CRD

COMPUTATIONAL RESEARCH DIVISION

Benchmarking BGL, UPC, Checkpoint/Restart

Future Technologies Group

Lawrence Berkeley National Laboratory

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October 15th, 2003

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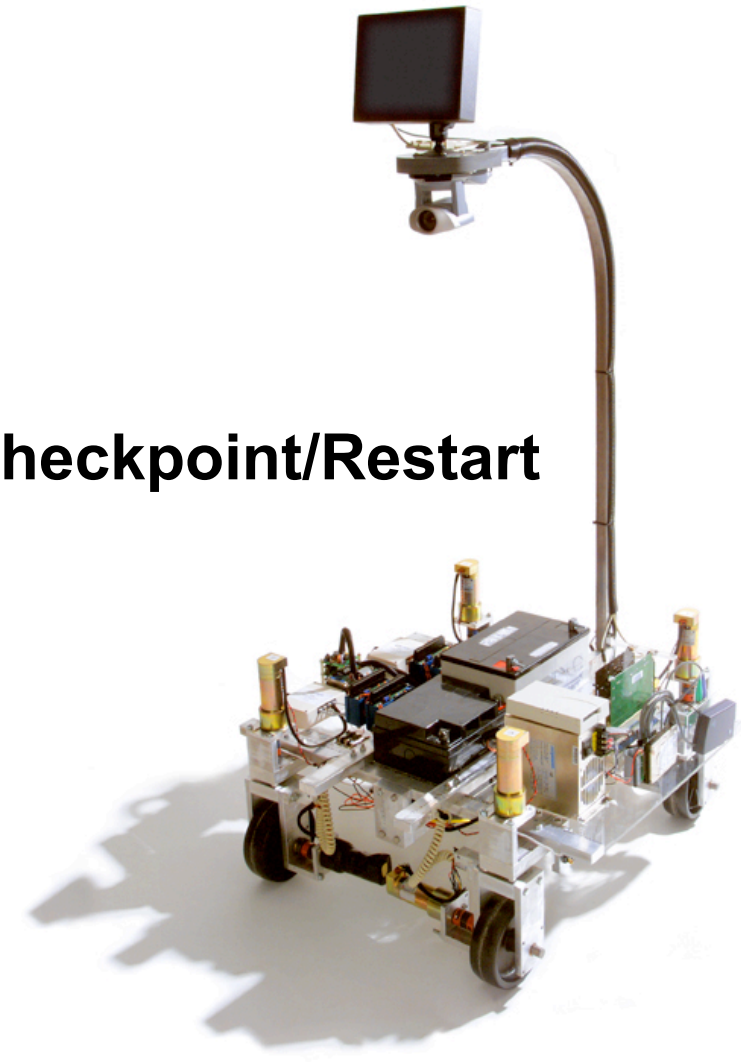
Outline

- HPC @ LBNL/NERSC
- FTG's purpose
- Performance studies, UPC, Checkpoint/Restart
- Follow-up



