High Performance Multi-Paradigm Messaging Runtime Integrating Grids and Multicore Systems

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Abstract

eScience applications need to use distributed Grid environments where each component is an individual or cluster of multicore systems. These are expected to have 64-128 cores 5 years from now and the need to support scalable parallelism. We expect users will want to compose heterogeneous components into single jobs and run seamlessly in both distributed fashion and on a future "Grid on a chip" with different subsets of cores supporting individual components. We propose an elegant programming model exhibiting the "efficiency" and "productivity" layers in Patterson's description of the Berkeley approach to parallel computing [1]. The efficiency layer finds traditional high performance parallel computing paradigms including OpenMP, MPI, dynamic threading and discrete event simulation. The "productivity" layer accessible to a broader range of programmers can be implemented in many ways including scripting, MapReduce [2], service workflow and Web 2.0 Mashups. In this paper, we look at a Cheminformatics application where compute intensive services running on multicore systems are linked together and to data sources such as PubChem and to visualization interfaces. A common underlying runtime that supports the different paradigms in each layer appears to be one important part of future computing environments integrating grid and multicore parallelism. Here we examine CCR or the Concurrency and Coordination Runtime from Microsoft as a multi-paradigm runtime

supporting It is an attractive multi-paradigm candidate as it was designed to support general dynamic message "efficiency layer" patterns with high performance and already has a distributed "productivity layer" runtime known as DSS (Decentralised Software Services) built on top of it. Here we present performance measurements on 4 and 8 core systems for MPIstyle, dynamic threading and workflow. Our work uses managed code (C#) and our results on AMD and Intel processors show around a factor of 5 better performance than Java (for MPJ [3] and Axis2) with MPI pattern and dynamic threading latencies of a few microseconds. We are building a suite of data mining services using these ideas which will further test the runtime and suggest extensions to MPI to support the rich messaging needed in this hybrid Grid-multicore environment.

1. Introduction

Grids and multicore [4-6] systems are contemporary technologies that will have great impact on eScience. Grids integrate the myriad of distributed resources needed by modern science and multicore will certainly allow very high performance simulation engines. However multicore is also a dominant feature of the next generations of commodity systems and this will motivate a new generation of software environments that will address commodity client and server applications and programmers at the "efficiency" and "productivity" layers. Future client systems are not likely to need large scale

simulations and an analysis by Intel [7] identifies gaming and more broadly datamining as critical client-side applications with latter including speech, image and video analysis as well processing of local sensors and data fetched the web. These datamining algorithms often use "classic" scientific algorithms for matrix arithmetic or optimization at their core and will need good support for both dynamic threads and MPI style loosely synchronous applications [8]. We note that it will be the data deluge that drives eScience in the large and the commodity software on the multicore "small". Note that almost certainly the software environments developed for commodity multicore systems will be the most attractive for (specialized) eScience applications due to the excellent support for commodity software. We follow the model proposed by Berkeley [1] and indeed used traditionally in parallel computing with a few experts working at the "efficiency" layer building libraries (packaged as services) that implement good parallel algorithms. We see excellent approaches several to the "productivity" layer which was often termed coarse grained functional parallelism in the old literature and supported by systems like AVS, Khoros, SciRUN and HeNCE [9]. Nowadays workflow, Mashups, MapReduce [2], or just scripting languages provide popular productivity models and we expect these to improve but no breakthroughs are needed to provide a good programming model at this layer. We believe that the efficiency layer still needs much work and we need to integrate support for it with the productivity laver and between the different models in the efficiency layer; these include MPI style, threading and discrete event simulations built on dynamic threading. This motivates our research which is looking at a variety of datamining algorithms and the underlying runtime which allow jobs to be composed from multiple, data sources and visualizations and to run efficiently and seamlessly either internally to a single CPU or across a tightly coupled cluster or distributed Grid. In this paper we focus on one part of this puzzle - namely investigating the runtime that could span these different environments and different platforms that would be used by the expected heterogeneous composite applications. Note that managed code will be important for desktop commodity applications and so C# (mainly used here) and Java (only a quick comparison here) could become more important than now for parallel programming.

We first present the Cheminformatics example a powerful with clustering datamining application. This would traditionally use MPI but here we use the CCR runtime running in MPI mode. CCR [10-11] was designed for robotics applications [12] but also investigated [13] as a general programming paradigm. CCR supports efficient thread management for handlers (continuations) spawned in response to messages being posted to ports. The ports (queues) are managed by CCR which has several primitives supporting the initiation of handlers when different message/port assignment patterns are recognized. Note that CCR supports a particular flavor of threading where information is passed by messages allowing simple correctness criteria. However this paper is not really proposing a programming model but examining a possible low level runtime which could support a variety of different parallel programming models that would map down into it. In particular the new generation of parallel languages [14] from Darpa's HPCS High Productivity Computing System program supports the three execution styles (dynamic threading, MPI, coarse grain functional parallelism) we investigate here.

