

# Computer Systems Performance Analysis and Benchmarking (37-235)

**Analytic Modeling**

**Simulation**

**Measurements / Benchmarking**

**Lecture/Assignments/Projects:**

Dr. Christian Kurmann

**Textbook:**

Raj Jain, "The Art of Computer Systems Performance Analysis", 1991 Wiley & Sons, New York

**Topic of Today:**

- **Memory Systems Benchmarks (ECT-memperf)**
- **Modelling of an application (OPAL)**

# Performance Evaluation, -Modeling and -Prediction of a Message Passing Molecular Simulation Code

M. Taufer, T. Stricker

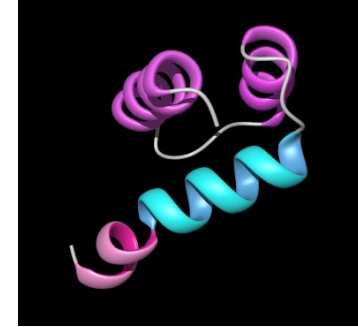
Laboratory for Computer Systems

ETH - Swiss Institute of Technology

CH-8092 Zurich

## Motivation

- Molecular simulation code: Opal



- Different parallel platforms to run on:



Cray J90



Cray T3E



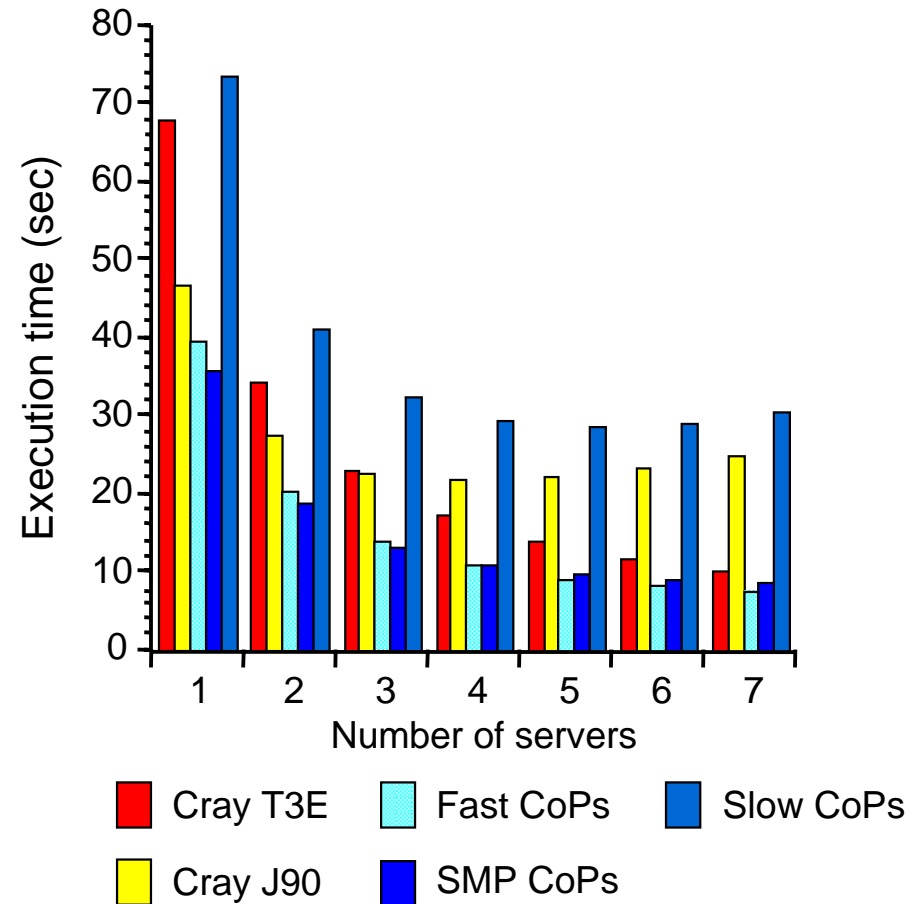
Different Clusters of PCs

which ones will work?

which one is most cost effective?

# Motivation

- Little is known about the **interaction between the application and the platform**
- Our solution is using:
  - analytical modeling
  - measurementsduring:
  - application design
  - parallelization
  - performance analysis



# Outline

- Introduction to the code
  - application: Opal
  - middleware: Sciddle, PVM
- Performance modeling
  - parameter space
  - time complexity
  - measurements
  - calibration
- Performance prediction on different platforms
- Summary
- Conclusion

## Application: Opal

- Molecular dynamic simulation of proteins and nucleic acids
  - P.Luginbühl, P.Güntert, M.Billeter, K.Wüthrich. *The new program Opal...* Journal of Biomolecular NMR, [1996]
- Parallel version:
  - replicated-data (RD) method
  - client-server paradigm
  - list of active pairs (pairs of mass centers)
    - ◆ radius as cut-off parameter
  - simulation phases: update and energy computation

