Runtime Support for Multi-scale Applications on High-end Systems

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Motivation

- Programmer effort to develop complex high-performance applications is very high
- The majority of existing scalable parallel applications are written in MPI
  - Application programmers would prefer to use a parallel global address space framework IF they can get high performance
  - MPI will likely not be sufficient to achieve high performance on systems with significant multi-level parallelism (e.g. cluster of SMPs of 80-core CMPs)
- Can we provide runtime support that eases parallel programming and deliver high performance?
  - Focus on block-sparse computations
  - Motivating applications:
    - Tensor Contraction Engine – Domain-specific compiler for a class of ab-initio quantum chemistry models
    - MADNESS (Multiresolution ADaptive NumErical Scientific Simulation) – new quantum chemistry code from Robert Harrison

Tensor Contraction Engine

- Automatic transformation from high-level specification
  - Chemist specifies computation in high-level mathematical form
  - Synthesis system transforms it to efficient parallel program
  - Code is tailored to target machine
  - Code can be optimized for specific molecules being modeled
- Multi-institutional collaboration (OSU, LSU, Waterloo, ORNL, PNNL, U. Florida)
- Two prototypes of TCE are operational
  - a) Full exploitation of symmetry, but fewer optimizations, b) Dense tensors, but more sophisticated optimizations; Integrated version with all optimizations and exploitation of sparsity/symmetry is nearing completion
  - Used to implement over 20 models, included in latest release of NWChem
  - First parallel implementation for many of the methods
  - TCE Workshop at Sanibel 2007 meeting of quantum chemists generated much interest

$$A3A = \frac{1}{2}(X_{ce,af} Y_{ae,cf} + X_{\bar{c}\bar{e},\bar{a}\bar{f}} Y_{\bar{a}\bar{e},\bar{c}\bar{f}} + X_{c\bar{e},a\bar{f}} Y_{a\bar{e},c\bar{f}} + X_{\bar{c}e,\bar{a}f} Y_{\bar{a}e,\bar{c}f} + X_{\bar{c}\bar{e},\bar{a}\bar{f}} Y_{\bar{a}\bar{e},\bar{c}\bar{f}} + X_{\bar{c}e,\bar{a}\bar{f}} Y_{\bar{a}e,\bar{c}\bar{f}} + X_{\bar{c}\bar{e},\bar{a}f} Y_{\bar{a}\bar{e},\bar{c}f} + X_{\bar{c}\bar{e},\bar{a}\bar{f}} Y_{\bar{a}\bar{e},\bar{c}\bar{f}})$$

$$X_{ce,af} = t_{ij}^{ce} t_{ij}^{af} \qquad Y_{ae,cf} = \langle ab \| ek \rangle \langle cb \| fk \rangle$$

```
range V = 3000;
range O = 100;

index a,b,c,d,e,f : V;
index i,j,k : O;

mlimit = 10000000;

function F1(V,V,V,O);
function F2(V,V,V,O);

procedure P(in T1[O,O,V,V], in T2[O,O,V,V], out X)=

begin
   A3A == sum[ sum[F1(a,b,e,k) * F2(c,f,b,k), {b,k}]
                  * sum[T1[i,j,c,e] * T2[i,j,a,f], {i,j}],
                  {a,e,c,f}]*0.5 + ...;
end
```

