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# Trends in High Performance Computing, Enhancing Performance and the Computational Grid

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#### Outline

- Look at trends in HPC
  - ➤ Top500 statistics
- NetSolve
  - > Example of grid middleware
- Performance on today's architecture
  - > ATLAS effort
- Tools for performance evaluation
  - > Performance API (PAPI)

## **Background Information**

- Started in 6/93 by JD, Hans W. Meuer and Erich Strohmaier

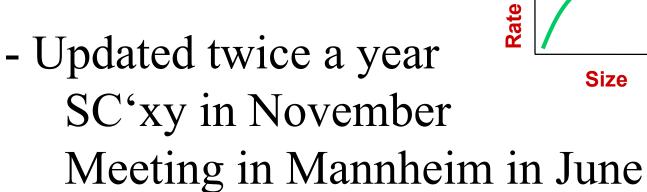
#### **TOP500 Motivation**

- Basis for analyzing the HCP market
- Quantify observations
- Detection of trends (market, architecture, technology)

#### **TOP500 Procedure**

- Listing of the 500 most powerful Computers in the World
- Yardstick: Rmax from LINPACK MPP

Ax=b, dense problem



- All data available from www.top500.org

#### TOP-500 List

- A way for tracking trends
  - >in performance
  - >in market
  - in classes of HPC systems
    - > Architecture
    - >Technology

- Original classes of machines
  - > Sequential
  - > SMPs
  - > MPPs
  - > SIMDs
- Two new classes
  - Beowulf-class systems
  - Clustering of SMPs and DSMs
    - Requires additional terminology
      - "Constellation"

#### "Constellation" Cluster of Clusters

- An ensemble of N nodes each comprising p computing elements
- The p elements are tightly bound shared memory (e.g. smp, dsm)
- The N nodes are loosely coupled, i.e.:
   distributed memory
   4TF Blue Pacific SST
- p is greater than N
- Distinction is which layer gives us the most power through parallelism