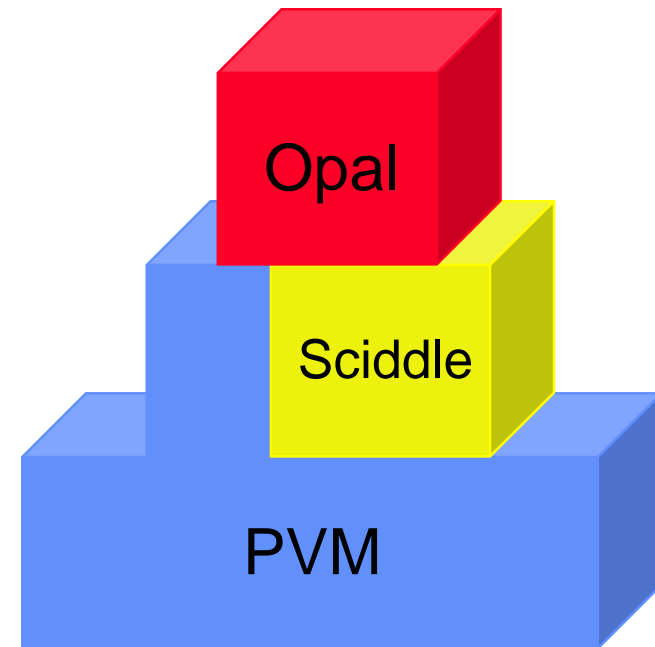
## Related Work

- Similar packages:
  - Amber
- Alternative parallelization:
  - replicated-data (RD) method
  - geometric- or space-decomposition (SD) method
  - force-decomposition (FD) method

Our work is only about performance modeling and not about computational chemistry or numerical algorithms.

# Middleware

- Sciddle for PVM:
  - remote procedure call system
  - extension to PVM
  - highly portable communication library
  - ☹ for a single J90 vector SMP  
shared memory support is better
  - 😊 for a cluster of *four* J90s:  
message passing over Hippi
  - 😊 for a cluster of PCs:  
message passing over
    - Ethernet (UDP/IP)
    - Myrinet (Fast Messages)



# Parameter Space of an Application Run

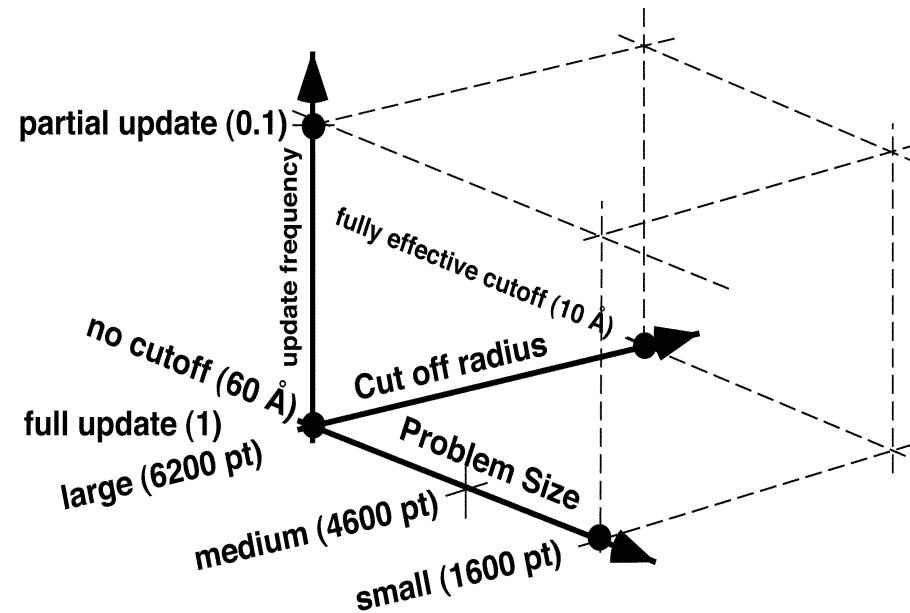
- Experimental factors

- problem size
- number of servers
- update parameter
- cut-off parameter

- Response variables

- parallel computation time
- sequential computation time
- communication time
- synchronization time
- idle time

- Full factorial design



## Analytical Modeling for the Execution Time of Opal

$$t_{opal} \approx s \begin{cases} \frac{1}{2p}(a_2 u(1-2\gamma)^2 + a_3)n^2 + \left(\frac{\alpha}{a_1}p(u+2) - \frac{1}{2p}(a_2 u(1-2\gamma) + a_3) + a_4\right)n + 2(u+1)(pb_1 + b_5) \\ \frac{1}{2p}(a_2 u(1-2\gamma)^2)n^2 + \left(\frac{\alpha}{a_1}p(u+2) + \left(\frac{1}{p}a_3\bar{n} - \frac{1}{2p}a_2 u(1-2\gamma)\right) + a_4\right)n + 2(u+1)(pb_1 + b_5) \end{cases}$$

- parallel computation time:

$$t_{par\_comp} \approx \begin{cases} O(n^2) \text{ no cut-off} \approx O(p^{-1}) \\ O(n) \text{ with cut-off} \end{cases}$$