CCSD Doubles Equation

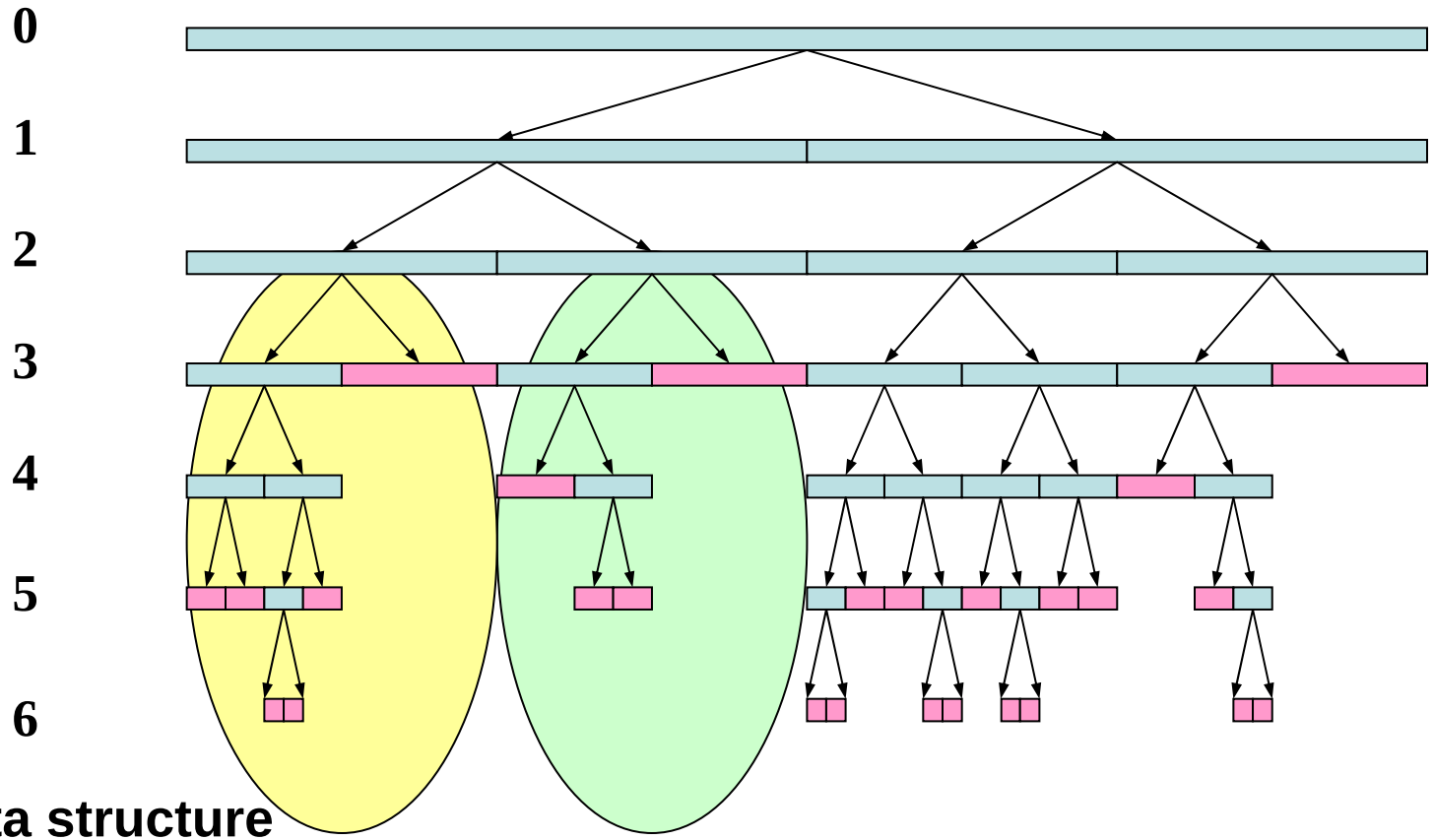
hbar[a,b,i,j] == sum[f[b,c]*t[i,j,a,c],{c}] -sum[f[k,c]*t[k,b]*t[i,j,a,c],{k,c}] +sum[f[a,c]*t[i,j,c,b],{c}] -sum[f[k,c]*t[k,a]*t[i,j,c,b],{k,c}] -sum[f[k,j]*t[i,k,a,b],{k}] -sum[f[k,c]*t[j,c]*t[i,k,a,b],{k,c}] -sum[f[k,i]*t[j,k,b,a],{k}] -sum[f[k,c]*t[i,c]*t[j,k,b,a],{k,c}] +sum[t[i,c]*t[j,d]*v[a,b,c,d],{c,d}] +sum[t[i,j,c,d]*v[a,b,c,d],{c,d}] +sum[t[j,c]*v[a,b,i,c],{c}] -sum[t[k,b]*v[a,k,i,j],{k}] +sum[t[i,c]*v[b,a,j,c],{c}] -sum[t[k,a]*v[b,k,j,i],{k}] -sum[t[k,d]*t[i,j,c,b]*v[k,a,c,d],{k,c,d}] -sum[t[i,c]*t[j,k,b,d]*v[k,a,c,d],{k,c,d}] -sum[t[j,c]*t[k,b]*v[k,a,c,i],{k,c}] +2*sum[t[j,k,b,c]*v[k,a,c,i],{k,c}] -sum[t[j,k,c,b]*v[k,a,c,i],{k,c}] -sum[t[i,c]*t[j,d]*t[k,b]*v[k,a,d,c],{k,c,d}] +2*sum[t[k,d]*t[i,j,c,b]*v[k,a,d,c],{k,c,d}] -sum[t[k,b]*t[i,j,c,d]*v[k,a,d,c],{k,c,d}] -sum[t[j,d]*t[i,k,c,b]*v[k,a,d,c],{k,c,d}] +2*sum[t[i,c]*t[j,k,b,d]*v[k,a,d,c],{k,c,d}] -sum[t[i,c]*t[j,k,d,b]*v[k,a,d,c],{k,c,d}] -sum[t[j,k,b,c]*v[k,a,i,c],{k,c}] -sum[t[i,c]*t[k,b]*v[k,a,j,c],{k,c}] -sum[t[i,k,c,b]*v[k,