3 x 480 4-way SMP nodes

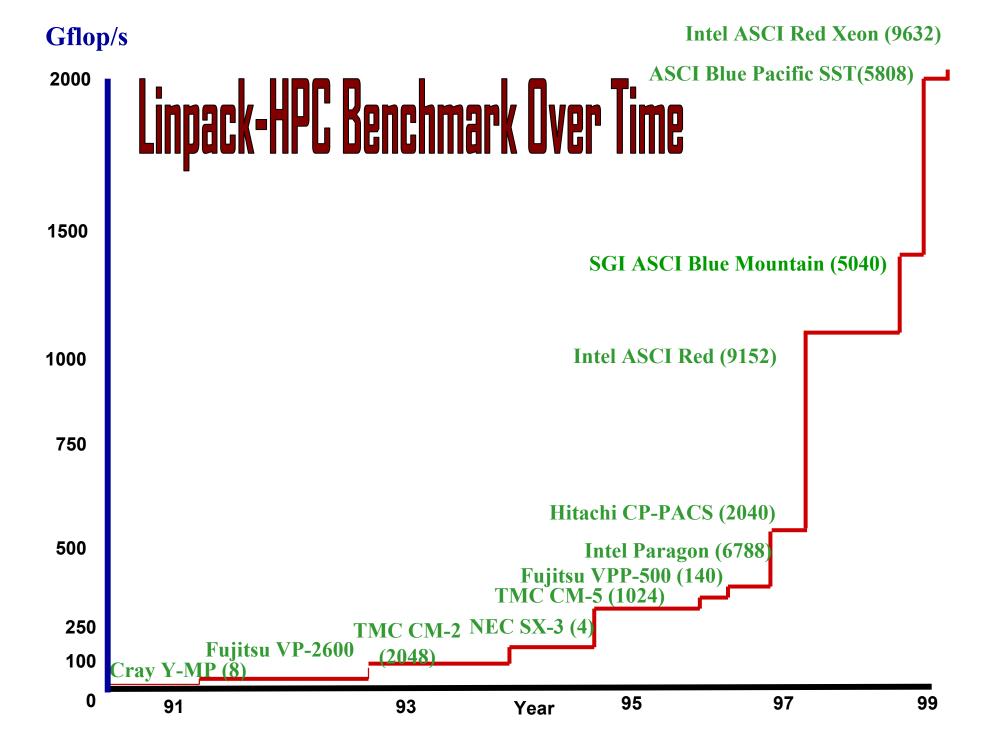
3.9 TF peak performance

2.6 TB memory

2.5 Tb/s bisectional bandwidth

62 TB disk

6.4 GB/s delivered I/O bandwidth

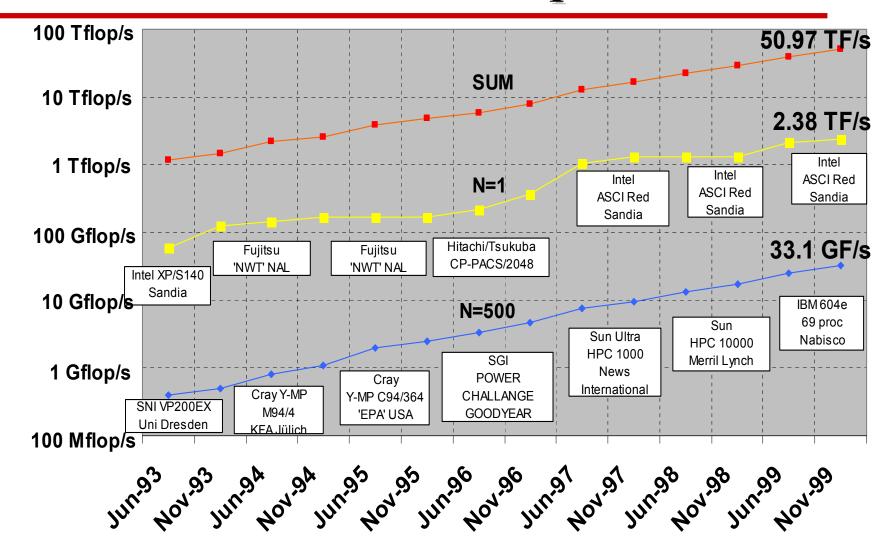


## TOP10 11/99

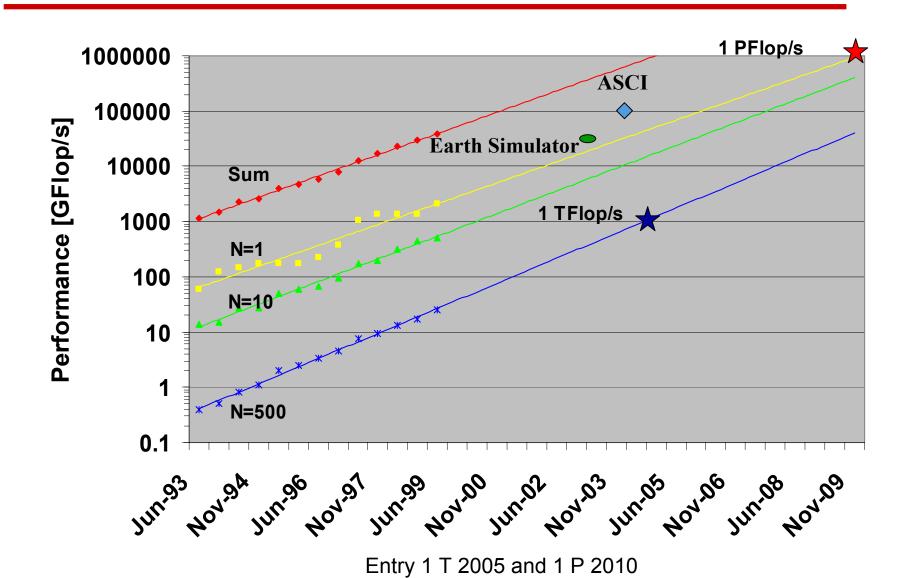
RANK	MANU- FACTURER	COMPUTER	RMAX [GF/S]	INSTALLATION SITE	COUNTRY	YEAR	AREA OF INSTALLATION	# PROC
1	Intel	ASCI Red	2379.6	Sandia National Labs Albuquerque	USA	1999	Research	9632
2	IBM	ASCI Blue- Pacific SST, IBM SP 604E	2144	Lawrence Livermore National Laboratory	USA	1999	Research	5808
3	SGI	ASCI Blue Mountain	1608	Los Alamos National Lab	USA	1998	Research	6144
4	SGI	T3E 1200	891.5	Government	USA	1998	Classified	1084
5	Hitachi	SR8000	873.6	University of Tokyo	Japan	1999	Academic	128
6	SGI	T3E 900	815.1	Government	USA	1997	Classified	1324
7	SGI	Orgin 2000	690.9	Los Alamos National Lab /ACL	USA	1999	Research	2048
8	Cray/SGI	T3E 900	<mark>675.7</mark>	Naval Oceanographic Office, Bay Saint Louis	USA	1999	Research Weather	1084
9	SGI	T3E 1200	<b>671.2</b>	<b>Deutscher Wetterdienst</b>	Germany	1999	Research Weather	812
10	IBM	SP Power3	558.13	UCSD/San Diego Supercomputer Center, IBM/Poughkeepsie	USA	1999	Research	1024



