypothesis generation is time consuming (boring and tricky)
- Idea: Automatically select best (scalability) model from predefined search space







### **Requirements modeling II: Automated best-fit modeling**

- Manual kernel selection and hypothesis generation is time consuming (and boring)
- Idea: Automatically select best model from predefined space

$$f(p) = \bigotimes_{k=1}^{n} c_{k} \times p^{i_{k}} \times \log_{2}^{j_{k}}(p)$$

$$i_{k} \cap I$$

$$i_{k} \cap I$$

$$i_{k} \cap J$$

$$i_{k}$$







### Talk: Fast Multi-Parameter Performance Modeling

A. Calotoiu, et al.

#### Tomorrow!!

10:30am Room: Grand Hall



Tutorial: Insighful Automatic Performance Modeling A. Calotoiu, F. Wolf, TH, M. Schulz

Sunday, November 13th 1:30pm - 5pm Room 355-C



[1] Download Extra-P at: http://www.scalasca.org/software/extra-p/download.html

[2] A. Calotoiu, D. Beckingsale, C. W. Earl TH, I. Karlin, M. Schulz, F. Wolf: Fast Multi-Parameter Performance Modeling, IEEE Cluster 2016

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# Requirements modeling III: Source-code analysis [1]

- Extra-P selects model based on best fit to the data
  - What if the data is not sufficient or too noisy?
- Back to first principles

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- The source code describes all possible executions
- Describing all possibilities is too expensive, focus on counting loop iterations symbolically







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LogP



### **Capability models for network communication**

### The LogP model family and the LogGOPS model [1]

A new parallel machine model reflects the critical technolog trends underlying parallel computers

# A PRACTICAL MODEL of PARALLEL COMPUTATION

UR GOAL IS TO DEVELOP A MODEL OF PARALLEL COMPUTATION THAT WILL serve as a basis for the design and analysis of fast, portable parallel algorithms, such as algorithms that can be implemented effectively on a wide variety of current and future parallel machines. If we look at the body of parallel algorithms developed under current parallel models, many are impractical because they exploit artificial factors not present in any reaPRAM consists of a collection of processors which compute synchronously in parallel and communicate with a global random access



### Finding LogGOPS parameters

Netgauge [2], model from first principles, fit to data using special PRTT(1,0,s) CPU 0 οi kernels Client GGGG 9 GGGG 9 ja a a aj Network GGGG 1 1 1 1 77777 Server CPU 0 0 0 0 (s-1)\*G (s-1)\*G (s-1)\*G L (s-1)\*G

#### Large scale LogGOPS Simulation



[1]: TH, T. Schneider and A. Lumsdaine: LogGOPSim - Simulating Large-Scale Applications in the LogGOPS Model, LSAP 2010, <a href="https://spcl.inf.ethz.ch/Research/Performance/LogGOPSim/">https://spcl.inf.ethz.ch/Research/Performance/LogGOPSim/</a> [2]: TH, T. Mehlan, A. Lumsdaine and W. Rehm: Netgauge: A Network Performance Measurement Framework, HPCC 2007, <a href="https://spcl.inf.ethz.ch/Research/Performance/Netgauge/">https://spcl.inf.ethz.ch/Research/Performance/LogGOPSim/</a>





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# Capability models for cache-to-cache communication





TH: Bridging Performance Analysis Tools and Analytic Performance Modeling for HPC

# Part III: Understand

### Use models to

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- 1. Proof optimality of real implementations
  - Stop optimizing, step back to algorithm level
- 2. Design optimal algorithms or systems in the model
  - Can lead to non-intuitive designs
- Proof optimality of matrix multiplication
  - Intuition: flop rate is the bottleneck
  - t(n) = 76ps \* n<sup>3</sup>
  - Flop rate R = 2flop \* n<sup>3</sup>/(76ps \* n<sup>3</sup>) = 27.78 Gflop/s
  - Flop peak: 3.864 GHz \* 8 flops = 30.912 Gflop/s
     Achieved ~90% of peak (IBM Power 7 IH @3.864GHz)
- Gets more complex quickly
  - Imagine sparse matrix-vector



Time [s]









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# 2) Design optimal algorithms – small broadcast in LogP

L=2, o=1, P=7



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S. Ramos, TH: "Modeling Communication in Cache-Coherent SMP Systems - A Case-Study with Xeon Phi", ACM HPDC'13





