A Unified Runtime Infrastructure for Exascale Programming Models

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(with input from others at Argonne, Oak Ridge, Lawrence Berkeley, Pacific Northwest, Lawrence Livermore, Sandia, UIUC, UH, OSU, Rice, IBM and Cray)

Presentation Layout

- **State of Programming Models**
- Application Requirements for the Exascale Era
- The Vision for a Unified Programming Infrastructure
- Technical Challenges
- Concluding Remarks

Current State of Programming Models

- Three broad categories
  - High-level Compilers/Languages
    - UPC, Chapel, CAF, …
  - High-level Libraries
    - Global data space models (Global Arrays, Global Trees) and Global computation space models (ADLB, Scioto, Charm++)
  - Low-level Runtime Systems
    - MPI, ARMCI, GASNET, OSPRI, accelerator models (OpenCL, CUDA), …
- Each model provides unique capabilities, but comes with its set of challenges as well

Application Challenges for Exascale Systems

- Applications have so far relied on more-or-less a single model
  - Most applications use MPI (either directly or through high-level domain-specific libraries)
  - Some applications use alternate models such as Global Arrays (NWChem) or UPC (NSA applications)
- As we move forward to exascale, applications will need more!
  - While the programming models that exist today lack capabilities to handle exascale challenges, we are not yet at a point where we need a completely new model
    - Each model has its flaws, but each model has its strengths too
    - Each model is very good at the set of things it is built for
  - Instead of redesigning a completely new programming model, we should leverage the strengths of the different models

Cherry-picking Programming Models

- Multi-model programming
  - For multimodule applications primarily based on MPI, how can a new module be written using alternate models such as UPC or CAF in such a way that it can interoperate with the rest of the application?
  - How can an application written in Cray Chapel or IBM X10 utilize math libraries written in MPI, such as PETSc, that have had close to a hundred man-years of development invested in them?
  - Can an MPI application directly move data from a local accelerator device to another physical node without explicitly using accelerator programming models to stage data locally before using MPI to move it outside the node?
  - If you have an ADLB application using work stealing and task migration, can it interact with Global Arrays to provide a globally accessible data region?

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Application Requirements for the Exascale Era

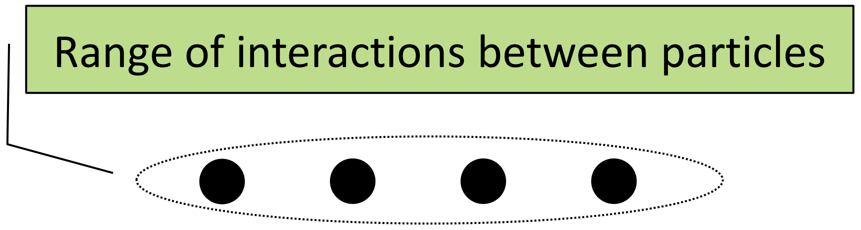
- Applications need to deal with two dimensions of problems:
  - The science they are trying to solve is becoming more complex (hence the need for exascale computing)
    - More data requirements, more computation
  - Hardware architectures are becoming more complex (hierarchical architectures, heterogeneous systems)
    - Current machines cannot just scale up because of cost and power constraints
- Current computation and communication methodologies used by applications cannot just migrate to exascale architectures
  - Too many variables here; everything will not magically scale