	Table 1: Machines Used
Ī	AMD4: HPxw9300 workstation, 2 AMD Opteron
	CPUs Processor 275 at 2.19GHz, L2 Cache 4x1MB,
	Memory 4GB, XP Pro 64bit 4 cores
	Benchmark Computational unit: 1.388 µs
Ī	Intel4: Dell Precision PWS670, 2 Intel Xeon CPUs at
	2.80GHz, L2 Cache 2x2MB, Memory 4GB, XP Pro
	64bit 4 cores
	Benchmark Computational unit: 1.475 µs
Ī	Intel8A: Dell Precision PWS690, 2 Intel Xeon CPUs
	E5320 at 1.86GHz, L2 Cache 4x2M, Memory 8GB,
	XP Pro 64bit 8 cores
	Benchmark Computational unit: 1.696 µs
Ī	Intel8B: Dell Precision PWS690, 2 Intel Xeon CPUs
	x5355 at 2.66GHz, L2 Cache 4x2M, Memory 4GB,
	Vista Ultimate 64bit 8 cores
	Benchmark Computational unit: 1.188 µs

We used four machine types in this study with details recorded above in table 1. Each machine had two processors; one used the AMD dual core Opteron, one dual Intel Xeons and there were two models of quad core Intel Xeons. As well as basic hardware, the table indicates performance on a computational unit used in performance test.

In the next section, we discuss the clustering application and then in section 3 CCR and DSS. Section 4 defines more precisely our three execution models. Section 5 presents our basic

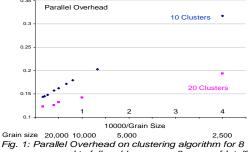
performance results that suggest one can build a single runtime that supports the different execution models and so implement the hybrid productivity-efficiency environment. Future work and conclusions are in section 6.

3. Clustering

Clustering on chemical properties is an important tool [15] for finding for example a set of chemicals similar to each other and so likely candidates for a given drug. We present in fig. 1, initial results from a parallel clustering implemented on the 8 core Intel machine labeled Intel8A in table 1. We chose an improved Kmeans [16] algorithm whose structure can be straightforwardly parallelized using MPI style programming. This method [17] uses a multiscale approach to avoid false minima and has a parallel overhead [18] that decreases asymptotically like 1/grain size as the data set increases. Here grain size is the dataset size divided by the number of processors (cores) which is here 8. Putting T(n) as the execution time on n cores. we can define

> Overhead f = (PT(P)-T(1))/T(1)Efficiency $\varepsilon = 1/(1+f)$

Note that the advent of multicore systems is likely to prompt a re-examination of algorithms with preference being given to those that can be efficiently parallelized. Our results required arrangement of data in memory to avoid any interference in cache lines accessed by different cores; such interference increased memory traffic and produced factors of 2 variations in runtime. The presented results in fig. 1 are reproducible and show overheads decreasing (efficiency tending to 1 and speedups to 8) as the grain size increases.



cores compared to full problem run on 8 cores of Intel8a. Results for 10 and 20 cluster problems are shown

The detailed analysis is affected by cache issues which we will discuss elsewhere. Further these results use CCR for all inter process communication and messaging and will improve when we have finished primitives optimized for multicore systems for the equivalent of MPI reduction operations. These initial results confirm that we can get good performance with CCR and are encouraging for the basic strategy of building a suite of high performance datamining algorithms with CCR. Now we look in detail at CCR and DSS performance (DSS encapsulates this clustering application in the "productivity" layer) so we can compare with more familiar technology.

3. Overview of CCR and DSS

CCR provides a framework for building general collective communication where threads can write to a general set of ports and read one or more messages from one or more ports. The framework manages both ports and threads with optimized dispatchers that can efficiently iterate over multiple threads. All primitives result in a task construct being posted on one or more queues, associated with a dispatcher. The dispatcher uses OS threads to load balance tasks. The current applications and provided primitives support what we call the dynamic threading model with capabilities that include:

- 1) *FromHandler:* Spawn threads without reading ports
- 2) *Receive:* Each handler reads one item from a single port
- 3) *MultipleItemReceive:* Each handler reads a prescribed number of items of a given type from a given port. Note items in a port can be general structures but all must have same type.
- 4) *MultiplePortReceive:* Each handler reads a one item of a given type from multiple ports.
- 5) *JoinedReceive:* Each handler reads one item from each of two ports. The items can be of different type.
- 6) *Choice:* Execute a choice of two or more port-handler pairings
- 7) Interleave: Consists of a set of arbiters (port -- handler pairs) of 3 types that are Concurrent, Exclusive or Teardown (called at end for clean up). Concurrent arbiters are run concurrently but exclusive handlers are not.