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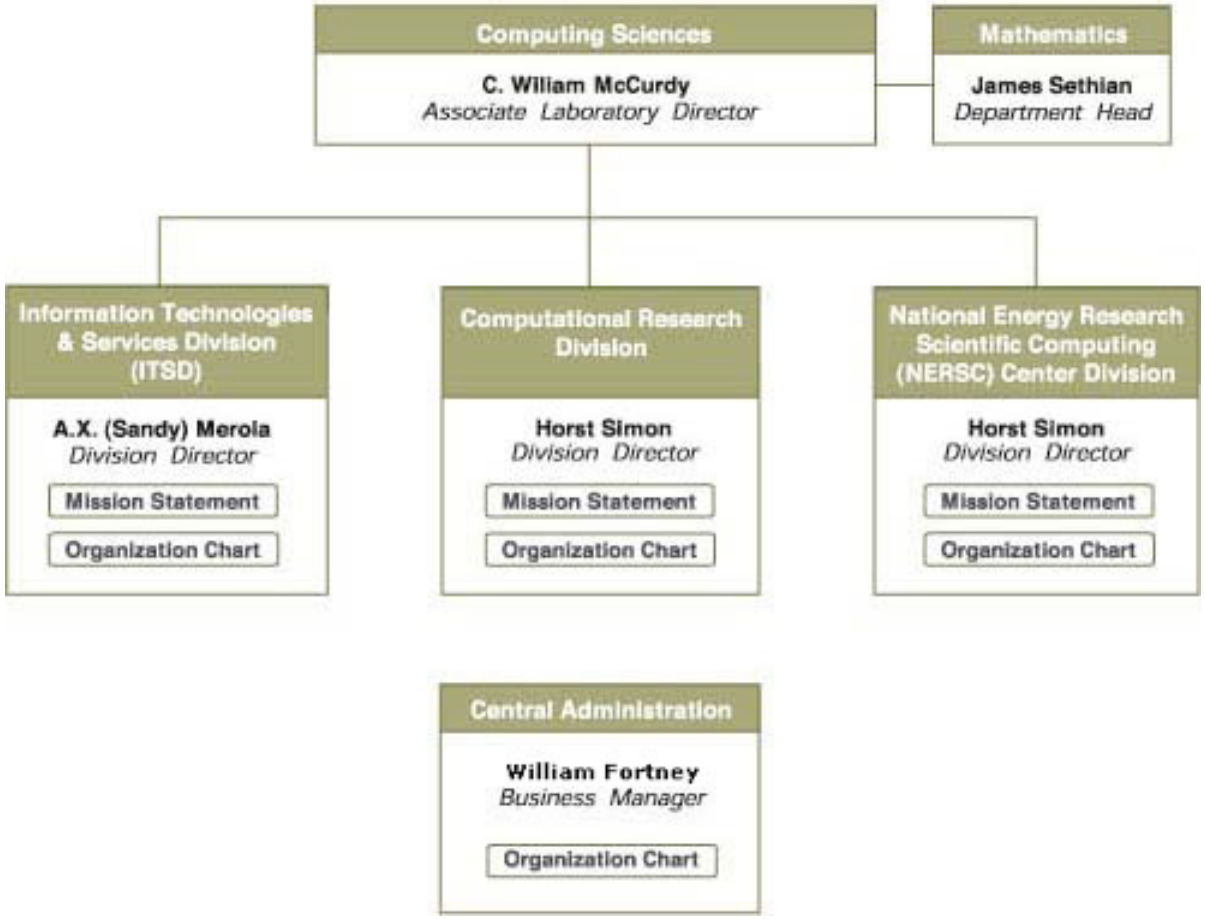
LBNL