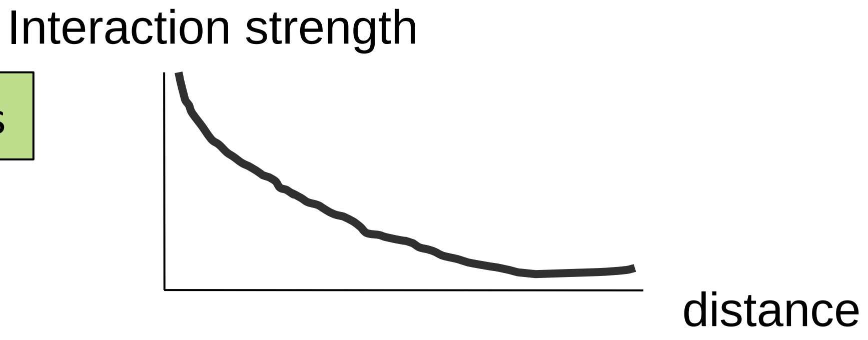
N-Body Coulomb Interactions

- Current applications have been looking at small-to-medium molecules consisting of 20-100 atoms
  - Amount of computation per data element is reasonably large, so scientists have been reasonably successful decoupling computation and data movement
- For exascale systems, scientists want to study molecules of the order of a 1000 atoms or larger
  - Coulomb interactions between the atoms is much stronger in the problems today than what we expect for exascale-level problems
  - Larger problems will need to support short-range and longer-range components of the coulomb interactions (possibly using different solvers)
    - Diversity in the amount of computation per data element is going to increase substantially
    - Regularity of data and/or computation would be substantially different

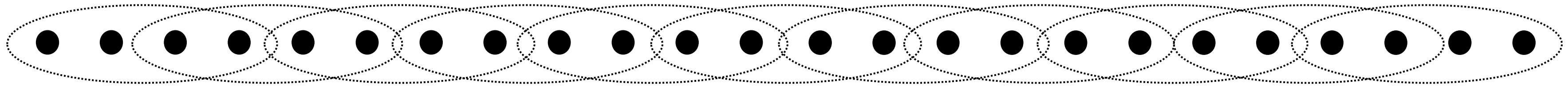
Quantum mechanical interactions are near-sighted (Walter Kohn)

Traditional quantum chemistry studies lie within the nearsighted range where interactions are dense:





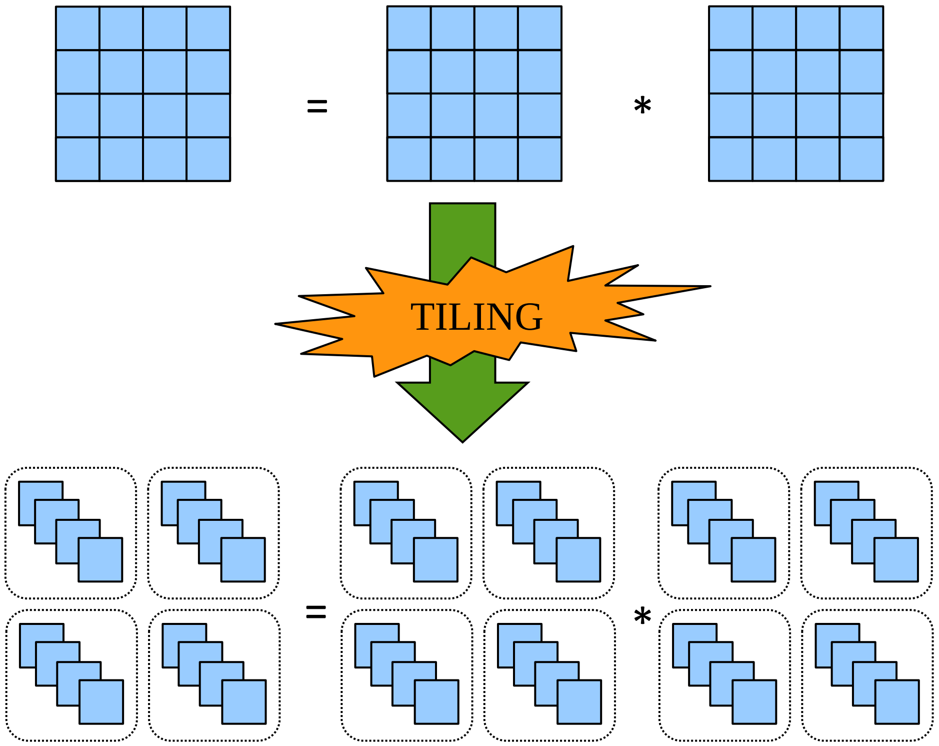
Future quantum chemistry studies expose both short- and long-range interactions:



Note that the figures are phenomenological. Quantum chemistry methods treat correlation using a variety of approaches and have different short/long-range cutoffs.

