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

\[
A3A = \frac{1}{2} (X_{ce,af} Y_{ae,cf} + X_{ce,af} Y_{ae,cf}) + X_{ce,af} Y_{ae,cf}
\]

\[
X_{ce,af} = t_{ij}^{ce} t_{ij}^{af}
\]

\[
Y_{ae,cf} = \langle ab\|ek\rangle \langle cb\|fk\rangle
\]

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

\[ hbar[a,b,i] = \sum[f[b,c]*t[i,j,a,c],{c}] - \sum[f[k,c]*t[i,j,a,c],{k,c}] +\sum[f[a,c]*t[i,j,c,b],{c}] - \sum[f[k,c]*t[i,j,a,b],{k,c}] - \sum[f[j,k,b,a],{k,c}] +\sum[f[a,b,c]*t[i,j,a,c],{c}] - \sum[f[k,a,b],{k,c}] \]

\[ +\sum[t[i,c]*t[j,d]*v[a,b,c,d],{c,d}] +\sum[t[i,c]*v[a,b,c,d],{c,d}] +\sum[t[i,j,c,d]*v[a,b,c,d],{c,d}] -\sum[t[i,c]*t[j,k,a,b],{k,c}] -\sum[t[i,c]*t[j,k,a,b],{k,c}] \]

\[ +\sum[t[i,c]*v[a,b,c,d],{c,d}] +\sum[t[i,c]*v[a,b,c,d],{c,d}] -\sum[t[i,j,c,d]*v[a,b,c,d],{c,d}] -\sum[t[i,c]*t[j,k,a,b],{k,c}] -\sum[t[i,c]*t[j,k,a,b],{k,c}] \]

\[ -\sum[t[i,c]*t[j,k,a,b],{k,c}] -\sum[t[i,c]*t[j,k,a,b],{k,c}] \]
<table>
<thead>
<tr>
<th>MADNESS</th>
<th>New quantum chemistry code from Robert Harrison</th>
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<tbody>
<tr>
<td></td>
<td>Multiresolution Adaptive Numerical Scientific Simulation</td>
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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 address 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