Parallel, Adaptive Scientific Computation in Heterogeneous, Hierarchical, and Non-Dedicated Computing Environments

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Yet another Powerpoint-free presentation!

Overview

- Why parallel computing?
 - solve larger problems in less time: clusters, supercomputers
 - recent trends: clock speed increases slowing, more processors per node
- Target computational paradigm: parallel adaptive methods
 - distributed data structures and partitioning
 - dynamic load balancing algorithms
 - load balancing software: Zoltan Toolkit
- Heterogeneous, hierarchical and non-dedicated computing environments
 - target environments, including Bullpen cluster
 - what can be adjusted? who can make the adjustments?
 - what can we do at just the load balancing step?
- Resource-aware parallel computation
 - Dynamic Resource Utilization Model (DRUM)
 - other approaches: hierarchical partitions, process migration, operating system migration





Participants

- Rensselaer Polytechnic Institute
 - Ph.D. students: Jamal Faik (now at Oracle), Luis Gervasio
 - Faculty: Joseph Flaherty
 - Undergraduates: Jin Chang
 - Various SCOREC students/postdocs/staff
- Sandia National Laboratories
 - Karen Devine and the Zoltan group
- Williams College undergraduates



- Most recent summers: Laura Effinger-Dean '06, Arjun Sharma '07, Bartley Tablante '07
- Previous: Kai Chen '04, Lida Ungar '02, Diane Bennett '03
- 2006 honors thesis student: Travis Vachon '06

Why Parallel Computation?

Parallelism adds complexity, so why bother?

Traditionally, there are two major motivations.



solve the same problem but in less time than on a single processor solve larger problems than could be solved *at all* on a single processor within time or space constraints

Recent Trends

• Until recently, computational scientists could assume that faster processors were always on the way



- Manufacturers are hitting the limits of current technology
- Focus now: multiple processors, hyperthreading, multi-core processors
- Today: dual core is common Soon: 4, 8 or more cores per chip
- Parallel computing is needed to use such systems effectively!

Figure used with permission from article *The Mother of All CPU Charts 2005/2006*, Bert Töpelt, Daniel Schuhmann, Frank Völkel, Tom's Hardware Guide, Nov. 2005, http://www.tomshardware.com/2005/11/21/the_mother_of_all_cpu_charts_2005/

Target Applications: Finite Element and Related Methods

- More elements \implies better accuracy, but higher cost
- Adaptivity concentrates computational effort where it is needed
- Guided by error estimates or error indicators
- h-adaptivity: mesh enrichment



- \bullet *p*-adaptivity: method order variation; *r*-adaptivity: mesh motion
- Local refinement method: time step adaptivity
- Adaptivity is essential

A Simple Adaptive Computation

Refine the underlying mesh to achieve desired accuracy



Parallel Strategy

- Dominant paradigm: Single Program Multiple Data (SPMD)
 - distributed memory; communication via message passing (usually MPI)
- Can run the same software on shared and distributed memory systems
- Adaptive methods lend themselves to linked structures
 - automatic parallelization is difficult
- Must explicitly distribute the computation via a domain decomposition





- Distributed structures complicate matters
 - interprocess links, boundary structures, migration support
 - very interesting issues, but not today's focus

Mesh Partitioning

• Determine and achieve the domain decomposition



- "Partition quality" is important to solution efficiency
 - evenly distribute mesh elements (computational work)
 - minimize elements on partition boundaries (communication volume)
 - minimize number of "adjacent" processes (number of messages)
- But.. this is essentially graph partitioning: "Optimal" solution intractable!

Why dynamic load balancing?

Need a rebalancing capability in the presence of:

- Unpredictable computational costs
 - Multiphysics
 - Adaptive methods









Initial balanced partition

Adaptivity introduces imbalance

Migrate as needed

Rebalanced partition

- Non-dedicated computational resources
- Heterogeneous computational resources of unknown relative powers

Load Balancing Considerations

- Like a partitioner, a load balancer seeks
 - computational balance
 - minimization of communication and number of messages
- But also must consider
 - cost of computing the new partition
 - * may tolerate imbalance to avoid a repartition step
 - cost of moving the data to realize it
 - * may prefer incrementality over resulting quality
- Must be able to operate in parallel on distributed input
 - scalability
- It is *not* just graph partitioning no single algorithm is best for all situations
- Several approaches have been used successfully

Geometric Mesh Partitioning/Load Balancing

Use only coordinate information

• Most commonly use "cutting planes" to divide the mesh



- Tend to be fast, and can achieve strict load balance
- "Unfortunate" cuts may lead to larger partition boundaries