### Measured results – small broadcast and reduction



All which is a start of the start of the







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# **Part IV: Build**





### **Case study: Network Topologies**

- **Observe:** optimize for cost, maintain performance:
  - router radix, number of cables, number of routers  $\rightarrow$  cost
- number of endpoints, latency, global bandwidth  $\rightarrow$  capabilities
- Model: system as graph
- Understand: degree-diameter graphs
- Build: Slim Fly topology
- Result: non-trivial topology that outperforms all existing ones









Parating an





#### copper cables, small radix switches



fiber, high-radix switches

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International Symposium on Computer Architecture

#### Technology-Driven, Highly-Scalable Dragonfly Topology\*

ber of cables, and particularly the num

bles should be minimized to realize a

this paper, we introduce the dragonfly

group of high-radix routers as a virtue

effective radix of the network. With minimally routed packet traverses at m By reducing global channels, a dragonf

compared to a flattened butterfly and l

We also introduce two new variants

ing that enable load-balanced routing

router in a dragonfly must make an ac

folded Clos network in configurations

John Kim Northwestern University	William J. Dally Stanford University	Steve Scott Cray Inc.	Dennis Abts Google Inc.						
jjk12@northwestern.edu	2010 18th IEEE Symposium on High Performance Interconnects								
Abstract	The PERCS High-Performance Interconnect								
vate the use of high-radix routers to re									
tency, and cost of interconnection netw works, however, require longer cable,	Baba Arimilli *,	, Ravi Arimilli *, Vicent	te Chung *, Scott Clark *, Wo	olfgang Denzel <sup>†</sup> , Ben Drerup <sup>*</sup> , Torsten Hoefler <sup>‡</sup> ,					
works, however, require longer cable. counterparts. Because cables dominate	Baba Arimilli *, Kavi Arimilli *, Vicente Chung *, Scott Clark *, Wolfgang Denzel <sup>†</sup> , Ben Drerup *, Torsten Hoeffer +, Jody Joyner *, Jerry Lewis *, Jian Li <sup>†</sup> , Nan Ni * and Ram Rajamony <sup>†</sup>								

Jody Joyner \*, Jerry Lewis \*, Jian Li<sup>T</sup>, Nan Ni \* and Ram Rajamon \* IBM Systems and Technology Group, 11501 Burnet Road, Austin, TX 78758 <sup>†</sup> IBM Research (Austin, Zurich), 11501 Burnet Road, Austin, TX 78758 <sup>‡</sup> Blue Waters Directorate, NCSA, University of Illinois at Urbana-Champaign, Urbana, IL 61801 E-mail: arimilli@us.ibm.com, rajamony@us.ibm.com, htor@illinois.edu

Abstract-The PERCS system was designed by IBM in response to a DARPA challenge that called for a high-productivity high-performance computing system. A major innovation in the PERCS design is the network that is built using Hub chips that are integrated into the compute nodes. Each Hub chip is about 580 mm<sup>2</sup> in size, has over 3700 signal I/Os, and is packaged in a module that also contains LGA-attached optical electronic devices.

The Hub module implements five types of high-bandwidth interconnects with multiple links that are fully-connected with a high-performance internal crossbar switch. These links provide over 9 Tbits/second of raw bandwidth and are used to construct a two-level direct-connect topology spanning up to tens of thoubandwidths do not scale accordingly. For instance, while High Performance Linpack performance [5], [10] shows a steady improvement over time, interconnect-intensive metrics such as G-RandomAccess and G-FFTE [5] show very little improvement.

The challenge of building a high-performance, highly productive, multi-Petaflop system forced us to recognize early on that the entire infrastructure had to scale along with the microprocessor's capabilities. A significant component of our scaling solution is a new switchless interconnect with very high fanout organized into a two-level direct connec





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### **A** BRIEF HISTORY OF NETWORK TOPOLOGIES

copper cables, small radix switches



### fiber, high-radix switches

Key insight:



- "It's the diameter, stupid"
- Lower diameter:
- $\rightarrow$  Fewer cables traversed
- $\rightarrow$  Fewer cables needed
- $\rightarrow$  Fewer routers needed

