The Loci Multithreading System

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This document details the current (2016) design and implementation of the multithreading system and related supporting infrastructure in the Loci framework. It provides documentation support for future developers of the Loci system wishing to understand, extend, and maintain the multithreading modules. Such developers are also encouraged to read through the related source files in the Loci code base, as those files contain additional comments and information pertaining to the implementation and coding considerations of the multithreading system. Relevant source files will be outlined later in this document.

1 Overview

The main goal of the multithreading modules is to extend the Loci framework to better support next generation high performance computing systems. The Loci framework already supports distributed memory and runs well on pure distributed memory systems. It however lacks support of multithreading scheduling and code generation, making it less than ideal to run on mixed distributed and shared memory systems, which is the main architecture employed today. The multithreading system adds the thread level parallelism to the Loci framework, making it able to exploit a hybrid form of parallelism consisting of MPI and threads. When both enabled, Loci applications will be first distributed to MPI processes and then further partitioned to multiple threads within a single MPI process. The initiation of the multithreading system will also hopefully pave the way for future enhancements to the system such as addressing the vector parallelism paradigm that is also on the rise in recent time.

The Loci multithreading system has been tested and verified using the Chem test suite. Although it is considered ready for real production use, there has not been large-scale production run using the multithreading system. Future developers may need to perform careful studies and evaluations of the multithreading system to observe its behavior for large-scale real-world problems.

Also preliminary performance testing and evaluation has been conducted for the multithreading system. In the preliminary evaluation, it has been found that the multithreading system is generally effective, though its raw peak performance cannot compete equally well with a pure MPI parallelism. Much work has been conducted to try to identify the performance bottleneck in the multithreading system. Although there is currently no definitive conclusion to this question (due to the complexity and nature of non-trivial multi-threading programs), the most plausible cause seems to be the data locality issues. There are also several current Loci internal designs that may also degrade threading performance. Another issue is that current performance evaluation has been carried out on relative small-scale (up to dozens of threads). The performance behavior of the multithreading system under large-scale thread parallelism (e.g., up to hundreds or thousands of threads) is unknown. This document together with the comments in the source code will try to point out several important issues that may be affecting the threading performance.

During the design and development of the Loci multithreading system, several new thoughts and ideas have also emerged. Some of these relate mainly to the multithreading system itself (but was not implemented due to current software architecture constraints or lack of time), while several others offer potential improvements to the Loci system in general. This document will also try to point out some of these thoughts so that future developers may consider to adopt/adapt some of them in the Loci system as it continues to evolve.

2 Installation, setup, and source code organization

The multithreading modules are fully integrated within the Loci framework. There is no separate installation requirement. Once the Loci framework is installed, the multithreading modules are also installed. By default, the multithreading functionality is not enabled. To compile the multithreading code into the Loci library, the `PTHREADS` macro has to be defined for the compiler to see, and the `pthread` library needs to be linked to the object code. Since the current Loci installation uses configuration files, it is suggested to add the following section into the file `sys.conf`. And then add these macro definitions to the relevant sections in the `comp.conf` and `sys.conf` files. In the future, when the multithreading system is deemed sufficiently robust, it may be compiled into the Loci framework by default by removing these requirements.

```
#########################
THREADS = -DPTHREADS
THREAD_LIB = -lpthread
THREAD_INCLUDE =
#########################
```

Figure 1 is a diagram of the organization of the main source code files containing the implementation of the multithreading modules within the current Loci code base. The brief comments within the parentheses provide a summary of the main purpose of that particular source code file in the multithreading implementation. The most important files are `thread.h` and `thread.cc`. These files are specifically created from scratch and contain the overall architecture and major scheduling and execution mechanisms of the multithreading system. All other related files mentioned in Figure 1 contain specific patches and enhancements to previous codes that support multithreading functionality. These patches and enhancements can be roughly sorted into the following categories:

- Fix of existing code so that thread safety issues are not violated. Most of the fixes occur in the original event dispatch code.
- Enhancements made specifically to improve multithreading function and performance. These mainly include removing thread blocking requirements in some of the container classes (see section 5.2 for more discussion), and changes to the rule kernel executions to better suit multithreading.
- Patches made to each rule compiler and execution module so that a special multithreaded module will be compiled and generated when multithreading is enabled. For example, the file `comp_chomp.cc` contains chomping related modules that generate Loci execution back-end for chomping scheduling. In the multithreaded version, it also includes code that determines when and how to generate multithreaded versions of chomping scheduling.
- Changes made to the Loci scheduler to incorporate multithreading scheduling.