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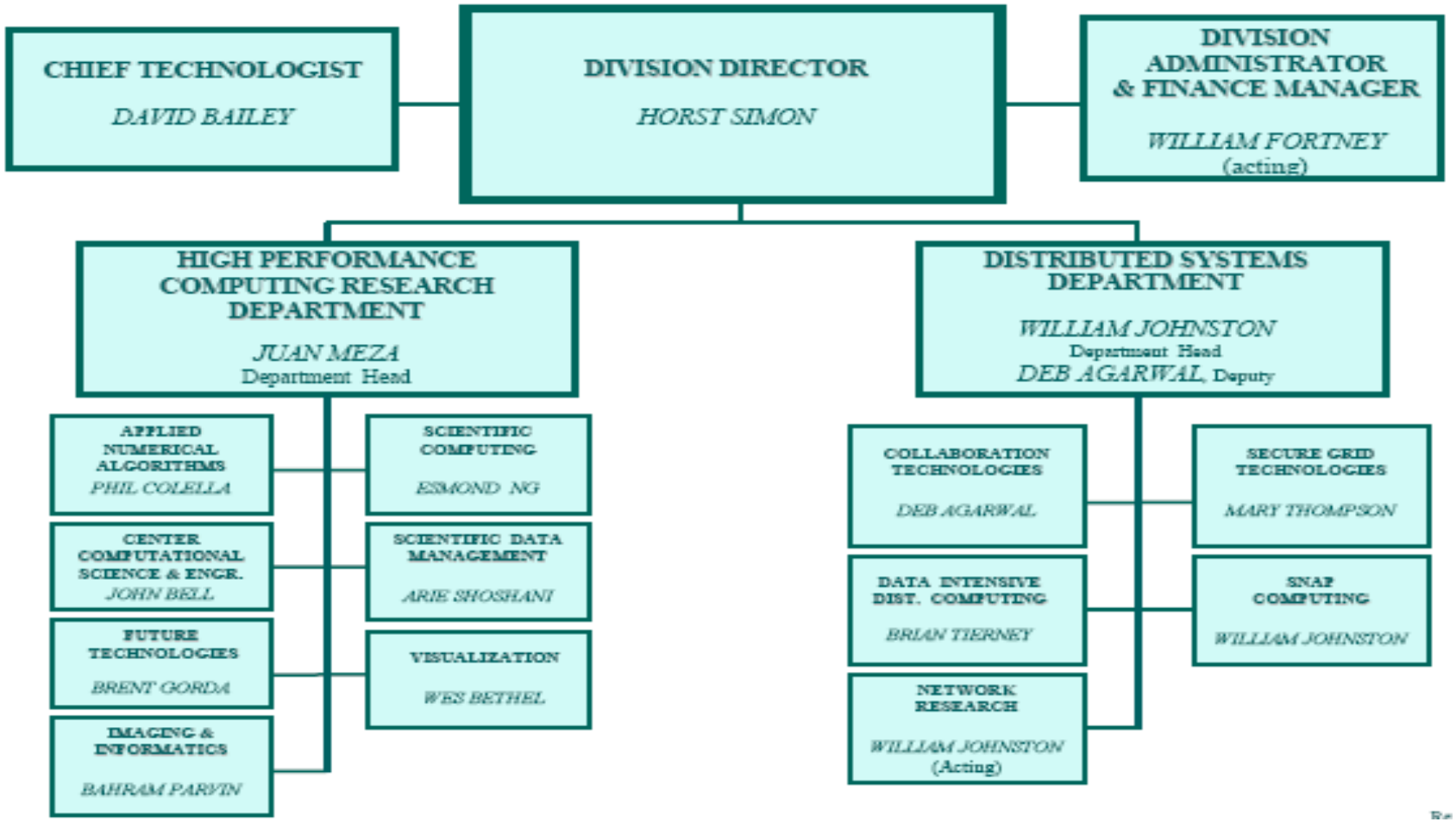

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CRD NERSC Production Center

DOE Office of Science flagship Computing Center

Supports open, unclassified, basic research

- **~2000 Users, ~400 Projects**

- **Main computational facility (Seaborg) consists of:**
  - **416 16-way Power 3+ nodes**
  - **6,656 CPUs – 6,080 for computation @ 1.5 Gflop/s each**
  - **Peak Performance of 10 Teraflop/s**
  - **7.8 TB Memory, 44TB GPFS disk (+15TB local disk)**

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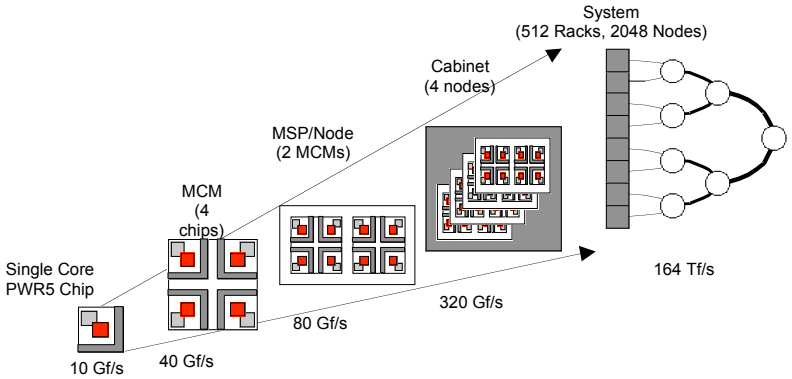
Future Technologies Group

BERKELEY LAB

LBNL's Future Technologies Group (FTG) is focused on performance aspects of High Performance Computing (HPC).



FTG's focus is the 5+ year timeframe.

