Many-Task Computing and Blue Waters

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Abstract

This report discusses many-task computing (MTC), both generically and in the context of the proposed Blue Waters systems. Blue Waters is planned to be the largest supercomputer funded by NSF when it begins production use in 2011–2012 at NCSA. The aim of this report is to inform the Blue Waters project about MTC, including understanding aspects of MTC applications that can be used to characterize the domain and understanding the implications of these aspects to middleware and policies on Blue Waters.

Many MTC applications do not neatly fit the stereotypes of high-performance computing (HPC) or high-throughput computing (HTC) applications. Like HTC applications, by definition MTC applications are structured as graphs of discrete tasks, with explicit input and output dependencies forming the graph edges. However, MTC applications have significant features that distinguish them from typical HTC applications. In particular, different engineering constraints for hardware and software must be met in order to support these applications.

HTC applications have traditionally run on platforms such as grids and clusters, through either workflow systems or parallel programming systems. MTC applications, in contrast, will often demand a short time to solution, may be communication intensive or data intensive, and may comprise very short tasks. Therefore, hardware and software for MTC must be engineered to support the additional communication and I/O and must minimize task dispatch overheads.

The hardware of large-scale HPC systems such as Blue Waters, with its high degree of parallelism and support for intensive communication, is well suited for achieving low turnaround times with large, intensive MTC applications. However, HPC systems often lack a dynamic resource-provisioning feature, are not ideal for task communication via the file

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system, and have an I/O system that is not optimized for MTC-style applications. Hence, additional software support is likely to be required to gain full benefit from the HPC hardware.
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1 Introduction

As computers have become more powerful, both simulation and data-processing applications have become increasingly complex. Simulations have increased in dimension (1D to 2D to 3D), both in the equations being simulated (one equation to multiple equations in one domain to multiple equations in multiple domain) and in the number of time scales being studied simultaneously. Similarly, data-processing applications have increased in terms of complexity of the analyses being run. In both cases, the next natural step seems to be to increase the number of such applications that fit into a meta-application. This may involve adding another layer around the initial application, such as in optimization or uncertainty quantification or in a parameter sweep. Such applications can be considered many-task computing (MTC) applications, since they are assembled of a series of tasks, each of which may be a full application or something simpler. In a recent talk David Keyes identified reasons why today’s computational scientists want performance: resolution, fidelity, dimension, artificial boundaries, parameter inversion, optimal control, uncertainty quantification, and the statistics of ensembles [1]. The last four of these can be addressed by MTC.

The term MTC first appeared in the literature in 2008, introduced to describe a class of applications that did not fit neatly into the categories of traditional high-performance computing (HPC) or high-throughput computing (HTC) [2]. Also in 2008, a workshop titled “Many-Task Computing on Grids and Supercomputers” was held; this workshop subsequently has been run at the SC08, SC09, SC10, and SC11 conferences.

As with traditional HPC, a defining aspect of MTC is the emphasis on performing a large amount of computation in a timespan of days or even hours, in order to provide important results in a timely manner. However, in contrast to traditional HPC applications, which tend to be a single program (e.g., using MPI) run simultaneously on many nodes of a single cluster or supercomputer, an MTC application is a set of many distinct tasks with interdependencies, often viewed as a directed graph of data dependencies. In many cases, the data dependencies will be files that are written to and read from a file system shared between the compute resources; however, MTC does not exclude applications in which tasks communicate in other manners.

For many applications, a graph of distinct tasks is a natural way to conceptualize the computation and is often a natural way to build the application, particularly if some tasks can be performed by existing, standalone programs. Structuring an application in this way also gives increased flexibility. For example, it allows tasks to be run on multiple sites simultaneously; it simplifies failure recovery and allows the application to continue when nodes fail, if tasks write their results to disk as they finish; and it permits the application to be tested and run on varying numbers of nodes without any rewriting or modification.

MTC applications can greatly benefit from being run on high-end HPC systems such as Blue Waters, and candidate applications for HPC—those that require high-performance hardware and timely results—may benefit from incorporating ideas from MTC into their design. The hardware of HPC systems
such as Blue Waters, with its high degree of parallelism and high-performance communication networks, is well suited to achieve low turnaround times for large-scale, intensive MTC applications. As we discuss in detail in this report, however, many MTC applications may not be viable on HPC systems such as Blue Waters without hardware and software systems support for specific features. For example, HPC systems often lack a fine-grained dynamic resource provisioning feature and have I/O systems that are not optimized for MTC-style applications. MTC applications also generally require a node operating system (OS) that supports full POSIX fork() and exec() semantics, in order that worker-node provisioning agents can execute the widest possible range of arbitrary application programs. This report discusses problems presented by MTC applications as a whole as well as by specific design patterns commonly present in MTC applications. Many of these problems can be solved by using appropriate middleware, but others may place additional requirements on the underlying Blue Waters hardware and software environment.

The initial design of Blue Waters was an IBM Power7-based system, with multiple levels of hierarchy, going from cores that can run multiple threads through chips, nodes, supernodes (drawers), and multirack building blocks, up to the full system, all network connected, with different types of connections at different levels (see Figure 1). It was to have a systemwide, shared global file system (running GPFS) that would be embedded and distributed within the network. The global file system was to have integrated hierarchical storage management via HPFS for archival data retention. Blue Waters was going to run a full Linux kernel on each 32-core compute node. Our understanding was that the nodes would boot off of the global shared file system and would have only RAM-disk for limited, node-local file storage. Nodes were to have approximate 4 GB total RAM available per core. IBM and NCSA recently announced, however, that this initial version of Blue Waters will not be built [3]. Instead, NCSA is planning a new design for the Blue Waters systems, but no details are currently public.

1.1 Motivation: Making More Things Easy

Petascale scientific computing poses multiple challenges that must be addressed by the deployment teams who intend to deliver these exceptional resources to application users. Porting and optimizing tightly coupled applications on new machines will be a time-consuming endeavor and may not succeed in all cases. Worthy applications that can quickly be promoted to petascale should be addressed first, regardless of the technologies used. Beyond petascale, systems researchers have identified challenges in communication, fault tolerance, and other areas that will make continued increases beyond Blue Waters-class systems difficult.

MTC offers the ability for domain scientists and system providers to rapidly develop and deploy applications that can gain near-peak hardware performance because of the nature of the application and software structure. Although not every application may be structured as an MTC application, many can.
found scientifically worthy of allocations on petascale resources, these applications should be provided with the most practical tools to do the job.

Some of the challenges petascale applications face, and the reasons MTC applications can meet these challenges, are as follows:

- **Expression of natural parallelism**: Many algorithms found in applications from a wide variety of scientific domains are naturally divisible into cleanly separated task executions. In their simplest form, these tasks are constructed as collections of independent POSIX processes, each of which consumes and produces data files over POSIX interfaces.

- **Rapid application development**: The familiar POSIX computing model offers several advantages in the development of many-task applications. Developers do not need to learn a new API in the language. Individual tasks may be programmed as sequential programs, without threads or other multiprogramming models. Communication over traditional file system interfaces allows the use of customary file management techniques and tools. Additionally, these applications may be debugged on workstations or other computers by using standard methods and software.

- **Portability**: The ability to scale many-task applications from worksta-
tions up to petascale systems not only aids in development but also frees the science team to use multiple resources, multiplying the return on the initial development effort. Resources may then be selected by availability, the presence of specific performance-boosting hardware (e.g., GPUs), or other reasons. Portability also facilitates code sharing among groups with access to different computational infrastructures. Notably, this portability enables the use of grid resources such as the Open Science Grid.

- **Fault tolerance:** The partitioning of application procedures into individual processes with well-defined input and output parameters enables the use of robust fault handling mechanisms familiar in other settings (e.g., exit codes) and the development of simple fault response strategies (e.g., re-execution) as well as more complex techniques. Historically, this benefit is based on experience with wide-area computing techniques. On systems like Blue Waters, these time-tested patterns and methodologies will help users get real scientific applications up and running quickly, both during system shakeout and in the presence of ongoing faults.

### 1.2 Overview

In the remainder of this report, we discuss previous work with MTC applications (§2), the results of a survey of cyberinfrastructure providers regarding MTC applications on their systems (§3), a survey of MTC applications (§4), a categorization of MTC applications (§5), and the hardware and software needed to support MTC applications (§6). We present conclusions and recommendations in §7.

### 2 Previous Work

MTC applications have emerged as a result of the wide impact of distributed-computing and grid-computing application development in recent years. Applications developed for these platforms are necessarily loosely coupled; cooperating processors may be located in distributed locations, connected by wide-area networks. These use cases led to the development of programming languages and runtime systems that enabled users to run and manage ever more jobs at larger scales. However, the scale was ultimately limited by the constraints involved in shared access to resources, making relatively few (tens of) processors available to an individual at a time.

#### 2.1 System Software Support

Porting these applications to massively parallel HPC systems enabled individual users to run the same application at a very large scale, increasing to the range of thousands the number of processors that can be applied to a given application. These applications require new system support techniques to use the systems effectively. First, the scheduler must be able to quickly allocate
processors for jobs without using existing heavyweight system schedulers such as PBS [4]. An early solution, the Falkon [5] scheduler, achieves high job submission rates by allocating executor processes with the system scheduler, such as Cobalt [6], and scheduling tasks from the Falkon client to distributed task dispatchers and finally to the task executors themselves. This task scheduling mechanism bypasses the normal system scheduler for individual user jobs, reducing a job execution to the time it takes for a short interprocess communications (IPC) message exchange.