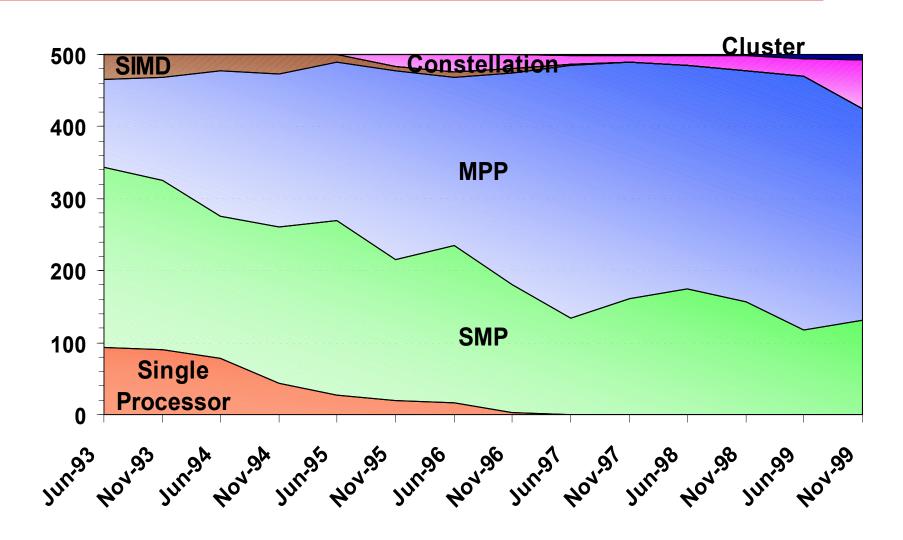
## Performance Development



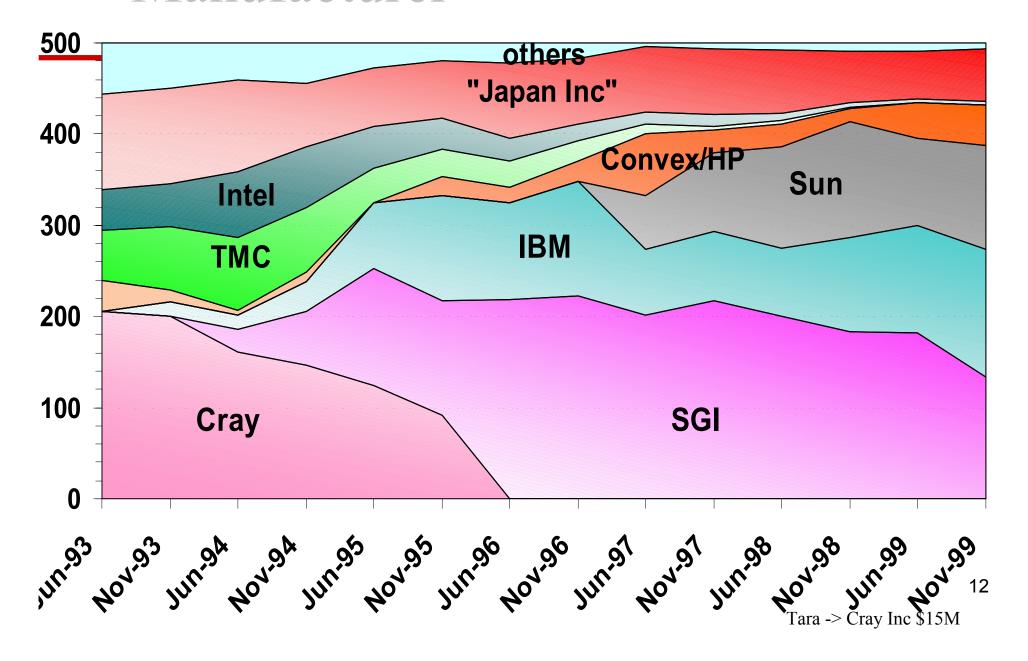
## Performance Development



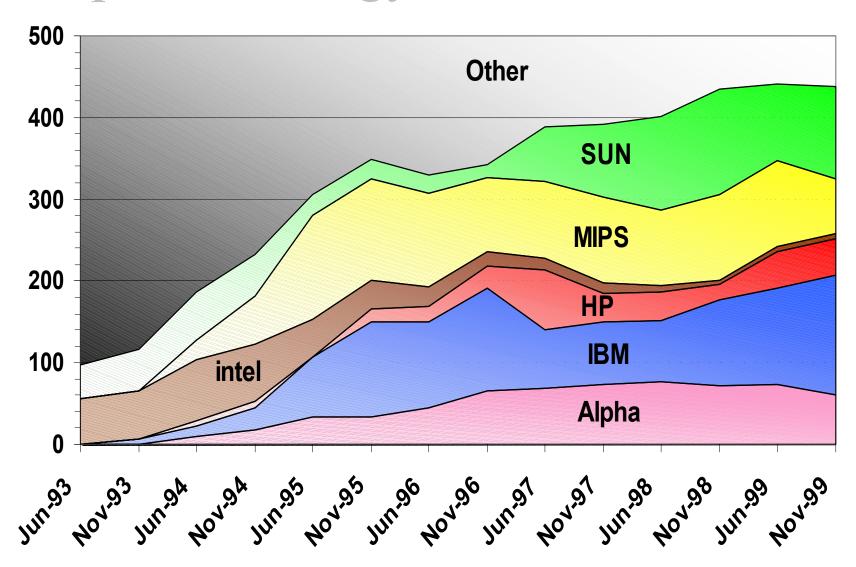
### Architectures



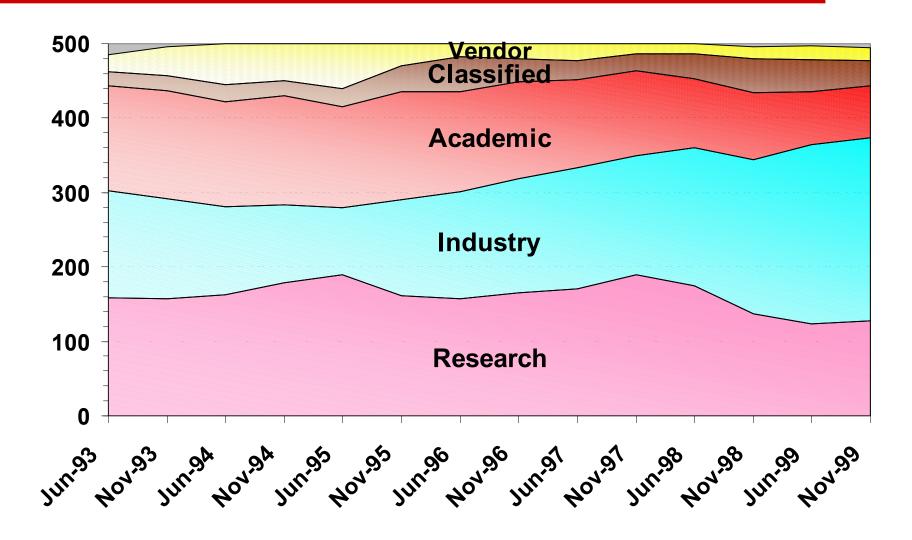
#### Manufacturer



## Chip Technology



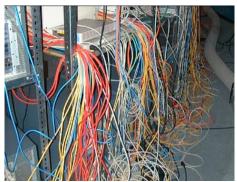
## Customer Type



# High-Performance Computing Directions

- Clustering of shared memory machines for scalability
  - > Emergence of PC commodity systems
    - > Pentium/Alpha based, Linux or NT driven
    - > "Supercomputer performance at mail-order prices"
  - Beowulf-Class Systems (Linux+PC)
  - Distributed Shared Memory (clusters of processors connected)
  - > Shared address space w/deep memory hierarchy
- Efficiency of message passing and data parallel programming
  - Helped by standards efforts such as PVM, MPI, Open-MP and HPF
- Many of the machines as a single user environments
- Pure COTS











