Charm++ & Adaptive MPI

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Exascale Applications

- Main challenge: variability
  - Hardware variation
    - Static/dynamic, heterogeneity, failures, power, etc.
  - Dynamic program behavior
    - AMR, particle movements, subscale simulations, …

- To deal with these, we must seek:
  - Not full automation
  - Not full burden on the app-developers
  - But a good division of labor between the app-developer and system

Charm++

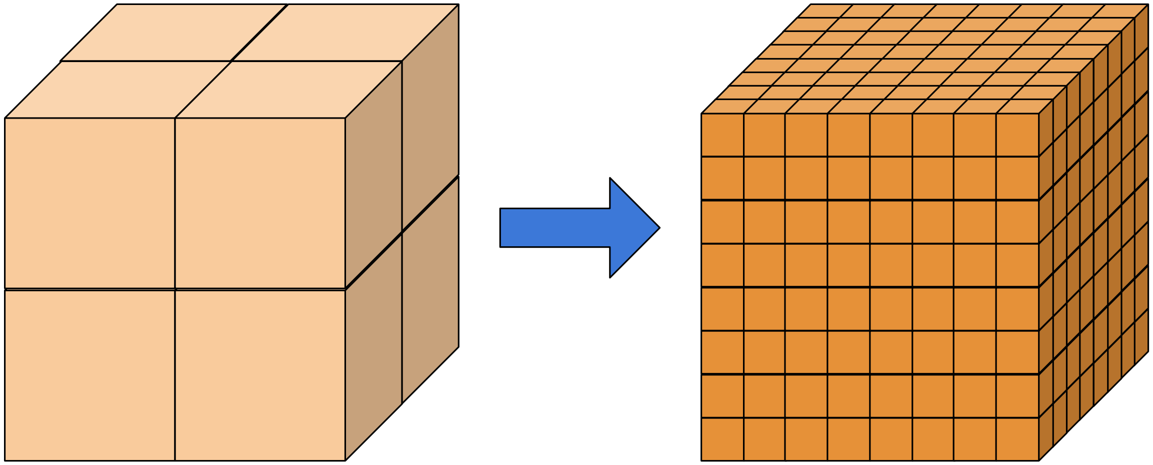
- Charm++ is a general-purpose object-oriented parallel programming system
  - Built on an adaptive runtime system

- Three principles that empower an adaptive runtime system:
  - Overdecomposition
  - Migratability
  - Asynchrony

Overdecomposition

- Decompose the work units & data units into many more pieces than execution units
  - Nodes/cores/…

- Not so hard: we do decomposition anyway

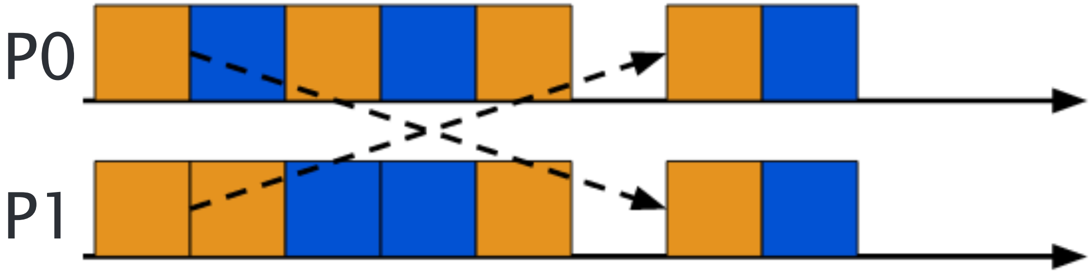


Migratability

- Allow these work and data units to be migratable at runtime
  - So the programmer or runtime can move them
- Consequences for users
  - Communication must be addressed to logical units with global names, not to processes
  - But this is a good thing
- Consequences for RTS
  - Naming and location management