Second, appropriate data management and movement mechanisms must be used to transfer data among HPC file services (e.g., GPFS [7]) and between intermediate system layers and user processes [8]. While MTC applications typically access parallel file systems over POSIX interfaces, they cannot directly benefit from parallel I/O optimizations [9] as made available in MPI-IO [10]. Their use of the file system typically appears as many small, uncoordinated accesses to the file system, resulting in poor performance. However, applications patterns may be observed and categorized [11] and then exploited by appropriate software [8]. More generally, aggressive caching may be used by distributing data items across caches on the compute sites [12] or by employing a distributed hash table [13].

2.2 Novel Infrastructures and Portability

New infrastructure such as compute clouds, installed at commercial data centers and research institutions, has additionally motivated the use of many-task methodologies. Compute clouds feature commodity hardware components organized and managed in a highly economical, scalable manner and emphasize flexibility through operating system virtualization and on-demand resource allocation [14]. This type of infrastructure is typically not associated with high-performance networks or other features found in HPC installations, making it a natural target for MTC-oriented applications such as workflows [15]. MTC applications are additionally often compatible with opportunistic computing systems such as Condor [16] and grids such as the Open Science Grid [17].

MTC applications offer this extreme portability by relying on widely portable languages and system interfaces. Typical use cases employ POSIX-related shells and other high-level, widely available languages such as Java and Python. MTC domain-specific languages such as Swift [18, 19] and Pegasus [20] are in turn developed with these tools. System interfaces used by these systems are limited to the widely available POSIX-like calls made available by these high-level languages. If an application can benefit from an infrastructure-specific optimization, it must be made available by the MTC language and runtime system; this is an active area of research.

2.3 The MTC Community

Current research, development, and production computing in MTC are performed by a broad community of researchers, institutions, and user groups.
MTC researchers are typically involved primarily in traditional distributed or high-performance computing and contribute to the MTC knowledge base tangentially. Similarly, application groups focus primarily on the specifics of their domain but contribute to the model by producing problems (both practical and conceptual) to be addressed by MTC systems, research, and development. The Many-Task Computing on Grids and Supercomputers (MTAGS) workshop at SC acts as one focus where these groups interact.

2.4 Task-Oriented Exploration and Problem Solving

A decade ago or earlier, it was recognized that applications composed of large numbers of tasks may be used as a driver for numerical experiments that may be combined into an aggregate method [21]. In particular, the following algorithm paradigms are well suited for MTC:

- **Optimization**: the process of exploring a parameter space to find extreme results. This model consists of the creation of many experiments that provide sparse information about the space; a higher-level method is applied to solve the optimization problem, possibly through the creation of additional experiments. MTC implementations treat individual experiments as tasks and use a higher-level program to make use of the results as a whole.

- **Data Analysis**: the concept of extracting aggregate or statistical information from existing data. Implementations are often structured to gain high I/O rates relative to computation, possibly on different data storage sites. MTC implementations provide a natural distribution of tasks and a model for generating useful final results.

- **Monte Carlo (MC)**: the exploration of a system by performing random experiments within it, followed by an integration of results. As in optimization, MTC implementations can be used to rapidly schedule randomly parameterized tasks and integrate results.

- **Uncertainty Quantification (UQ)**: the determination of the quality of a result. Computational results may be evaluated for sensitivity to perturbations in the input or numerical method used. MTC investigations into UQ may be structured by integrating results from batches of individual task executions, formulated as a Monte Carlo investigation or other method.

3 Production Grid and HPC Systems Survey

We have asked a number of infrastructure providers about MTC applications, and found the following.

TeraGrid providers responded with two applications: work on hurricane ensembles from NOAA and work on an ensemble Kalman filter inverse problem.
for oil reservoir simulation that has tasks distributed over Abe, Queen Bee, and Ranger [22].

Regarding the NOAA application, Bill Barth at TACC reported:

“We had, over the last two hurricane seasons, teams from NOAA doing ensemble weather forecasting for hurricane track prediction. These simulations were done both at the global and regional level using FIM and WRF, respectively. In these simulations, multiple runs of each case are simulated with slightly different initial conditions and incorporating the latest data from aircraft, satellites, buoys, and weather stations, and the results are averaged in clever ways to give a prediction of the hurricane path. The results of these simulations turned out to be much better than the methods NOAA was using at the time.

“Obviously, predicting the path of a hurricane directly can save both lives and dollars. The better the prediction, the few people who have to evacuate, and the more accurate the evacuation orders can be.”

Open Science Grid providers mentioned two applications: the Large Hadron Collider [23] and the Laser Interferometer Gravitational Wave Observatory [24]. Both have been well studied and well characterized in previous publications.

From the Department of Energy, David Skinner at LBL stated: “Most of the parameter sweeps I have been involved with in QCD and chemistry have had MPI codes underneath. For example in quantum Monte Carlo one often allows one task (or set of tasks) to quickly cancel and reschedule work running on other tasks which results in rapid pruning and growth of who is doing what. It’s not deterministic but rather like a workflow.”

David also discussed another case: “Replica exchange MD is another case where an ensemble of parallel MD runs rapidly communicate small pieces of information between each other. It requires a parallel computer but there are two scales to the level of interconnection.”

Katherine Riley at the Argonne Leadership Computing Facility highlighted the work of David Baker at the University of Washington as “a great example of a parameter sweep/ensemble set.” His laboratory focuses on the prediction and design of protein structures and protein-protein interactions. Baker’s group created the Rosetta application [25], which has a BOINC-based Rosetta@home version [26] and supports a server called Robetta [27]. Katherine also mentioned the work of Benoit Roux and Andrew Binkowski, who use the DOCK application in a manner similar to what we describe in §4.4.

Katherine described as another promising MTC application area the materials science research in ‘rational materials design led by Larry Curtis and Jeff Greeley. Theory-aided design of novel materials is a growing area of research that has the potential to revolutionize the materials discovery process. Until recently, however, the ability to characterize many materials has been hampered by the lack of computer resources and by the difficulty for smaller organizations to harness large amounts of distributed resources and novel petascale systems. That situation is beginning to change with the introduction of petascale computers that allow for the rapid computational characterization of many candidate materials. For example, in catalysis studies it is possible to characterize 1,000 candidate surface compositions within a few hours on the Argonne Blue...
Gene/P machine. Moreover, the development of new density functional codes is enabling scientists to run more accurate computations in parallel on thousands of processors on large cluster, grid, petascale, and cloud systems. One such approach is being pioneered by Jens Norskov and his colleagues [28, 29], who are collaborating with Argonne’s Center for Nanoscale Materials and Mathematics and Computer Science (MCS) Division to develop these codes for use on the Blue Gene. Orchestrating the large numbers of computations demanded by the rational design process, whether on petascale computers or on other platforms such as scientific clouds, is a clear application for the MTC programming model.

Speculating on applications of MTC in finer-grained mathematical algorithms, Todd Munson of Argonne’s MCS Division described five scenarios in which mathematical applications will require MTC execution patterns as they expand to petascale and exascale computing levels. These applications are summarized below, in order of their “shovel readiness.” The application descriptions were edited for inclusion here from a private communication [30].

Sequential Monte Carlo with Reweighting for Climate Model Assessment
Purpose: uncertainty quantification
Algorithm: Generate an ensemble of initial conditions and weights; run a climate simulation on each element of the ensemble in parallel, where each climate simulation runs on 128–1024 processors; analyze the results to compute uncertainty information and recompute weights; rerun the climate simulations with the new weights.

An interesting point here is that the analysis phase can sometimes be run in parallel with the climate simulations. It does not always need the full set of results to compute the new weights, limiting the amount of synchronization required. Moreover, a weight can be zero, in which case the corresponding element of the ensemble no longer needs to be run and can be removed from the queue. (If it is currently running, it can be stopped.) It is possible that the weights may provide priorities and indicate the order in which to compute the elements of the ensemble (i.e., one may need a priority queue where the weights can be adjusted).

In this application, the number of processors required should be constant and known ahead of time.

Uncertainty Quantification Using the Adjoint Method
Purpose: uncertainty quantification
Algorithm: Run a PDE simulation forward in time on, say, 1024 processors (the forward simulation checkpoints at regular intervals); run an adjoint simulation backward in time on, say, 1024*1024 processors. The adjoint simulation runs the forward PDE starting from one of the checkpoints to gather required information. Then the adjoint computation is rerun backwards.
An interesting resource utilization characteristic here is the ramp-up: one needs a relatively small number of processors initially, but then more processors later.

**Optimal Design with Integer Variables Using Branch and Bound**

**Purpose:** parameter estimation and design for partial differential equations

**Algorithm:** Generate a set of subtrees using strong branching: for each integer variable solve two independent optimization problems (each problem is a PDE-constrained optimization problem that runs on say 1024 processors). Once the subtrees are generated, run branch and bound on each of them independently. Each independent branch and bound on the subtree solves, for example, 1024 optimization problems with PDE constraints, each of which requires 1024 processors.

An interesting MTC characteristic for this algorithm is that some coordination is required in the branch-and-bound process to prune subtrees and so forth. Once the PDE-constrained optimization problems are communicated, the additional communication required for the branch-and-bound procedure is minimal.