- communication time:

$$t_{comm} \approx O(n) \approx O(p)$$

# Measurements on Cray J90

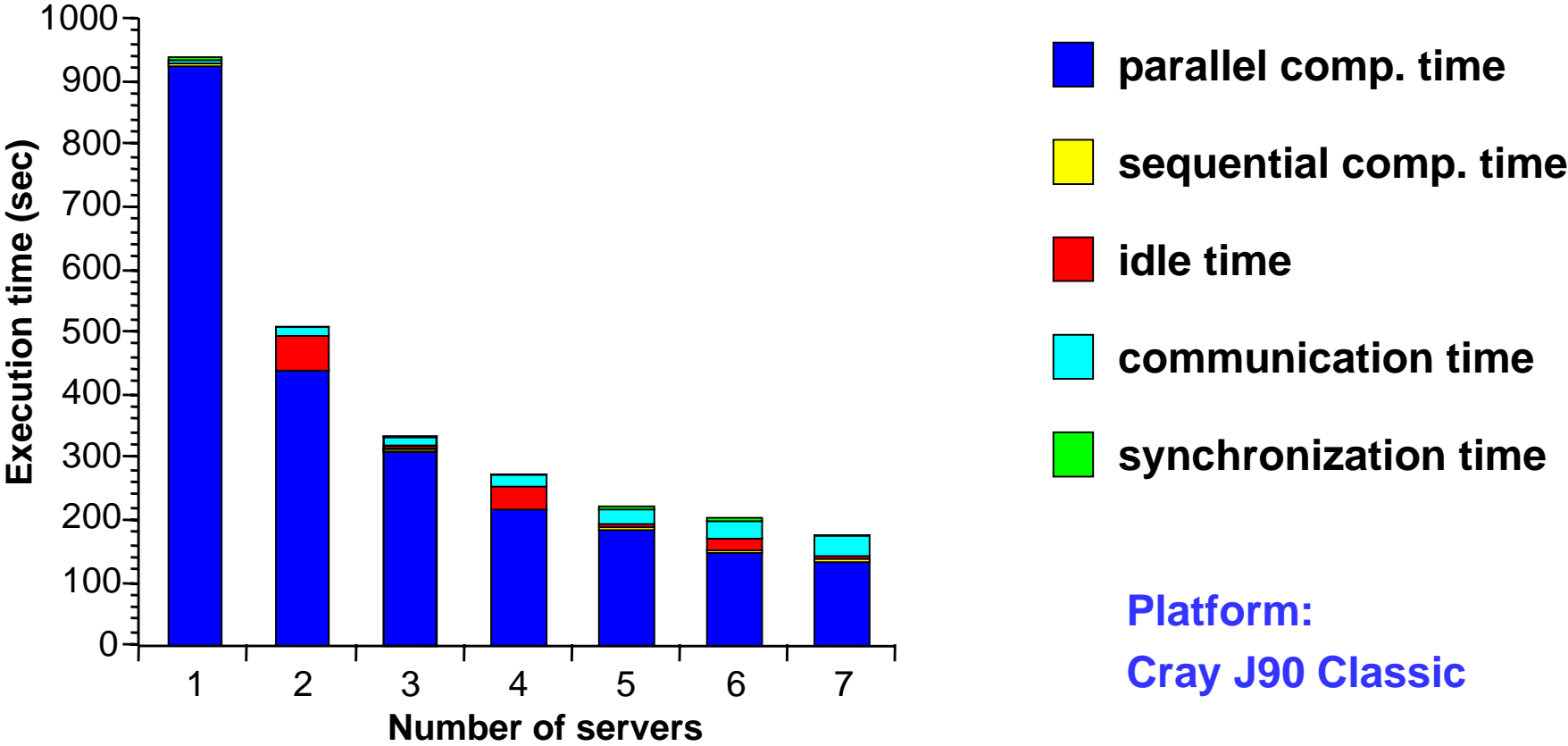
## Problem with middleware

- High overlap of computation and communication
  - no support for:
    - ◆ detailed quantification of elapsed time
    - ◆ correct accounting of elapsed time
- Precise timing model
  - give up some overlap
  - introduction of additional synchronization: PVM barrier