- cut through a highly refined region

- May be the only option when only coordinates are available
- May be especially beneficial when spatial searches are needed
 - contact problems in crash simulations

Recursive Bisection Mesh Partitioning/Load Balancing

Simple geometric methods

• Recursive methods, recursive cuts determined by



- Simple and fast
- RCB is incremental
- Partition quality may be poor
- Boundary size may be reduced by a post-processing "smoothing" step

SFC Mesh Partitioning/Load Balancing

Another geometric method

- Use the locality-preserving properties of space-filling curves (SFCs)
- Each element is assigned a coordinate along an SFC
 - a linearization of the objects in two- or three-dimensional space





• Hilbert SFC is most effective





• Related methods: octree partitioning, refinement tree partitioning

Graph-Based Mesh Partitioning/Load Balancing Use connectivity information

Partition 3

Subdomain 4

- Spectral methods (Chaco)
 - prohibitively expensive and difficult to parallelize
 - produces excellent partitions
- Multilevel partitioning (Parmetis, Jostle)
 - much faster than spectral, but still more expensive than geometric
 - quality of partitions approaches that of spectral methods
- May introduce some load imbalance to improve boundary sizes

Load Balancing Algorithm Implementations

- Again, no single algorithm is best in all situations
- Some are difficult to implement
- Bad: implementation within an application or framework
 - likely usable only by a single application
 - at best, usable by a few applications that share common data structures
 - unlikely that an expert in load balancing is the developer
- Better: implementation within reusable libraries
 - load balancing experts can develop and optimize implementations
 - application programmers can make use without worrying about details
 - but...how to deal with the variety of applications and data structures?
 - * require specific input and output structures
 - applications must construct them
 - * data-structure neutral design
 - applications only need to provide a small set of callback functions

Zoltan Toolkit

Sandia

Includes suite of partitioning algorithms, developed at Includes algorithms

- General interface to a variety of partitioners and load balancers
- Application programmer can avoid the details of load balancing
- Interact with application through callback functions and migration arrays
 - "data structure neutral" design
- Switch among load balancers easily; experiment to find what works best
- Provides high quality implementations of:
 - Coordinate bisection, Inertial bisection
 - Octree/SFC partitioning (with Loy, Gervasio, Campbell RPI)
 - Hilbert SFC partitioning
 - Refinement tree balancing (Mitchell NIST)
 - Hypergraph partitioning
- Provides easier-to-use interfaces for:
 - Metis/Parmetis (Karypis, Kumar, Schloegel Minnesota)
 - Jostle (Walshaw Greenwich)
- Freely available: http://www.cs.sandia.gov/Zoltan/

Zoltan Toolkit Interaction with Applications



Typical Computation Flow



Example Parallel Adaptive Software

We wish to run several applications.

- Rensselaer's "LOCO"
 - parallel adaptive discontinuous Galerkin solution of compressible Euler equations in C.
 - using Parallel Mesh Database
 - "perforated shock tube" problem
- Rensselaer's "DG"
 - also discontinuous Galerkin methods, but in C++
 - using Algorithm-Oriented Mesh Database
 - Rayleigh-Taylor flow instabilities and others
- Mitchell's PHAML
 - Fortran 90, adaptive solutions of various PDEs
- Simmetrix, Inc. MeshSim-based applications
- Real interest for parallel computing is in 3D transient problems



Target Computational Environments

- FreeBSD Lab, Williams CS: 12 dual hyperthreaded 2.4 GHz Intel Xeon processor systems
- *Bullpen Cluster*, Williams CS: 13 node Sun cluster, total of 4 300 MHz and 21 450 MHz UltraSparc II processors
- *Dhanni Cluster*, Williams CS: 14 nodes, 8 with 2 hyperthreaded 2.8 GHz Intel Xeon processors, 2 with 2 dual-core hyperthreaded 2.8 GHz Intel Xeon processors, 1 with dual hyperthreaded 2.4 GHz Intel Xeon processor (compile node), and 3 with 1 1GHz Intel Pentium III
- *Medusa Cluster*, RPI: 32 dual 2.0GHz Intel Xeon processor systems
- ASCI-class supercomputers: large clusters of SMPs
- Grid computers "clusters of clusters" or "clusters of supercomputers"

This is just a small sample of the wide variety of systems in use.