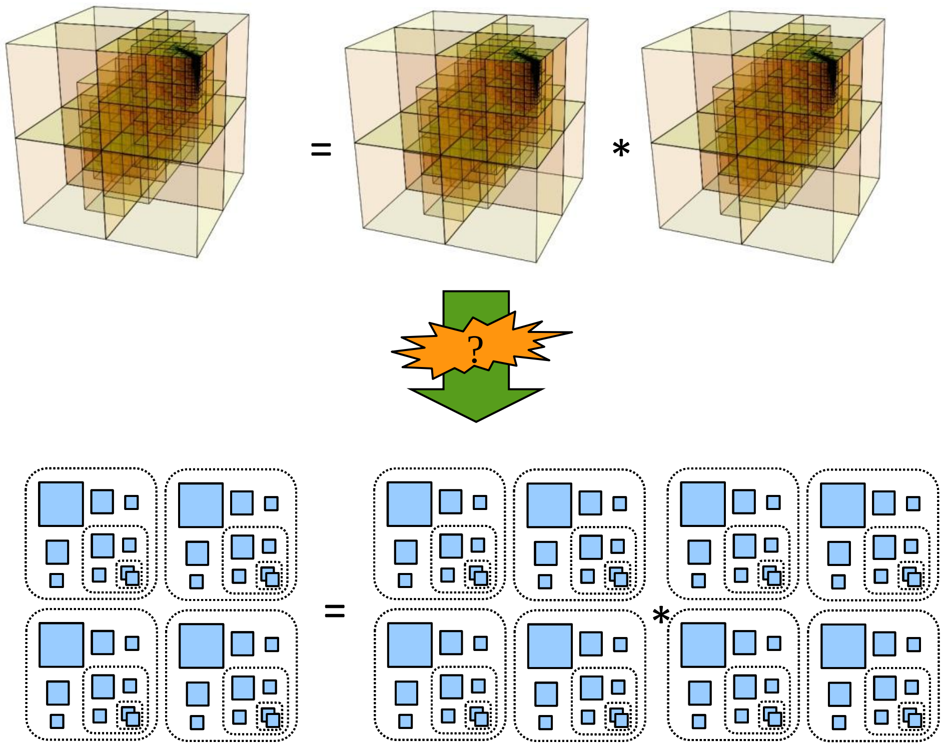
Courtesy Jeff Hammond, Argonne National Laboratory

Current: Regular Dense Computation



- Traditional models such as MPI or GA alone have been sufficient for this model of computation
  - Fetch data locally and compute

Exascale: Irregular Dense/Sparse Computation



- Traditional models "individually" are no longer sufficient
  - MPI or GA like model is good for dense parts of the data (fetch data locally and compute)
  - Charm++, ADLB or Scioto like model is good for the sparse parts

Another Motivating Example: GFMC

- Green's Function Monte Carlo -- the "gold standard" for *ab initio* calculations in nuclear physics at Argonne
- A non-trivial master/slave algorithm, with assorted work types and priorities; multiple processes create work; large work units
- Scaled to 2000 processors on BG/L a little over two years ago, then hit scalability wall
- Need to get to 10's of thousands of processors at least, in order to carry out calculations on ^{12}C, an explicit goal of the UNEDF SciDAC project
- The algorithm has had to become even more complex, with more types and dependencies among work units, together with smaller work units
- Want to maintain master/slave structure of physics code
- This situation called for the invention of a new library -- ADLB, the Asynchronous Dynamic Load Balancing Library (written in MPI)
  - Attacking general problem: how to devise a programming model that makes things simpler and more scalable at the same time

Memory Scalability of GFMC

- GFMC's view of ADLB is that of a "generalized master-worker"
  - Each worker provides tasks to the "master" (physically distributed set of servers), and other workers can steal this work
  - Issues related to task dependencies/load-balancing are handled within ADLB (GFMC gives hints, but doesn't explicitly handle it)
- As GFMC moved to larger elements, the memory available to each task was no longer sufficient (factorial of atomic weight)
- First solution was MPI + OpenMP: allowed GFMC to scale to C-12
- Next steps forward are C-14 and O-16, and a simple task-based model such as ADLB is no longer sufficient
  - We need to investigate using ADLB in conjunction with GA or UPC, …
  - MPI to move data within an address space, but GA or UPC to expand the address space available to each process (global space)