Less than 5% slowdown over the code with overlap

# Understanding the Execution Time

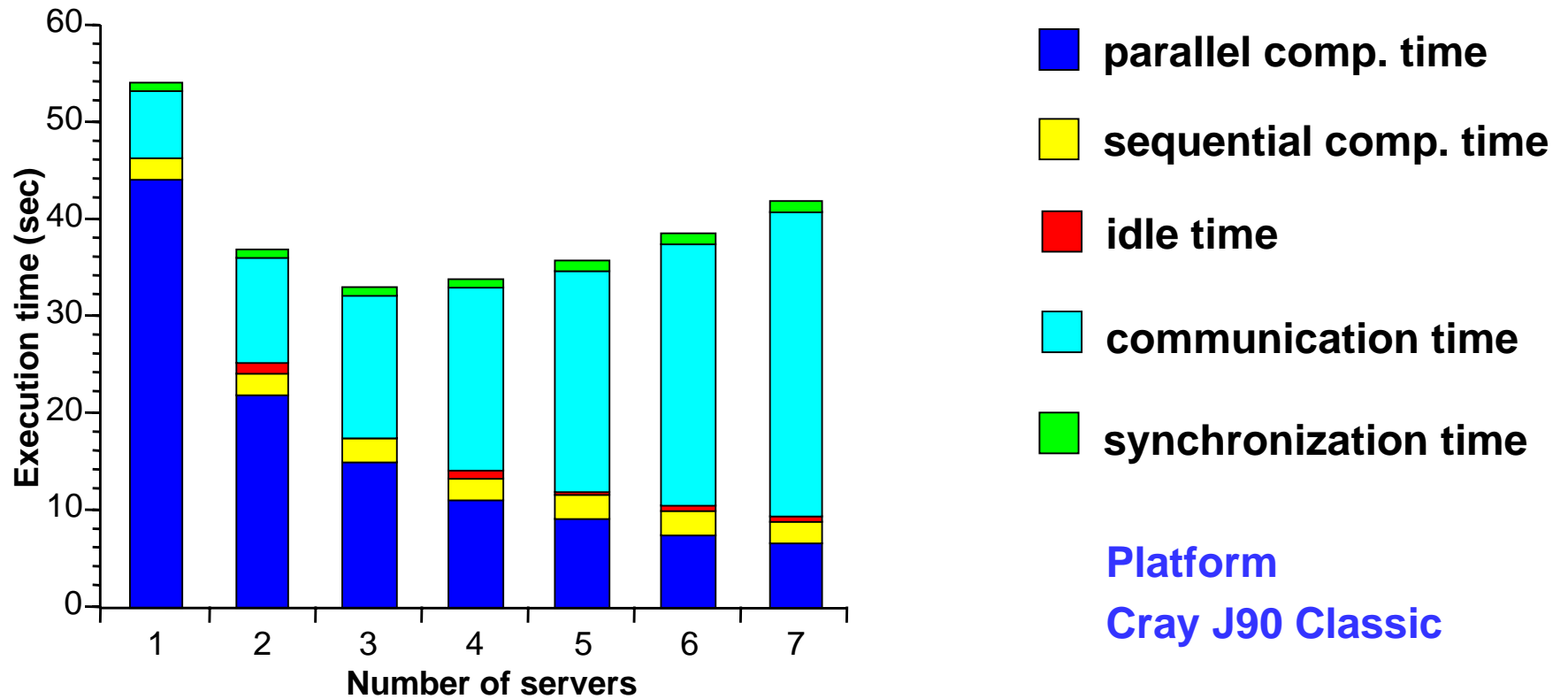
No cut-off



Platform:  
Cray J90 Classic

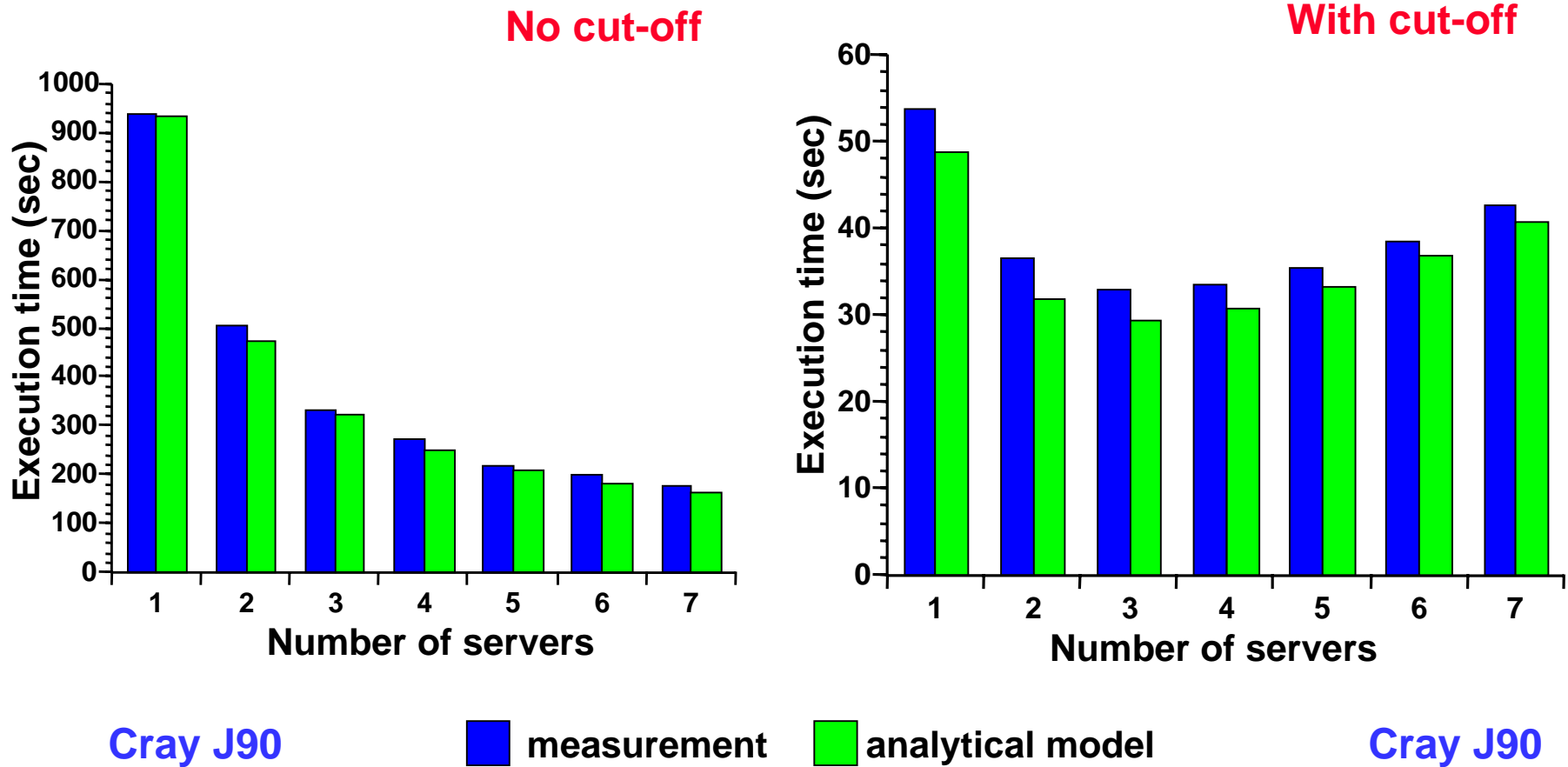
# Understanding the Execution Time

With cut-off



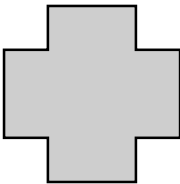