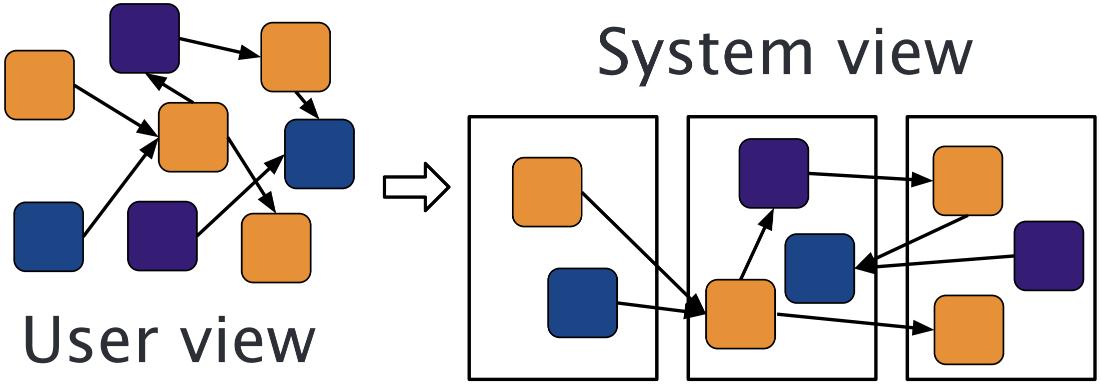
Asynchrony

- We have multiple units on each processor
- They address each other via logical names
  - How do we schedule them?
- Message-driven execution:
  - Let the work-unit that happens to have data ("message") available for it execute next
  - Let the RTS select among ready work units

