# BLUE WATERS SUSTAINED PETASCALE COMPUTING

Performance Modeling for Systematic Performance Tuning

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with inputs from William Gropp, Marc Snir, Bill Kramer

Invited Talk RWTH Aachen University March 30<sup>th</sup>, Aachen, Germany

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#### The Perspective of a Computing Center

- Performance = "completed science per cost and time"
- Optimizing this metric can be manifold:
  - Application optimization (support application teams)
  - Architecture optimization (select best hardware)
  - Optimize Middleware (scheduler, libraries etc.)
  - Optimize Policies (scheduling, charging etc.)
  - ... and many more





#### **Performance Modeling – State of the Practice**

- Delivers the "science per cost/time" metric
  - Can be used to drive optimizations!
- Who does performance modeling?
  - Mostly computer scientists, in-house teams
- BUT: most development is done by application developers and/or domain scientists
  - They should develop performance models during software development
    - See performance modeling panel @3:30 in TCC 101





# (Ideal) State of the Practice @NCSA

- Propose to use simple performance modeling to characterize the behavior of applications
  - Enables rough optimization (cf. "80/20 rule")
- We provide a set of simple modeling guidelines
  - Semi-analytic performance modeling
  - Small number of parameters, use other techniques where necessary



Hoefler, Gropp, Snir, Kramer: Performance Modeling for Systematic Performance Tuning





# **Overview of Performance Modeling**

- Analytic modeling:
  - Determine application requirements and system speeds to compute time (e.g., bandwidth)
- Empirical modeling (e.g. [1,2]):
  - "Black-box" approach: machine learning, neural networks, statistical learning ...
- Semi-empirical modeling:
  - "White box" approach: find asymptotically tight analytic models, parameterize empirically (curve fitting)

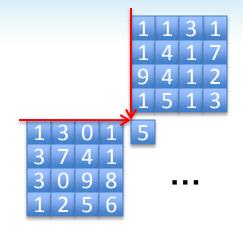
[1]: Barnes, Rountree, Lowenthal, Reeves, Supinski, Schulz: A regression-based approach to scalability prediction [2]: McKee, Singh, Supinski, Schulz: Constructing Application Performance Models Using Neural Networks



# A Quick Example - MM

• Matrix multiplication (N<sup>3</sup> algorithm)

for(int i=0; i<N; ++i)
for(int j=0; j<N; ++j)
for(int k=0; k<N; ++k)
C[i+j\*N] += A[i+k\*N] \* B[k+j\*N];</pre>

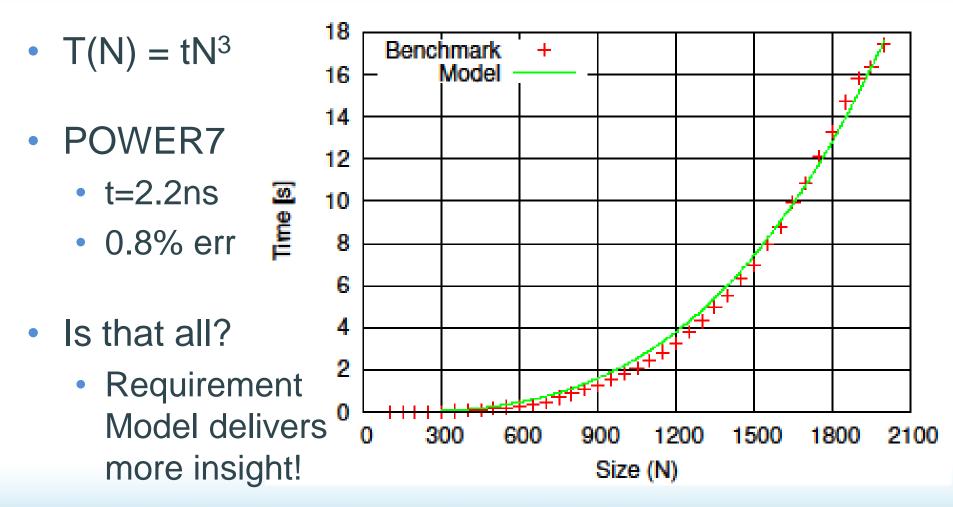


- Trivial (non-blocked) algorithm
- Analytic Model:
  - N<sup>3</sup> FP add/mult, 4N<sup>3</sup> FP load/store, +int ops
  - How can we get to an execution time?  $\rightarrow$  very hard!