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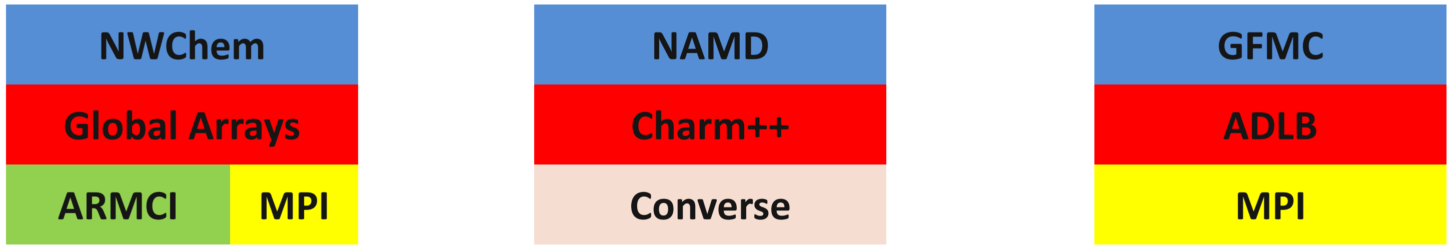
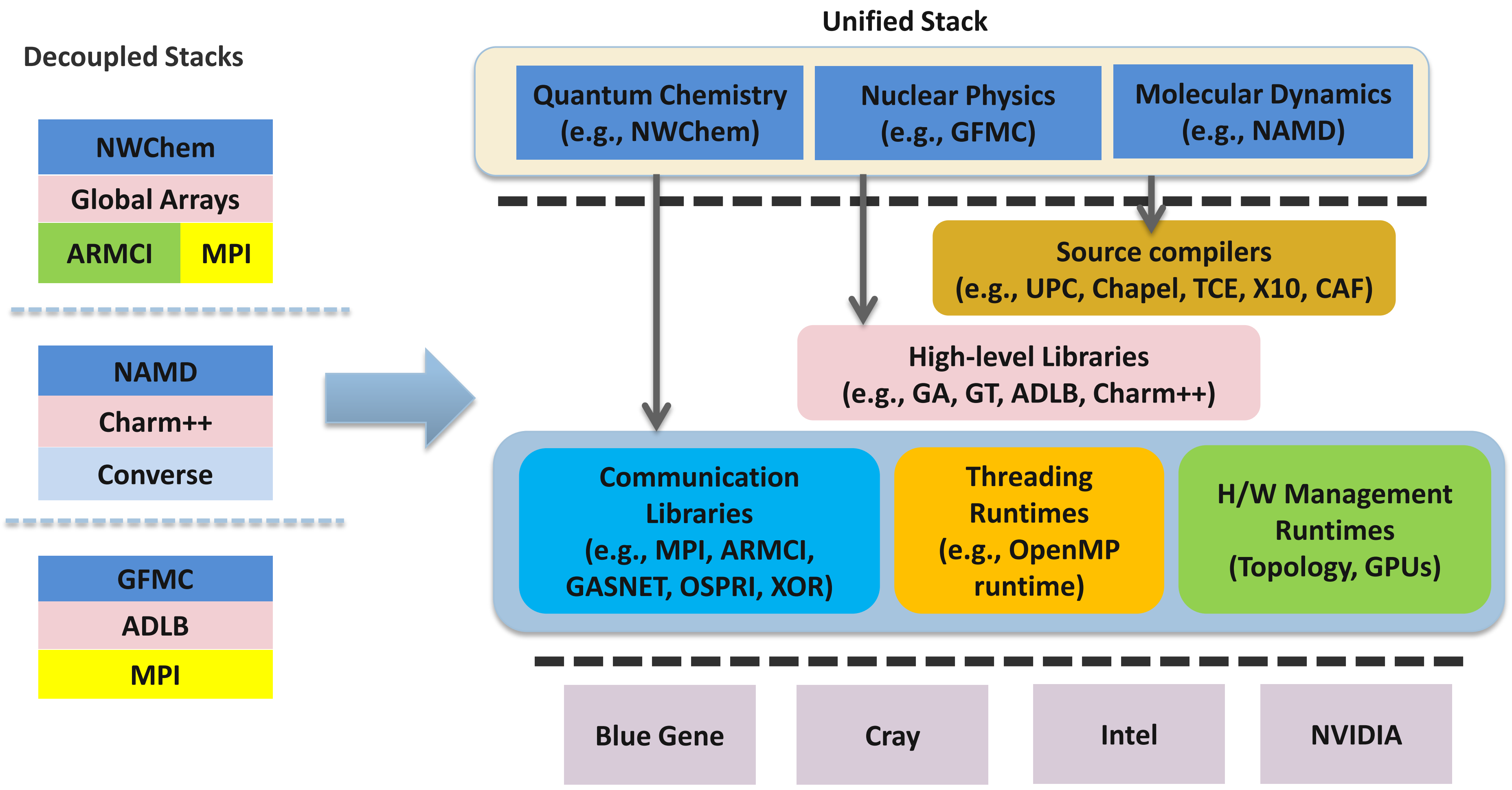
A Separate Runtime System for each Application