- long-term "resource-aware computation" goal: software that can run efficiently on any of them
- work described here is one step toward this goal, current focus on systems found at places like Williams

Resource-Aware Computing Motivations

- Heterogeneous processor speeds
 - seem straightforward to deal with
 - does it matter? computation proceeds only as fast as the *slowest* process
- Distributed vs. shared memory
 - some algorithms may be a more appropriate choice than others
- Non-dedicated computational resources
 - can be highly dynamic, transient
 - will the situation change by the time we can react?
- Heterogeneous or non-dedicated networks
- Hierarchical network structures
 - message cost depends on the path it must take
- Relative speeds of processors/memory/networks
 - important even when targeting different homogeneous clusters

What Can Be Adjusted?

- Choice of solution methods and algorithms
 - different approaches for multithreading vs. distributed memory
- Parallelization paradigm
 - threads vs. message passing vs. actor/theater model vs. hybrid approaches
 - "bag-of-tasks" master/slave vs. domain decomposition
- Ordering of computation and/or communication
- Replication of data or computation
- Communication patterns (*e.g.*, message packing)
- Optimal number of processors, processes, or threads
 - not necessarily one process/thread per processor
- Our focus: partitioning and dynamic load balancing
 - tradeoffs for imbalance vs. communication volume
 - variable-sized partitions
 - avoid communication across slowest interfaces

Bullpen Cluster at Williams College





All nodes contain (aging) Sun UltraSparc II processors http://bullpen.cs.williams.edu/

Resource-Aware Load Balancing

- Goal: account for environment characteristics in load balancing
- Idea: build a model of the computing environment and use it to guide load balancing
 - represent heterogeneity and hierarchy
 - * processor heterogeneity, SMP
 - * network capabilities, load, hierarchy
 - static capability and dynamic monitoring feedback
- Use existing load balancing procedures to produce, as appropriate
 - variable size partitions
 - "hierarchical" partitions
- Longer-term: tailor other parts of the computation to the environment
- Alternate approach: process-level or system-level load balancing



- Run-time model encapsulates the details of the execution environment
- Supports dynamic load balancing for environments with
 - heterogeneous processing capabilities
 - heterogeneous network speeds
 - hierarchical network topology
 - non-dedicated resources
- Not dependent on any specific application, data structure, or partitioner

http://www.cs.williams.edu/drum/

Computation Flow with DRUM monitoring





- Tree structure based on network hierarchy
- Computation nodes, assigned "processing power"
 - UP uniprocessor node
 - SMP symmetric multiprocessing node
- Communication nodes
 - network characteristics (bandwidth, latency)
 - assigned a processing power as a function of children

- Static capabilities
 - gathered by benchmarks or specified manually once per system
 - processor speeds, network capabilities and topology
- Dynamic performance monitoring
 - gathered by "agent" threads managed through a simple API
 - communication interface (NIC) monitors
 - * monitor incoming and outgoing packets and/or available bandwidth
 - CPU/Memory monitors
 - * monitors CPU and memory usage and availability
- Combine static capability information and dynamic monitoring feedback
- Straightforward to use powers to create weighted partitions with existing procedures
- Optional Zoltan interface allows use by applications with no modifications
- More details and computational results in recent papers: *Applied Numerical Mathematics*, 52(2-3), pp. 133-152, 2005 *Computing in Science & Engineering*, 7(2), pp. 40-50, 2005

DRUM Setup and Configuration

- DRUM needs some information about the environment to construct its model
- Some may be detected at run time, some must be specified
- DRUM reads a "cluster description file" in XML format

```
<machinemodel>
<machinemodel>
<machinemodel>
<mode type="NETWORK" nodenum="0" name="" IP="" isMonitorable="false"
parent="-1" imgx="361.0" imgy="52.0">
<lbmethod lbm="HSFC" KEEP_CUTS="1"></lbmethod></mode>
<mode type="SINGLE_COMPUTING" nodenum="2" name="mendoza.cs.williams.edu"
IP="137.165.8.140" isMonitorable="true" parent="0"
benchmark="52.43" imgx="50.0" imgy="138.0"></mode>
<mode type="MULTIPLE_COMPUTING" nodenum="3" name="rivera.cs.williams.edu"
IP="137.165.8.130" isMonitorable="false" parent="0"
imgx="74.64" imgy="263.0" benchmark="82.55" numprocs="4">
```

- XML file needs only be updated if the cluster changes
- Arjun Sharma project Summer '04: improve generation of these files

DRUMhead: Model Creation Tool



- Build topology description
- Run benchmark suite to determine static capabilities
- Specify hierarchical balancing parameters
- Write XML file description

DRUM Monitoring Capabilities

- DRUM needs to gather performance statistics at run time
- Some available through kernel statistics

- specific to Solaris and Linux

• Some available through Simple Network Management Protocol (SNMP)

– not all environments make SNMP information available

- Similar information is available through the Network Weather Service (NWS)
 DRUM can use NWS information (Laura Effinger-Dean, Summer '04)
- DRUM's modular design allows other monitoring tools to be used in the future