If multithreading support is compiled into the Loci framework, it can be activated using the command-line switch "`--threads`." For example, suppose "`app`" is the name of a Loci application, then issuing the command: `app --threads 8` will launch the `app` program using eight threads. If the option "`--threads`" is not provided, then the program will only run in a single thread (the default one in a process). Currently a maximum of 24 threads may be used within a single application process. If in the future, large-scale thread parallelism performance is proved to be sufficiently good, then this limit can be removed (in file `scheduler.cc`). Issuing the command: `mpirun -np 4 ./app --threads 8` will launch the program `app` using four MPI processes (working in parallel) and eight threads within each MPI process (for a total parallelism of 32 execution units). In addition, the following command-line options are also provided to fine tune multithreading behavior:

- `--thread_blocks <n>`, where `n` is a number used to provide maximum blocks to be used within a single thread. See section 4.5 for discussions of thread blocking. If this option is not provided, then a default value of ten is used. The current maximum value of the `n` that can be used is 99.

```
src/
 ├─ include/
 │   ├─ Tools/
 │   │   ├─ cptr.h (thread safety fix)
 │   │   ├─ Handle.h (thread safety fix)
 │   │   └─ lmutex.h (thread safety fix)
 │   ├─ execute.h (threading/non-threading rule kernel interface)
 │   ├─ rule.h (threading/non-threading rule kernel interface)
 │   ├─ parameter_def.h (non-blocking fast_copy)
 │   ├─ parameter_impl.h (non-blocking fast_copy)
 │   └─ store_rep.h (non-blocking fast_copy)
 ├─ Tools/
 │   └─ eventNotify.cc (thread safety fix)
 └─ System/
     ├─ thread.h (main impl)
     ├─ thread.cc (main impl)
     ├─ comp_chomp.cc (chomping rule related changes)
     ├─ comp_impl.cc (pointwise rule related changes)
     ├─ comp_recurse.cc (recursive rule related changes)
     ├─ comp_reduce.cc (reduction rule related changes)
     ├─ comp_tools.cc (misc changes)
     ├─ Initialize.cc (scheduler related changes)
     ├─ rule.cc (threading/non-threading rule kernel interface)
     ├─ sched_comp.cc (scheduler related changes)
     ├─ sched_tools.h (threading/non-threading rule kernel interface)
     ├─ scheduler.cc (scheduler related changes)
     └─ store_rep.cc (non-blocking fast_copy)
```

Figure 1: Loci multithreading implementation source code organization

- `--no_threading_pointwise`. If provided, then all of the Loci pointwise rules will not be scheduled using multithreading.
- `--no_threading_global_reduction`. If provided, then all of the Loci global reduction rules will not be scheduled using multithreading.
- `--no_threading_local_reduction`. If provided, then all of the Loci local reduction rules will not be scheduled using multithreading.
- `--no_threading_chomp`. If provided, then all of the Loci chomping rules will not be scheduled using multithreading.
- `--no_threading_recursion`. If provided, then all of the Loci recursive rules will not be scheduled using multithreading.

3 Overall design considerations

This section discusses the overall design choices and considerations related to high-level multithreading facility. First of all, the multithreading modules continue to use data parallelism in the same way as the existing distributed memory implementation.

Figure 2 shows the task and data parallel view of multithreading execution of a set of Loci rules. Task parallelism assigns entire rule computation to different threads, while data parallelism assigns sub-domains in each rule to different threads. These are the two major forms of thread level parallelization strategies in use today. In all of current Loci applications, the task parallelism level is quite small since there will only be a small set of independent rules at a given scheduling step. Therefore in the current implementation, data parallelism is used since the domain of each rule is usually very large. And therefore data parallelism supports a much larger thread level concurrency. It is possible to mix the two forms of thread level parallelism in the Loci framework and it may provide some benefits for certain types of applications. This is left as a future improvements. At the present time, only data parallelism is beneficial to any multithreading scheduling of Loci applications.