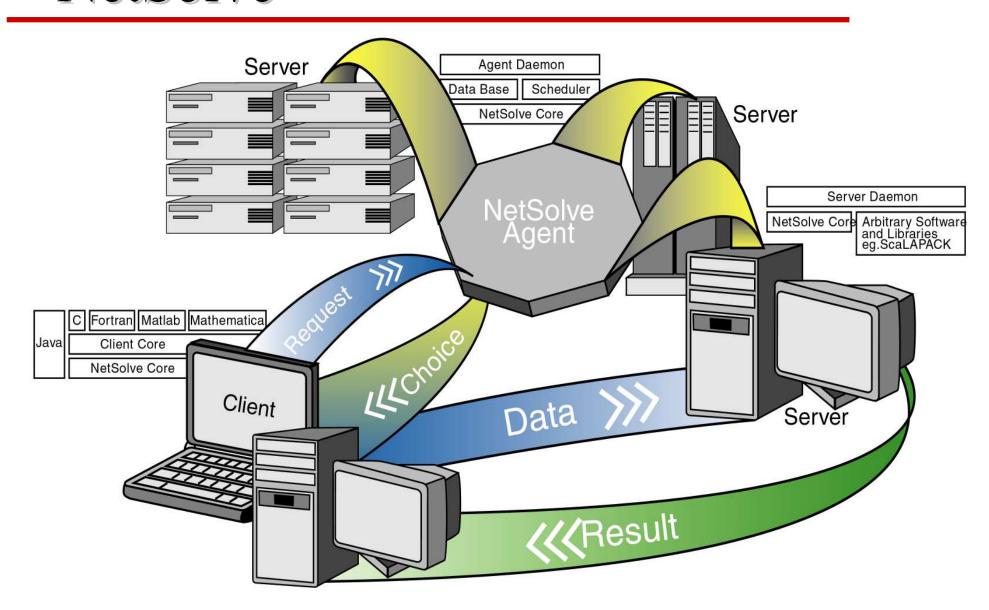
## Clusters on the TOP500

RANK	MANU- FACTURER	COMPUTER	RMAX	INSTALLATION SITE	COUNTRY	YEAR	AREA OF INSTALLATION	# PROC
33	Sun	HPC 450 Cluster	272.1	Sun, Burlington	USA	1999	Vendor	720
34	Compaq	Alpha Server SC	271.4	Compaq Computer Corp. Littleton	USA	1999	Vendor	512
•••			•••		•••			•••
44	Self-made	Cplant Cluster	232.6	Sandia National Laboratories	USA	1999	Research	580
•••			•••		•••			•••
169	Self-made	Alphleet Cluster	61.3	Institute of Physical and Chemical Res. (RIKEN)	Japan	1999	Research	140
					•••		•••	
265	Self-made	Avalon Cluster	48.6	Los Alamos National Lab/ CNLS	USA	1998	Research	140
•••					•••	•••		•••
351	Siemens	hpcLine Cluster	41.45	Universitaet Paderborn/PC2	Germany	1999	Academic	192
454	Self-made	Parnass2 Cluster	34.23	University of Bonn/ Applied Mathematic	Germany	1999	Academic	128

## NetSolve -Network Enabled Servers

- Allow networked resources to be integrated into the desktop.
- Not just hardware, but also make available software resources.
- Locate and "deliver" software or solutions to the user in a directly usable and "conventional" form.
- Part of the motivation software maintenance

### NetSolve



#### NetSolve

- Three basic scenarios:
  - Client, servers and agents anywhere on Internet (3(10)-150(80-ws/mpp)-Mcell)
  - > Client, servers and agents on an Intranet
  - Client, server and agent on the same machine
- "Blue Collar" Grid Based Computing
  - > User can set things up, no "su" required
  - Doesn't require deep knowledge of network programming
- Focus on Matlab users
  - >00 language, objects are matrices (pse, eg os)
  - One of the most popular desktop systems for numerical computing, 400K Users

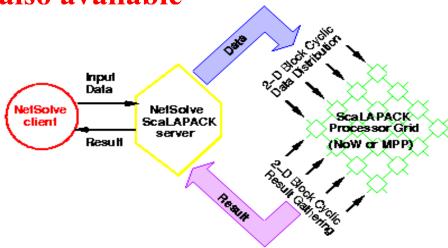
#### **NetSolve** - The Client

- No knowledge of networking involved
- Hide complexity of numerical software
- Computation location transparency
- Provides access to Virtual Libraries:
  - Component grid-based framework
  - Central management of library resources
  - User not concerned with most up-to-date version
  - Automatic tie to Netlib repository in project
- Provides synchronous or asynchronous calls (User level parallelism)

#### NetSolve - Interface

- >> define sparse matrix A
- >> define rhs
- >> [x, its] = netsolve('itmeth','petsc', A, rhs, 1.e-6

**Asynchronous Calls also available** 



#### NetSolve - The Server Side

#### **Computational Server:**

- Various Software resources installed on various Hardware Resources
- Configurable and Extensible:
  - Framework to easily add arbitrary software ...
  - Many numerical libraries being integrated by the NetSolve team
  - Many software being integrated by users

#### Agent:

- Gateway to the computational servers
- Performs Load Balancing among the resources

## NetSolve - Load Balancing

#### **NetSolve agent:**

**predicts** the execution times and **sorts** the servers

#### Prediction for a server based on:

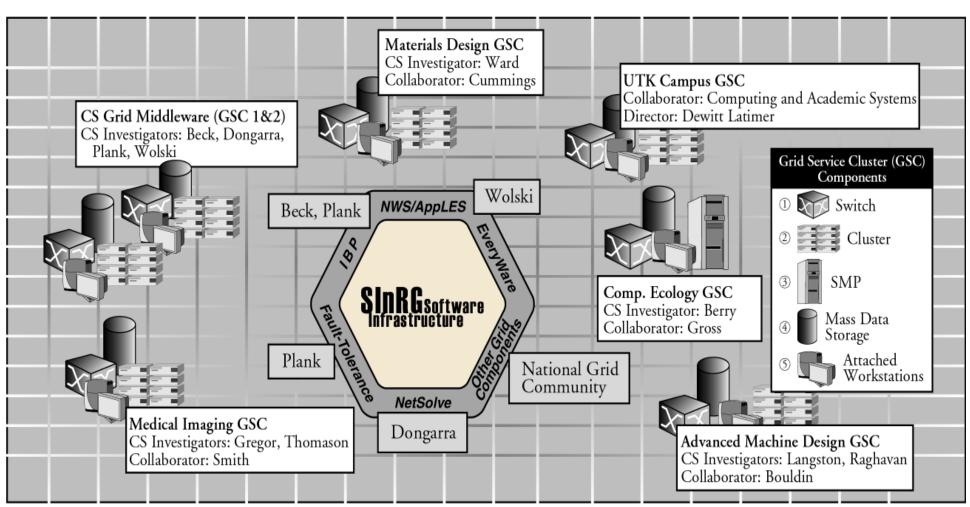
- Its distance over the network
  - Latency and Bandwidth
  - Statistical Averaging
- Its performance (LINPACK benchmark)
- Its workload
- The problem size and the algorithm complexity