# Calibration between Analytical Model and Measurements

## Measured time vs. analytical model time



# Performance Prediction on different Platforms

Analytical Model



Standard Performance Data

Opal	Cray T3E
Performance	Cray J90
on	Fast CoPs
different	SMP Cops
Computer	Slow CoPs
Platforms	

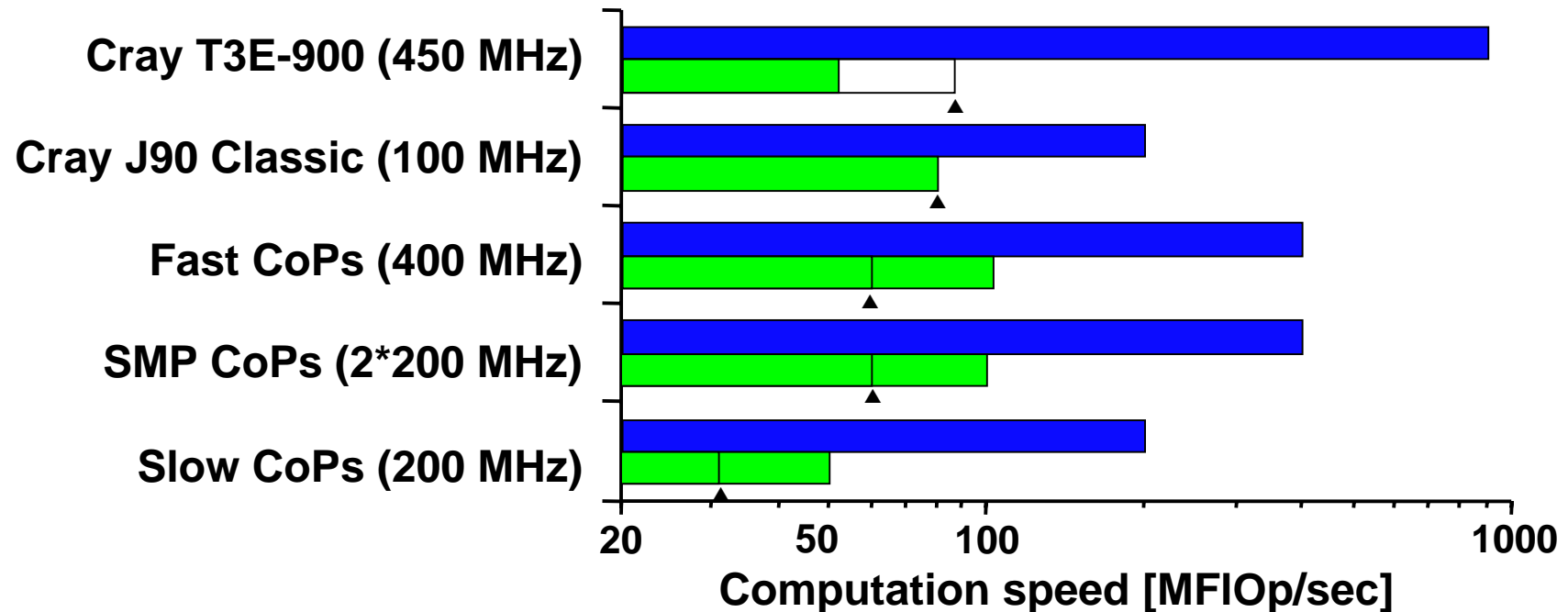
## Performance Prediction on different Platforms