- Each application packaged with its own high-level programming library (GA, Charm++, ADLB, MADNESS runtime) on top of a different low-level runtime (MPI, ARMCI, GASNET)
- This model is fundamentally not sustainable at Exascale
  - *Interoperability between application models is difficult* – underlying runtime infrastructure has to be either interoperable or integrated
  - *Research optimizations are either redundant or not interoperable*
    - GA, GT, Data Spaces, etc., mostly do the same optimizations
    - For what's not repeated (e.g., if GA does something DS doesn't), they are not interoperable
  - *Commercial support impractical* – vendors will not support five runtime libraries – hard enough to get support for MPI + <anything else>



Vision for a Unified Programming Infrastructure



Decoupled Stacks
NWChem
Global Arrays
ARMCI
MPI
NAMD
Charm++
Converse
GFMC
ADLB
MPI
Unified Stack
Quantum Chemistry (e.g., NWChem)
Nuclear Physics (e.g., GFMC)
Molecular Dynamics (e.g., NAMD)
Source compilers (e.g., UPC, Chapel, TCE, X10, CAF)
High-level Libraries (e.g., GA, GT, ADLB, Charm++)
Communication Libraries (e.g., MPI, ARMCI, GASNET, OSPRI, XOR)
Threading Runtimes (e.g., OpenMP runtime)
H/W Management Runtimes (Topology, GPUs)
Blue Gene
Cray
Intel
NVIDIA

The key is to provide a unified architectures with multiple levels of capabilities and ALLOW APPLICATIONS TO BREAK THE LAYERING → transition path for applications!

Fundamental Concept of the Unified Stack

- Integrated runtime infrastructure
  - One single, unified stack that can provide multiple interfaces: MPI, ARMCI, GASNET, OSPRI, threading models
  - Extensions for capabilities not directly available in any model: hardware topology information, accelerator-specific extensions
- High-level libraries utilize the unified runtime infrastructure making interoperability simpler
  - Global Arrays can interoperate with ADLB, or Charm++ can interoperate with Data spaces
- High-level languages (such as UPC, CAF) can utilize either high-level libraries or the unified runtime infrastructure as their target runtime infrastructure

Community-wide Collaborative Effort

- DOE Laboratories
  - Argonne National Laboratory
  - Oak Ridge National Laboratory
  - Lawrence Berkeley National Laboratory
  - Lawrence Livermore National Laboratory
  - Pacific Northwest National Laboratory
  - Sandia National Laboratory
- Universities
  - University of Illinois at Urbana-Champaign
  - Rice University
  - Ohio State University
  - University of Houston
- Industry
  - IBM
  - Cray