Cached data

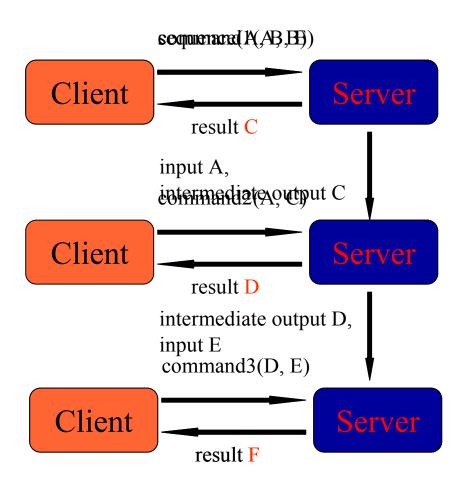


http://www.cs.utk.edu/netsolve

#### University of Tennessee's Grid Prototype: Scalable Intracampus Research Grid: SInRG

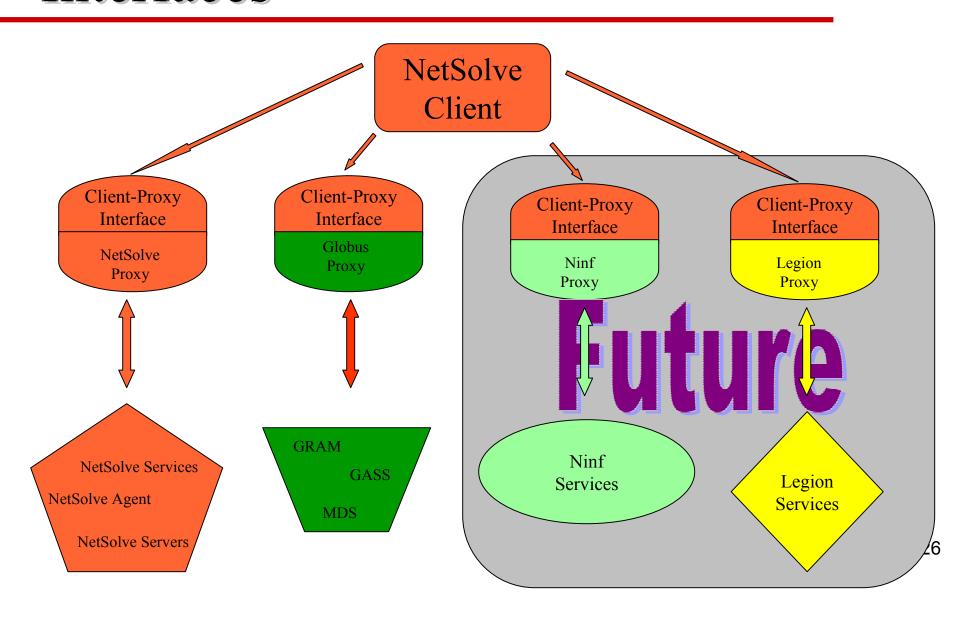


## Data Persistence (cont'd)



```
netsl_begin_sequence();
netsl("88mmand1"; A; B; E);
netsl("88mmand2"; A; E; E);
netsl("88mmand3"; B; E; E);
netsl_end_sequence(C, D);
```

## Developing Client Proxies Interfaces



# NetSolve Authentication with Kerberos

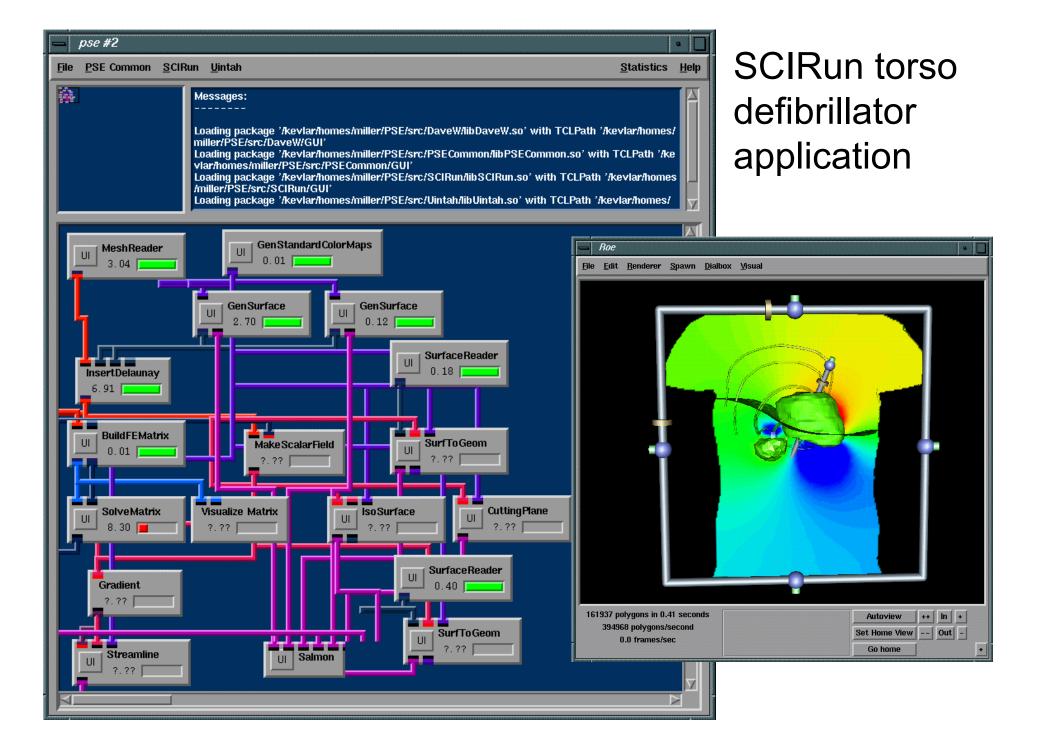


- Kerberos used to maintain Access Control Lists and manage access to computational resources.
- NetSolve properly handles authorized and non-authorized components together in the same system.
- In use by DOD Modernization program at Army Research Lab

## Task Farming

Multiple requests to single problem.

- Previous Solution:
  - Many calls to netslnb(); /\* non-blocking \*/
- New Solution:
  - Single call to netsl\_farm();



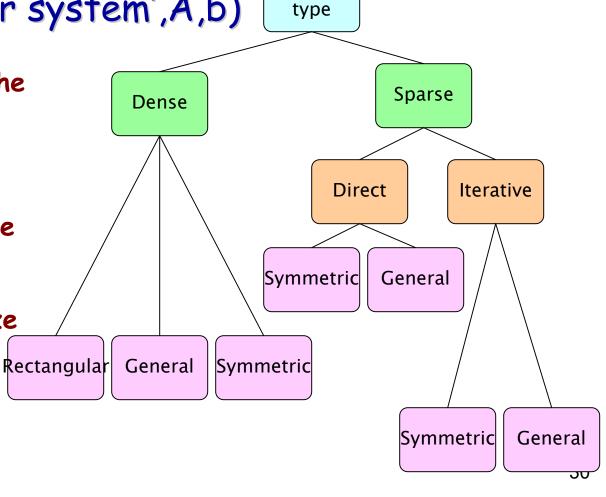
# NetSolve to Determine the Best Algorithm/Software (A bit in the future)

\*x = netsolve('linear system',A,b)

NetSolve examines the user's data together with the resources available (in the grid sense) and makes decisions on best time to solution dynamically.