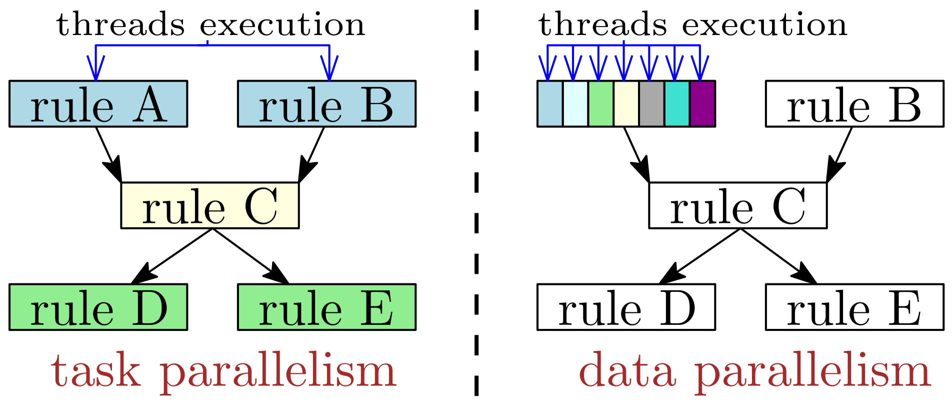


Figure 2: Task and data parallelism

Another issue is load balancing. We do not perform any dynamic load balancing to the current multithreading schedules. The reason is the same as we do not have dynamic load balancing in the current distributed memory schedules — the cost of computation kernel applied to each entity in a rule domain is usually uniform. Load balancing is another reason why we have only adopted the data parallelism form for multithreading schedules. The task parallelism would usually require some form of dynamic load balancing to distribute the work evenly to all threads as the cost of different rule computations may indeed be dramatically different.

In recent development of multithreading programming, an important class of technique called "logic parallelism" is increasingly gaining widespread adoption. Representative languages and systems that use such concurrency paradigm include the Intel Cilk and Threading Building Blocks, the Java executer and fork/join frameworks, as well as a number of other research products. Systems using logic parallelism employ a scheduling layer that sits between the program specification and the machine hardware. In the program specification, the programmer uses language and system constructs to indicate at a high level where parallelism *might* occur, and/or where executions *can* happen concurrently. These special constructs provide the middle layer hints how and where parallel execution can be scheduled and they usually also support recursive and nested logic parallelism. In the logic view of the program, the total number of threads can be unbounded. The middle layer then schedules these logic threads onto a given set of low level system threads (such as real hardware threads or threads provided by certain libraries). The scheduler can usually also be configured in different ways and works transparently in the background from the programmer's perspective. Several such systems also employ provably optimal scheduling policies that generate asymptotically guaranteed thread scheduling performance.

The Loci framework can also be structured to take advantage of such logic parallelism. For example, all the entities that form the domain of a Loci rule can be partitioned into large numbers of small chunks each contains a few (maybe on the order a few dozens) entities. Then each such chunk together with the computational kernel can be treated as a "logic" task and handed over to the thread scheduler. The runtime thread scheduler will take care of the mapping, scheduling, and load balancing issues. Another way to restructure a Loci rule computation would be to split the rule domain in half recursively and let the system scheduler deal with the management of nested parallelism on a fixed number of hardware threads. Using such an approach can dramatically simplify taking advantage of multithreading concurrency as the middle layer scheduler takes care of vast number of important issues automatically. It also provides a means of dynamic load balance within the participating threads. Loci rules under this paradigm will only be viewed as collections of small chunks and each chunk is computed independently. So long as the dependency that produces correct results is respected, the scheduler is free to mix and reorder the execution of all these chunks as it sees fit.