One can spawn handlers that consume messages as is natural in a dynamic search application where handlers correspond to links in a tree. However one can also have long running handlers where messages are sent and consumed at a rendezvous points (yield points in CCR) as used in traditional MPI applications. Note that "active messages" correspond to the spawning model of CCR and can be straightforwardly supported. Further CCR takes care of all the needed queuing and asynchronous operations that avoid race conditions in complex messaging. For this paper, we did use the CCR framework to build a custom optimized collective operation corresponding to the MPI "exchange" operation but used existing capabilities for the "reduce" and "shift" patterns. We believe one can extend this work to provide all MPI messaging patterns.

Note that all our work was for managed code in C# which is an important implementation language for commodity desktop applications although slower than C++. In this regard we note that there are plans for a C++ version of CCR which would be faster but prone to traditional un-managed code errors such as memory leaks, buffer overruns and memory corruption. CCR is very portable and runs on both CE (small devices) and desktop windows.

DSS sits on top of CCR and provides a lightweight, REST oriented application model that is particularly suited for creating coarse grain applications in the Web-style as compositions of services running in a distributed environment. Services are isolated from each other, even when running within the same node and are only exposed through their state and a uniform set of operations over that state. The DSS runtime provides a hosting environment for managing services and a set of infrastructure services that can be used for service creation. discovery, logging, debugging, monitoring, and security. DSS builds on existing Web architecture and extends the application model provided by HTTP through structured data manipulation and event notification. Interaction with DSS services happen either through HTTP or DSSP [19] which is a SOAP-based protocol for managing structured data manipulations and event notifications

4. MPI and the 3 Execution Models

MPI – Message Passing Interface – dominates the runtime support of large scale parallel applications for technical computing. It is a complicated specification with 128 separate calls in the original specification [20] and double this number of interfaces in the more recent MPI-2 including support of parallel external I/O [21-22]. MPI like CCR is built around the idea of concurrently executing threads (processes, programs) that exchange information by messages. In the classic analysis [18, 23-25], parallel technical computing applications can be divided into four classes:

- a) **Synchronous** problems where every process executes the same instruction at each clock cycle. This is a special case of b) below and only relevant as a separate class if one considers SIMD (Single Instruction Multiple Data) hardware architectures.
- b) Loosely Synchronous problems where each process runs different instruction streams (often using the same program in SPMD mode) but they synchronize with the other processes every now and then. Such problems divide into stages where at the beginning and end of each stage the processes exchange messages and this exchange provides the needed synchronization that is scalable as it needs no global barriers. Load balancing must be used to ensure that all processes execute for roughly (within say 5%) the same time in each phase and MPI provides the messaging at the beginning and end of each stage. We get at each loose synchronization point a message pattern of many overlapping joins that is not usually seen in commodity applications and represents a new challenge.
- c) **Embarrassingly or Pleasingly parallel** problems have no significant inter-process communication and are often executed on a Grid.
- d) Functional parallelism leads to what were originally called metaproblems that consist of multiple applications, each of which is of one of the classes a), b), c) as seen in multidisciplinary applications such as linkage of structural, acoustic and fluid-flow simulations in aerodynamics. These have a coarse grain parallelism.

Classes c) and d) today would typically be implemented as a workflow using services to represent the individual components. Often the components are distributed and the latency requirements are typically less stringent than for synchronous and loosely synchronous problems. We view this as functional parallelism corresponding to the "productivity layer" and use DSS already developed for Robotics [10] on top of CCR for this case and idealized in fig. 2(a). Note in this paper, we only discuss run-time and do not address the many different ways of expressing the "productivity layer" i.e. we are discussing runtime and not languages.

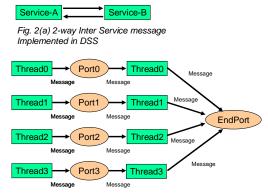


Fig. 2(b) Pipeline of Spawned Threads followed by a Reduction implemented using CCR Interleave

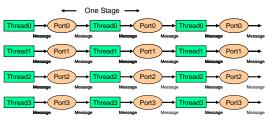


Fig. 3: Illustration of multiple stages used in CCR Performance Measurements

We use CCR in a mode where multiple identical stages are executed and the run is completed by combining the computations with a simple CCR supported reduction as shown in fig. 2(b). This also illustrates the simple Pipeline Spawn execution that we used for basic performance measurements of the dynamic threading performance. Each thread writes to a single port that is read by a fresh thread as shown in more detail in fig. 3.

