

ExM: High level dataflow programming for extreme-scale systems

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Abstract

We present here the ExM (extreme-scale many-task) programming and execution model as a practical solution to the challenges of programming the higher-level logic of complex parallel applications on current petascale and future exascale computing systems. ExM provides an expressive high-level functional programming model that yields massive concurrency through implicit, automated parallelism. It comprises a judicious integration of dataflow constructs, highly parallel function evaluation, and extremely scalable task generation. It directly addresses the intertwined programmability and scalability requirements of systems with massive concurrency with a programming model that may be attractive and feasible for systems of much lower scale. We describe here the benefits of the ExM programming and execution model, its potential applications, and the performance of its current implementation.

1 Introduction

Exaflop computers capable of 10^{18} floating-point operations/s are expected to provide concurrency at the scale of $O(10^9)$ threads on $O(10^6)$ cores [22]. Such extreme-scale systems will enable and demand new problem-solving methods that do not follow today’s dominant single program, multiple data (SPMD) paradigm but instead involve many (often a time-varying number) concurrent and interacting tasks. Writing correct, scalable programs at this level can be an onerous task, with significant investment of programmer time required to make a program run efficiently on hundreds or thousands of cores. Applications at this scale can have a development cycle approaching a decade.

For some applications, intricate high-level coordination logic is necessary; but in other cases, the high-level coordination pattern is relatively straightforward and may be expressed as the composition of a number of computational tasks. In practice, the composition takes the form of scripted dataflow logic, in which tasks are linked together through their input and output data sets; the tasks themselves are developed separately as libraries or external programs. Important applications in methodologies such as rational design, uncertainty quantification, parameter estimation, and inverse modeling all

have this many-task property. Many will have aggregate computing use cases that require exascale computers. The ExM computing model draws on recent trends that emphasize the identification of coarse-grained parallelism as a first and separate step in application development [14, 23, 24]

Currently, many-task applications are programmed in one of two ways. In the first approach, the logic associated with the different tasks is integrated into a single, tightly coupled application. Load-balancing libraries based on MPI [15], such as the Asynchronous Dynamic Load Balancing Library, ADLB [12], or on Global Arrays [18], such as Scioto [8], have recently emerged as promising solutions to aid in this approach. They provide a master/worker system with a put/get API for task descriptions, thus allowing workers to add work dynamically to the system. However, they lack a comprehensive programming model, data model, and other features required for high-productivity programming. In the second approach, a script or workflow is written that invokes the tasks, in sequence or in parallel, with each task reading and writing input and output files or streams. However, performance can be poor, since existing many-task scripting languages are implemented with *centralized evaluators* that cannot sustain the high overall task rate necessary to efficiently communicate with and utilize $O(10^6)$ cores.

Our view is that the programming of a significant fraction of extreme-scale applications will require a hierarchy of programming models. An implicitly parallel, functional, dataflow-based programming model is well suited for programming the higher levels of such applications, while many diverse and finer-grained parallel models will be used in hybrid approaches to program the cores of such applications. This view is based on our significant experience with the Swift parallel scripting language [25], which has been used extensively to program the “outer loops” of such applications and to compose existing programs into larger and more sophisticated applications such as simulation or analysis pipelines, parameter sweeps, ensemble methods, and complex workflows graphs. The contribution of this paper is a comprehensive strategy to perform such high-level application coordination at extreme scales with greater programmability.

Previous approaches to workflow execution on high-performance resources have involved deploying a toolkit developed for distributed systems on the target infrastructure. Software systems relevant for this model include Dryad [10], Skywriting [16]/CIEL [17], and Swift [25]. This approach is convenient for the user, particularly when each task is a distinct executable program. However, this approach faces multiple performance challenges, including the ability to rapidly launch independent processes [21], manage large numbers of pilot jobs [13], communicate over an emulated TCP network [11], and coordinate data access [26].