Planning Steps

- Collaboration between different laboratories, universities and industry labs
  - Effort includes programming model leads (co-producers of the unified stack) and co-design centers (consumers of the unified stack)
  - Everyone believes that is the right step forward, and we as a community need to make it happen
- We are having a few workshops to plan how this unified programming infrastructure will shape up
- IBM graciously hosted the first workshop in October
  - Initial discussions on what the goals of the unified stack would be
- We are working on a white paper that details what applications should expect from this effort

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Technical Challenges and Key Functionality

- Memory Consistency
- Computation Management and Load Balancing
- Unified Communication Runtime and Progress Model
- Coordinated Management of Shared Resources
- Hybridization and Interoperability
- Heterogeneous/Accelerator Computing
- Memory Hierarchy and Threading
- Fault Tolerance
- Interaction with Performance and Debugger Tools

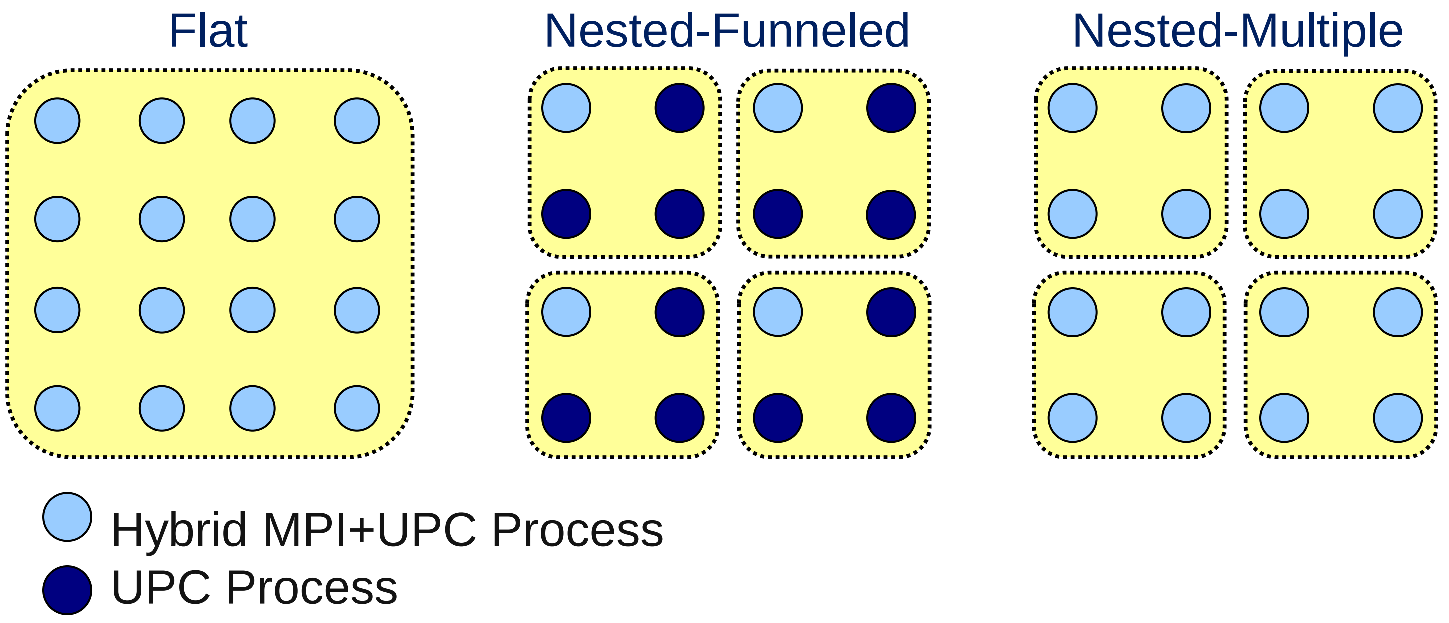
Challenges for the Unified Programming Infrastructure