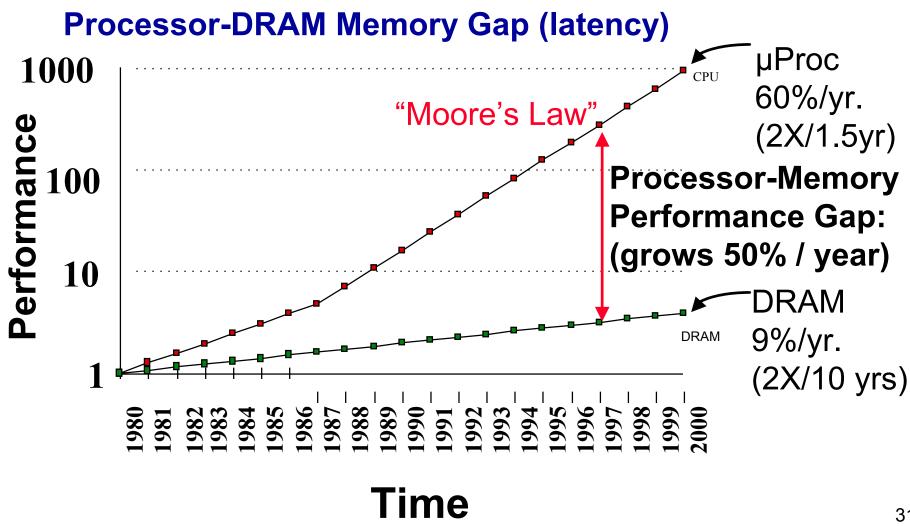
Decision based on size of problem, hardware/software, network connection etc.

Method and Placement



Matrix

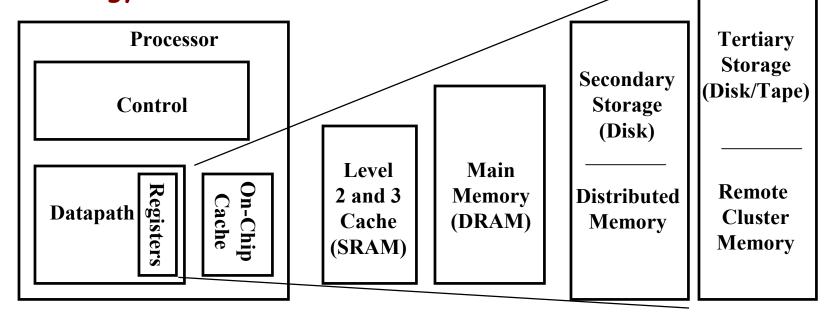
#### Where Does the Performance Go? or Why Should I Cares About the Memory Hierarchy?



## Memory Hierarchy

- By taking advantage of the principle of locality:
  - > Present the user with as much memory as is available in the cheapest technology.

> Provide access at the speed offered by the fastest technology.



Speed (ns): 1s	10s	100s	10,000,000s	10,000,000,000s
Size (bytes): 100s			(10s ms)	(10s sec)
Size (bytes). 100s	Ks	Ms	100,000 s	10,000,000 s
			(.1s ms)	(10s ms)
			Gs	Ts

## How To Get Performance From Commodity Processors?

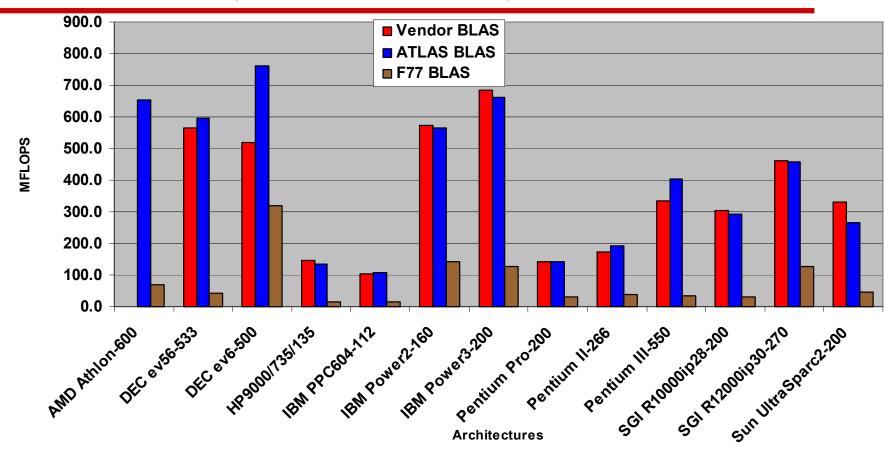
- Today's processors can achieve high-performance, but this requires extensive machine-specific hand tuning.
- Hardware and software have a large design space w/many parameters
  - Blocking sizes, loop nesting permutations, loop unrolling depths, software pipelining strategies, register allocations, and instruction schedules.
  - > Complicated interactions with the increasingly sophisticated micro-architectures of new microprocessors.
- About a year ago no tuned BLAS for Pentium for Linux.
- Need for quick/dynamic deployment of optimized routines.
- ATLAS Automatic Tuned Linear Algebra Software
  - PhiPac from Berkeley
  - > FFTW from MIT (http://www.fftw.org)

#### **ATLAS**

- An adaptive software architecture
  - >High-performance
  - >Portability
  - > Elegance

 ATLAS is faster than all other portable BLAS implementations and it is comparable with machine-specific libraries provided by the vendor.