## **Semi-Empiric Model for MM**

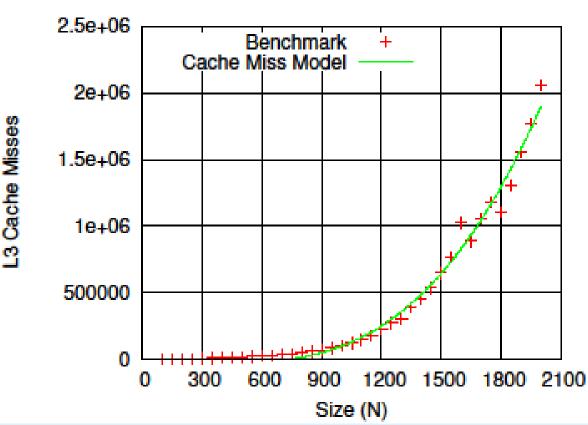






## **Requirements Model for MM**

- Required floating point operations: 2N<sup>3</sup> (verified)
- Cache misses?
  - Semi-analytic!
  - $C(N) = aN^3 bN^2$
- POWER7
  - a=3.8e-4
  - a=2.7e-1



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# **Our Ubiquitous Modeling Philosophy**

- Modeling during each phase of SW development:
  - Analysis pick right method (asymptotic models)
  - Design pick right algorithms (asymptotic models)
  - Implementation show good usage of machine, e.g., blocking in MM (semi-empirical models)
  - Testing fulfilling model expectations as correctness criterion (compare tests with models)
  - Maintenance monitor performance on different architectures (compare times with models)





# More uses of Models

- Performance Optimization
  - Identify bottlenecks and problems during porting
- System Design



- Co-design based on application requirements
- System Deployment and Testing
  - Know what to expect, find performance issues quickly
- During System Operation
  - Detect silent (and slow) performance degradation





# **Six-Steps to a Model**

- Our <u>very</u> high-level strategy consists of the following six steps:
  - 1) Identify input parameters that influence runtime
  - 2) Identify application kernels
  - 3) Determine communication pattern
  - 4) Determine communication/computation overlap
  - 5) Determine sequential baseline
  - 6) Determine communication parameters

Analytic

Empiric

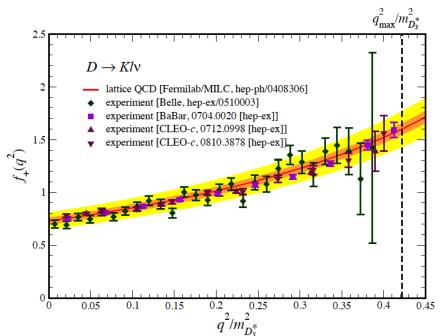




# All Steps By Example – MILC

- MIMD Lattice Computation
  - Gains deeper insights in fundamental laws of physics
  - Determine the predictions of lattice field theories (QCD & Beyond Standard Model)
  - Major NSF application
- Challenge:
  - High accuracy (computationally intensive) required for comparison with results from experimental programs in high energy & nuclear physics

Bernard, Gottlieb et al.: Studying Quarks and Gluons On Mimd Parallel Computers







# **Step 1: Critical Parameters**

- Best way: ask a domain expert!
  - Or: look through the code/input file format
- For MILC (thanks to S. Gottlieb):