- Unified semantics
  - What does it mean to have a non-blocking UPC collective followed by an MPI collective? How is it expected to behave?
  - Does an **ARMCI_FENCE** call guarantee completion of GASNET operations?
  - How are operations ordered between MPI and CAF?
- Interoperability of Data Objects
  - I should be able to do MPI operations on GASNET allocated memory regions – how will this work?
- Integrated Resource Management
  - Progress threads, buffer allocations, memory registration

Ad-hoc interactions being studied currently

- Some form of: MPI + threads, MPI + UPC, ADLB + MPI
- But we need a more truly unified (drag-and-drop) model
  - Migration path for applications to start using other models (any other model!) in conjunction with what they are already doing

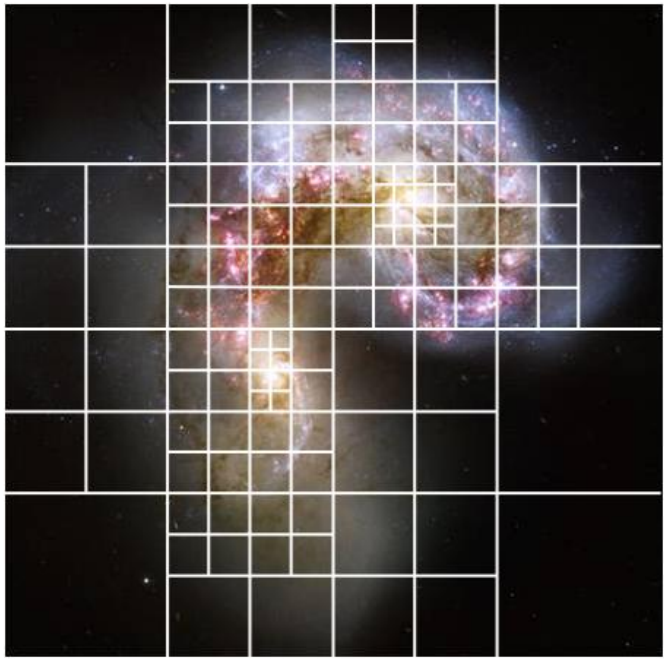
Case Study: Hybrid MPI+UPC Programming



- Many possible ways to combine MPI
  - Flat: One global address space
  - Nested: Multiple global address spaces (UPC groups)