**Derivative-Free, Least-Squares Parameter Estimation**

**Purpose:** estimate parameters for a nuclear physics application

**Algorithm:** Generate a prioritized list of trial points; run the trial points in parallel (each run with a trial point requires the evaluation of say 1024 independent computations that can take vastly different amounts of time to complete); gather the results, update the priorities for the trial points, and add new trial points.

The interesting feature here is that running the trial points, updating the priorities, and adding new trial points can run in tandem. Also, the 1024 independent calculations for each trial point have priorities. By observing the output from some of the initial calculations, we can sometimes say immediately that the point is useless and that one should stop the rest of the calculations and pick the next trial point.

**Hierarchical, Asynchronous Dynamic Programming**

**Purpose:** solve dynamic programming problems in parallel

**Algorithm:** Solve a large set of optimization problems; gather the results to compute a new functional approximation; resolve a set of optimization problems.

The interesting MTC aspect here is that the data transfers are small. Under certain assumptions, solving the optimization problems can be done simultaneously with updating the functional approximation. A hierarchy also would need to be exploited. This is the least understood of the five applications and will need considerable mathematical analysis to assess its feasibility.
4 MTC Applications Details

This section discusses the details for a set of MTC applications, describing 12 applications, their science domain, their history, and their computational characteristics. Included is a discussion of how they were programmed, what infrastructure they use, what processing paradigm they use, and what their data and computing requirements are. Many of these applications have been previously discussed, either individually as noted below or in summary [18].

4.1 AstroPortal

AstroPortal [31] is an application that provides astronomers with the ability to dynamically combine astronomical data sets to create new, “stacked” composite images. Often, by combining images of different wavelengths or images taken at different times, one can detect astronomical objects that may be too faint or indistinguishable from noise in a single image only.

4.1.1 Science Domain

Astronomy

4.1.2 History

AstroPortal was developed from 2005-2007 to provide a service to astronomers and also to investigate the dynamic analysis on-demand of large data sets (in this case the Sloan Digital Sky Survey).

4.1.3 Computational Characterization

- **Language:** Java
- **Infrastructure:** The system uses SDSS data, accessed from a GPFS file system. A SDSS database is used to locate objects. Globus Toolkit 4 services are used for transferring data and launching jobs.
- **Processing Paradigm:** A master-worker paradigm is used. Each stacking is data-parallel.
- **Data:** The size of the data set used in the development of AstroPortal (SDSS DR4) is approximately 3 terabytes when compressed. However, the amount of this image data that is actually used in a given stacking job varies. The data set is divided into images of \(2048 \times 1489\) pixels of approximately 2 MB each. The number of images that need to be stacked for a typical query invocation is uncertain, but we can estimate the data size would be in the range of 5 to several hundred megabytes, depending on the region of the sky.
• **Processing Time:** The amount of processing required for each stacking is small. Less than a second per stacking was required on 2006-era commodity hardware.

### 4.2 PTMap

Many biological processes are controlled by post-translational modifications (PTMs) of proteins; such PTMs are studied in order to understand the mechanisms of cell regulation. PTMap [32] is used for mapping sites of PTMs using mass spectrometry data and databases of protein sites. Commonly, the algorithm will be invoked on all pairs of input data. Results are combined, selected by quality, and reprocessed until high-quality results are obtained.

#### 4.2.1 Science Domain

Biochemistry

#### 4.2.2 History

PTMap originated from a group at the Department of Biochemistry and Pharmacology, University of Texas Southwestern Medical Center. As members of the team moved to the Ben May Department of Cancer Research at the University of Chicago, it is now a joint effort of Ben May Department of Cancer Research and the Computation Institute. The Cancer Department team is in charge of PTMap code development and maintenance, while the Computation Institute group parallelizes the code.

#### 4.2.3 Computational Characterization

- **Language:** C++
- **Infrastructure:** Cluster computing
- **Processing Paradigm:** All-Pairs: Each spectroscopy given file is compared to each given protein sequence (FASTA) file. Further processing is derived from these results.
- **Data:** Overall, 1.1 TB of data is read from the file system. For each protein, approximately 120 MB must be read. Each pair of spectroscopy datasets requires approximately 150 KB to be read. The intermediate files, used for communication between tasks, are of the order of 100 KB per task. The final output is very small.
- **Processing Time:** Each pair requires 5–10 minutes on IBM BG/P, which has a 850-MHz quad-core CPU. Typical use case of the program may involve 50,000 or more tasks [11].
4.3 OOPS: Protein Structure Prediction

The Open Protein Simulator (OOPS) builds on the Protein Library (PL). Both have been developed at the University of Chicago. OOPS is multipurpose and allows extensions to perform various simulation tasks relevant for life scientists, such as protein folding or protein structure prediction.

4.3.1 Science Domain

Biochemistry

4.3.2 History

OOPS research can be traced back to 2006, when it started as the Open Protein Simulator, which was created by a group of chemical and biological scientists. In 2008, it became a joint effort of Department of Chemistry, the University of Chicago and the Computation Institute.

4.3.3 Computational Characterization

One situation where OOPS has been used in an MTC context is for protein structure prediction using Monte Carlo–based simulated annealing (MCSA), a technique that requires many randomized, independent computations [33]. This is the use case discussed here.

- **Language:** C++ for application code, Swift for coordination
- **Infrastructure:** Swift interpreter and a compatible task dispatcher deployed on the computational infrastructure; shared file system.
- **Processing Paradigm:** MTC, communicating via shared file system
- **Data:**
  - Input: Common input data of 27 MB. Per protein datasets (shared between iterations of each task in the same proteins) in several files of sizes ~1 KB
  - Output: ~1 MB (verbose mode), ~1 KB (regular mode) per task.
- **Processing Time:** 0.5 to 3 CPU-hours per MCSA task; approximately 1000 CPU-hours overall for a typical protein on a ~2.33-GHz x86 CPU.

4.4 DOCK

The DOCK6 molecular dynamics application identifies the low-energy binding modes of a small molecule (ligand) within the active site of a macromolecule (receptor). A compound acts as a drug if it inhibits the function of the receptor it binds to. DOCK6 is used for the following purposes:
- Predict binding modes of small molecule-protein complexes
- Search databases of ligands for compounds that inhibit enzyme activity
- Search databases of ligands for compounds that bind a particular protein
- Search databases of ligands for compounds that bind nucleic acid targets
- Examine possible binding orientations of protein-protein and protein-DNA complexes
- Help guide synthetic efforts by examining small molecules that are computationally derived

4.4.1 Science Domain

Bioinformatics

4.4.2 History

The DOCK application family can be traced back to the 1980s, with a variety of versions, including DOCK3, DOCK4, DOCK5 and DOCK6. The DOCK program has been executed in parallel both in an MPI implementation and in a grid environment. As stated in [2], DOCK6 has scaled up to 128,000 CPU cores on BG/P with the scheduling support of Falkon.

4.4.3 Computational Characterization

- **Language:** C++
- **Infrastructure:** Swift interpreter and a compatible task dispatcher deployed on the computational infrastructure. Shared file system.
- **Processing Paradigm:**
  - HTC Mode: Each DOCK6 run is completely independent from others
  - HPC Mode: (massively parallel) An MPI version of the master-worker model is implemented for DOCK6.
- **Data:**
  - Input: 1 ligand file ~10 KB, 1 grid.nrg file ~10 MB, 1 dock.in file ~1 KB, 1 selected_spheres.sph file ~1 KB, 1 vdw_AMBER_parm99.defn file ~10 KB, 1 flex.defn file ~1 KB, 1 flex_drive.tbl file ~1 KB.
  - Output: 1 scored ligand file ~10 KB, 1 standard output file ~1 KB.
- **Processing Time:** Processing time varies from seconds to hours on BG/L, with an average of 713±560 seconds [2].
In HPC mode, the performance of DOCK6 starts to decrease significantly at the scale of 16,483 cores on BG/L [34], due to

1. Scheduling capability of a single master node
2. Data-processing capability of a single master node, as all input files are read in by the master node then randomly distributed to slave nodes
3. Unpredicted load balancing caused by random data distribution
4. I/O capability between compute nodes to GPFS

To improve the load balancing, we could sort the input files according to the running time, as the running time could be predicted by “the greatest number of rotatable bonds” and “the number of atoms per ligand”.

In HTC mode, there is linear scalability up to 16,384 cores [34]. Work with Falkon showed a sustained utilization of 99.6% in the first 5700 seconds out of 7200 second run on 128,000 cores. [2]

4.5 Montage

The purpose of Montage (http://montage.ipac.caltech.edu/) [35, 36] is to build astronomic image mosaics, while preserving image accuracy. That is, the amount of energy in the input images is conserved and the position of the energy is preserved.

4.5.1 Science Domain

Astronomy

4.5.2 History

Montage development began in 2002, with the first production release in 2003 (v. 1.7). The current version (v 3.0) was released in 2007. Version 3.2b6 is the current release.

4.5.3 Computational Characterization

- **Language:** C for application code, MPI or Pegasus for infrastructure
- **Infrastructure:** shared file system for MPI, with Pegasus handling file transfers
- **Processing Paradigm:** Many-task computing, communicating via shared file system
- **Data:** A benchmark problem is generating a mosaic of 2MASS data from a 6 degree × 6 degree region around M16. Construction of this mosaic requires 1,254 2MASS images as input, each having about 0.5 megapixels, for a total of about 657 megapixels input (or about 5 GB, with 64 bits per
pixel double-precision floating-point data). The output is a 3.7 GB FITS file with a 21,600-pixel × 21600 pixel data segment and 64 bits per pixel double-precision floating-point data. Note that the output data size is a little smaller than the input data size because of some overlap between neighboring input images.