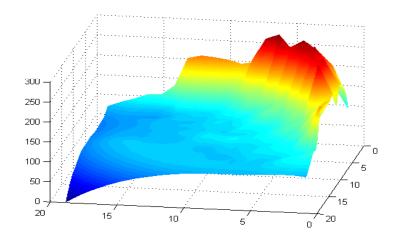
### ATLAS (DGEMM n = 500)



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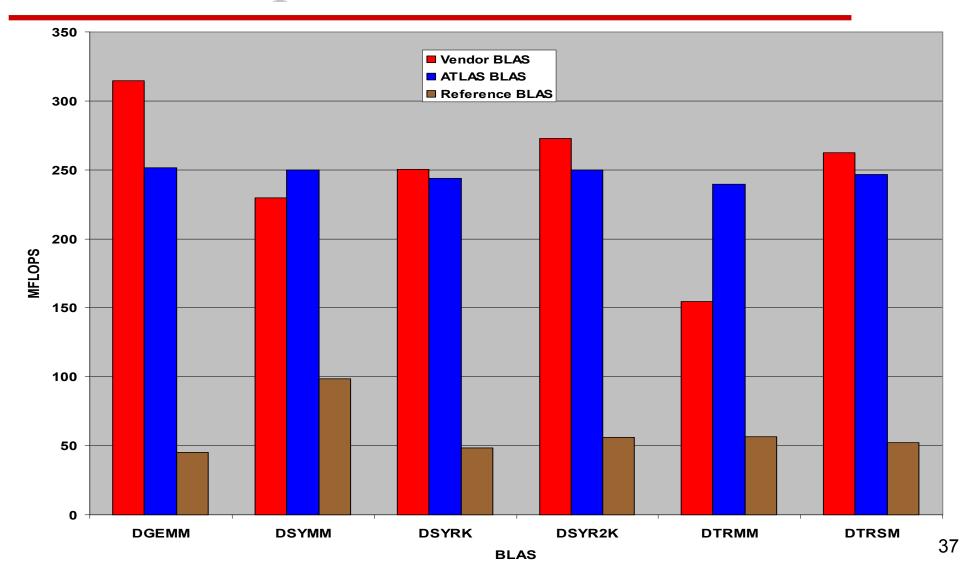
## Code Generation Strategy

- Two phases:
  - Probes the systems for system features
  - > Does a parameter study
- On-chip multiply optimizes for:
  - > TLB access
  - > L1 cache reuse
  - > FP unit usage
  - > Memory fetch
  - Register reuse
  - Loop overhead minimization
- New model of HP programming where critical code is machine generated using parameter optimization.

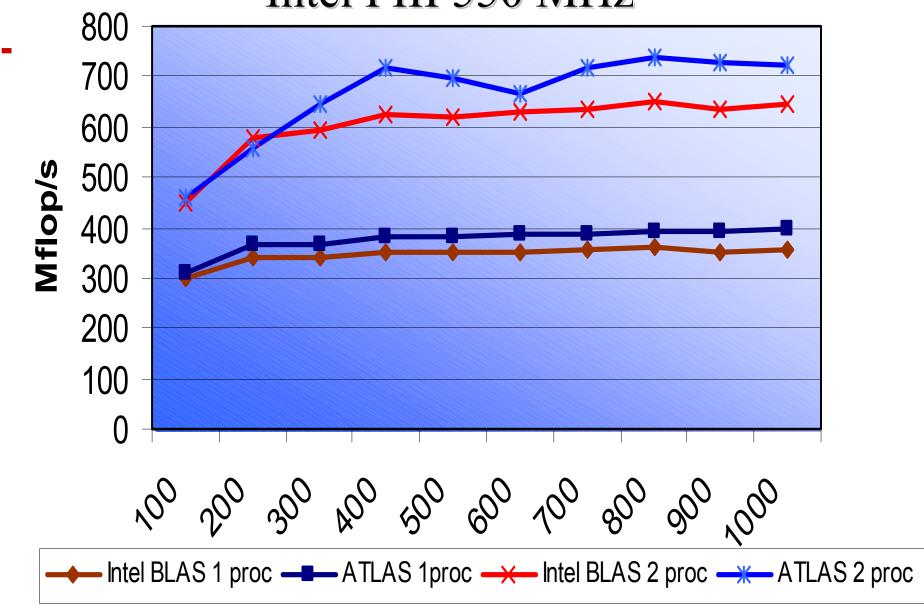


- Code is iteratively generated & timed until optimal case is found. We try:
  - > Differing NBs
  - Breaking false dependencies
  - > M, N and K loop unrolling
- Designed for RISC arch
  - > Super Scalar
  - Need reasonable C compiler
- Takes ~20 minutes to run

# 500x500 Recursive Level 3 BLAS on UltraSparc 2 200



## Multi-Threaded DGEMM Intel PIII 550 MHz



## Plans for ATLAS

- Software Release, available today:
  - Level 1, 2, and 3 BLAS implementations
  - > See: www.netlib.org/atlas/
- Near Future:
  - Multi-treading
  - Optimize message passing system
  - > Extend these ideas to Java directly
  - Sparse Matrix-Vector ops
- Futures:
  - > Runtime adaptation
    - > Sparsity analysis
    - > Iterative code improvement
  - > Specialization for user applications
  - > Adaptive libraries



# Tools for Performance Evaluation

- Timing and performance evaluation has been an art
  - > Resolution of the clock
  - >Issues about cache effects
  - > Different systems
- Situation about to change
  - > Today's processors have internal counters

## **Performance Counters**

- Hidden from users.
- On most platforms the APIs, if they exist, are not appropriate for a common user, functional or well documented.
- Existing performance counter APIs
  - > Cray T3E
  - > SGI MIPS R10000
  - > IBM Power series
  - > DEC Alpha pfm pseudo-device interface
  - > Windows 95, NT and Linux



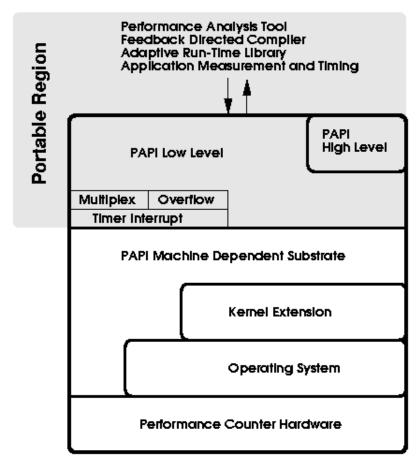
# Performance Data (cont.)