a,j,c],{k,c}] -sum[t[i,c]*t[j,d]*t[k,a]*v[k,b,c,d],{k,c,d}] -sum[t[k,d]*t[i,j,a,c]*v[k,b,c,d],{k,c,d}] -sum[t[k,a]*t[i,j,c,d]*v[k,b,c,d],{k,c,d}] +2*sum[t[j,d]*t[i,k,a,c]*v[k,b,c,d],{k,c,d}] -sum[t[j,d]*t[i,k,c,a]*v[k,b,c,d],{k,c,d}] -sum[t[i,c]*t[j,k,d,a]*v[k,b,c,d],{k,c,d}] -sum[t[i,c]*t[k,a]*v[k,b,c,j],{k,c}] +2*sum[t[i,k,a,c]*v[k,b,c,j],{k,c}] -sum[t[i,k,c,a]*v[k,b,c,j],{k,c}] +2*sum[t[k,d]*t[i,j,a,c]*v[k,b,d,c],{k,c,d}] -sum[t[j,d]*t[i,k,a,c]*v[k,b,d,c],{k,c,d}] -sum[t[j,c]*t[k,a]*v[k,b,i,c],{k,c}] -sum[t[j,k,c,a]*v[k,b,i,c],{k,c}] -sum[t[i,k,a,c]*v[k,b,j,c],{k,c}] +sum[t[i,c]*t[j,d]*t[k,a]*t[l,b]*v[k,l,c,d],{k,l,c,d}] -2*sum[t[k,b]*t[l,d]*t[i,j,a,c]*v[k,l,c,d],{k,l,c,d}] -2*sum[t[k,a]*t[l,d]*t[i,j,c,b]*v[k,l,c,d],{k,l,c,d}] +sum[t[k,a]*t[l,b]*t[i,j,c,d]*v[k,l,c,d],{k,l,c,d}] -2*sum[t[j,c]*t[l,d]*t[i,k,a,b]*v[k,l,c,d],{k,l,c,d}] -2*sum[t[j,d]*t[l,b]*t[i,k,a,c]*v[k,l,c,d],{k,l,c,d}] +sum[t[j,d]*t[l,b]*t[i,k,c,a]*v[k,l,c,d],{k,l,c,d}] -2*sum[t[i,c]*t[l,d]*t[j,k,b,a]*v[k,l,c,d],{k,l,c,d}] +sum[t[i,c]*t[l,a]*t[j,k,b,d]*v[k,l,c,d],{k,l,c,d}] +sum[t[i,c]*t[