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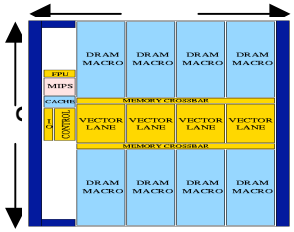
CRD FTG Activities: Architecture

FTG seeks to understand performance of new architectures:

PERC

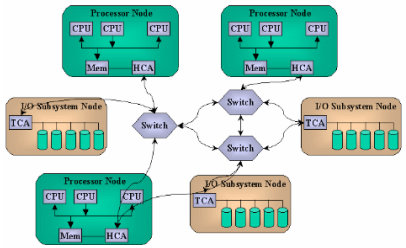


THE BLUE PLANET

BLUEGENE/L

HPCS

APEX



The Answer To ...

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CRD Modern Vector Evaluation

Principal Investigator: Lenny Oliker

- Study performance of SX6, X1, Earth Simulator
- Study of key factors of modern parallel vector systems: runtime, scalability, programmability, portability, and memory overhead while identifying potential bottlenecks
- microbenchmarks, kernels, and application codes

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Performance Studies on BGL

Leverage current work:

- Micro benchmarks in communications, memory access issues/patterns/conflicts
- Application kernels – glimpse at performance expectations
- If able: select application codes for in-depth capability-oriented study

✓ Can BGL enable science for the Office of Science?

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Applications of interest

- **Astrophysics:**
  - **MADCAP Microwave Anisotropy Dataset Computational Analysis Package. Analyses cosmic microwave background radiation datasets to extract the maximum likelihood angular power spectrum. Julian Borrill LBNL**
  - **CACTUS Direct evolution of Einstein's equations. Involves a coupled set of non-linear hyperbolic, elliptic equations with thousands of terms. John Shalf LBNL**
- **Climate:**
  - **CCM3 Community Climate Model Michael Wehner LBNL**

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More …

Fusion

- GTC Gyrokinetic Toroidal Code. 3D particle-in-cell code to study microturbulence in magnetic confinement fusion. Stephane Ethier Princeton Plasma Physics Laboratory
- TLBE Thermal Lattice Boltzmann equation solver for modeling turbulence and collisions in plasma. Jonathan Carter LBNL

Material Science

- PARATEC PARAllel Total Energy Code. Electronic structure code which performs ab-initio quantum-mechanical total energy calculations. Andrew Canning LBNL

Molecular Dynamics

- NAMD Object-oriented molecular dynamics code designed for simulation of large biomolecular systems. David Skinner LBNL

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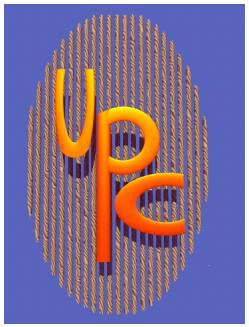
Berkeley UPC compiler



Principal Investigator: Kathy Yelick (UCB)
Joint project between LBNL and UC Berkeley