- **Processing Time:** For the benchmark problem above, about 280 minutes on a single 1.5 GHz core, and about 20–30 minutes on 64 such cores.

Montage takes a number of image files as input and builds an output file (possibly tiled) as output. The output image can be almost as large as the input images (minus the overlaps in the inputs), or it can be smaller if the resolution/projection of the output is significantly different from that of the input.

**Typical steps in Montage:**

- Reprojection of input images to a common spatial scale, coordinate system, and WCS projection (multiple tasks can be done in parallel)
- Modeling of background radiation in images to achieve common flux scales and background levels by minimizing the interimage differences (initially multiple tasks can be done in parallel, followed by a sequence of tasks that must be done in order)
- Rectification of images to a common flux scale and background level (multiple tasks can be done in parallel)
- Co-addition of reprojected, background-corrected images into a final mosaic (can be done in parallel in MPI but is single task)

### 4.6 Social Learning Strategies

Computer simulations can be used to provide insight into the role social learning plays in evolution, and human behavior. One simulation places two different kinds of learning agents—social and asocial—on a two-dimensional grid, with reproduction, environmental change, movement, and learning playing a role in the simulation [37].

Another application, a tournament [38], involves competitions between a number of autonomous agents submitted by a number of different participating groups. Each match in the tournament is a contrived game, where each agent follows its own strategy to maximize its payoff according to the rules of the game. The choices each agent must make at each step are designed to be somewhat analogous to those a person must make when learning and performing a new task.

In both the simulation and the tournament, the relative success and failure of different learning strategies were used to derive insight into the role and importance of social learning to humans.
4.6.1 Science Domain
Psychology, Evolution

4.6.2 History
Similar tournaments focusing on simulated social behavior were initially organized in the 1980s by Robert Axelrod [38].

4.6.3 Computational characterization
- **Language**: Matlab/GNU Octave
- **Infrastructure**: A desktop computer was used for the simulation. The UK National Grid Service (NGS) was used for the tournament.
- **Processing Paradigm**: All-Pairs: each pair of strategies was tested against each other, with multiple randomized simulations performed for each pair.
- **Data**: Minimal size. The tournament required strategy definitions as input. The output is statistics about the success of different strategies.
- **Processing Time**: In both cases, 5–20 minutes per simulation instance on a single ~2.5-GHz core was required.
  - **Simulation**: Each simulation involved 2,000 rounds, simulating several thousand agents. There were 20 instances of a simulation per parameter combination. The simulations were run in batches of about 600 parameter combinations to investigate different factors; each batch took 2–3 days on a single-core machine [39].
  - **Tournament**: The first stage of the tournament involved pairwise competitions among 104 strategies, with 10,000 rounds in each competition. The second stage involved the 10 best strategies, where they all competed in the same simulation rather than in pairwise matches. Approximately 65,000 CPU-hours were used on the NGS for the entire tournament [39].

4.7 BLAST
The Basic Local Alignment Search Tool (BLAST) finds regions of local similarity between biological sequences. The program compares nucleotide or protein sequences to sequence databases and calculates the statistical significance of matches. BLAST can be used to infer functional and evolutionary relationships between sequences as well as help identify members of gene families.

A number of varieties of BLAST exist:
- nucleotide blast: Search a nucleotide database using a nucleotide query
- protein blast: Search protein database using a protein query
• blastx: Search protein database using a translated nucleotide query
• tblastn: Search translated nucleotide database using a protein query
• tblastx: Search translated nucleotide database using a translated nucleotide query

4.7.1 Science Domain
Bioinformatics

4.7.2 History
The BLAST program was designed by Eugene Myers, Stephen Altschul, Warren Gish, David J. Lipman, and Webb Miller at the NIH and was published in J. Mol. Biol. in 1990 [40]. BLAST is one of the most widely used bioinformatics programs, because it addresses the fundamental problem of sequence alignment, with an emphasis on speed. This emphasis on speed is vital for making the algorithm practical on the huge genome databases currently available, although later algorithms can be even faster. Before fast algorithms such as BLAST and FASTA were developed, doing database searches for protein or nucleic sequences by using a full alignment procedure like Smith-Waterman was very time consuming. BLAST cannot guarantee the optimal alignments of the query and database sequences as Smith-Waterman does, but the results have proven to be sufficiently accurate to prompt widespread adoption of BLAST by scientists.

4.7.3 Computational characterization
• Language: C++
• Infrastructure: The Swift version requires a Swift interpreter and a compatible task dispatcher deployed on the computational infrastructure. Shared file system.
• Processing Paradigm:
  – HTC Mode: Each BLAST run is completely independent from others.
  – HPC Mode: (Massively Parallel) An MPI version of BLAST is implemented by Wu Feng, director of the Synergy Lab at Virginia Tech.
• Data:
  – Input: 1 database file \(~1\) GB (a common database file is \(6\) GB), 1 query string file \(~1\) KB
  – Output: 1 text output file \(~1\) KB
• Processing Time: A simple query may take \(~1\) minute on BG/P. If multiple queries are wrapped in one transaction, the running time is longer.
In HPC mode, mpiBLAST showed a 93% efficiency performance on 32,768 cores on IBM BG/P at Argonne [41].

In HTC mode, no productive measurements have been published. The machine utilization of current HTC implementations of BLAST is unacceptably low on supercomputers, because of load-balancing problems and due to BLAST’s need to share the typically large search database in-RAM between cooperating SMP cores. [41]

In summary, BLAST is a perfect example of an application for which MTC processing on petascale systems can be highly desirable and scientifically important and which is best accomplished as a hybrid application of many independent executions of tightly coupled mpiBLAST runs. This approach provides the workflow flexibility of restart and variable-sized work units while leveraging the efficient data sharing of tightly coupled MPI application kernels.

4.8 CIM-EARTH

CIM-EARTH is a collaborative, multi-institutional project to design a large-scale integrated modeling framework as a tool for decision makers in climate and energy policy. CIM-EARTH is intended to enhance economic detail and computational capabilities in climate change policy models and to create and support a broad interdisciplinary and international community of researchers and policymakers.

4.8.1 Science Domain

Economics, Earth Systems, Climate

4.8.2 History

The CIM-EARTH project originated as a collaboration of researchers from University of Chicago, Argonne National Laboratory, and the Hoover Institute. Discussion about CIM-EARTH started around 2008. In 2009, a \( \sim 50,000 \) CPU-hour run of the v0.1 CIM-EARTH model, expressed in the AMPL mathematical programming language, was performed on the TeraGrid Ranger supercomputer at TACC and on several OSG sites, including Firefly at the University of Nebraska-Lincoln and TeraPort at the University of Chicago.

The model is executed in large ensemble runs of 1,000 to 10,000 model executions with stochastic inputs, to perform uncertainty quantification. A first v0.5 CIM-EARTH model coded as a native C++/FORTRAN app is under development, which will enable far greater portability of the model to an abundant set of petascale systems, including the BG/P, where we are currently unable to execute the binary AMPL application.

4.8.3 Computational characterization

- **Language:** AMPL and TAO libraries for numerical programming and optimization, Swift for parallel processing.
• **Infrastructure:** The workflow is written in Swift, execution is done on clusters. Requires data to be accessible on shared file system.

• **Processing Paradigm:**
  - HTC Mode: Each AMPL run is completely independent from others.
  - HPC Mode: N/A

• **Data:**
  - Input: 6 input files, ~10 KB–100 KB each.
  - Output: 6 output files, 2 of which are ~10 MB size, 1 ~100 KB, 2 ~10 KB, with a ~1 MB standard output.

• **Processing Time:** ~10 minutes to ~1 hour using ~2.5-GHz cores.

Some experimental results have been published [42], but no performance results have been presented.

### 4.9 SYNAPPS

The purpose of SYNAPPS is to estimate the properties of a particular class of supernovae in such a way that they match an observed spectrum. SYNAPPS uses the SYNOW spectrum synthesis fitter to estimate the spectrum of a supernova using a model with over 50 input parameters. Previously, SYNOW was typically utilized in a human-supervised manner, with a human in the loop adjusting the input parameters until a reasonable fit was found, guided by experience and intuition rather than any systematic approach. SYNAPPS replaces the human with the APPSPACK optimization code to iteratively explore the parameter space with many parallel instances of SYNOW [43].

#### 4.9.1 Science Domain

Astronomy

#### 4.9.2 History

The original version of SYNOW was released in 1995. It is still being maintained, with an updated version 2.0 described in a 2007 paper [44]. It has been used in a number of investigations of supernovae.

SYNOW is in frequent use in the astronomy community. A Google Scholar search for “SYNOW supernova” returns 187 results, almost all of which describe SYNOW being used for astronomical research.