However we have decided to not adopt such "logic parallelism" in our implementation of multithreading in Loci. The first reason is that this will add dependency and make the Loci code base rely on more external libraries and packages, whose future status and standard comformance plans are not entirely clear. We want to maintain as minimal dependence as possible and as much standard compliant as possible. The more important reason is that these logic threading parallel programming libraries, while increasingly being adopted, are mainly targeting application development. We have a unique situation where we ourselves are developing a runtime system and programming tools (and not application level software). Thus if we employ some of these libraries to do multithreading, we will lose some opportunities to customize and optimize the code for our own case. Loci can be viewed as on the same abstraction level as those logic threading parallel libraries. Thus essentially we would want to develop our own equivalent version of those parallel libraries. Doing so also provides us chances where we can take advantage of special Loci features to better support its applications.

Another notable recent development is the modern C++ standard (c++11 and c++14, and the upcoming c++17). These are quite major updates to the C++ language. The current standard also added multithreading support as standard libraries in the `std` namespace. In terms of c++11 threads support, there are three main components. The first is essentially the same mechanism as the older POSIX-thread programming mechanism, wrapped in nicer C++ constructs. The second part is the support of asynchronous programming through the `std::future`, `std::promise`, and `std::packaged_task` mechanism.[1] The third

[1]It would be nice to have these constructs support the logic parallelism discussed early. They appear to be mostly mirroring similar constructs and mechanisms on the Java platform. Unfortunately at this writing, these new c++11 constructs do not (yet) support true logic parallelism. The current C++ thread implementation does not appear to use a sophisticated thread scheduler to support dynamic thread scheduling. We would hope however, that implementations in the future would catch up

part is the addition of a set of atomic variables and an associated memory model that guarantees sequential consistency behavior if certain rules are followed.

Since Loci was developed in C++, this will have a major impact on how we actually implement our multithreading infrastructure. We have not adopted in using modern C++ so far. One major reason is that the adoption relies on all our clients willing to upgrade to the newest C++ compiler and libraries. Fully upgrading Loci framework to modern C++ probably also means that some of the previous code will break and it will take time to fix everything. Secondly, for the same reason that we are not developing application level software means that we are less dependent on many features. For example, so far we do not need the asynchronous threading support from the new C++ thread library. However we would stress that although we did not incorporate modern C++ into the current Loci multithreading infrastructure, moving towards the adoption of it is inevitable. Fully employ the modern C++ facility in the near future is advised. This has the benefit of staying current and relevant to the programming language we use. In addition, several C++ threads features (such as the atomic variable and standardized memory semantics) will be very helpful as well to support our development.

4 Thread architecture design and implementation

This section provides discussions on the high level implementation of the current Loci multithreading modules. It outlines the major algorithms in use in the multithreading system. The Loci code base contains additional comments about actual code that implements these algorithms. A major goal of this development is to keep the public interface of the Loci framework the same as before. In this way, users and all existing Loci programs do not have to make any significant changes to utilize the new threads capability. Currently the new threads implementation follows the same Loci software architecture and is made to be extensible.

4.1 Overall software architecture

Since we schedule and manage low level threads in the Loci framework, the top-level and most important software architecture in our threads infrastructure is the ability to generate and manage threads. For this purpose, we designed an interface for such requirements.

```
// in file "src/System/thread.h"
class ThreadControl {
public:
  virtual void create_threads() = 0;
  virtual void shutdown() = 0;
  virtual void restart(vector<ThreadedExecutionModule>&) = 0;
  virtual void wait_threads() = 0;
};
```

Figure 3: The abstract thread manager

The `ThreadControl` type serves as a required interface that the thread manager in Loci should be able to support (only partial interface shown in Figure 3). This essentially models a thread pool, where low level threads are not created and destroyed as the lifetime of the tasks put on them. Instead, a fixed number of low level threads are created and reused all the time for all computations in the system. The reason is clear because creation and destruction of low level threads are generally expensive. We want to reuse a low level thread whenever possible.

There are two types of threads in the system, the main control thread and the work threads. There is only one control thread in the system and it is created by the process. There can be multiple work threads

to provide true logic parallelism and dynamic threading support.

existing at the same time. Work threads are all created by the main control thread. The control thread only invokes methods defined in the ThreadControl type and does not participate in any computation. The work threads are managed by the control thread and they only participate in actual computation.

The create_threads() method will create all the low level threads necessary (the exact number is defined at the construction time of a concrete thread manager). After creation, each thread will be in a suspended state waiting for any work to come.