- Cray T3E → high-end MPP supercomputer
- Cray J90 → low cost vector supercomputer
- fast CoPs → medium cost solution  
Gigabit/s Myrinet interconnection
- SMP CoPs → built with commodity components  
SCI shared memory interconnection
- slow CoPs → low cost solution  
Ethernet 100BaseT

## Opal as Micro-benchmark

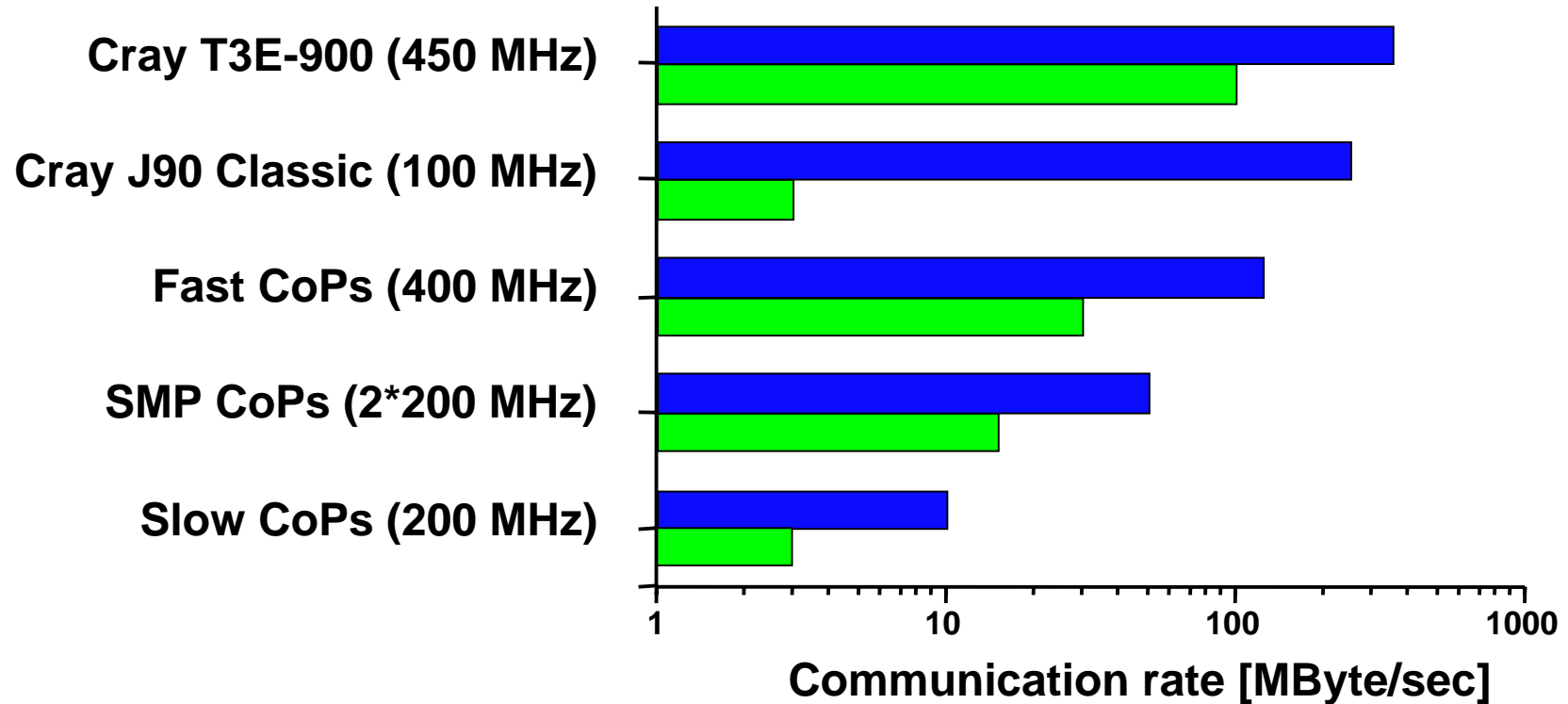
- Inner loop of Opal on one processor
- 64 bit arithmetic (IEEE, Cray) - correct results
- Amount of work for 10 iterations
  - CoPs, Pentium II: **327 MFLOp**
  - Cray J90: **497 MFLOp**
  - Cray T3E, Alpha 21164 **811 MFLOp**
- Measured with performance counting hardware

## Machine Parameters: CPU Speed [MFIOp/sec]



- Theoretical peak speed per processing node [MFIOp/sec]
- Measured and adjusted computation speed per node [MFIOp/sec]