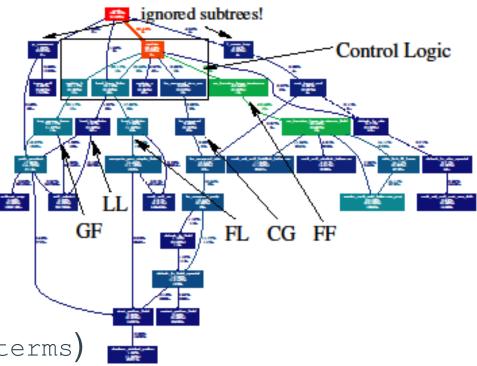
Name	Description
Р	number of PEs (intrinsic parameter)
nx, ny, nz, nt	size in x, y, z, t dimension
warms, trajecs	warmup rounds and trajectories (outer loop)
traj_between_meas	measurement "frequency"
steps_per_trajectory	number of "steps" in each trajectory
beta, mass1, $\dots$	physics parameters that influence CG iterations
max_cg_iterations	limits the conjugate gradient iterations





# **Step 2: Find Kernels**

- E.g., investigate call-tree or source-code
- Control logic
  - update
- MILC's kernels:
  - LL (load\_longlinks)
  - **FL**(load\_fatlinks)
  - CG (ks\_congrad)
  - **GF** (imp\_gauge\_force)
  - FF (eo\_fermion\_force\_twoterms)







# **Step 4: Sequential Performance**

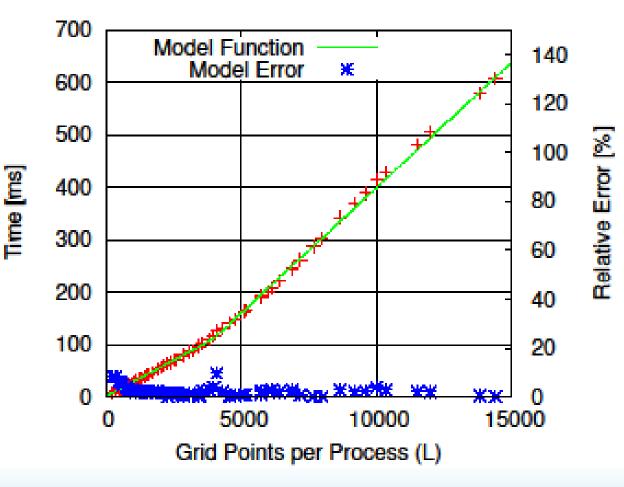
- MILC "only" loops over the lattice  $\rightarrow \Theta(V)$
- > T(V) = tV
  - Wait, it's not that simple with caches  $\boldsymbol{\boldsymbol{\Im}}$
  - Small V fit in cache!
- $> T(V) = t_1 * min(s, V) + t_2 * max(0, V-s)$ 
  - Cache holds s data elements
  - Three parameters for each kernel





## An Example Kernel: GF (Gauge Force)

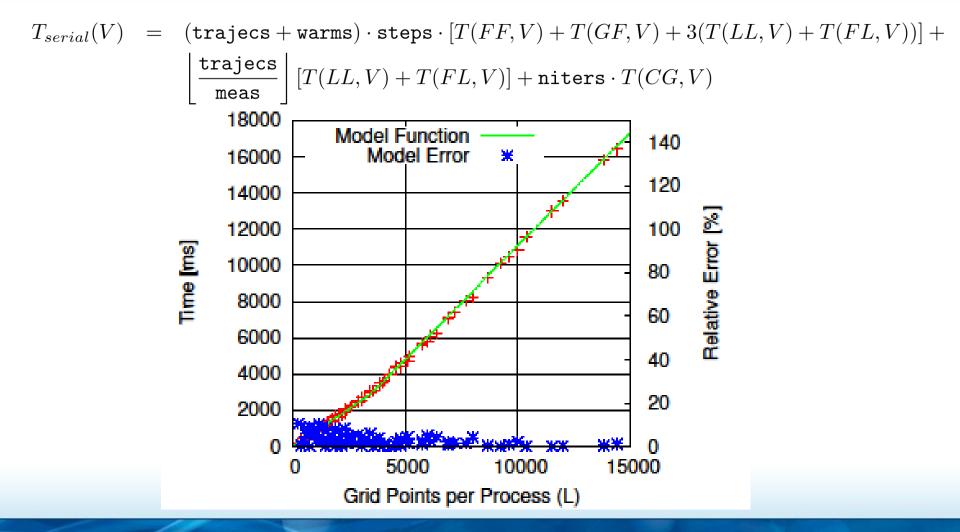
- On POWER7:
  - t<sub>1</sub>=62.4 µs
  - t<sub>2</sub>=92 µs
  - s=4.000
- Errors
  - Max <10%
  - Cum <3%







