ALCF Early Science Program

Enabling Petascale Science on BG/Q: Tools, Libraries, Programming Models & Other System Software

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Motivation

- **Lessons learnt from BG/P – Reduce bring up time after production**
- **Provide a familiar (BG/P) environment to users**
- **Increase success of ESP projects**
  - Single node performance
  - Scalability

Projects - Tools, Debuggers

- **Peformance Tools**
  - PAPI (Dan Terpstra, Shirley Moore)
  - HPCToolkit (John Mellor-Crummey, Nathan Tallent)
  - TAU (Sameer Shende, Allen D. Malony)
  - Scalasca (Bernd Mohr, Brian Wylie)
  - Open|Speedshop (Jim Galarowicz)
  - FPMPI2 (Bill Gropp)
- **Debuggers**
  - Allinea (DDT)
  - Rogue Wave (Totalview)

Projects - Libraries

- **Libraries**
  - FFT, BLAS (Franz Franchetti)
  - PetSc (Barry Smith, Satish Balay)
  - Parallel I/O – PnetCDF, HDF5 (Rob Ross, Rob Latham)
  - Chombo (Phil Colella, John Bell)
  - Visualization (Rob Ross, Tom Peterka)
- **Other System Software**
  - OS Stacks (Kamil Iskra)

Projects - Libraries

- **Programming Models**
  - Charm++, AMPI (Sanjay Kale)
  - GA Toolkit (Jeff Hammond)
  - Coarray Fortran (John Mellor-Crummey, William Scherer, Guohua Jin))
  - UPC (Paul Hargrove, Yili Zheng)
  - GASnet (Paul Hargrove, Yili Zheng)
  - MPI (Rusty Lusk, Rajeev Thakur, Pavan Balaji)

Library and Tool Usage

NOT SHOWN: MPI, MPI-IO, OpenMP

	ESP Projects Using
NetCDF	3
HDF	5
VisIt	2
ParaView	2
IDL	1
FFTW, FFTPACK5, P3DFFT, ESSL FFT	5
BLAS, ESSL BLAS	4
LAPACK	2
ScaLAPACK	1
MASS, MASSV, ESSL	1
parMETIS	1
PETSc	1
Python	1
TAU, Scalasca, HPCToolkit	0
Charm++	2
Chombo	1
GASNet	1

COLORS: BG/Q PORT
Kumar's tool effort
IBM
Other efforts

Plan for Next 6 Months Effort

- **Help find and hire a project postdoc**
- **Working groups with IBM, Argonne and Tool developers**
- **Educate users on use of tools and libraries. Collect feedback**