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UPC language

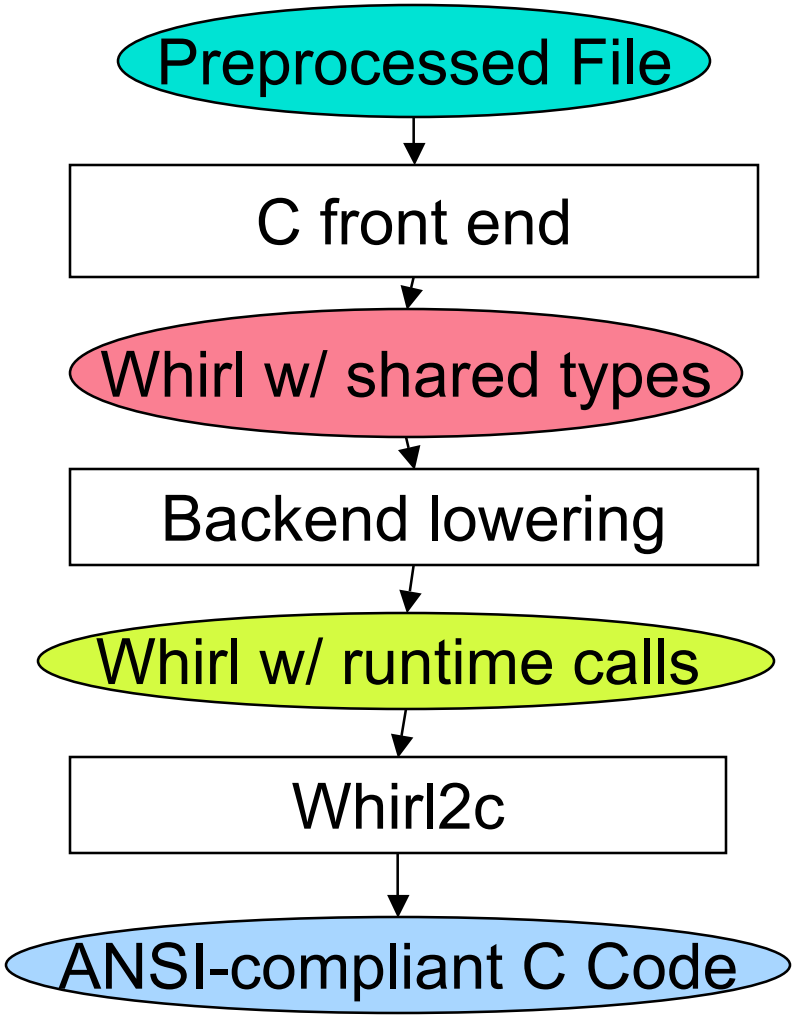
- **UPC is an explicitly parallel global address space language with SPMD parallelism**
  - **An extension of C**
  - **Shared memory is partitioned by threads**
  - **One-sided (bulk and fine-grained) communication through reads/writes of shared variables**

UPC has a "forall" construct for distributing computation:

Ex: Vector Addition

```
shared int v1[N], v2[N], v3[N];
upc_forall (i=0; i < N; i++; &v3[i] ) {
    v3[i] = v2[i] + v1[i];
}
```

CRD Compiler Implementation



- Based on the Open64 compiler
- Source to source transformation
- Convert shared memory operations into runtime library calls
- Designed to incorporate existing optimization framework in open64
- Communicate with runtime via a standard API

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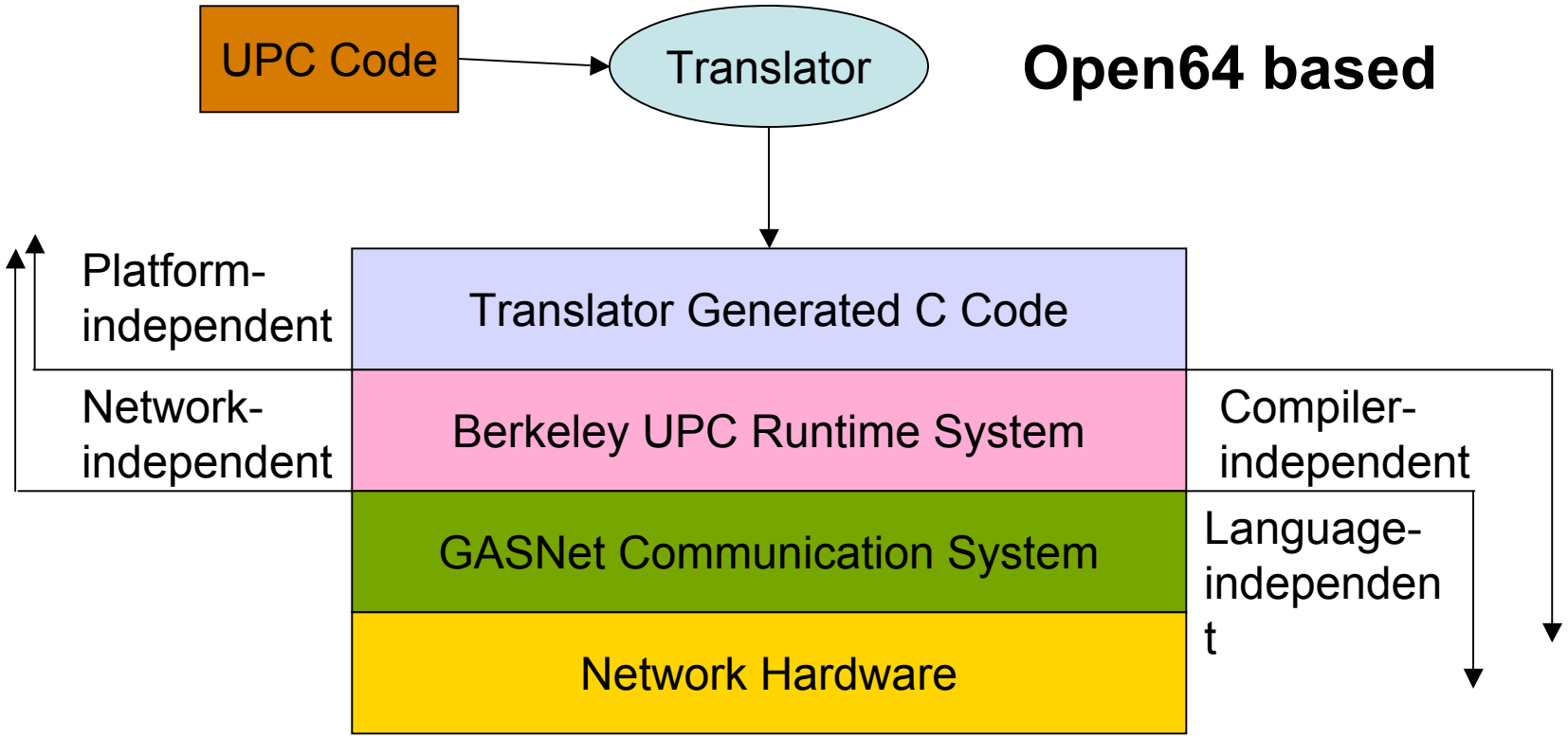
Gasnet