SYNAPPS was developed more recently and has been used to generate published results since at least 2008.
4.9.3 Computational Characterization

- **Language:** SYNOW is written in FORTRAN. APPSPACK is written in C++/MPI.
- **Infrastructure:** MPI
- **Processing Paradigm:** Master/Worker. Each worker is assigned a task, which is to calculate the “figure of merit” for a single point in the parameter space.
- **Data:**
  - Input: Observed spectrum (same for all tasks) of ~60 KB, plus the model parameters for each task, which are ~1 KB in size.
  - Output: Figure of merit, which is a single number
- **Processing Time:** A few seconds for each task; less than two hours of wall-clock time total on a 96 Opteron processor cluster

4.10 Deem’s Database of Hypothetical Zeolite Structures

Deem’s database is a repository for zeolite structures (a kind of mineral) that have been computationally predicted to have some reasonable chance of existing in nature or being synthesizable [45]. There are various applications for such a database, such as identifying materials, searching for materials with certain properties, or researching the properties of Zeolite structures. Populating this database has been a computationally expensive task, requiring an extremely computationally expensive Monte Carlo search.

Constructing the database required over 3 million Condor jobs to be run, each of which is a single core task that takes between 10 and 60 minutes on an x86 processor. There are no dependencies between jobs. Various platforms were used to scavenge cycles for this application. Over the 40-day period these 3 million jobs were run in, on average 200+ processors, which were used for a workflow involving three primary applications.

4.10.1 Science Domain

Physical Chemistry

4.10.2 History

Computationally predicting the structure of zeolites has been of interest since at least 1992, when a Monte Carlo method for structure prediction was show to be valid in predicting real-world structures. Public and proprietary databases have grown in size since then; there were 600,000 hypothetical zeolites known in 2006. The work on Deem’s database has been ongoing since at least 2006, with large computing allocations on TeraGrid [45].
4.10.3 Computational Characterization

An earlier paper describes some of the computational work done in order to populate the database [46].

- **Language**: DAGMan for workflows
- **Infrastructure**: Condor for task dispatch, MyCluster as middleware, running on several TeraGrid resources
- **Processing Paradigm**: HTC workflow, using a directed acyclic graph (DAG) to represent data dependencies
- **Data**:
  - Input: a set of parameters describing a region in the space of possible zeolite structures
  - Output: 3 million hypothetical zeolite structures, a few kilobytes each
- **Processing Time**: 2 million CPU-hours on ~2.5-GHz cores. Each task ran for a highly variable amount of time, from a minimum of few minutes to 3–4 hours for typical tasks. It was possible for some simulations to run for an extremely long period of time, in which case they were terminated after 10 hours and not rerun.

4.11 fMRI

The fMRI application analyzes brain regions for response to experimental stimuli. A relational database of responses for a given subject may be queried for analysis, providing statistical connections to be made between MRI data and brain function. The fMRI script pulls records from the MRI database, performing statistical tests on each brain region using the statistical analysis language R, then writes the result.

4.11.1 Science Domain

Neuroscience

4.11.2 History

The papers related to this research can be traced back to 1994 [47, 48].

4.11.3 Computational Characterization

- **Language**: R for statistical computation, Swift for parallel processing
- **Infrastructure**: The workflow is written in Swift, execution is done on TeraGrid. Requires data to be accessible on a shared file system.
• **Processing Paradigm:**
  - HTC Mode: Each fMRI task is independent. Then a summary stage is applied to all previous results.

• **Data:**
  - Input: 1 input file, 1 KB each
  - Output: 1 output file, 2 KB each for first stage, 1 2-GB output file for the second stage

• **Processing Time:** ~10 minutes to ~1 hour on ~2.5-GHz cores.

In HTC mode, fMRI along with Swift has run on TACC’s Ranger at the scale of 65,536 jobs in about 16 hours.

### 4.12 Model SEED: Genome-scale Metabolic Models

Genome-scale metabolic models are a valuable resource to understand the genome, phenotypes, and behavior of the cells in an organism. These metabolic models are invaluable as they can be used to understand the function and importance of different genes and can model the organism’s behavior under different conditions. The models make testable predictions that can be checked experimentally. A key component of each model is a set of gene-protein-reactions mappings, which represent a theory about which metabolic reactions occur in the organism’s cells, which enzymes catalyze the reactions, and which genes encode those enzymes. In addition, the models require further information about the reactions that play a role in the organism’s metabolism and require a biomass objective function capturing the molecules required for growth [49].

High-throughput sequencing of genomes has meant that the pace at which genome sequences are assembled exceeds the pace at which metabolic models can be manually constructed using the genomes [49]. Manually reconstructing these models can take 96 steps under at least one published protocol [50].

Model SEED ([http://blog.theseed.org/model_seed/](http://blog.theseed.org/model_seed/)) is an online resource that automates much of the process of constructing metabolic models from sequenced genomes. It reconstructs a preliminary metabolic model based on existing genome annotations, automatically filling in gaps in the model. This preliminary model can be checked manually, after which Model SEED can automatically optimize it through various analysis steps that check the viability of the model, validate it against experimental data, and perform optimizations to refine the set of reactions included in the model [50].

The majority of the computation performed is in the form of optimization problems. The most computationally intensive steps are those that attempt to add to or remove reactions from the model, which are formulated as complex mixed-integer linear optimization problems (MILPs). These require from one minute to one day per organism to solve running on eight processors in...
parallel [49]. Other steps, such as simulations of an organism in different environments or with different genes removed, can be formulated as less computationally intensive linear programs. However, these steps may require many more problem instances to be solved. For example, a simple growth simulation of an organism with a set of genes removed in a particular medium can be completed in around 20 milliseconds, but a user might want to perform that simulation for millions or billions of gene combinations in hundreds of different media per organism. More complex growth simulations, which check that predictions are thermodynamically feasible, can take much longer: around 4 seconds per simulations [49]. All these computational steps may need to be performed for hundreds or thousands of genomes, motivating the use of HPC.

4.12.1 Science Domain

Bioinformatics

4.12.2 History

The model SEED has its origins in the Project to Annotate 1,000 Genomes, which was initiated by the Fellowship for Interpretation of Genomes in December 2003. The stated goal of this project was to produce and make freely available high-quality annotations and metabolic models for the first 1000 sequenced genomes [51].

4.12.3 Computational characterization

- **Language**: C/C++
- **Infrastructure**: [52]
  - Scheduling and distribution of work used for customized MPI code
  - GLPK and CLP solvers used for linear optimization
  - CBC and Scip solvers used for mixed integer linear optimization
  - MySQL database used for data storage
- **Processing Paradigm**: Master-worker and static scheduling approaches both used within MPI
- **Data**: Input and output files are in the range of 1–4 MB. Some stages require the input to be broadcast to all tasks; some stages have different per task input files. Task outputs are typically at most 2 MB [49, 52].
- **Processing Time**: [49]
  - Up to 24 hours (on BG/P) per MILP task for automatic filling of gaps or generation of gaps
  - 10–20 milliseconds for simple simulation tasks
Minutes to hours for more complex simulation tasks

Gene knockout simulation have scaled to 65,536 processors on Blue Gene/P Intrepid [49].

We note that as more high-quality options become available for various mathematical programming and optimization approaches, and these tools can be portably compiled across a broader set of system architecture and Linux/GCC/Libc variants, new opportunities will be made available for MTC applications across the newest and continually expanding set of petascale machines. In particular, the ability to run such tools on non-Intel architectures has been a limiting factor on petascale systems such as BG/P and will be limiting on Blue Waters as well, until such tools enter the open source toolkit.

5 Categorizing MTC Applications

We present two methods for characterizing MTC applications. In §5.1, we discuss some general issues about the applications and the resources on which they run. In §5.2, we discuss a set of patterns that are found in MTC applications.

5.1 Abstract Issues of Applications

One method for analyzing MTC applications is to ask a set of questions about the application. An issue that occurs during this process is defining “the application.” Is the application the source code? Or the algorithm? Or the combination of the code and the general system it is defined to run on? What happens when an application has variants for multiple systems? Unfortunately, this issue dramatically complicates discussions about the application. Here, we discuss abstract issues about the application, but we also discuss some issues about the resources used, and we focus on a particular “production” use of the application, as defined in §4.

Some of the issues are properties of the application:

- What is the type of task involved: sequential or parallel (MPI) or both?
- Is the communication at the start and end of the tasks (likely via files), or continuous within the tasks (via messages)?
- How intense is the communication? (This leads to two types of parallelism, tightly coupled and loosely coupled, neither of which is rigorously defined.)
- How many tasks does the application comprise?
- Is the number of tasks defined at build time or runtime? If it is defined at runtime, is it a function of the amount of input data or of the values of that data?
- What is the shape of the graph of tasks?
– Are any of the control-flow or data-flow patterns from §5.2 present in the graph?
– Is the graph divided up into distinct stages, with each stage dependent on the previous?
– Are there tasks that depend on the output of other tasks? If so, how deep is the graph? That is, what is the length of the longest path from start to end?
– Are there higher-level patterns in the graph, for example, MapReduce or AllPairs?
– Does the graph have cycles in it? Is there a subgraph that is iterated over and unfolded into a DAG at runtime?
– How does the degree of parallelism (i.e., the width of the graph) change as execution of the workflow proceeds?
– Is the graph shape static or dynamic? That is, can tasks be added or removed from the graph during runtime?

• How much computation and communication are there in the application?

Other issues are properties of the environment or resources on which the application is run:

• How long do tasks run?
• Is computation or communication the limiting factor in application performance?
• Is the resource model static or dynamic? That is, can the set of resources that the application uses be changed during execution?