Alternatively, the developer may hand-code a work distribution system using available high-performance tools, communicating through MPI messaging in distributed memory or function calls (as in the parallel version of the Common Component Architecture [2].) This approach uses familiar technologies but can be inefficient unless much effort is spent incorporating load-balancing algorithms into the application. Moreover, the approach can involve considerable programming effort if multiple component codes are to be integrated. Partitioned global address space (PGAS) [20] language features provide a partial solution to the data model but do not offer notifications and other features necessary for the construction of high-level scripts.

Our approach integrates these two models. First, we provide a very high-level, naturally concurrent programming model in the previously developed Swift language. Second, we developed translation strategies to render Swift semantics into a distributed-memory model, based on efficient primitives compatible with the highly scalable ADLB library - the primary focus of this paper.

2 modFTDock: A sample application

Running many-task applications, such as ensembles of protein analysis codes, efficiently, reliably, and easily on large-scale machines is challenging. *modFTDock* [19], a relatively simple application analyzing protein docking, highlights these challenges. As shown in Figure 1, *modFTDock* starts with M input files and N input parameters. Each of these $M \times N$ combinations is processed by the sequential *modftdock* task. The resulting docking data is stored and processed later by tasks *merge* and *score*, which produce the requisite results. All the application stages communicate only through their input and output data. Figure 2 illustrates the simple specification of this dataflow in Swift. Quantitative information for a contemporary *modFTDock* run is tabulated in Table 1; conceivable future experiments could be composed of trillions of tasks.

The challenge is to efficiently, reliably, and scalably coordinate the million tasks generated by the *modFTDock* application while at the same time using a com-

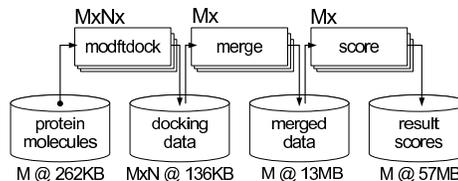


Figure 1: Dataflow schematic for modFTDock. The output sizes are for a single run of an application task.

```

1  dock_score scores[];
2  foreach (p1, i in proteins) {
3    dock_result docked[];
4    foreach (p2, j in proteins) {
5      if (i < j) {
6        docked[j] = modftdock(p1, p2);
7      }
8    }
9    scores[i] = score(merge(docked));
10 }

```

Figure 2: Swift implementation of modFTDock.

pact, programmer-friendly specification that can support the integration of legacy code.

3 Swift: A dataflow language to support many-task applications

The canonical applications for which Swift was originally designed had most of the sequential computation code already written and encapsulated as command-line binaries that needed to be coordinated as a workflow. Traditionally UNIX shell scripts have been used to this end, but Swift was designed to better support running such applications in distributed and parallel contexts, where synchronization, data movement, explicit task scheduling, and fault-tolerance are necessary.

The Swift execution model may be split into two processes: *task generation*, the interpretation of the user dataflow script, generating concurrent tasks and *task execution*, which distributes the resulting side-effect free *leaf tasks* and orchestrates their execution. *Leaf tasks* may be implemented as procedures and correspond to library call invocations, or standalone executables, in which case they correspond to launching a new process. Leaf tasks themselves may use multiple cores or even multiple nodes.

To link the above to our sample application, we treat the components of the modFTDock as leaf tasks coordinated by a Swift script. For modFTDock, the leaf tasks

Table 1: Statistics for a full modFTDock application run.

Task	Number of Tasks	Duration
modftdock	1,200,000	1,000s
merge	12,000	5s
score	12,000	6,000s

are single-process executables, yet concurrency is exposed by Swift semantics. Data dependencies, task distribution, and data movement are managed by the system as follows.

In Swift, unlike in shell scripts, all inputs and outputs of a (side-effect free) leaf task must be explicitly defined, so that the Swift runtime has enough information to manage its input and output. A Swift app function definition such as the one below converts a standalone executable (the `convert` utility) to a Swift function with arguments and return values (such as image files or `int` parameters).

```
app (image out) rotate(image in, int angle) {
    convert "-rotate" angle @in @out;
}
```

We will provide an extension mechanism to allow functions from other languages to be defined and compiled/linked as Swift tasks as well. In addition to these external functions, functions can also be defined within Swift, comprising multiple Swift statements.