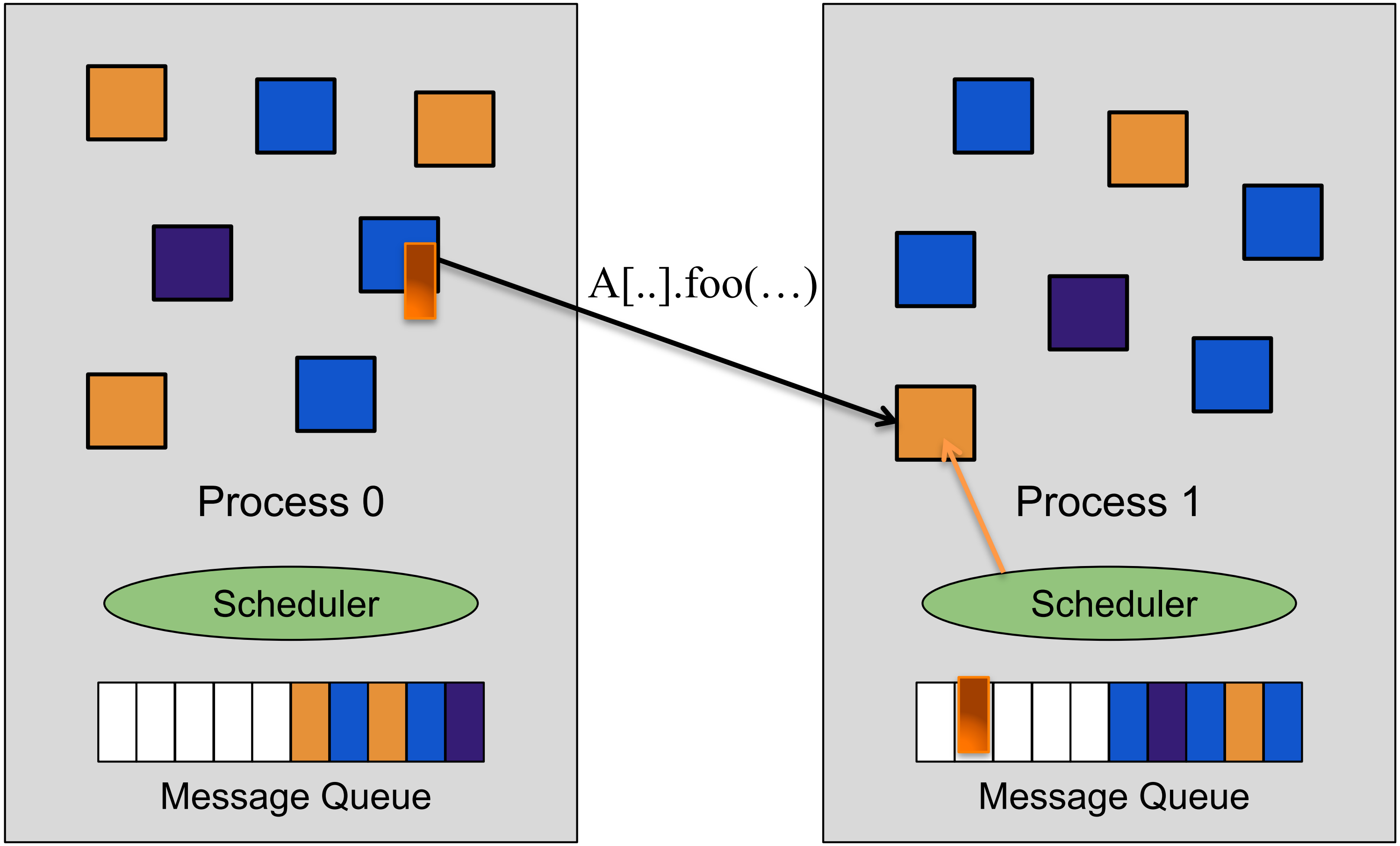


Charm++: Object-based overdecomposition

- Multiple indexed collections of C++ objects
  - Indices: multidimensional and/or sparse
- Programmer expresses communication between objects
  - Objects communicate via asynchronous remote method invocation
  - With no reference to processors: A[i].foo(…)