l,b]*t[j,k,d,a]*v[k,l,c,d],{k,l,c,d}] +sum[t[i,k,c,d]*t[j,l,b,a]*v[k,l,c,d],{k,l,c,d}] +4*sum[t[i,k,a,c]*t[j,l,b,d]*v[k,l,c,d],{k,l,c,d}] -2*sum[t[i,k,c,a]*t[j,l,b,d]*v[k,l,c,d],{k,l,c,d}] -2*sum[t[i,k,a,b]*t[j,l,c,d]*v[k,l,c,d],{k,l,c,d}] -2*sum[t[i,k,a,c]*t[j,l,d,b]*v[k,l,c,d],{k,l,c,d}] +sum[t[i,k,c,a]*t[j,l,d,b]*v[k,l,c,d],{k,l,c,d}] +sum[t[i,c]*t[j,d]*t[k,l,a,b]*v[k,l,c,d],{k,l,c,d}] +sum[t[i,j,c,d]*t[k,l,a,b]*v[k,l,c,d],{k,l,c,d}] -2*sum[t[i,j,c,b]*t[k,l,a,d]*v[k,l,c,d],{k,l,c,d}] -2*sum[t[i,j,a,c]*t[k,l,b,d]*v[k,l,c,d],{k,l,c,d}] +sum[t[j,c]*t[k,b]*t[l,a]*v[k,l,c,i],{k,l,c}] +sum[t[l,c]*t[j,k,b,a]*v[k,l,c,i],{k,l,c}] -2*sum[t[l,a]*t[j,k,b,c]*v[k,l,c,i],{k,l,c}] +sum[t[l,a]*t[j,k,c,b]*v[k,l,c,i],{k,l,c}] -2*sum[t[k,c]*t[j,l,b,a]*v[k,l,c,i],{k,l,c}] +sum[t[k,a]*t[j,l,b,c]*v[k,l,c,i],{k,l,c}] +sum[t[k,b]*t[j,l,c,a]*v[k,l,c,i],{k,l,c}] +sum[t[j,c]*t[l,k,a,b]*v[k,l,c,i],{k,l,c}] +sum[t[i,c]*t[k,a]*t[l,b]*v[k,l,c,j],{k,l,c}] +sum[t[l,c]*t[i,k,a,b]*v[k,l,c,j],{k,l,c}] -2*sum[t[l,b]*t[i,k,a,c]*v[k,l,c,j],{k,l,c}] +sum[t[l,b]*t[i,k,c,a]*v[k,l,c,j],{k,l,c}] +sum[t[i,c]*t[k,l,a,b]*v[k,l,c,j],{k,l,c}] +sum[t[j,c]*t[l,d]*t[i,k,a,b]*v[k,l,d,c],{k,l,c,d}] +sum[t[j,d]*t[l,b]*t[i,k,a,c]*v[k,l,d,c],{k,l,c,d}] +sum[t[j,d]*t[l,a]*t[i,k,c,b]*v[k,l,d,c],{k,l,c,d}] -2*sum[t[i,k,c,d]*t[j,l,b,a]*v[k,l,d,c],{k,l,c,d}] -2*sum[t[i,k,a,c]*t[j,l,b,d]*v[k,l,d,c],{k,l,c,d}] +sum[t[i,k,c,a]*t[j,l,b,d]*v[k,l,d,c],{k,l,c,d}] +sum[t[i,k,a,b]*t[j,l,c,d]*v[k,l,d,c],{k,l,c,d}] +sum[t[i,k,c,b]*t[j,l,d,a]*v[k,l,d,c],{k,l,c,d}] +sum[t[i,k,a,c]*t[j,l,d,b]*v[k,l,d,c],{k,l,c,d}] +sum[t[k,a]*t[l,b]*v[k,l,i,j],{k,l}] +sum[t[k,l,a,b]*v[k,l,i,j],{k,l}] +sum[t[k,b]*t[l,d]*t[i,j,a,c]*v[l,k,c,d],{k,l,c,d}] +sum[t[k,a]*t[l,d]*t[i,j,c,b]*v[l,k,c,d],{k,l,c,d}] +sum[t[i,c]*t[l,d]*t[j,k,b,a]*v[l,k,c,d],{k,l,c,d}] -2*sum[t[i,c]*t[l,a]*t[j,k,b,d]*v[l,k,c,d],{k,l,c,d}] +sum[t[i,c]*t[l,a]*t[j,k,d,b]*v[l,k,c,d],{k,l,c,d}] +sum[t[i,j,c,b]*t[k,l,a,d]*v[l,k,c,d],{k,l,c,d}] +sum[t[i,j,a,c]*t[k,l,b,d]*v[l,k,c,d],{k,l,c,d}] -2*sum[t[l,c]*t[i,k,a,b]*v[l,k,c,j],{k,l,c}] +sum[t[l,b]*t[i,k,a,c]*v[l,k,c,j],{k,l,c}] +sum[t[l,a]*t[i,k,c,b]*v[l,k,c,j],{k,l,c}] +v[a,b,i,j]