The parallelism in a Swift script is exposed implicitly, with the order of execution of Swift statements determined entirely by data dependencies. Multiple statements and subexpressions can execute in parallel, given no data dependencies and sufficient parallel computing resources. Consider the following example:

```
(datafile result) process (datafile in) {
    datafile foo; datafile bar;
    foo = f(in);
    // g and h below can run concurrently with f
    bar = g(in);
    result = j(foo, h(bar));
}
```

Each iteration of a `foreach` loop in Swift runs independently, but data dependencies may serialize execution.

```
int out[];
foreach f, i in myfiles {
    // Each iteration is completely independent
    out[i] = readData(process(f));
}

int out[];
foreach f, i in myfiles {
    // But these are serialized by data dependencies
    if (i > 0) {
        out[i] = readData(process2(f, out[i-1]));
    } else {
        out[i] = readData(process(f));
    }
}
```

The Swift language design ensures that even high concurrency programs are *deterministic by default* [4]. The core Swift language constructs are deterministic and non-determinism can only originate from non-Swift code. A valid Swift program always produces the same

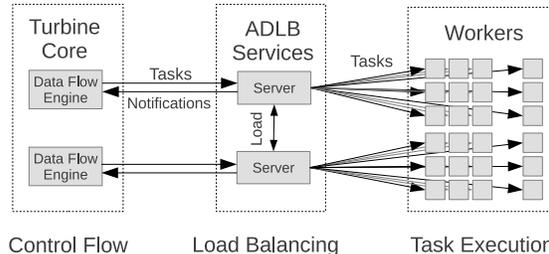


Figure 3: Task distribution in the Turbine runtime system.

output (although the ordering of side-effects such as log messages can vary).

The main feature that enables this property is the use of write-once variables: each Swift variable can be written to only once. Writing twice causes a compile or runtime error.

Write-once variables give programming in Swift a nonimperative programming flavor and eliminate the possibility of many concurrency bugs. A Swift compiler can automatically detect or warn of many classes of errors such as deadlocks from circular dependencies or unassigned variables. Including arrays in the language allows more runtime errors because of the impossibility of deciding statically if a particular array index is modified (cf. the halting problem), but these quasi-imperative arrays of write-once variables are more expressive than purely functional alternatives [3] and are less of a leap for programmers familiar with imperative languages.

In summary, Swift programs are well suited for expressing the upper-level concurrency of complex applications that integrate a variety of other functional components (often written in other diverse parallel programming models). The Swift runtime provides the scalability and performance necessary to manage millions of task definitions and input/output data objects. This allows the use of distributed memory to store script control variables and cache user datasets, while resolving the data dependencies that coordinate independent processes.

4 ExM architecture

We are developing a new implementation of Swift based on the ExM extreme-scale many-task execution model. This implementation performs fully distributed execution of a Swift program with no centralization of control flow.

The full ExM system comprises a distributed version of Swift and MosaStore, a distributed in-memory file system [6]. We discuss only the former in this paper, which is implemented as two subsystems: the runtime system (called Turbine) and the Swift-to-Turbine compiler (called *stc*).

We think of the intermediate code, the crucial inter-

```

1 | main {
2 |   int x;
3 |   int y;
4 |   int z = 1;
5 |   (x, y) = f(z);
6 |   if (x != 0) {
7 |     trace(y);
8 |   } else {
9 |     trace(z);
10 |   }
11 | }