- Straightforward to give less work to slower or busy processors
- Idea: also give less work to processes that communicate over slow or busy network interfaces
- Compute the "power" for a process as the weighted sum

 $power = w^{comm}c + w^{cpu}p, \quad w^{comm} + w^{cpu} = 1$

of processing power \boldsymbol{p} and communication power \boldsymbol{c}

- how to choose p and c?
- how to choose weights?
- can we do something better than a weighted sum?
- Processing power based on static benchmark plus monitored CPU usage and idle times
- Communication power based on interface packet counts or available bandwidth measures
- Communication and processing weights currently set manually

- Processing power, $p_{n,j}$, for process j on node n based on:
 - the node's "MFLOPS" rating obtained from benchmarking, b_n
 - per-process CPU utilizations, $u_{n,j}$
 - usable idle time
 - \ast monitor fraction of idle time of CPU t (of m CPUs in node), i_t
 - * compute the overall idle time in node n, $\sum_{t=1}^{m} i_t$
 - * compute total usable idle time on node n, $\min(k_n \sum_{j=1}^{k_n} u_{n,j}, \sum_{t=1}^m i_t)$
 - Compute average CPU usage and idle times per process:

$$\overline{u}_n = \frac{1}{k_n} \sum_{j=1}^{k_n} u_{n,j}, \quad \overline{i}_n = \frac{1}{k_n} \min(k_n - \sum_{j=1}^{k_n} u_{n,j}, \sum_{t=1}^m i_t)$$

- processing power estimated as:

$$p_{n,j} = b_n(\overline{u}_n + \overline{i}_n), \ j = 1, 2, \dots, k_n$$

- Communication power, c_n , for interface *i* (of *s* interfaces) based on:
 - communication activity factor, $CAF_{n,i}$
 - software loopback interfaces and interfaces with CAF = 0 are ignored

$$c_n = \frac{1}{\frac{1}{s}\sum_{i=1}^{s} CAF_{n,i}}$$

- or, NWS-measured "available bandwidth" (Effinger-Dean, Summer '04)
- Effectively just need a way to specify *relative* communication powers
- Considering other ways to determine a communication power and weight

DRUM: Early Computational Example

- Execution environment
 - eight processors of Williams College "Bullpen" cluster
 - five "fast" (450MHz), three "slow" (300MHz) processors
- Computation
 - 2D discontinuous Galerkin solution of R-T instability
 - 200 adaptive mesh refinement/rebalancing steps
 - maximum of 6320 elements
- DRUM resource-aware load balancing results
 - assigning 50% more work to fast nodes: theoretical 24% improvement
 - straightforward Octree/SFC partitioning: 9507 seconds
 - dynamic monitoring and partition-weighted Octree/SFC: 7351 seconds
 - 22.6% improvement, 94.1% of theoretical



Example results on a heterogeneous cluster

- Using Mitchell's PHAML software to solve 2D Laplace equation
- Combination of "fast" (450 MHz) and "slow" (300 or 333 MHz) processors
 - 2, 4, 6, 8 fast processors
 - -0, 2, 4 slow processors
- Adaptive simulation for 17 refinement steps, resulting in 524,500 nodes
- \bullet Straightforward DRUM-aware HSFC partitioning used, vary w^{comm}



DRUM on a Heterogeneous Cluster



- Runs on a homogeneous subset of nodes indicate low overhead
- Adding 2 or 4 "slow" nodes to a run on "fast" nodes slows the computation without DRUM, but with DRUM these processors can be used effectively
- Here, accounting for communication ($w^{comm} > 0$) is usually not helpful
 - the computation is latency-dominated

DRUM on a Heterogeneous Cluster



- Grey bars: "ideal" relative change speedup we could get under perfect conditions by accounting only for processor speeds
- Red bars show best achieved on each combination of nodes across all attempted w^{comm} values
- A significant part of the ideal change is achieved

Example computation in a dynamic system

- Same cluster and application parameters, *but*
 - external computational load on nodes running two of the processes
- Demonstrates DRUM's dynamic capabilities
- DRUM dynamically adjusts the powers appropriately



Modified Bullpen Cluster

When is a non-zero communication weight beneficial?