5.2 Patterns

Summarizing the §4 discussion of application characteristics, Table 1 shows that many applications make use of computational and dataflow patterns. These patterns, known to the developer, may be used as a guide when developing MTC middleware, enabling developers to gain access to toolkits optimized for particular implementations. In this report, we focus on optimizations made possible by the advanced technologies available on Blue Waters. We outline some patterns here:

• Control Flow Patterns:

– Parameter sweep: when the same code is run many times in parallel with only difference being input parameters. Randomized simulations can also be considered parameter sweeps, with the crucial parameter being the random seed.
Table 1: MTC applications discussed in this report and corresponding patterns.

|                | Parameter Sweep | Data-intensive | Scatter | Gather | Repartition | Iteration | Task Pruning | Pipeline | Coordination of MPI Apps | Variable Runtimes |
|----------------|-----------------|---------------|---------|--------|-------------|-----------|--------------|----------|--------------------------|---------------------|
| AstroPortal    | ×                | ×             | ×       | ×      |             |           |              |          |                          | ×                   |
| PTMap          | ×                | ×             | ×       | ×      | ×           |           |              |          |                          | ×                   |
| OOPS           | ×                | ×             | ×       | ×      | ×           | ×         |              |          |                          | ×                   |
| DOCK           | ×                | ×             | ×       |         | ×           | ×         |              |          |                          | ×                   |
| Montage        | ×                |               | ×       |         |             |           |              |          |                          | ×                   |
| Social learning strategies | ×         |               |         |         |             |           |              |          |                          | ×                   |
| BLAST (MTC version) | ×         | ×             |         |         |             |           |              |          |                          | ×                   |
| CIM-EARTH      | ×                |               |         |         |             |           |              |          |                          | ×                   |
| SYNAPPS        | ×                |               |         |         |             |           |              |          |                          | ×                   |
| Deem’s database | ×                |               |         |         |             |           |              |          |                          | ×                   |
| SEM            | ×                |               |         |         |             |           |              |          |                          | ×                   |
| Metabolic Models (SEED) | ×        | ×             |         |         |             |           |              |          |                          | ×                   |

- Iteration: when a section of the job is iterated a number of times, and the number is often unknown at the outset of the job, as it is determined by some loop completion criteria.

- Task pruning: when tasks are speculatively executed, and can be “pruned” dynamically before completion. Typically, this would occur when one task determines that the result of another concurrent task is no longer necessary. An example is a branch-and-bound algorithm, where branches are speculatively explored in parallel.

- Dataflow Patterns:

  - Scatter: At a stage of the MTC computation, a single item of data must be broadcast to all subsequent tasks, or multicast to some number of subsequent tasks. This could be the output of a previous task, or it could be a data file from the global file system (e.g., the sequence for a BLAST query).

  - Gather: A small number of tasks take as input the output from a large number of tasks. Examples include a task that checks the results of previous tasks for a convergence criterion and a task that calculates summary statistics from the output of many tasks.

  - Pipeline: A set of tasks operate on given data in sequence, with the output of one task becoming the input of the next.
- Data reuse: Bulk data is reused by task after task.

- Other Features:

  - User toolkits with compositional flexibility: Many applications are structured as a set of tools (often, “command line” invocable) with moderately complex usage patterns, which benefit from a workflow language in which one can concisely and easily specify the execution patterns. The more declaratively these patterns of composition can be specified, the more work has been moved from the user to that of the workflow automation tool. An excellent example of such applications is the Montage suite (§4.5), which gives astronomers a very general set of software modules that are efficiently and flexibly linked through loosely coupled file exchange.

  - Coordination of MPI applications: Instead of sequential tasks, the unit of execution is a tightly coupled MPI application. Note that we contrast here applications of MPI in which the communicating processes conduct many message exchanges over their mutual lifetimes, from applications in which a communicating entity is a single task that gets its input, performs a process to completion, and either terminates or awaits a similar task. The former class we categorize as tightly coupled applications, while the latter are more loosely coupled and often exhibit MTC patterns. Again, Montage provides an excellent illustration of both these degrees of coupling. Some uses of MPI within Montage leverage repetitive tightly coupled message exchange, while others follow the input-process-output model and are well suited for MTC execution via file exchange. Enabling the loose coupling to be specified by a declarative functional workflow language, as we have done by specifying Montage workflows using Swift, illustrates the flexibility and scientific productivity afforded by the MTC model to manage the complex data dependency graphs that such applications entail.

  - Variable runtimes: Concurrent tasks in the application can run for variable, possibly unpredictable lengths of time.

6 Support for MTC Applications

This section enumerates a range of key challenges that arise when attempting to run many-task applications on HPC systems. We first describe (§6.1) the basic requirements needed to run a typical many-task application. We then discuss (§6.2) design choices of the requirements. We conclude the section with a discussion (§6.3) of commonly occurring patterns of data movement and communication, the challenges in efficiently supporting them, and how we address those challenges with the design choices covered in §6.2.
6.1 Basic Hardware and Software Environment

We describe the requirements of MTC in three categories: hardware requirements, operating system requirements, and MTC middleware requirements.

- **Hardware Requirements:**
  - **Local Storage:** Local storage for compute nodes could be in the form of RAM disk, hard disk, or solid state disk. Local storage is used for local data caching and intermediate data storage. The data policy for local storage varies. For most supercomputers, the availability of local storage is synchronized with the allocation of compute resources, meaning that data on local storage is erased as the compute allocation is released.
  - **Network:** Compute nodes require networks for communication and data collection. The network is usually a global network through which compute nodes can reach all their peers. Vendors have different network configurations: for example, some machines are built with specialized technologies such as InfiniBand, while others are built with commodity network technologies. Since a network is required for Message Passing, it is available on every high-end machine.
  - **Persistent Storage:** A global shared file system is required to store the input and output of MTC applications. Ideally, the shared file system can handle huge amounts of concurrent read/write operations.

- **OS Requirements:**
  - **Full OS kernel:** Many scientific applications have been written assuming that various features are provided by the operating system on the compute node. Many applications will make use of some subset of system calls and functions from one of the POSIX standards. Others will also use OS-specific extensions, such as Linux-specific systems calls or functions from the glibc library.
  - **fork()/exec() support:** The fork()/exec() family of system calls is necessary for MTC middleware to run on supercomputers, as the MTC middleware requires these calls to start tasks. Some supercomputer node operating systems, for example CNK on Blue Gene systems, do not provide this functionality. In the case of CNK, this meant that the compute node has to be rebooted before starting each new task.
  - **Dynamic Linking:** Dynamic linking is required by many applications to load shared libraries at runtime. The absence of dynamic linking will add an undesirable barrier to compiling standard open source applications, especially those in which high performance packages written in C and FORTRAN are dynamically linked into high-productivity, front-end driver language frameworks such as Python. We see this, for example, on the Open Protein Simulator and on other chemistry codes based on its framework.
POSIX-Compatible File System Access: The OS should provide POSIX-compatible file system access to both local storage and persistent storage, since existing applications typically use POSIX libraries and assume POSIX semantics when accessing files. Compute nodes—even those lacking hard disks and utilizing RAM or FLASH for local file systems—should make sufficient local file system space available to permit fast exchange of files for the inputs and outputs of MTC applications. Ideally, locally shared file systems will be made available on which collective data management strategies can implement intermediate file systems (IFSs) situated between the compute nodes and global file systems (GFSs). Such IFSs should be efficient and free of the costly locking and integrity guarantees that make GFSs problematic for efficiently managed file sharing.

Intermediate Utility Nodes: Intermediate utility nodes provide access to intermediate I/O processors for the execution of MTC middleware, as described in experiences based on Falkon [2]. Also, utility worker nodes on the periphery of the system, with efficient interconnect access to the entire system and with sufficient resources in terms of RAM and CPU cores and speed, can run workflow managers. Such nodes should be assignable to specific user jobs and should not impact other users or jobs.

Middleware Requirements:

Resource Provisioner: A resource provisioner functions as a negotiator between the MTC middleware and the default resource manager on the supercomputer. Common resource managers include PBS, SGE, and Cobalt. A resource provisioner uses the default resource manager to both allocate and release resources. Additionally, in a dynamic approach, the resource provisioner can/may adjust the size of allocated resources according to the utilization of the allocation.

Job Scheduler and Load Balancer: A job scheduler dispatches jobs to available computing resources. A load balancer can be either a scheduling strategy in the job scheduler or an independent module. The load balancer avoids the starving situation when some busy compute nodes have jobs in the queue while other compute nodes are idle.

Data Manager: The data manager implements a data policy that decides when and where to move each type of data. The types are common input data, unique input data, intermediate data, and output data. The data manager must decide whether to move the input and output data synchronously at the beginning and end of the job or, alternatively, to prestage the input data or delay writing back the output data. The data manager also must decide the destination of a file movement: whether the local file system, intermediate file system, the global file system, or some other resource.
Resilience: Typically, we expect MTC middleware to provide resilience to intermittent faults and failures. The middleware should be able to recover from the incomplete execution of a run or individual task failures. A run can be terminated because of hardware/software failure or concern about system utilization. Resilience requires the components of the system—the job scheduler, the load balancer, and the data manager—to be able to recover enough state to continue execution of the run after a failure.

Programming Interface: A programming interface is required so that users can flexibly generate an MTC workload. The MTC middleware programming interface could be in the form of a library that allows a user to express an MTC workflow in an existing language, or a custom programming language that expresses a workflow. Not only could a library, compiler, or interpreter execute the MTC workload, but they could also identify the various MTC patterns explored (stated in §5.2) and perform appropriate optimizations.