```

Figure 4: Swift script to be compiled by *stc*.

```

1 | # Main program fragment-
2 | # starts on a single process
3 | main {
4 |   # allocate data in global data store
5 |   integer x
6 |   integer y
7 |   integer z literal 1
8 |
9 |   # post call to f, with input x and output x, y
10 |  statement call_composite f [ z ] [ x y ]
11 |
12 |   # post call to conditional expression
13 |  statement conditional if-0 [ x y z ]
14 | }
15 |
16 | # This program fragment executes sometime after x
17 | # is written, maybe in another process
18 | block if-0 { x y z } {
19 |   # retrieve x from the global data store
20 |   integer_get x
21 |   if (x) {
22 |     statement builtin trace [ y ]
23 |   } else {
24 |     statement builtin trace [ z ]
25 |   }
26 | }

```

Figure 5: Generated Turbine intermediate code. Each fragment is sequentially evaluated, with each statement command creating an asynchronous task.

face between the two, as the instructions for an abstract workflow machine. The set of runtime system primitives for task management, data management and synchronization is kept as minimal as possible, in order to make the Turbine runtime as robust and flexible as possible. Figures 4–7 illustrate how Swift code is translated into intermediate code for Turbine’s consumption.

The Turbine runtime system currently is built on top of MPI, running on a cluster with all communication between components using messages. Using MPI made it easy to port to several cluster architectures, including IBM Blue Gene/P, Cray, and SiCortex systems. The MPI processes are divided among three roles: ADLB servers that manage the task queue and data store; Turbine rule engines that track data dependencies and execute intermediate code; and workers that exclusively execute leaf tasks. Typically the bulk of processes are workers, since the bulk of computation occurs in leaf tasks.

```

1 | # int A[];
2 | container A integer integer # container with int keys, vals
3 |
4 | # test[0]=1;
5 | integer _t0 literal 1
6 | container_insert immediate A 0 _t0
7 |
8 | # test[f]=g();
9 | integer _t1
10 | statement call_composite g [] [ _t1 ]
11 | integer _t2
12 | statement call_composite f [] [ _t2 ]
13 | container_insert future A _t2 _t1
14 |
15 | # trace(test[1]);
16 | reference _t3
17 | container_lookup_ref immediate A 1 _t3
18 | integer _t4
19 | dereference _t3 _t4
20 | statement builtin trace [ _t4 ]
21 |
22 | # cleanup operation: decrement container writer count
23 | container_decr_writers A

```

Figure 6: Generated Turbine intermediate code for array operations, with the corresponding Swift code in comments.

```

1 | int A[]; int B[];
2 | A = constructArray();
3 | foreach x, i in A {
4 |   B[i] = f(x);
5 | }

```

```

1 | main {
2 |   container A integer integer
3 |   container B integer integer
4 |   statement call_composite constructArray [] [ A ]
5 |   loop A loop1_body [ B ]
6 | }
7 |
8 | block loop1_body { B x i } {
9 |   integer _t0
10 |  statement call_composite f [ _t0 ] [ x ]
11 |  container_insert immediate B i _t0
12 | }

```

Figure 7: Swift script with foreach loop to be compiled by *stc*, and the corresponding intermediate code.

5 Implementation progress and challenges

At the time of writing, we have a working compiler and runtime system that can handle a significant subset of the language, including functions, recursive function calls, conditionals, expressions, arrays and structures. We are focusing currently on scalability, running Swift scripts on tens of thousand of cores.

A number of challenges arise in making the Turbine interpreter scale. ADLB provides a strong base on which to implement task distribution, but a naive approach to task generation can put unnecessary strain on load balancing and data dependency management processes. A naive foreach loop, without throttling or loop splitting could create hundreds of thousands of tasks simultaneously, swamping ADLB. Long data dependency chains between tasks in the runtime also occurs with a naive ap-

proach. Static analysis is necessary to defer task creation until data is ready and to coalesce tasks if possible.