Message-driven Execution

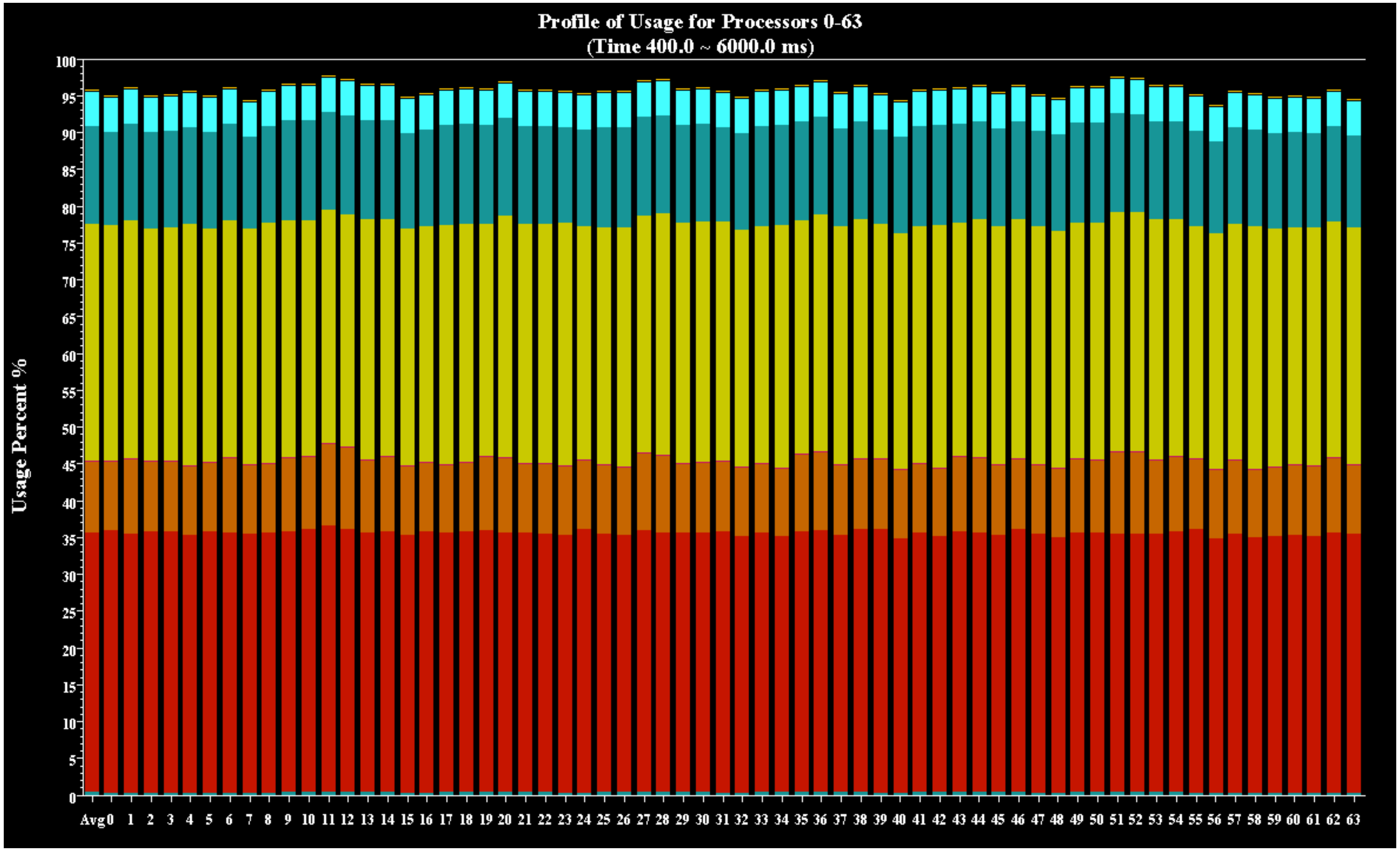


Adaptive Runtime Systems

- Decomposing a program into a large number of migratable objects empowers the RTS to:
  - Map and migrate objects at will
  - Schedule tasks when they have work
  - Instrument computation and communication
    - Object A communicates x bytes to B every iteration
  - Maintain historical data to track changes in application behavior
    - i.e. to trigger load balancing

Projections

- Performance visualization tool for Charm++

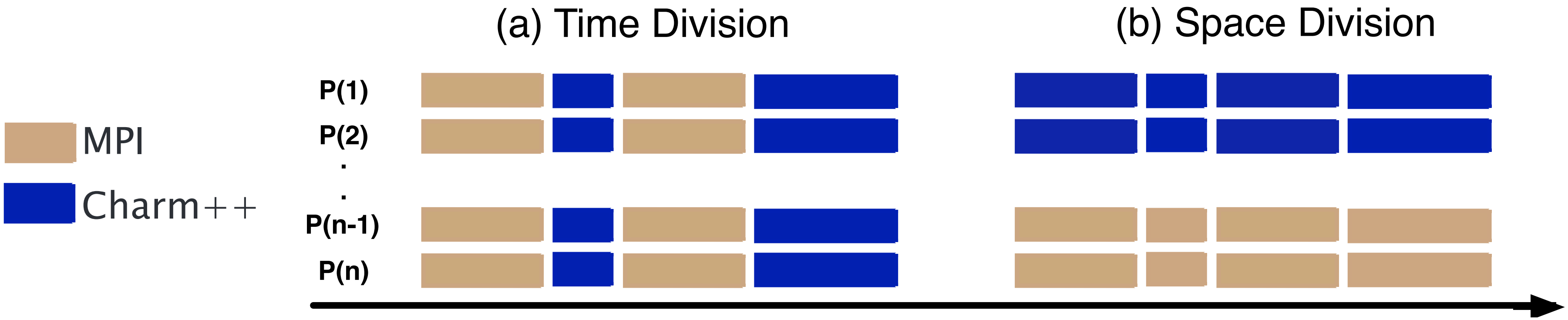


Fault Tolerance

- Basic Ideas:
  - Checkpoints are just migrations to storage
  - Underlying storage can be various things
  - Can be used in concert with load balancing
- Four approaches available:
  - Disk-based checkpoint/restart
  - In-memory double checkpoint w/ auto restart
  - Proactive object migration
  - Message-logging