MADNESS

Multiresolution
Adaptive
Numerical
Scientific
Simulation

New quantum chemistry code from Robert Harrison

Sub-Tree Parallelism in MADNESS



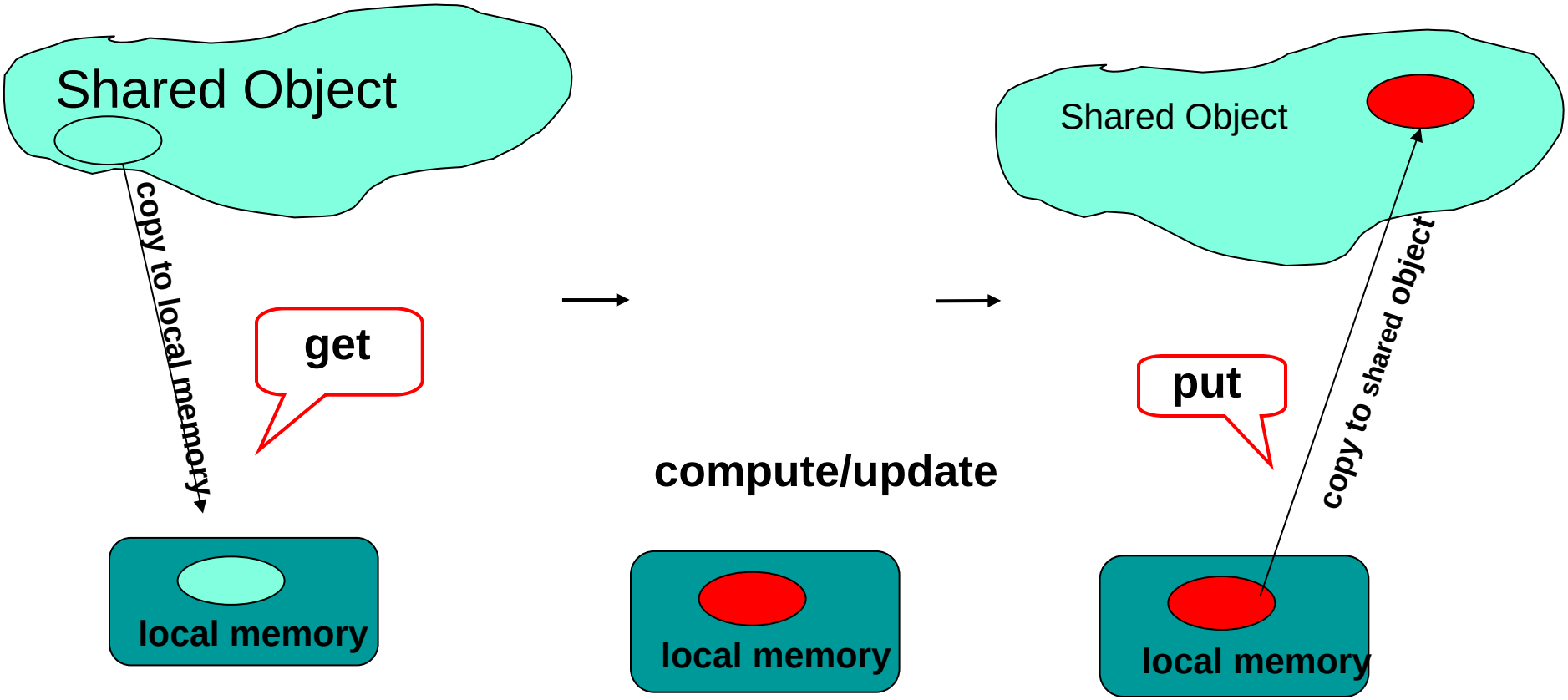
Data structure

- Tree representation of spatial functions, adaptively refined for necessary precision
- Distributed in a global address space

Operations

- Algebraic operations, integration, differentiation, etc.
- Tree traversals requiring parent-child and neighbor relationships
- Dynamically created and destroyed

Global Arrays Model of Computations



- Shared memory view for distributed dense arrays
- MPI-Compatible; Currently usable with Fortran, C, C++, Python
- Data locality and granularity control similar to message passing model
- Used in large scale efforts, e.g. NWChem (million+ lines/code)

Extensions to the GA Model

DATA: Beyond dense multi-dimensional arrays

- More complex data-structures: block sparse arrays; tree structures
- Globally addressable, but locality aware

COMPUTATION: Beyond static process-centric parallelism

- Some applications are easier to program with a task based message-driven model
- Support for load-balancing

ARCHITECTURE: Simplify programming explicitly managed memory hierarchies.

- Automatically schedule data movement
- Locality-aware load-balanced computation scheduling
- Transparent Memory Hierarchy Management
  - Non-collective I/O on local disks
  - Shared memory-style programming across distinct adress spaces, but locality-managed for performance

Non-collective I/O on local disks

- Data distributed on local disks of nodes
  - Scalable with number of nodes
- Control over data distribution
  - Better exploitation of data locality
- Any processor can non-collectively access any data on disk
  - Global address space for data on disk
  - Simplifies out-of-core programming
- Global Procedure Calls (GPC)
  - Mechanism to invoke a procedure in a remote processor
  - Provides portable active messages support in GA suite
- Non-collective I/O implemented by leveraging GPC

Transparent Memory Hierarchy Management for Independent Tasks

- Problem: Schedule computation and disk I/O operations
- Objective: Minimize disk I/O
- Constraint: Available physical memory
- Solution: Hypergraph partitioning formulation
  - Efficient solutions to the hypergraph problem exist
  - Typically used in the context of parallelization
    - Number of parts known
  - No constraints such as memory limit
    - Only balancing constraint