Goals: Portability and High-Performance

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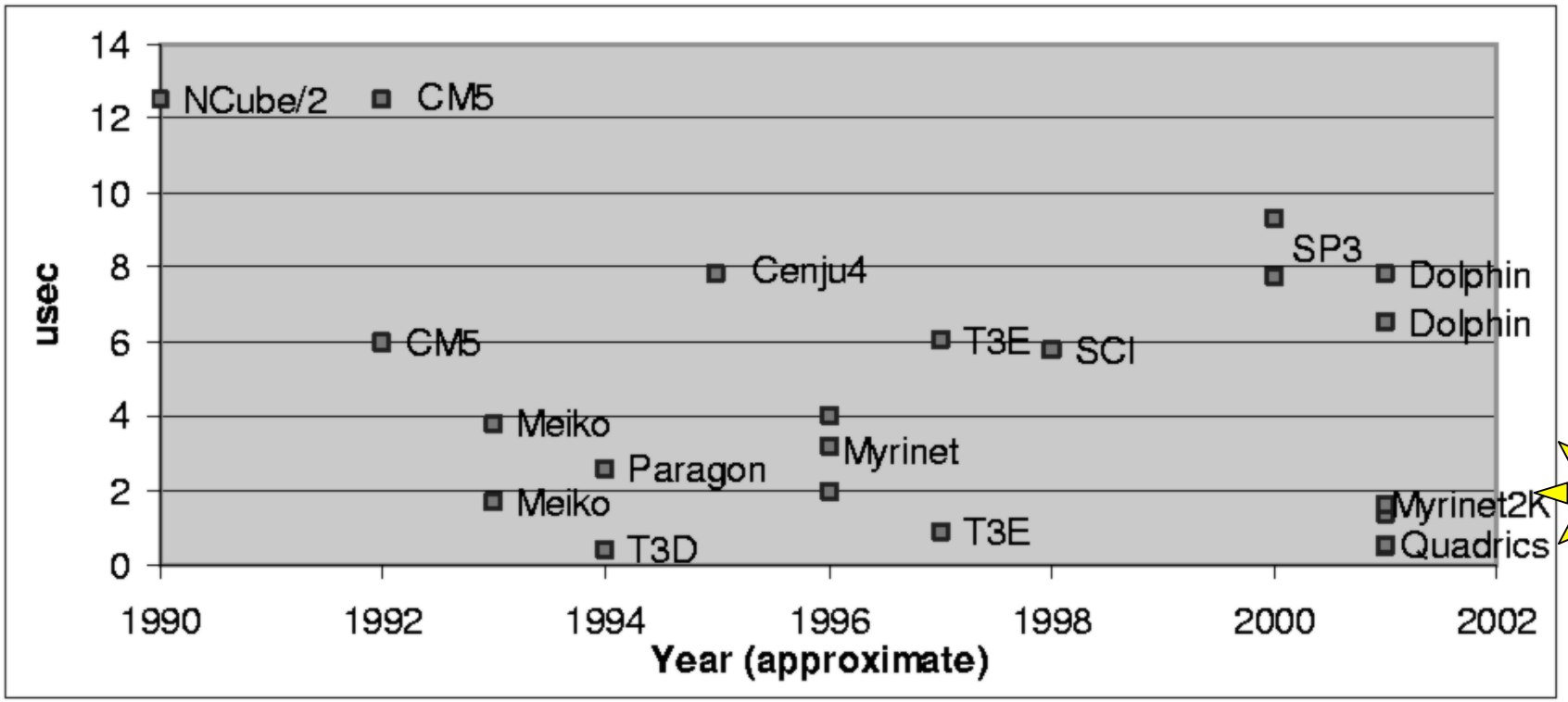
CRD Single word transfer is key