- > Cycle count
- > Floating point instruction count
- > Integer instruction count
- > Instruction count
- > Load/store count
- Branch taken / not taken count
- > Branch mispredictions

- Pipeline stalls due to memory subsystem
- Pipeline stalls due to resource conflicts
- >I/D cache misses for different levels
- > Cache invalidations
- > TLB misses
- > TLB invalidations

# **PAPI** Implementation

- Performance Application Programming Interface
- ◆ The purpose of PAPI is to design, standardize and implement a portable and efficient API to access the hardware performance monitor counters found on most modern microprocessors
- Used by Tau (A. Malony) and SvPablo (D. Reed)

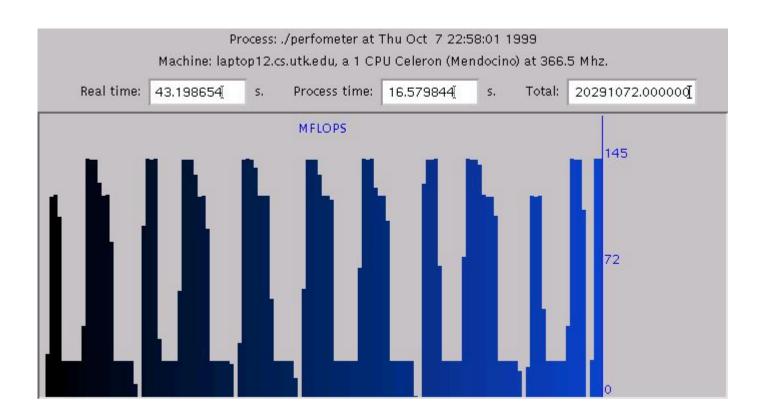


# Perfometer Usage

- ◆ Application is instrumented with PAPI
   ➤ One simple "call"
- Will be layered over the best existing vendor-specific APIs for these platforms
- Sections of code that are of interest are designated with specific colors
  - Using a call to mark\_perfometer('color')
- Application is started and a Java window containing the Perfometer application is also started

## Perfometer Screenshot

### Call Perfometer()



## Contributors to These Ideas

#### ◆ Top500

- > Hans W. Meuer, Mannheim U
- > Erich Strohmaier, UTK

#### NetSolve

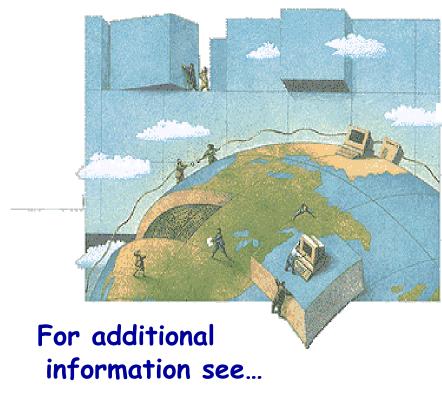
- > Dorian Arnold, UTK
- > Susan Blackford, UTK
- > Henri Casanova, UCSD
- > Michelle Miller, UTK
- > Ganapathy Raman, UTK
- > Sathish Vadhiyar, UTK

#### ATLAS

- > Clint Whaley, UTK
- > Antoine Petitet, UTK

#### PAPI

- > Shirley Browne, UTK
- > Nathan Garner, UTK
- > Kevin London, UTK
- > Phil Mucci, UTK



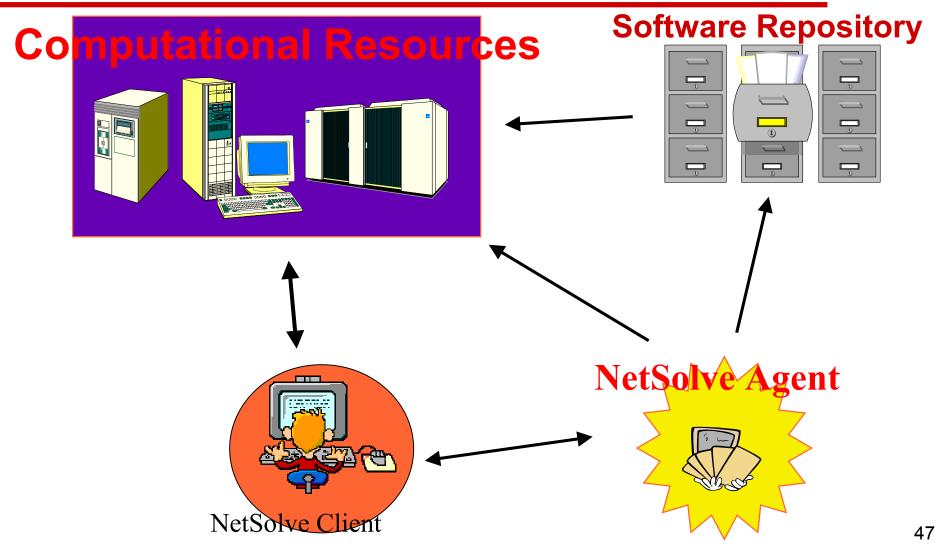
www.top500.org

www.netlib.org/atlas/

www.netlib.org/netsolve/

www.cs.utk.edu/~dongarra/

# Next Step: Hardware & Software Servers



http://www.cs.utk.edu/netsolve/

## **Futures**

### List of Top 100 Clusters

- > IEEE Task Force on Cluster Computing
- Interested in assembling a list of the Top n Clusters
- > Based on current metric
- > Starting to put together software to facilitate running and collection of data.

### Sparse Benchmark

- Look at the performance in terms of sparse matrix operations
- > Iterative solvers
- > Beginning to collect data

# NetSolve Applications and Interactions



#### Tool integration

- > Globus Middleware infrastructure (ANL/SSI)
- > Condor Workstation farm (U Wisconsin)
- > NWS Network Weather Service (U Tennessee)
- > SCIRun Computational steering (U Utah)
- > Ninf NetSolve-like system, (Tsukuba U)

#### Library usage

- > LAPACK/ScaLAPACK Parallel dense linear solvers
- > SuperLU/MA28 Parallel sparse direct linear solvers(UCB/RAL)
- > PETSc/Aztec Parallel iterative solvers (ANL/SNL)
- > Other areas as well (not just linear algebra)

#### Applications

- MCell Microcellular physiology (UCSD/Salk)
- > IPARS Reservoir Simulator (UTexas, Austin)
- Virtual Human Pulmonary System Model (ORNL)
- RSICC Radiation Safety sw/simulation (ORNL)
- > LUCAS Land usage modeling (U Tennessee)
- > ImageVision Computer Graphics and Vision (Graz U)

# Sparse Matrices/Solvers

- Iterative and direct solvers:
   PETSc, Aztec, SuperLU, Ma28, ...
- Support for compressed row/column sparse matrix storage -significantly reduces network data transmission
- Sequential and parallel
   Implementations available

**MA28** 