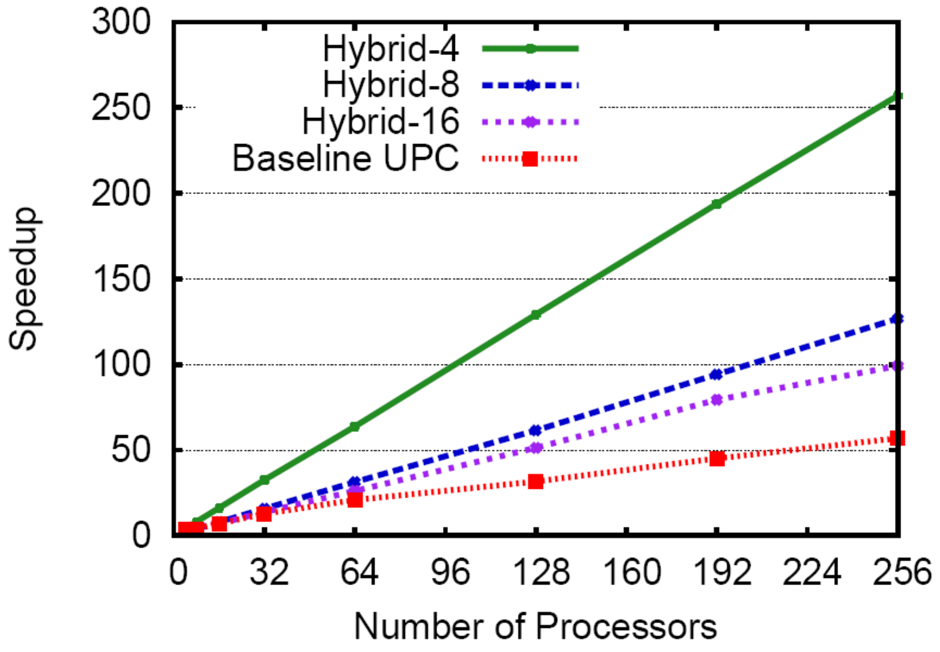
Barnes-Hut n-Body Simulation

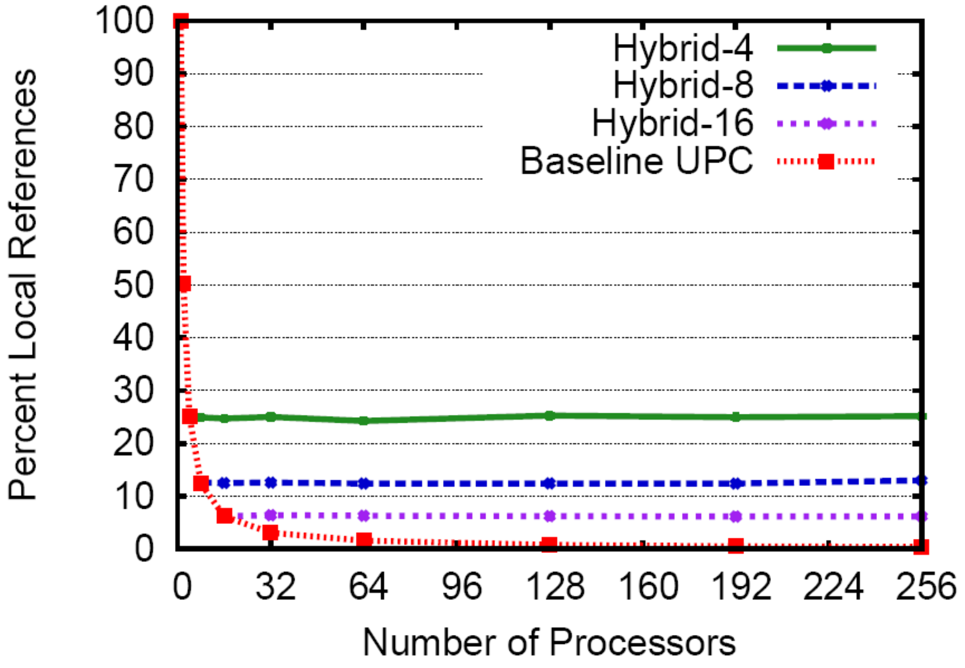
- Simulate motion and gravitational interactions of *n* astronomical bodies over time
- Represents 3-d space using an oct-tree
  - Space is sparse
- Summarize distant interactions using center of mass

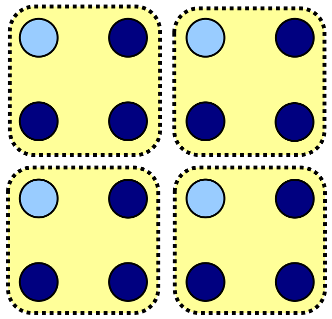


Colliding Antennae Galaxies (Hubble Space Telescope)

Hybrid MPI+UPC Barnes-Hut







- Nested-funneled model
  - Tree is replicated across UPC groups
- 51 new lines of code (2% increase)
  - Distribute work and collect results

Case Study: MPI + ARMCI (collaboration with ORNL and PNNL)

- Understanding what parts of ARMCI can sit on top of MPI-2 RMA and what parts need to be natively implemented for each platform
- Guide what is needed in MPI-3 RMA
- MPI-3 RMA functionality might encompass a lot of the features required by ARMCI (and even GASNET)

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Concluding Remarks

- Several programming models out there, but applications might need more than what each of the provides
- It might be time for us to be able to allow applications to use multiples of these models together
  - While there has been some work that performs ad-hoc interactions between select model, we need a focused effort in combining the capabilities of many (or all) of these models
  - Applications should be able to pick and choose what they want to use based on application characteristics and requirements
- The unified programming infrastructure is a community-wide effort to bring together the capabilities of virtually all of the existing programming models available today

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Argonne Programming Models Group

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