We take a fixed computation that takes from 12 to 17 seconds $(10^7 \text{ stages of time complexity})$ listed in table 1) depending on hardware and execution environment to run sequentially on the machines we used in this study. This computation was divided into a variable number of stages of identical computational complexity and then the measurement of execution time as a function of number of stages allows one to find the thread and messaging overhead. Note that the extreme case of 10^7 stages corresponds to the basic unit execution times of 1.188 to 1.696 µs given in table 1 and is a stringent test for MPI style messaging which can require microsecond level latencies. We concentrated on small message payloads as it is the latency (overhead) in this case that is the critical problem. As multicore systems have shared memories, one would often use handles in small messages rather than transferring large payloads.

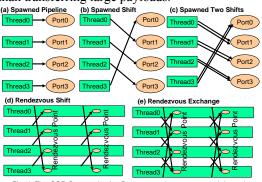


Fig. 4: Five CCR Communication Patterns used to test spawned dynamic threading (a,b,c) and MPI style Rendezvous's (d,e) and shown for 4 cores

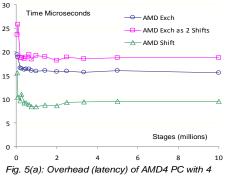
We looked at three different message patterns for the dynamic spawned thread case choosing structure that was similar to MPI to allow easier comparison of the rendezvous and spawned models. These spawned patterns are illustrated in fig. 4(a-c) and augment the pipeline of fig. 2(b) and 2 with a "nearest neighbor" shift with either one or two messages written to ports so we could time both the *Receive* and *MultiItemReceive* modes of CCR. We note that figures 2 to 4 are drawn for 4 cores while our tests used both 4 and 8 core systems.

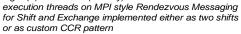
For our test of the final execution style, namely the MPI style runtime, we needed rendezvous semantics which are fully supported by CCR and we chose to use patterns corresponding to the MPI SENDRECV interface with either toroidal nearest neighbor shift of fig. 4(d) or the combination of a left and right shift, namely an exchange, shown in fig. 4(e). Note that posting to a port in CCR corresponds to a MPISEND and the matching MPIRECV is achieved from arguments of handler invoked to process the port. MPI has a much richer set of defined methods that describe different synchronicity options, various utilities and collectives. These include the multi-cast (broadcast, gather-scatter) of messages with the calculation of associative and commutative functions on the fly. It is not clear what primitives and indeed what implementation will be most effective on multicore systems [1, 26] and so we only looked at a few simple but representative cases in this initial study. In fact it is possible that our study which suggests one can support in the same framework a set of execution models that is broader than today's MPI, could motivate a new

look at messaging standards for parallel computing.

5. Performance of CCR in 3 Execution Models

5.1 CCR Message Latency and Overhead





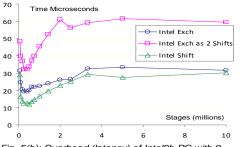


Fig. 5(b): Overhead (latency) of Intel8b PC with 8 execution threads on MPI style Rendezvous Messaging for Shift and Exchange implemented either as two shifts or as custom CCR pattern

We performed detailed benchmark measurements on 3 machines labeled AMD4 Intel4 and Intel8b in table 1 with results shown in table 2 and figs. 5(a) and (b). Table

2 looks at seven messaging modes shown in fig. 3 with rendezvous exchange implemented either as two separate shifts or as a custom CCR primitive which is faster especially on Intel8b. We also show pipeline implemented in both spawned and rendezvous fashion. The results correspond to a computation stage between messaging that is 20 times the values of table 1 i.e. from 23 (Intel8b) to 29 μ s(Intel4). The newer Intel8b on 8 cores shows significantly lower overheads than the older Intel4 on 4 cores and the AMD4 Opteron on 4 cores has slightly lower overheads than Intel8b on 8 cores.

We see the dynamic threading has an overhead that is around 5 μ s for pipeline and shift for both AMD4 and Intel8b on 4 or 8 cores respectively. The MPI style rendezvous overheads increase to

9.36(11.74) μ s for Shift and 16.3(20.16) μ s for the optimized exchange operation on AMD4 (Intel8b) on 4(8) cores. We have performed identical measurements on the recent MPJ [3] on AMD4 which gives overheads of 185 μ s for Rendezvous and 104 μ s for Shift with the full MPI. It appears that C# is the by far the fastest managed code for messaging.