Swift’s data model also presents challenges, with data potentially shared by many tasks. With load balancing it is essential that any data remain accessible to tasks after relocation. Turbine provides a global data store to this end. Primitive data types such as numbers or strings are stored directly in the data store. Arrays and structures also reside in the data store as Turbine *containers*, a dictionary data type, with linked containers supporting more complex data structures. Containers are specialized to support the deterministic semantics of a Swift script, such as the requirement that any ordering of reads and writes to an array index should result in the same outcome and that a read should eventually fail if an array index will never be written to. Hence, the interpreters need to reach a consensus on when a container is *closed* (i.e. no more writes will occur). To this end, we use static analysis in the compiler and special reference counting operations in Turbine. For scalability, Turbine supports *distributed* containers, with the container split between data servers by index range.

Logically all Swift variables are values, rather than references; but for efficiency we want to avoid doing excessive copies-by-value, particularly of arrays. Copying references, however, introduces the problem of garbage collection. Various techniques exist for distributed garbage collection [1]; distributed reference counting is the most straightforward candidate for Swift but can be inefficient. Most Swift variables are unneeded beyond the lifetime of a procedure stack frame, so we anticipate that escape analysis [5] should be sufficient to keep the reference counting overhead manageable.

In general static analysis techniques in the compiler will be important for scalability and performance, with efficiency of individual runtime operations playing a secondary role. Often a naive approach to compilation results in severe inefficiencies, such as repeated redundant lookups of variable values or other inefficient usage patterns of the Turbine runtime. Static analysis of Swift is fortunately straightforward because of write-once semantics for variables, thus making it easy to convert a Swift program to a simple version of the standard Static Single Assignment form [7] and deploy many code optimization techniques.

The current Turbine design with processes divided into three roles has been easy to scale up, but it may eventually prove to limit the efficiency of task distribution. Past work on building extremely efficient task-parallel runtime systems (for example, Cilk [9]) has tended to use a symmetrical design, where each process cooperates equally in load balancing and task execution, with work-stealing providing load balancing. For ExM, moving to this model could reduce internode communication

significantly, with tasks and data remaining local except when load balancing occurs.

6 Performance results

In this section, we demonstrate the ability of the ExM task distributor to run a synthetic user application that performs nontrivial script logic. This benchmark carries out an algorithm similar to a recursive search and emulates user work at the leaf function calls.

We wrote a Swift script to evaluate the n th Fibonacci number `fib(n)` according to the recursive formulation $\text{fib}(0) = 0$; $\text{fib}(1) = 1$; $\text{fib}(n) = \text{fib}(n - 1) + \text{fib}(n - 2)$.

In the Swift model, these recursive calls generate a data-dependent workflow to be evaluated among the control flow components in the runtime system. As the workflow progresses, many recursive procedure invocations are triggered, exercising the control flow functions of Turbine. At the base cases $n = 1$ or $n = 0$, leaf tasks sleep for 10 seconds to emulate user computation time.

We ran this benchmark on the IBM Blue Gene/P *Inrepid*, a system with 40,960 nodes of 4 cores each. We used varying core counts, with one MPI process per core, with the workload and number of leaf tasks increased by increasing the input parameter n . We obtained a utilization result by dividing the user time (time spent in sleep) by the wall time of the run. Results are shown in Table 2.

Table 2: Detailed statistics for `fib` runs

Cores	n	Leaf Tasks	Time (s)	Util.
4,096	23	46,368	129.0	87.6%
8,192	26	196,418	168.7	87.8%
16,384	27	317,811	217.9	89.0%
32,768	29	832,040	284.1	89.3%
65,536	30	1,346,269	233.3	88.0%

7 Conclusion and future work

We have motivated and described the ExM distributed execution model for running Swift dataflow applications. Swift makes it easy to express massive coarse-grain parallelism, and ExM is capable of executing Swift applications with extreme scalability. While much work remains to complete and validate the full Swift language on ExM and to achieve exascale performance targets, the system will soon be capable of supporting real scientific applications. We will use current petascale systems to extend testing to the 160K core range and to simulate its performance at over 1M core concurrency. We believe ExM’s many-task execution model and distributed hierarchical data model makes it well suited to address the resilience and energy-aware load balancing that will be required at the exascale. We will evaluate these potential benefits as the implementation proceeds.

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