# Machine Parameters: Communication Speed [MByte/sec]

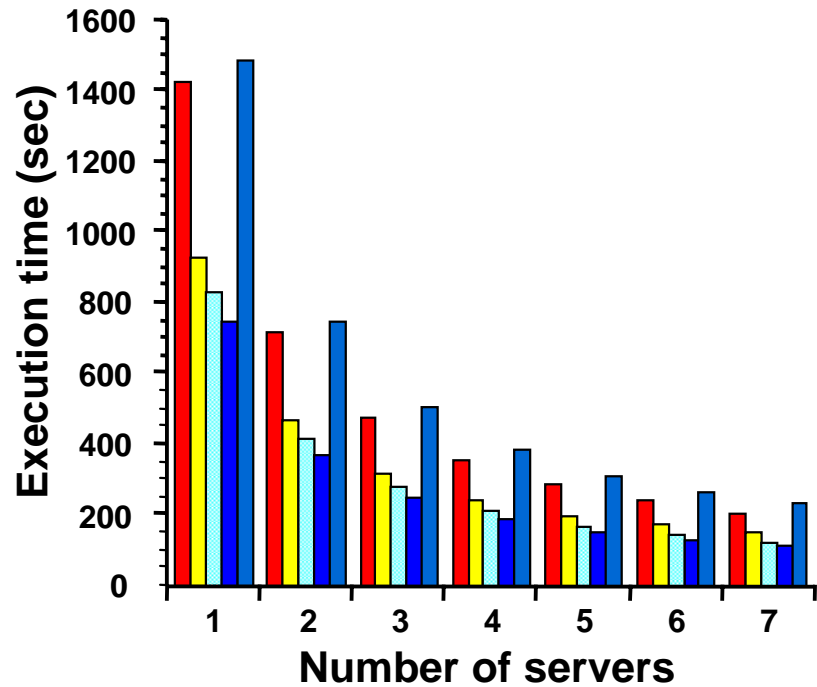


- Theoretical peak communication speed on a link [Mbyte/sec]
- Observed communication speed in PVM / MPI / Sciddle [Mbyte/sec]

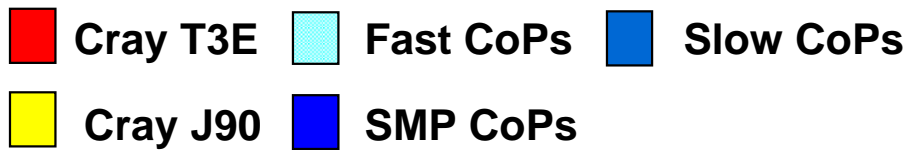
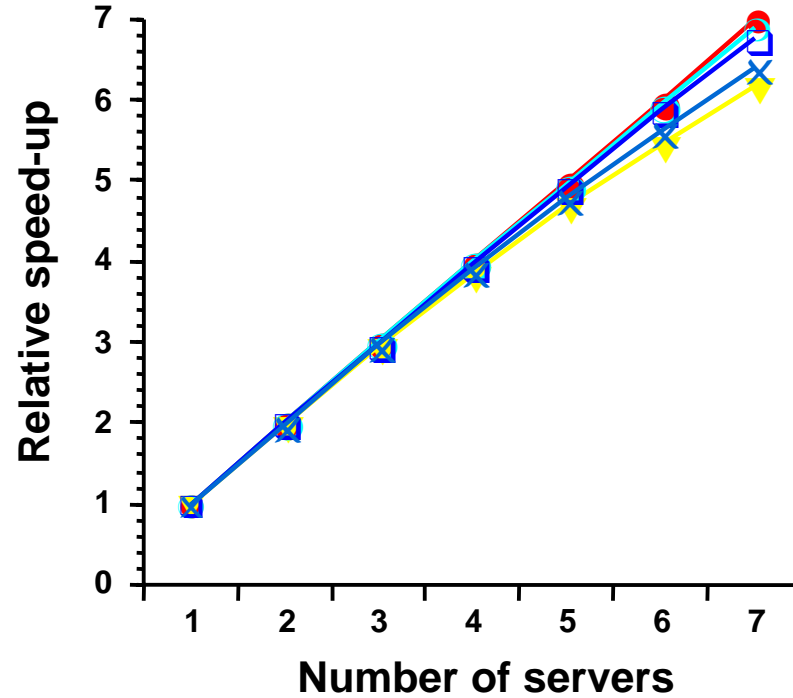
# Performance Prediction on different Platforms