Flexible Scheduler Granularity: A flexible, systemwide scheduling granularity enables portions of a larger resource allocation to be freed.

Communication Fabric Access Primitives: These primitives support user access—via convenient APIs and command line interfaces—to the full power of the system’s communication fabric and, in particular, to broadcast and multicast capabilities at both the file and the message level.

### 6.2 Design Choices for Middleware

Executing and optimizing MTC applications could, in most cases, be done separately for each MTC application, for example by writing custom MPI code or by using MPI library functions for collective I/O operations or dynamic load balancing [53]. In doing so, however, we would lose many advantages that MTC applications gain from being represented as an abstract graph (in some cases, a DAG). Arguably, it is best to implement middleware that can execute a properly specified graph, for example in the form of a Pegasus DAX file [20] or a Swift script [18, 19], and apply appropriate optimizations (as we will describe in §6.3).

MTC middleware may provide some or all of the following functions:

- Programming interface – providing a flexible interface for users to compose MTC workloads
- Task scheduling and dispatch – including load balancing
- I/O scheduling and coordination – transferring data between nodes, and staging data in and out from a global file system
• Data management and caching – tracking the availability and location of input and output files. Many optimizations such as caching, prestaging of data, and multicasting of data could be implemented here.

• Resilience – detecting and recovering from failures.

An MTC middleware system would typically incorporate separate components running on different parts of a supercomputer. Falkon, which provides task dispatch and some data management services, has an multilevel architecture with a central coordinator on a login node, lightweight task executors on compute nodes, and another layer of task dispatchers that act as intermediates between the task executors and the central coordinator [5].

In the remainder of this subsection, we discuss some characteristics and choices for the MTC middleware:

• Programming Interface:
  The scope of the functionality provided by a MTC middleware system is the first and most important design decision that must be made. It is also intrinsically tied to the programming interface that the middleware exports. One basic strength of MTC is that it can abstract away many of the implementation problems inherent in taking existing codes and running them in a massively parallel way. Hiding implementation details under layers of abstraction can cause problems, however, if an application programmer requires lower-level control.

For example, writing robust code to correctly and efficiently stage data between file systems and nodes in a parallel computer as required for an MTC workflow is a significant task that can be implemented in the middleware and reused for many different workflows. For most applications, this significantly reduces the effort required to get an application up and running in parallel on a supercomputer. However, if the details of data movement are entirely abstracted away by the middleware, the programmer will lose some control and may have difficulty implementing application-specific requirements or performance improvements.

Further examples of problems that can be abstracted away by the middleware are site selection, fault tolerance, job submission to different schedulers, and throttling of job submissions. Abstracting away implementation details in a workflow can also permit dataflow optimizations by the middleware, for example, grouping jobs into batches or implementing more efficient communication patterns, such as multicast trees or reduction trees.

• Resource Provisioning:
  – Dynamic vs. Static: With a dynamic resource provisioning strategy, the number of computational resources devoted to a workflow is determined by the present demands of the workflow and fluctuates according to the number of ready tasks available. In contrast, with
a static strategy, the number of resources is fixed for the duration of the workflow.

An obvious advantage of a dynamic strategy is that higher utilization of resources can typically be achieved. Given an scientific application with various task lengths (running time), the static resource provisioning strategy would result in a “long tail” at the end of the processing, when most of the resources go idle and only a small number of jobs are still running. A dynamic strategy can release resources as they become idle, thus yielding a higher utilization. (The variable runtimes paragraph in §6.3 further discusses this “long tail” issue, which is discussed in even greater detail in [54].)

– Granularity: Different dynamic resource provisioning strategies will request resources in batches of different sizes.

The strategy is first constrained by the granularity provided by the parallel computer’s scheduler. Many parallel computers have hundreds to tens of thousands of nodes. On some HPC systems, allocating these nodes individually to jobs is neither efficient nor effective. Thus, some vendors design their systems with a greater resource provisioning granularity. For example, BG/L has a 32-node granularity, while BG/P has a granularity of 64 compute nodes. TACC’s Ranger has a granularity of 1 compute node.

Given such system constraints, a resource provisioning strategy must decide how many nodes to request at a time. Making many individual requests of the minimum granularity imposes overhead in provisioning and tracking all the requests. It also interacts badly with most batch scheduling systems and scheduling policies, discouraging users from flooding queues with many small requests, for example by limiting the number of active jobs per user. Many strategies are possible: nodes can be requested in increments of constant size as a workflow ramps up, in increments forming an arithmetic progression, or increments forming a geometric progression.

● Job Scheduling and Load Balancing:

  – Centralized vs. Decentralized: Falkon [2] was originally designed as a centralized task scheduler in the grid environment, with all scheduler state stored on a single computer. When it was deployed on BG/P, the centralized architecture didn’t fit the scale of the machine. Falkon’s performance dropped drastically at 1,000 compute nodes. Thus, it was altered to have a more hierarchical design, in order to better schedule large numbers of jobs on supercomputers. Falkon’s three-tier architecture consists of a submit host, a group of schedulers, and numerous workers.

  – Push vs. Pull: One principle when designing ultrascale software is avoiding any centralized point that could be a bottleneck. Falkon
uses a combined model to dispatch tasks, where the submit host pushes tasks to schedulers and workers pull tasks from the scheduler once they are free. The scheduler here is a partial centralized point in the system, as it holds a number of tasks in the queue.

An alternative to a pull model is a push architecture. Here, the submit host and schedulers tries to push available tasks to all workers uniformly. The scheduler have a lighter load, since it no longer needs to keep the task queue in its memory. One drawback of the push model’s scheduler is that there is no guarantee that the input data for a task is ready. And there is a risk of a starving situation, where busy nodes have jobs while idle nodes don’t have jobs to run. To compensate for this drawback, one could use “work stealing” to load balance, where a worker would ask its neighbors for tasks if it is idle.

• Data Management:
  – Common Input, Pull vs. Push: Broadcasting common input files among compute nodes could be done via a pull or a push model. The source of a common input is either the shared file system or a compute node’s local storage. In a push model, the broadcast operation can be done by a direct broadcast over the network. This approach is good for broadcasting from a shared file system, since it is already supported by machine hardware because the message-passing paradigm also requires it. An alternative solution is broadcasting through a tree topology to balance the data transfer load. This approach is useful when broadcasting from one compute node to others. A pull model fetches the data on the demand of a task. An optimization of multiple fetches from the same compute nodes could be done by checking the availability of the data before fetching.
  – Intermediate Data:
    * Data-Aware Scheduling vs. Distributed Coherence Protocol: Falkon has a data-aware scheduling feature. The goal is to route a task to the worker that has the input data needed for its task. This is a typical scenario in multistage scientific applications. The advantage of this scheme is that, at some level, performance can benefit by decreasing the amount of data movement that occurs. On the other hand, it poses new challenges for the task scheduler. First, in order to route the tasks to the right workers, the scheduler has to keep a map of the global data and its location. This is feasible at some level, but eventually the scheduling will become highly inefficient as querying the map will take an unacceptable length of time. Second, if multiple input data is needed for a given task, finding the optimal will be challenging.
    In order to avoid the disadvantages of data aware scheduling and to avoid centralized point, a distributed coherence protocol could be used. Each coherence protocol server would keep information
about a certain part of the data, using a hashing function. When a worker checked for the availability of a piece of data, it could use the same hash function, then look up the data at the right server in O(1) time.

∗ Location Lookup vs. Data Store: To support intermediate data caching, one could either use location lookup to find out where the data is and then move it in a peer-to-peer style or build an intermediate file system on the fly. A location lookup service would have a smaller amount of data movement since it only would need to copy from the source to the destination, whereas the data store would double the amount of data movement, with one copy needed from the source to the data store and another copy needed from the data store to the destination. By implementing a POSIX interface, the data store strategy has less coding complexity than does the location lookup service.

– Synchronized Data Movement vs. Collective Data Management: The data movement strategy must manage four types of data: common input data, unique input data, intermediate data, and output data. Both of the proposed strategies share common techniques for common/unique input data. They broadcast common input data to compute nodes, and workers pull unique input data from persistent storage when it is demanded by a job. Intermediate data management has been covered in the preceding paragraph. Synchronized data movement and collective data management differ when handling output data. Collective data management stores output data in a temporary shared file system, and the file system periodically backs up the data to the persistent file system. On the other hand, synchronized data movement copies output data to the persistent file system synchronously when each job finishes.

• Resilience:

MTC failures can be categorized as: hardware failure, OS failure, application failure, and strategic failure. A hardware failure happens when the power is cut or hardware becomes unavailable. OS failure includes environment variable misconfiguration and out of memory. An application failure could be caused by a programming error in the application code. A strategic failure happens when the run is shut off for specific purpose, such as in “tail chopping,” where in order to achieve high utilization on supercomputers, a current run may be killed when 90% of the jobs finish; then a smaller allocation of resource may be used for the rest of the jobs, restarting the killed jobs, until the whole run is completed.

With any of the above failures, the states of the services need to be reestablished, so that the remaining jobs can resume and finish. A number of technologies exist for failure recovery, including retry strategy and checkpointing. Also, a group of services need to be recovered: job scheduler,
data lookup service, intermediate file system. To recover the job scheduler, one could simply retry the failed and unreturned jobs. The data lookup service requires use of checkpointing, since it needs to know both the location and the state of the intermediate data. If a different group of resources is being used after the restart, the intermediate data on GPFS must be consistent with the information of the data lookup services, as well as information migration from larger to smaller allocation. The intermediate file system (e.g., MosaStore [55]) should provide the functionality of checkpointing recovery, so that when the intermediate file system is restarted on a different allocation, it can recover the data there.