The shutdown() method terminates all created low level threads. And the restart() procedure will restart all suspended threads, feeding each with a new work. The type ThreadedExecutionModule defines what a thread work is (to be explained later in section 4.2).

Work threads do not automatically go away after finishing their assigned work. They just become inactive. All the work threads are explicitly created and destroyed by the create_threads() and the shutdown() calls from the main control thread.

The wait_threads() causes the main control thread to suspend waiting for all the active work threads to finish their current work and then it wakes up. This also implies that after this function returns, all work threads will be in a suspended state.

Such a thread control also includes implicit synchronizations among all the work threads, i.e., all active work threads will implicitly synchronize after each restart() call (when they finish all assigned work in the current step, typically a rule). See section 4.3 for a discussion how this is implemented. This form of bulk synchronization is the same mechanism used in the current MPI implementation of the distributed memory parallelism (since both are a form of data parallelism). It is unclear at this moment whether removing or relaxing some of the barriers will enhance the performance. For example, if it is determined that two sequential restart()s do not share dependency, then we might be able to remove the barrier between the restart()s. But since we package entity sets to be handed to work threads, we can equally create a new task that combines computations in multiple Loci rules and feed it to the threads. This is equivalent to removing the implicit synchronization between rules. This is an overall complicated optimization problem, whose solution may require extensive evaluation.

```
// in file "src/System/thread.h"
class ThreadControl_pthread: public ThreadControl {
public:
  void create_threads() { pthread_create(/* ... implementation */) }
  // ... other implementations
private:
  // ... details
};
```

Figure 4: A concrete thread manager

We currently use POSIX-threads as our underlying low level thread generator. We have implemented a concrete thread manager that instantiates the abstract interface as presented in Figure 4. Other threading mechanism can also be packaged as similar concrete classes that will allow easy switch of the underlying threading choice (for example, one can also implement a ThreadControl_cpp to use the thread library from the c++11 standard as an implementation).

In the file src/System/thread.cc, there is a global variable thread_control (whose type is ThreadControl*, a pointer to the ThreadControl type). This global variable should point to a concrete thread controller that is initialized in the file src/System/sched_comp.cc. Currently if multithreading is enabled for an application, the global variable thread_control is initialized with a ThreadControl_pthread object.

The file src/System/thread.h also contains two classes StartThreads and ShutDownThreads. They are subtypes of the Loci execute_modules type (whose respective execute() method invokes the corresponding ThreadControl interfaces, create_threads() and shutdown()) and are used to start and shut down the thread controller (pointed to by the global variable `thread_control`). These execution modules are inserted into the overall Loci execution list in the file `src/System/sched_comp.cc`.

4.2 Integrating threads into existing software architecture

The current Loci framework compiles each rule specification into a functional block (called "compiler" in the Loci code base). All of these functional blocks are then arranged in a linear order as a list ("scheduling"). Finally each of these functional blocks in the list is then converted into an execution module, which is an abstract type with an `execute()` interface that can be called to carry out the original rule's specification when supplied with a set of entities (the "context") and a place to read/write the data associated with the rule's definition (usually the `fact_db`).

For example, a Loci `pointwise` rule is usually converted into an `impl_compiler` object, which when called, generates the execution context (represented as a Loci sequence) for the corresponding `pointwise` rule. The `impl_compiler` object is then linearized in a list of similar compilers objects and eventually converted to an `execute_rule` object, whose `execute()` interface when invoked, finds the rule context and applies the `pointwise` kernel to the context and stores the associated data in the Loci `fact_db`. This is the main architecture and mechanism of the Loci framework scheduling.

The multithread implementation reuses such an organization. When we detect multithreading is enabled, for each functional block in the scheduling list where threads can be applied, we will create a special multithreaded execution module instead of a conventional execution module. Such special multithreaded execution module is also a subtype of the common abstract `execute_modules` type. When the `execute()` interface of such multithreaded execution module is called, it applies the corresponding rule kernel over the entire computation context using multiple threads (instead of a single thread as in the conventional schedule). For example, for a Loci `pointwise` rule and its associated `impl_compiler`, instead of producing an `execute_rule` object, the multithreading code produces a `Threaded_execute_rule` object, which is also a subtype of the `execute_modules` type. Figure 5 shows how a `Threaded_execute_rule` type is implemented in the current Loci base.