Cost and energy savings: → Up to 50% over Fat Tree → Up to 33% over Dragonfly







Optimize towards the Moore Bound [1]: the upper bound on the *number of vertices* in a graph with given *diameter D* and *radix k.* 

$$MB(D,k) = 1 + k + k(k-1) + k(k-1)^{2} + \cdots$$

$$MB(D,k) = 1 + k \sum_{i=0}^{D-1} (k-1)^{i}$$



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### **CONNECTING ROUTERS: DIAMETER 2**

Example Slim Fly design for *diameter* = 2: *MMS graphs* [1]







[1] B. D. McKay, M. Miller, and J. Siráň. A note on large graphs of diameter two and given maximum degree. Journal of Combinatorial Theory, Series B, 74(1):110 – 118, 1998





**CONNECTING ROUTERS: DIAMETER 2** 



Groups form a fully-connected bipartite graph





**CONNECTING ROUTERS: DIAMETER 2** 



2 Construct a finite field  $\mathcal{F}_q$ . Assuming *q* is prime:  $\mathcal{F}_q = \mathbb{Z}/q\mathbb{Z} = \{0, 1, ..., q - 1\}$ with modular arithmetic.

E Example: q = 550 routers network radix: 7  $\mathcal{F}_5 = \{0, 1, 2, 3, 4\}$ 







**CONNECTING ROUTERS: DIAMETER 2** 



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**CONNECTING ROUTERS: DIAMETER 2** 

4 Find primitive element  $\xi$   $\xi \in \mathcal{F}_q$  generates  $\mathcal{F}_q$ : All non-zero elements of  $\mathcal{F}_q$ can be written as  $\xi^i$ ;  $i \in \mathbb{N}$ 

5 Build Generator Sets  

$$X = \{1, \xi^2, ..., \xi^{q-3}\}$$
  
 $X' = \{\xi, \xi^3, ..., \xi^{q-2}\}$ 

Example: q = 5  $\mathcal{F}_5 = \{0, 1, 2, 3, 4\}$   $\xi = 2$   $1 = \xi^4 \mod 5 =$   $2^4 \mod 5 = 16 \mod 5$   $X = \{1, 4\}$  $X' = \{2, 3\}$ 







**CONNECTING ROUTERS: DIAMETER 2** 

### 6 Intra-group connections

Two routers in one group are connected iff their "vertical Manhattan distance" is an element from:

$$X = \{1, \xi^2, ..., \xi^{q-3}\} \text{ (for subgraph 0)}$$
$$X' = \{\xi, \xi^3, ..., \xi^{q-2}\} \text{ (for subgraph 1)}$$

Example: 
$$q = 5$$
  
Take Routers (0,0,.)  
 $X = 14$ 









**CONNECTING ROUTERS: DIAMETER 2** 

### 6 Intra-group connections

Two routers in one group are connected iff their "vertical Manhattan distance" is an element from:

 $X = \{1, \xi^2, ..., \xi^{q-3}\} \text{ (for subgraph 0)}$  $X' = \{\xi, \xi^3, ..., \xi^{q-2}\} \text{ (for subgraph 1)}$ 

Example: 
$$q = 5$$
  
Take Routers (1,4,.)  
 $X' = \{2,3\}$ 









**CONNECTING ROUTERS: DIAMETER 2** 



Example: q = 5Take Router (1,0,0)  $(1,0,0) \leftrightarrow (0, x, 0)$ Take Router (1,1,0) m = 1, c = 0 $(1,0,0) \leftrightarrow (0, x, x)$ 

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### **COST COMPARISON**





🔀 Slim Fly





#### A LOWEST-DIAMETER TOPOLOGY

- $\rightarrow$  Approaching the Moore Bound
- → Resilient



#### A COST & POWER EFFECTIVE TOPOLOGY

 $\rightarrow$  25% less expensive than Dragonfly,

all the second

 $\rightarrow$  26% less power-hungry than Dragonfly









### How to continue from here?

### Parallel Language



[1]: M. Besta, TH: Accelerating Irregular Computations with Hardware Transactional Memory and Active Messages, ACM HPDC'15

[2]: R. Belli, TH: Notified Access: Extending Remote Memory Access Programming Models for Producer-Consumer Synchronization, IPDPS'15

[3]: S. Di Girolamo, P. Jolivet, K. D. Underwood, TH: Exploiting Offload Enabled Network Interfaces, IEEE Micro'16































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# Backup