6.3 Hardware and Software Support of Patterns

In this section, we discuss the demands each of the patterns described in §5.2 has for the MTC middleware:

- Control Flow Patterns:
  - Parameter Sweep: Parameter sweeps are perhaps the most straightforward use of MTC to support. They require little more from software and hardware beyond the basic ability to launch parallel tasks on worker nodes. However, the parameter sweep workload is “flat”: all job specifications are available in advance. Thus they may be efficiently organized and scheduled as a whole and dispatched to worker sites using high-performance messaging techniques.
  - Iteration: Iteration requires support from the MTC runtime. Some systems that assume that the DAG of tasks is static, such as Condor’s DAGMan, cannot support iteration without augmentation. Another challenge posed by iteration is that estimating the duration of the job may be difficult when requesting time on a machine, and providing an upper bound on the length of a job may be especially difficult: if a reservation runs out before the job ends, there is potential for the computational results to be lost. Fortunately, MTC supports the resumption of incomplete jobs, since results of each completed task can be written out to a file system.
  - Task Pruning: Task pruning requires support from the MTC middleware to allow a running task to signal another running task to stop without itself terminating.

- Dataflow Patterns:
  - Scatter: The major problem posed by the scatter pattern is that a very large load can be imposed on a single point in the system, either the GFS or the node with the data in its storage, since a large number of nodes will need to read the same item of data at the same time over the network.
In order to mitigate this problem, a mechanism is needed in the MTC middleware for efficiently disseminating data to many nodes, for example, by using a multicast tree, file replication, or special hardware support for broadcast/multicast.

- **Gather:** The naive implementation of a gather would involve writing all the files to a GFS and then reading them back in. A smarter implementation, which would require support from MTC middleware, would instead stage data directly from node to node, either through an intermediate file system (IFS), created by combining the storage capacity of worker nodes, or by staging data from one task to another directly. The node receiving all the data is likely to become a bottleneck, where the limiting factor may be network bandwidth, local storage availability, or compute performance. This bottleneck problem can be relieved by a compiler optimization. Instead of transferring all data to a single node where the data operation takes place, the compiler could generate a reduction tree of data operations. An important consideration here is whether the data is pushed to or pulled by the node. If data transfers to the bottleneck node can be initiated by the other side (“push”), there is a risk of overwhelming the node.

If data transfers can be staggered without causing delays, or if data can be reduced in size by processing it hierarchically, this approach is likely to improve performance.

- **Pipeline:** If a set of tasks is performed sequentially, with the output of each serving as the input to the next, this structure can be exploited to improve performance. The MTC middleware would ideally ensure that the set of tasks was assigned to the same node, allowing data to remain local to the node and to support efficient task dispatch so that there is minimal delay in executing one task once its predecessor is finished. An effective way to achieve this is to dispatch the set of tasks together as a group.

- **Data Reuse:** If the same data is reused by different tasks repeatedly, the potential exists for significant, unnecessary strain on the GFS if the data is repeatedly fetched.

  The use of a node’s local storage, or the use of an IFS can significantly reduce the stress on the GFS when used as a cache for intermediate files or files from the GFS. A data-aware task scheduler can then also move the computation to the data, reducing the amount of data that must be transferred.

- **Other Features:**

  - **Coordination of MPI Applications:** The MTC runtime would need to be able to request blocks of CPUs from the MTC scheduler on which to run MPI tasks. In this case, each worker in the allocated
block would receive information from the scheduler that would allow it to dynamically connect to other workers, dynamically constructing the MPI application from its component processes. Changes to the popular MPICH implementation have been made to support this mode of operation.

- Variable Runtimes: The primary problem that occurs in the presence of tasks with highly varying durations is that of efficiently utilizing available computer resources. MTC will keep worker nodes busy as long as sufficiently many parallel tasks are available. Even in the best case, however, utilization of the available resources is likely to drop off significantly at the end of a job or a phase, as the pool of available work shrinks and only a small “tail” of running jobs remain. This is particularly problematic when the distribution of task runtimes is skewed so that a significant proportion of tasks have runtimes much greater than the mean. If a supercomputer’s allocation policy requires compute nodes to be requested and released in large blocks, this can cause unacceptably inefficient use of allocated time on a supercomputer. We call this the “trailing task” problem; it is discussed in detail in a separate paper [54].

Where supported, the appropriate solution is to relinquish idle workers. However, supercomputer nodes typically must be allocated to jobs in blocks, and it may not be possible for a job to relinquish nodes individually when they are no longer needed.

Several solutions are possible. Dispatching tasks in order of longest to shortest runtime is effective in achieving a better schedule in most cases, but it is possible only if task runtimes are known ahead of time. Otherwise, reducing the number of worker CPUs allocated can improve utilization, but only at the cost of increasing time to solution. The terms of the trade-off between utilization and time to solution can be improved by “chopping off the tail” of tasks remaining once some number of CPUs have fallen unused. The MTC scheduler can terminate straggling tasks, allocate a smaller number of CPUs, and restart the work there, where it can complete without leaving as many resources idle. Specific scheduler and middleware features could be provided on a system such as Blue Waters to boost the effectiveness of tail chopping, thereby allowing scientists to obtain a quick time-to-solution while still using the machine efficiently. In particular, the ability to relinquish part of a CPU allocation without relinquishing the whole would allow tail chopping to proceed with no delay. The ability to migrate tasks between worker CPUs would further facilitate this, as it would enable longer-running tasks to be consolidated into smaller partitions of a supercomputer [54].
7 Conclusions

In this report, we have discussed the concept of MTC applications, a number of specific MTC applications, and the value of the MTC approach for enhanced scientific productivity. We believe that the number of MTC applications will continue to increase and that these applications will make up an important category of applications that will demand resources on large-scale systems such as Blue Waters.

We believe that all the application domains we have surveyed indicate an important progression and trend. The application starts out as a serial code. Such serial codes can almost always immediately benefit from execution as a many-task application because of a need to run the application on larger datasets and/or on an increasingly broad parameter space. Many of the algorithms involved also can be run in parallel with tightly coupled multiprocessing (e.g., MPI) or shared-memory multiprocessing (e.g., OpenMP). But in many cases, such fine-grained parallelism hits a ceiling of speedup between 1,000 and 10,000 cores, while the benefits of running many such application instances in parallel keeps increasing for the reasons above. Thus, we believe that many already parallel applications will benefit from a hybrid model of using MTC for the higher-level outer loops of a program, while using fine-grained parallel processing in the inner loops. We believe it will become increasingly beneficial—in terms of the scientific merits or reduced time-to-solution and hence to discovery—for Blue Waters to support such hybrid MTC-HPC applications.

In §5 we have presented a taxonomy for identifying MTC patterns, and in §6, we have provided insight into core features that the system needs to support, focusing on what will be needed to make Blue Waters an ideal platform for such applications. It appears that MTC applications will be able to make basic use of the Blue Waters system without demanding any changes to its intrinsic design. The following are some specific architectural recommendations that our study suggests for the Blue Waters system to benefit MTC applications:

- Providing full Linux semantics on its compute nodes, including multiprocessing (fork/exec) and dynamic loading, so that a broad set of applications can be readily compiled and executed, and so that MTC middleware can be readily deployed.
- Providing some (however limited) local file system, on compute node kernels, for use in passing datasets into and out of MTC applications.
- Providing access to intermediate I/O processors for the execution of MTC middleware, as described in experiences based on Falkon [2].
- Having a flexible, systemwide scheduling granularity that enables portions of a larger resource allocation to be freed.
- Supporting user access—via convenient APIs and command line interfaces—to the full power of the system’s communication fabric.
• Providing utility worker nodes on the periphery of the system on which workflow managers can be run with efficient interconnect access to the entire system and with sufficient resources in terms of RAM and CPU cores and speed. Such nodes should be assignable to specific user jobs and not impact other users or jobs.

We believe that all these recommendations can be met with minimal impact in the initial Blue Waters architecture, to the best of our knowledge based on current public information and experience on systems such as the BG/P, XT5, and Constellation.

Given the technical feasibility of efficient execution of MTC applications on Blue Waters-class systems, it thus becomes a matter of policy whether these applications are run on the system. We believe that the definition of “capability systems” should be interpreted by weighing the scientific merit of an application and its ability to efficiently use the system’s resources more than the application’s specific implementation approach. That is, the criteria for allocation should be scientific need/merit and the inability to achieve that science in a timely fashion using other more readily available resources. The fact that an MTC application could be run on smaller resources while a more traditionally implemented HPC application could not is, we believe, a criterion that does not reflect the true value and scientific opportunity presented by the resource request. Another reason to better support MTC applications is that urgent computing situations—perhaps arising from national or global health, climate, weather, or defense emergencies—may require the execution of MTC applications at a scale far greater than that which exists under normal conditions. For example, using petascale resources to run BLAST might be urgent in an emergency, requiring a more rapid time-to-solution than could be achieve by aggregating lower-performance resources.

In summary, MTC applications are here today, and they are increasing in number. Blue Waters technically can support such applications, as designed, and could better support them with some relatively small changes. Policies to support such applications on Blue Waters will lead to valuable science results that would otherwise be much delayed.

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