Four nodes removed from the main network and connected to the rest of the cluster through a slower 10Mbit Ethernet hub

Communication Weight Study

- Three-dimensional perforated shock tube problem on modified cluster
 - 4 processes on nodes connected to main switch
 - 4 processes on nodes connected to slower switch
- Vary communication weight w^{comm}



Communication Weight Study

- Best w^{comm} values in the 0.30-0.33 range
- More examples with finer adjustments to w^{comm}
- With $w^{comm} = 0.315$, processes on nodes connected to slow switch assigned power 0.09, others assigned 0.15



Hierarchical Partitioning and Load Balancing

• Goal:

- use different algorithms in different parts of the execution environment

- tailor mesh (or other) partitions for network hierarchy, SMP nodes



- Takes advantage of characteristics of available procedures
 - graph partitioners such as those in Parmetis
 - * minimize inter-partition boundaries, but may introduce imbalance
 - geometric methods such as inertial recursive bisection
 - * achieve strict balance, but may have large boundaries
 - studies with Ungar and Bennett at Williams
- Need ability to produce: variable-sized partitions, $k \neq p$ partitions

Hierarchical Load Balancing with the Zoltan Toolkit



- IHBS = internal hierarchical balancing structure
 - Parmetis-style arrays, augmented to maintain internal migration
- Can do any number of levels and use any combination of procedures
- Application is not modified; existing Zoltan procedures are not modified
- In Zoltan development version, expected to include in next release

Hierarchical Load Balancing



Strict BalanceMinimize BoundaryMixedMixed

- 1,103,018-element mesh of human arteries, partitioned using RIB and Parmetis
- Minimize communication across slow networks, balance strictly within SMPs

- for the 2 8-way node case, only 0.3% of faces are on "slow" boundary

Dhanni Cluster at Williams College





Legend: DC=dual core, HTT=hyperthreaded Blue nodes have 4 logical processors, red nodes have 8 logical processors

Processor Heterogeneity on Dhanni

- "Slow" vs. "Fast" nodes same issues as Bullpen
- But... hyperthreaded and multi-core nodes

Hyperthreading enabled

- A hyperthreaded processor appears to the OS as 2 "logical" processors

Hyperthreading disabled



Hyperthreading must be enabled/disabled in system BIOS before bootup

Processor Heterogeneity on Dhanni

- How does hyperthreading come into play?
 - Benefit of better hardware utilization must outweigh costs of cache misses
 - Initial tests with DRUM's 3D Cellular Automata example program
 - With hyperthreading disabled (in system BIOS):

4 nodes, 1 processes per node: 182.1 seconds 4 nodes, 2 processes per node: 91.9 seconds

– With hyperthreading enabled:

4 nodes, 1 processes per node: 182.4 seconds 4 nodes, 2 processes per node: 142.5 seconds 4 nodes, 3 processes per node: 110.1 seconds 4 nodes, 4 processes per node: 82.1 seconds

- Expectation: effect of hyperthreading can be difficult to predict
- Expectation: DRUM's dynamic monitors will "do the right thing"

Ongoing and Future Work in DRUM

- Apply DRUM to other applications (volunteers? *terescoj@cs.williams.edu*)
- Further DRUM management of the computation triggering load balancing
- Prepare a public release of DRUM (currently available by request)
- Apply to Grid environments
 - more heterogeneity: more need for and more benefit from DRUM
 - more hierarchy: hierarchical balancing
 - take advantage of other Grid-aware discovery and monitoring tools
- Hyperthreaded and dual-core nodes
 - test current DRUM version in these environments
 - enhance DRUM for such environments discovery, benchmarks
 - hierarchical partitions?

Balancing at Other Levels

- Process-level load balancing
 - migrate MPI processes among computing nodes
 - developing middleware MPI/IOS system with Varela and ElMaghraoui (RPI)
 - * uses MPI-2 functionality to migrate MPI processes
 - * migrate processes only at "convenient" times for the application using Process Checkpoint and Migration (PCM) library
 - migration is expensive
 - support for transient environments
- System-level load balancing
 - migrate entire virtual operating systems, enabled by Xen project
 - migration is expensive, but migrating systems can continue operating until the final step
 - just-completed senior honors thesis by Travis Vachon
 - initial focus on data center environments, but is this appropriate for HPC applications?

Closing Remarks

- Accounting for heterogeneity and hierarchy can improve efficiency
- DRUM and hierarchical balancing software are not dependent on specific application software or mesh structures
 - DRUM is a standalone library (but works well with Zoltan)
 - HIER is part of the Zoltan Toolkit
- DRUM and hierarchical balancing can be transparent to applications
- Tools like DRUM more important in more heterogeneous environments
- Heterogeneity was intentional here but will arise over time as nodes are added to clusters
 - "one man's trash is another man's new cluster node"
 - multi-core and hyperthreaded processors
 - also think of networks of workstations, grid environments
- Focus to date on application-level load balancing, but process- and systemlevel balancing may be appropriate in some circumstances

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