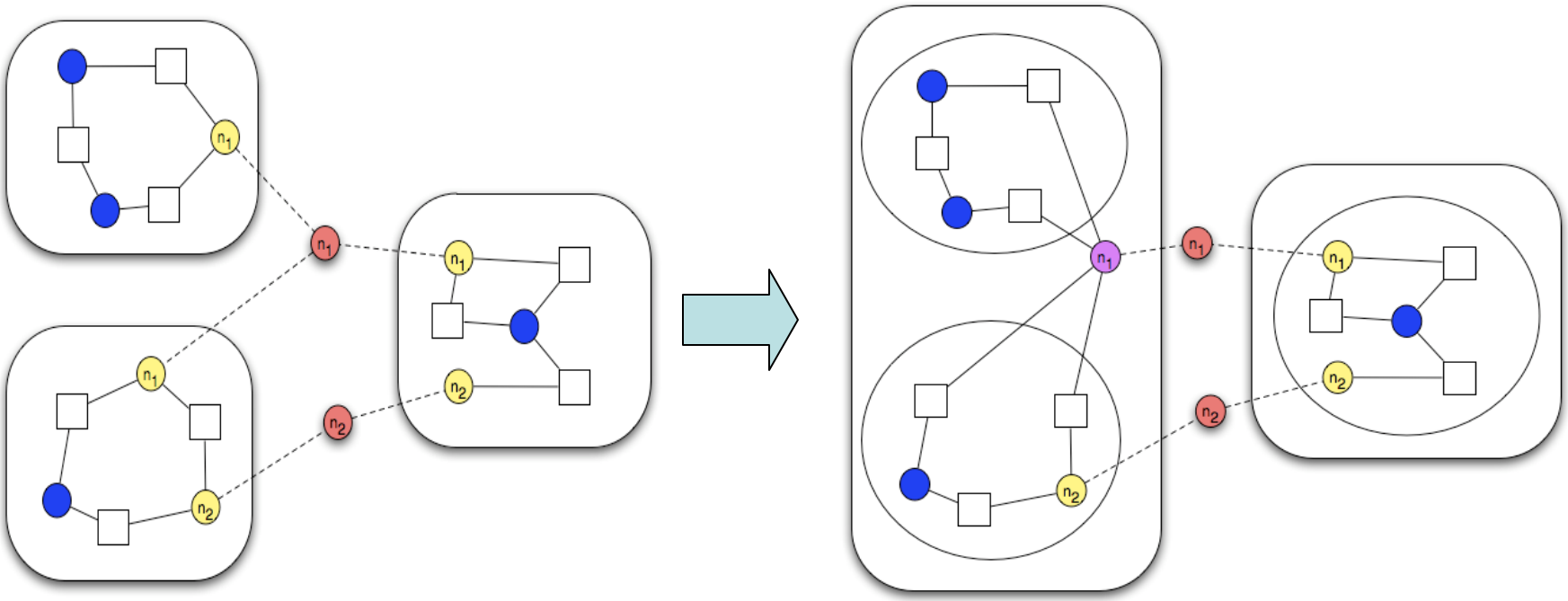
Hypergraph Formulation for Memory Management

- Formulation
  - Tasks -> vertices
  - Data -> Nets
  - No pre-assignment of nets to certain parts
  - Balance: Memory usage in the parts
    - Guarantees solution for some #parts, if it exists
  - Determine dynamically #parts
    - Modify the inherent recursive procedure of hypergraph partitioning.

Read-Once Partitioning

- Direct solution to above problem
  - Similar to approaches to parallelization
  - No refined reuse relationships
    - All tasks within a part have reuse, and none outside
- Read-Once Partitioning
  - Group tasks into steps
  - Identify data common across steps and load into memory
  - For each step, read non-common (step-exclusive) data, process tasks, and write/discard step-exclusive data
  - Better utilization of memory available -> reduced disk I/O

Read-Once Partitioning: Example



Disk I/O: 9 data elements

Disk I/O: 8 data elements

Summary

- Application-motivated approach to developing runtime support for scalable parallelism with global-address-space programming models
- Developing data and task abstractions that ease programming, but also achieve high performance
- Targeting systems with explicitly managed on-chip memory: Cell, GPGPU