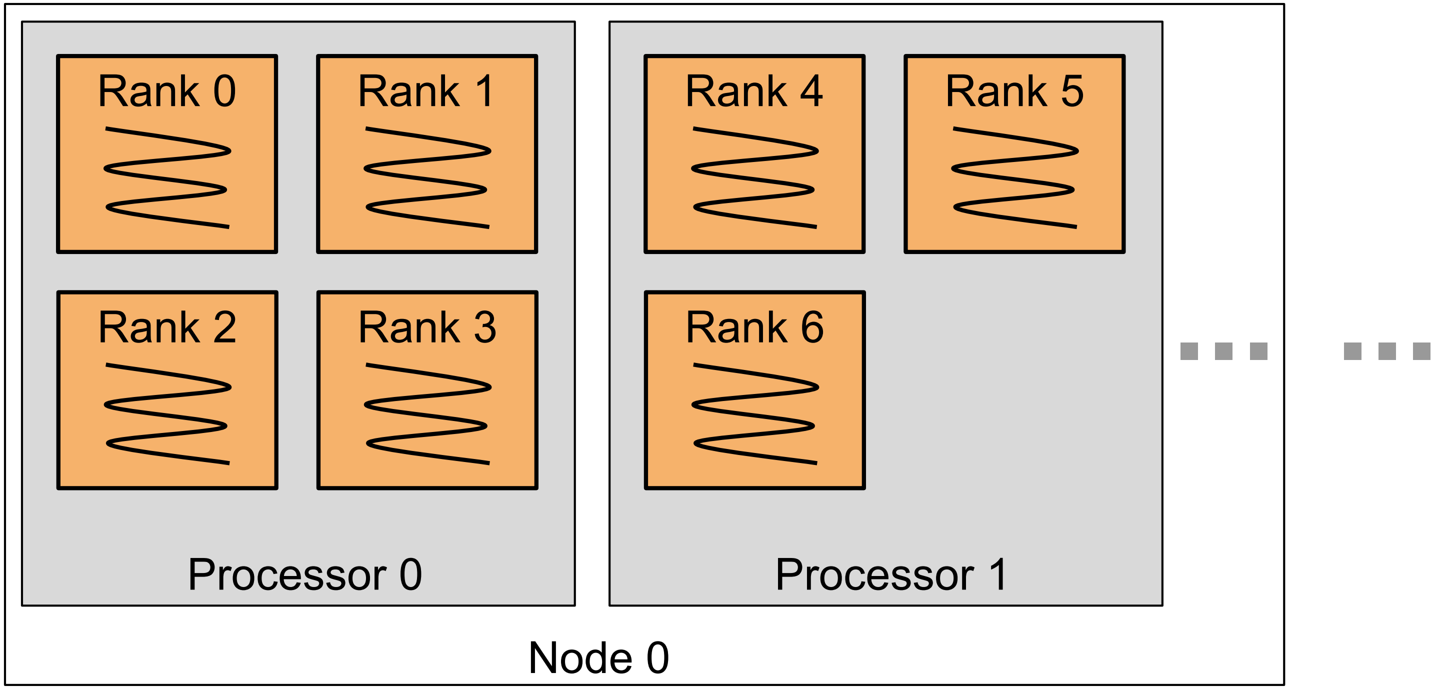
Interoperability with MPI

- Implement new libraries/modules in the model that fits it best
  - Reuse existing libraries
  - Incremental adoption path
  - Already in production use for petascale apps: NAMD, OpenAtom, EpiSimdemics