Table 2: Overheads per stage for CCR patterns on 0.5 million stages									
	MD4: 4 Core	Number of Parallel Computations							
- Al	(µs)	1	2	3	4	7	8		
pa	Pipeline	1.76	4.52	4.4	4.84	1.42	8.54		
wne	Shift	1.70	4.48	4.62	4.8	0.84	8.94		
Spawned	Two Shifts		7.44	8.9	10.18	12.74	23.92		
	Pipeline	3.7	5.88	6.52	6.74	8.54	14.98		
NOI	Shift		6.8	8.42	9.36	2.74	11.16		
Rendezvous	Exchange As Two Shifts		14.1	15.9	19.14	11.78	22.6		
В	Exchange		10.32	15.5	16.3	11.3	21.38		
In	ntel4: 4 Core	Number of Parallel Computations							
	(µs)	1	2	3	4	7	8		
ned	Pipeline	3.32	8.3	9.38	10.18	3.02	12.12		
Spawned	Shift		8.3	9.34	10.08	4.38	13.52		
Sp_{0}	Two Shifts		17.64	19.32	21	28.74	44.02		
s	Pipeline	9.36	12.08	13.02	13.58	16.68	25.68		
non	Shift		12.56	13.7	14.4	4.72	15.94		
Rendezvous	Exchange As Two Shifts		23.76	27.48	30.64	22.14	36.16		
Re	Exchange		18.48	24.02	25.76	20	34.56		
In	tel8b: 8 Core	Number of Parallel Computations							
	(µs)	1	2	3	4	7	8		
Spawned	Pipeline	1.58	2.44	3	2.94	4.5	5.06		
awı	Shift		2.42	3.2	3.38	5.26	5.14		
Sp	Two Shifts		4.94	5.9	6.84	14.32	19.44		
sn	Pipeline	2.48	3.96	4.52	5.78	6.82	7.18		
0/2	Shift		4.46	6.42	5.86	10.86	11.74		
Rendezvous	Exchange As Two Shifts		7.4	11.64	14.16	31.86	35.62		
R	Exchange		6.94	11.22	13.3	18.78	20.16		
	Figure 5 explores the dependence of the								

Figure 5 explores the dependence of the overhead on the number of stages for the MPI style rendezvous case i.e. on the amount of computation between each message with the extreme case of 10^7 stages corresponding to the 1.388 (1.188) µs computation value between messages of table 1 for AMD4 (Intel8b). The overheads remain reasonable even in these extreme conditions showing that an intense number of small messages will not be a serious problem. This fig. emphasizes that the CCR custom exchange (marked just Exch) can be much faster than the exchange implemented as a left followed by right shift (Marked Exch as 2 Shifts).

5.2 DSS Message Latency and Overhead

We now examine CCR for the third form of parallelism; namely the functional parallelism model represented in fig. 1(a). The Robotics release [12] includes a lightweight service environment DSS built on top of CCR and we performed an initial evaluation of DSS on the AMD4 machine. We time groups of requestresponse two way messages running on (different) cores of the AMD system. We find average times of 30-50 microseconds or throughputs of 20,000 to 25,000 two-way messages per second after initial start up effects are past. This result of internal service to internal service can be compared with Apache Axis 2 where the AMD PC supports about 3,000 messages per second throughput. This is not an entirely fair comparison as the measurements are internal to one machine so each service end-point has effectively just two cores. The Axis measurements used external clients interacting on a LAN so there is network overhead but now the service can access the full 4 cores. We will give more complete comparisons later and also examine the important one-way messaging case.

6. Conclusions and Futures

This study shows that CCR and DSS form an interesting infrastructure for eScience supporting with uniformly acceptable performance the hybrid efficiency-productivity lavered programming model from multicore through Grids. Current performance results are not as good as the best for MPI [28-31] but MPI has the benefit coming from many years of experience. CCR and the underlying Windows multicore scheduler have not before been applied to this style of messaging in intense environments and we expect significant improvements in CCR and DSS performance for both managed code and even more so C++ and native implementations. Further CCR supports the important dynamic threading and the coarse grain functional parallelism for which MPI is usually non optimal. We expect discrete event simulation to run well on a CCR base. We are also doing comparable multicore benchmarks on MPICH, OpenMPI and MPJ Express [3] (and mpiJava [27]) to cover the very best classic MPI's with in addition the extensions of initial Java results given in Sec. 5.1 corresponding to another managed code example. Further details of current analysis can be found in [32] which also studies in depth memory bandwidth and the Intel8a machine.

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