#### **Complete Serial Performance Model**



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# **Step 3: Communication Pattern**

- 4d domain is cut in all dimensions (cubic)
  - 4d nearest-neighbor communication (8 neighbors)
- Allreduce to check CG convergence
  - One per iteration on full process set
- We counted messages and sizes
  - Separate for each kernel
  - See paper for sizes and full model equation

	kernel	#Messages
	$\mathrm{FF}$	$(\texttt{trajecs} + \texttt{warms}) \cdot \texttt{steps} \cdot 1616$
	GF	$(\texttt{trajecs} + \texttt{warms}) \cdot \texttt{steps} \cdot 828$
	$\operatorname{LL}$	$(3 \cdot \texttt{steps} \cdot (\texttt{trajecs} + \texttt{warms}) + \lfloor \frac{\texttt{trajecs}}{\texttt{meas}} \rfloor) \cdot 8$
•	$\mathrm{FL}$	$(3 \cdot \texttt{steps} \cdot (\texttt{trajecs} + \texttt{warms}) + \lfloor \frac{\texttt{trajecs}}{\texttt{meas}} \rfloor) \cdot 288$





# **Step 6: Communication Parameters**

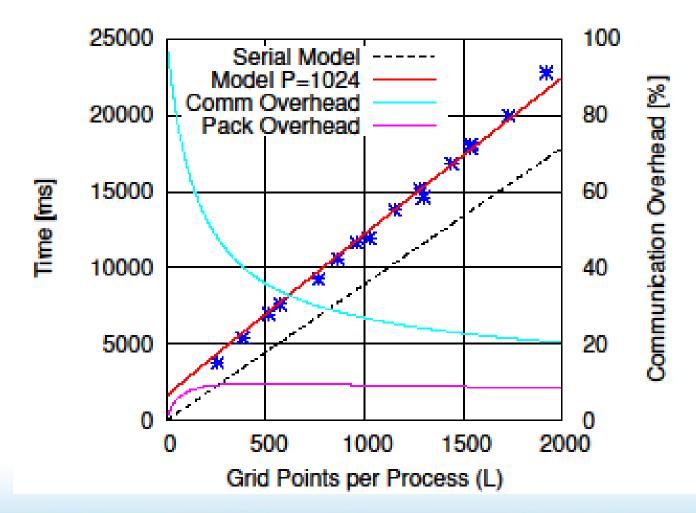
- Two options:
  - Semi-empiric fit measurements to get effective latency and bandwidth
    - Enables to check if they match expectations
  - Analytic derive parameters separately (e.g., documentation or separate benchmark)
    - Often problematic if they do not match expectations
- Our model was analytic
  - Uses LogGP parameters (measured by Netgauge [1])

[1] Hoefler et al.: Low-Overhead LogGP Parameter Assessment for Modern Interconnection Networks





#### **The Fully-Parameterized Parallel Model**



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# **Conclusions and Future Work**

- Models in use for predictions and optimizations
  - First successes: ~10-20% improved performance [1]
- Simple strategy enables application team models
  - Better chance to be maintained than external models
  - Critical for performance-centric software development
- We need (and work on):
  - More examples for irregular/dynamic codes
  - Better tool support for modeling

[1] Hoefler, Gottlieb.: Parallel Zero-Copy Algorithms for Fast Fourier Transform and Conjugate Gradient using MPI Datatypes

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