1. Scope
2. Goals for the long and short term
3. Progress by team
   - compilers, tools, libraries, systems, visualization, NT clusters
4. Collaborations with AT teams
5. The Future

http://www.cs.rice.edu/~ken/Presentations/Alliance98TeamA.pdf
Team A: Parallel, Visual Supercomputing

• Integrated Computing
  - single box
  - collection of homogeneous processors
  - visualization

• Architectures
  - Distributed shared memory (DSM)
  - Clusters of Homogeneous PCs
    Windows NT

• Challenges
  - Management of deep memory hierarchy
  - Portable programmability
  - Support for high performance visualization
General Goals

• Consistent Parallel Programming Environment
  - for all Alliance sites
  - special focus on DSM and PC Clusters
  - languages and tools
  - communication, math, and data structure libraries
  - scientific programming tools
    optimization, automatic differentiation, problem-solving
  - systems technologies
    schedulers, performance analysis

• Direct Collaboration with AT Teams
  - use of technologies in applications
  - feedback on usefulness of tools

• Wide Dissemination of Software
  - through repository and deployment teams
Specific Goals for the First Year

• Repository
  - **Goal:** All software available in distributable form with documentation up and running with software from over half the team (see demo)  
    http://www.nhse.org/rib/repositories/ncsa_teamA/
  - **Goal:** Software installed at NCSA  
    ScALAPACK, PETSc, PG HPF

• Collaboration
  - **Goal:** Each group actively working with at least one AT team  
    many connections established (see explicit slides)
  - **Goal:** Effective collaboration with central site  
    Scalable Computing initiative

• Deployment Team
  - **Goal:** Deployment team hired and working with NCSA and AT teams  
    not yet
Languages and Compilers

- HPF (Kennedy, Rice)
  - Goal: Improved HPF implementations for DSM
  - Strategies:
    - Build research prototype and work with vendor (PGI)
    - Use research tool in collaborations with applications
  - Activities:
    - First DSM prototype focuses on latency and bandwidth
    - Collaboration with Cosmology (Balsara) and Tools (Reed)

- HPC++ (Gannon, Indiana)
  - Goal: High performance on DSM systems
  - Strategy: Port HPC++Lib and tune to DSM
  - Activities:
    - Completed port of HPC++Lib to the SGI O2K using multithreaded shared-memory programming (version 10 by end of quarter)
• **SvPablo Performance Tool** *(Reed, Illinois)*

  - **Goals:**
    Connect performance analysis to high-level languages
    Employ advanced visualization

  - **Strategy:**
    Collaboration with compiler through documentation of transformations

  - **Activities:**
    Distributed and in wide use; supports C, Fortran, and HPF
    Experience: enables users to quickly identify and correct performance bottlenecks in large applications
    Collaboration with Cosmology AT team
    Beginning to explore ports of SvPablo interfaces to Windows NT
• General library interface (Johnsson, UH; Dongarra, Tennessee)
  - Goal: support for high-level languages (HPF and HPC++)
  - HPF interface to ScaLAPACK subset available on Team A repository

• ScaLAPACK (Dongarra, Tennessee)
  - Goal: dense linear algebra support, interfaced to high-level languages
  - Installed at NCSA, available via NHSE Team A repository
  - Working on out-of-core linear solvers and eigensolvers

• PETSc (Stevens, Argonne)
  - Sparse matrix-vector product and parallel preconditioners
  - Installed at NCSA, available via NHSE Team A repository

• FFTPACK (Johnsson, Houston)
  - Goal: general parallel FFTs for DSM
  - Implementation of 1D version
Advanced Tools

• **Optimization** *(Dennis, Rice; Stevens, Argonne)*
  - **Goals:**
    - Implement DSM version of Parallel Direct Search (PDS)
    - Implement parallel SLP and SQP on DSM
    - Parallel automatic differentiation (ADIFOR)
  - **Activities**
    - Parallel direct search on O2K by end of summer
    - ADIFOR available in Team A repository, tried and planned for use by Chemical Engineering AT team

• **Netsolve** *(Dongarra, Tennessee)*
  - **Goal:** Network-based problem solving
  - **Activities:**
    - Deployment of NetSolve on NCSA Alliance machines
    - ATLAS automatically tunes software for deep memory hierarchies
- **Communication** *(Stevens, Gropp, Lusk, Argonne)*
  - MPI
    - DSM and NT
    - MPICH and MPI-IO available on Alliance systems
  - Communication for adaptive irregular computations
    - SUMMA3D

- **Distributed Adaptive Data Structures** *(Browne, Texas)*
  - Goal: Support adaptive mesh refinement on parallel and distributed systems
  - Activities
    - DAGH available via Team A repository in May,
    - Tutorial offered, real manual in progress
    - Developing scripts to move DAGH to most common machines.
• Visual Supercomputing (DeFanti, Illinois Chicago)
  - Goals:
    Cave VR libraries on both DSM (done) and NT
    New VR technologies
  - Activities (see demos):
    Developed dual perspective VR
    Upgraded CAVE library to IR system and enable applications

• Systems for DSM
  - Scheduling (Vernon, Wisconsin)
    Goal: improved LSF across alliance
    Activity: software to generate performance metrics from LSF logs
  - DSM evaluation (Torrellas, Illinois)
    Goal: understand performance of DSM systems
    Activity: comparison of hand vs automatic parallelization on O2K
NT Clusters

- **HPVM (Chien, Illinois)**
  - **Goal:** complete HP computing environment on NT PC network
  - **Activities:**
    Design, integration, and demonstration of a 192-processor Windows NT "High Performance Virtual Machines" Cluster
    Running ZeusMP (Cosmology) code from Alliance, and others
    Performance analysis and tuning and HPF backend (PGI) underway.

- **TreadMarks (Zwaenepoel, Rice)**
  - **Goal:** software DSM on NT clusters
  - **Activities:**
    Completed port to NT clusters, but performance poor vs UNIX,
    tuning now in progress
    Collaborating with Chien to port onto HPVM/Fast Messages
    Evaluation with Cosmology of software DSM as alternative to HPF
Interactions with AT Teams I

- **Chemical Engineering**
  - ADIFOR client
  - Requests for large scale PDE simulations, large scale optimization, numerical linear algebra software, DSM performance analysis/tuning

- **Cosmology**
  - hpf-cosmo mailing list
  - Rice currently working on large code from Balsara, order of magnitude more complex than anything we've gotten through our research compiler before
  - Actively using HPC++ and DAGH on other codes
  - Much feedback to HPF and HPC++ about "less desirable features"

- **Environmental Hydrology**
  - Comparing standard versions of codes to PETSc version to understand performance, evaluate MPI
Interaction with AT Teams II

• Computational Biology
  - High performance parallel computation needed for Genome Informatics, Macromolecular structure, NMR databank, Molecular dynamics, Electrostatics/Brownian Dynamics
  - Specific requests for better FFTs, scalable n-body solvers, load balancing

• Nanostructures
  - Using DAGH for scalable multigrid solvers for real-space electronic structure
  - Considering HPF for kinetic lattice Monte Carlo for surface growth
  - Optimizing batch scheduling for O2K for better Monte Carlo throughput

• Scientific Instrumentation
  - 3-D FFTs needed on O2K for wide-field imaging algorithm (radio astronomy)
Summary

• Team A Head Start
  - Our job:
    Reap the harvest of HPCC software
    Install on alliance hardware and make available to NSF community
  - Where we stand
    Nearly halfway to goal

• The Future
  - Can we put ourselves out of business?
    Most Team A goals are near term
  - Long term— become subsidiary of Team B?
    Many problems reappear in more complex form