BGL

Software send overhead for 8-byte messages over time.

Not improving much over time (even in absolute terms)

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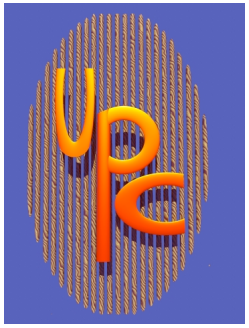
UPC on BGL

- Standard C compiler (optimizer good)
- Runtime support: GaSNet
- Low latency single word get/put operations

✓ **UPC Compiler is Open Source**
- V1.0 released early 2002
- Next release for SC03
- Strong BGL interest from UPC Team



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CRD Checkpoint-Restart for Linux

Principal Investigator: Paul Hargrove

- DOE Scalable systems software SciDAC
- Checkpoint/restart is a part of the larger resource management picture

- System initiated
- Apps needn't know (for the most part)
  - No recompile necessary
  - But: sockets, changing files, etc.

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C/R Motivation

- System Level Checkpoint facility enables:
  - Resource utilization: (NERSC T3D ~70%-90+%)
  - Fault tolerance for long running applications
  - System Maintenance / Upgrades
  - "Livermore Model"
    - Gang Scheduling – Moe Jette's work
    - Day vs. night use; debug vs long running
    - Capability + capacity

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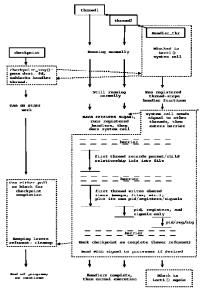
State of C/R

- Linux Kernel 2.4 (RedHat)
- Kernel Module – no kernel source modification
- LAM MPI
- Some details:
  - Standard I/O working
  - In process: pipes, special device files, full process groups, and sessions
  - Signals (and handlers) reinstated, files reopened
- Visit LBL booth @ SC03
- Soon: Initial (open source) release



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CRD C/R on BlueGene/L

- **Checkpoint:**
  - Coordination of compute & I/O nodes
  - Save state from compute node / BLRTS
  - Messages in flight: reliable delivery – just drop them?
  - Interaction with rest of BG/L system: batch system
- **Restart:**
  - I/O node: reinstate file pointers, reaquire locks, pid, session ID, process group, etc.
  - Compute nodes: recover memory, reestablish communications end-points

✓ **Checkpoint restart is Open Source**
- **Initial release for SC03**
- **C/R on BGL shouldn't be hard**

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Conclusion

- FTG is interested in whether BlueGene/L is an appropriate architecture for the Office of Science
- We have applicable projects and talent to contribute to the LLNL/IBM effort

Thank you!

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