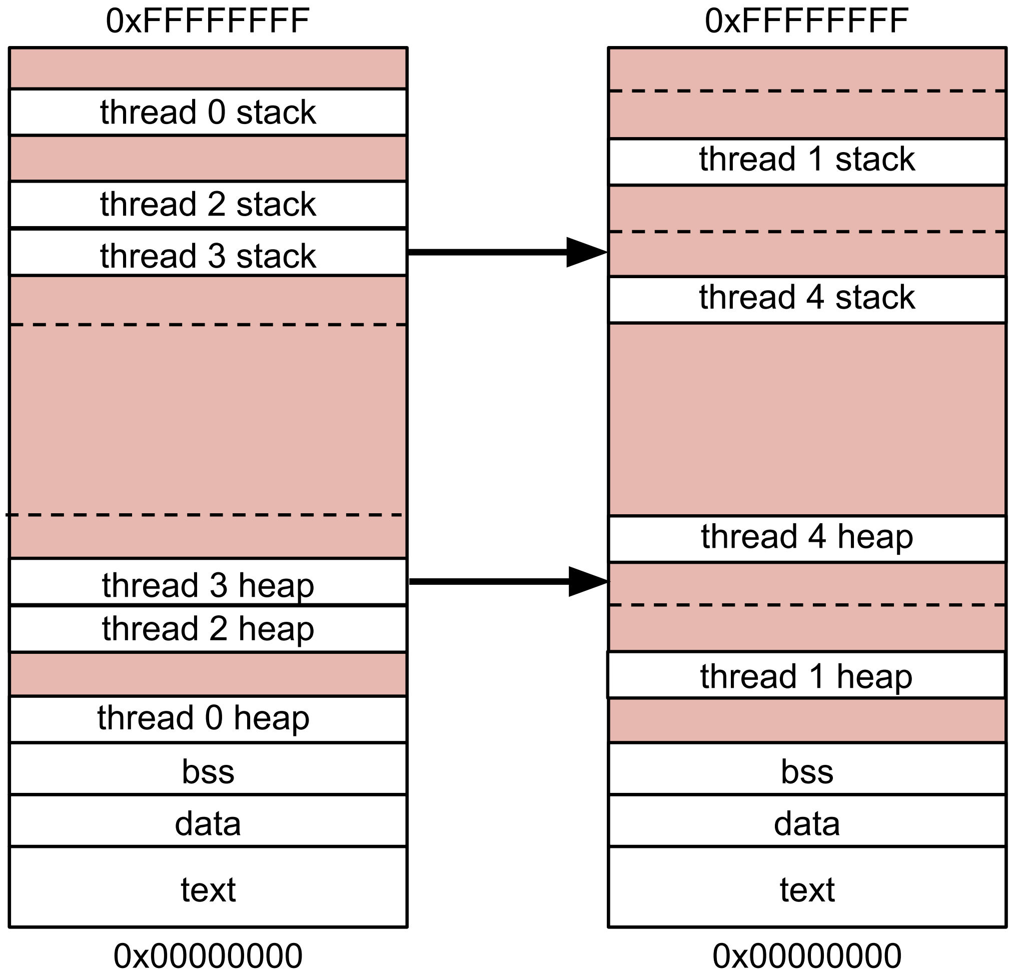
Adaptive MPI

- MPI-2.2 implementation on top of Charm++
  - MPI ranks are lightweight, migratable user-level threads associated with Charm++ objects



AMPI migration

- AMPI can transparently migrate ranks



Adaptive MPI

- Application-independent features:
  - Over-decomposition via process virtualization
  - Automatic overlap of comm. & comp.
  - Dynamic load balancing
  - Fault tolerance
- Issue: global/static variables are shared by all ranks in the same OS process
  - But we have automated compiler tools for privatization

Near Future Plans

- Merging now:
  - Improved GPU manager
  - Job shrink-expand
  - Online performance autotuning
  - Fine-grained message aggregation
- Ongoing work:
  - AMPI compliance with MPI-3.1
  - Improved node-level threading/tasking library
  - OpenMP thread/task scheduling integration

Summary

- Charm++ is a scalable, adaptive runtime system for asynchronous parallel computing
- Many applications have been developed using it
  - NAMD, ChaNGa, EpiSimdemics, OpenAtom, …
  - Many mini-apps and third-party apps
- Lesson: adaptivity developed for apps is useful for addressing exascale challenges
  - Adaptivity to hardware and software factors

Thank you

Charm++ production apps

Application	Domain	Previous parallelization	Scale
NAMD	Classical MD	PVM	500k
ChaNGa	N-body gravity & SPH	MPI	500k
EpiSimdemics	Agent-based epidemiology	MPI	500k
OpenAtom	Electronic Structure	MPI	128k
Spectre	Relativistic MHD		100k
FreeON/SpAMM	Quantum Chemistry	OpenMP	50k
Enzo-P/Cello	Astrophysics/Cosmology	MPI	32k
ROSS	PDES	MPI	16k
SDG	Elastodynamic fracture		10k
ADHydro	Systems Hydrology		1000
Disney ClothSim	Textile & rigid body dynamics	TBB	768
Particle Tracking	Velocimetry reconstruction		512
JetAlloc	Stochastic MIP optimization		480

AMPI codes (with no porting effort)

Mantevo 3.0

- CoMD 1.1
- HPCCG 1.0
- MiniFE 2.0
- MiniMD 2.0
- MiniXYCE 1.0

Other apps

- SNAP (C) 1.01
- PENNANT 0.8
- PRK 2.16

LLNL ASC Proxy Apps

- AMG 2013
- Kripke 1.1
- LULESH 2.0
- Lassen 1.0

LLNL Libraries

- HYPRE 2.10.1
- MFEM 3.0.1
- XBraid 1.1