No cut-off

Execution time

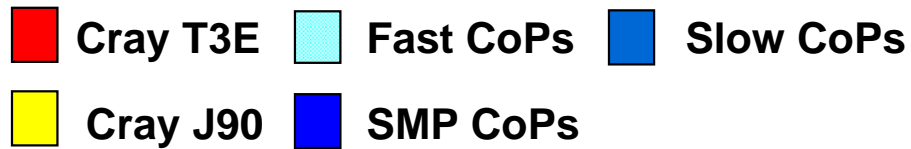
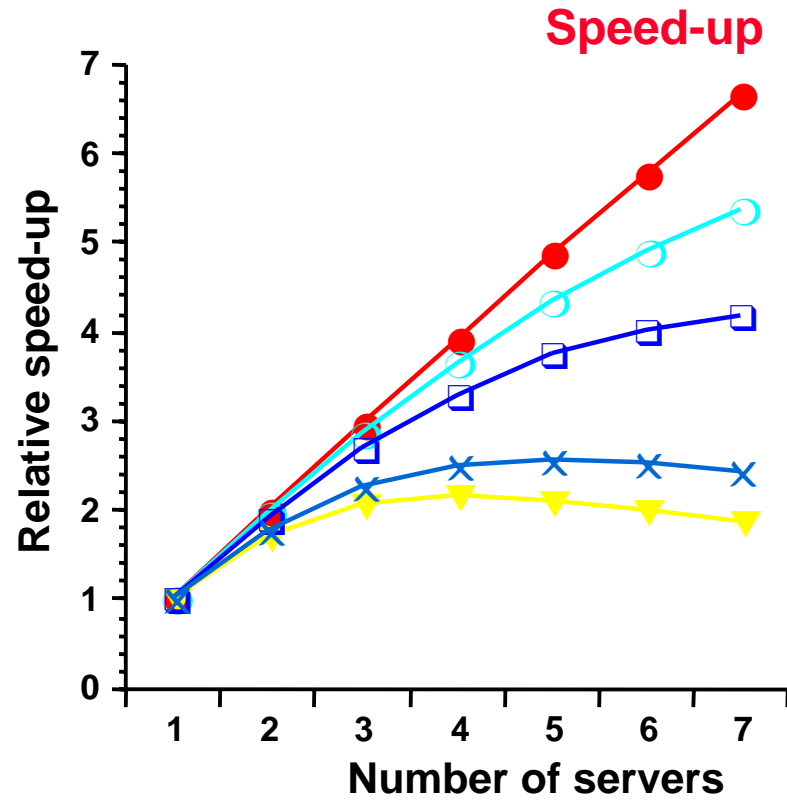
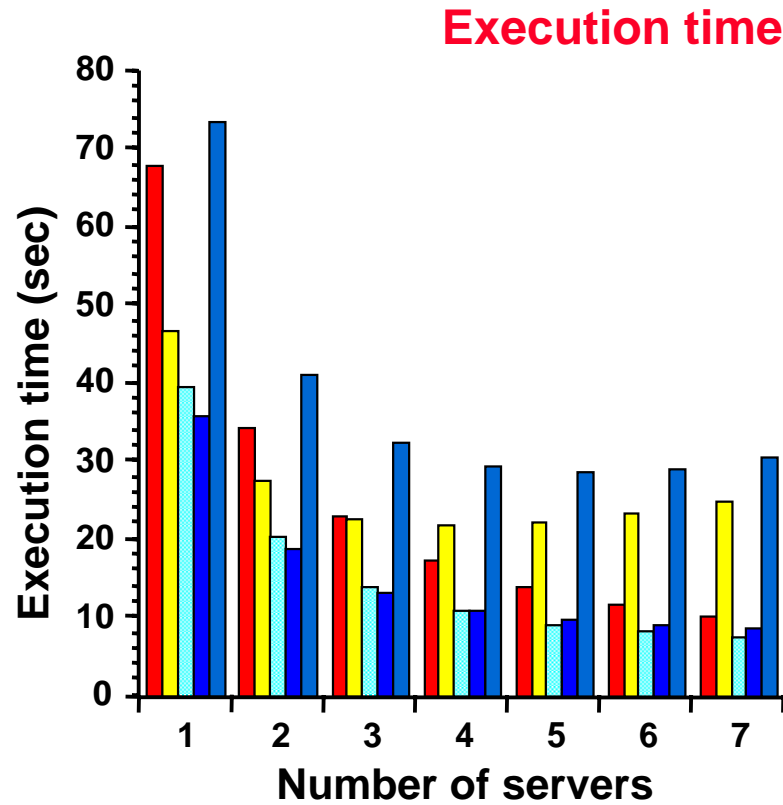


Speed-up



# Performance Prediction on different Platforms

With cut-off



## Summary

- An analytical complexity model and a careful instrumentation for performance monitoring leads to a better understanding of the resource demands of a parallel application.
- Interesting anomalies in the implementation:
  - load imbalance for even number of servers
  - differing number of floating point operations for different processor types
- Our model allows predictions with good certainty on different Platforms:
  - how would the application run on: fast CoPs, SMP CoPs, slow CoPs.

## Conclusion

- Middleware is dangerous:
  - it *interferes* with performance evaluation (i.e., the accounting of the execution time components).
- Looking just at speed-up is not sufficient to prove good performance:
  - keep an eye on the *total computation time*
- Prediction for execution times and speed-up figures indicate that a well designed *Cluster of PCs* can achieve an efficiency similar to the *Cray J90* and *Cray T3E for the application Opal*.