The `ThreadWork` in Figure 5 is a concrete implementation of the type `ThreadedExecutionModule` mentioned in section 4.1. This abstract type represents a unit of workload to be executed on a work thread managed by the thread controller. It also mandates an `execute()` interface that accepts a Loci `fact_db` and a `sched_db` as input parameters. These two parameters are not used in most current implementations. However they are supplied since the conventional Loci `execute()` interface in the `execute_modules` requires them and they may be used in the future. A concrete implementation of the `ThreadedExecutionModule` may simply execute its workload independently, or does some special internal processing on each different thread, or may require collective synchronization with other work threads. Such a detail is determined solely by the individual implementation. The multithreaded version of the `execute_modules` only generates and passes a `vector` of such `ThreadedExecutionModule` to the thread controller. Section 4.5 contains more information on how concrete `ThreadedExecutionModule`s are implemented for different types of Loci rule computations.

4.3 Thread synchronization

The thread controller (`ThreadControl`) also implements most of the thread synchronization operations. In the current implementation, all thread synchronizations are distributed, i.e., there is no global lock and memory space that is accessed by all the threads in the system. Also in order to reduce the cost of thread context switch, all locks used in the implementation are spin lock (a spin lock does not put a blocking thread into a suspended state, two context switches will occur if a thread goes into sleep and wakes up later). Since we use distributed locking mechanism and each lock is typically only shared between two threads, we anticipate the cost of spinning is small. The only place where threads are blocked is when all work threads finish computing a Loci rule. In that case, we put all work threads in a suspended state and transfer the control to the main control thread. When any of the work threads is active, the main control thread is suspended. Currently each thread (including the main control thread) has an associated POSIX semaphore

```
// simplified impl of Threaded_execute_rule, full version in file src/System/thread.h
class Threaded_execute_rule: public execute_modules {
public:
  Threaded_execute_rule(kernel k, Context c, Storage s) // construction
  { // thread_control is a ThreadControl*, see section 4.1 for details
    p = thread_control->num_threads();
    // partition the context into p parts, where p is the number of work threads
    partition = partition_context(c, p);
    for(i=0; i<p; ++i)
      tw.push_back(new ThreadWork(k, partition[i], s));
  }
  void execute()
  {
    thread_control->restart(tw);
    thread_control->wait_threads();
  }
private:
  vector<ThreadedExecutionModule> tw;
};
// ......
// we would replace any of the following code:
return new execute_rule(k,c,s);
// with the following code:
if(multithreading_is_enabled)
  return new Threaded_execute_rule(k,c,s);
else
  return new execute_rule(k,c,s);
```

Figure 5: Simplified version of a multithreaded execution module

that is used to block the corresponding thread. The pthread implementation `ThreadControl_pthread` in file `src/System/thread.h` defines the variable `main_block` (a `sem_t` type)to be used to regulate the state of the main control thread; and the variable `worker_block` (a `vector<sem_t>` type) to be used to regulate the state of all of the work threads.

The `restart` procedure presented in section 4.1 starts all of the work threads from their suspended state and feeds each one a thread work unit (i.e., `ThreadedExecutionModule`). Figure 6 illustrates the distributed restarting scheme used in the current pthread thread controller. This is a tree based starting mechanism. When it is time to start all work threads, the main control thread unblocks one of the work thread (typically the work thread with ID 0). The main control thread is then blocked (by calling the `wait_threads` interface). Subsequently all of the work threads are unblocked in a cascading fashion as illustrated in Figure 6. When the thread controller is constructed, it computes for each work thread a list of partners to unblock (the procedure `build_partner()` in file `src/System/thread.cc`). For example, thread 0 in Figure 6 has the following list: [4,2,1]. There are at most $\lceil \lg p \rceil$ elements in such a list, where p is the total number of threads. Also note that there is no implied synchronization between the steps in Figure 6. The distributed start mechanism is completely asynchronous, see Figure 7 for how the restart is currently implemented.

When all work threads finish computing a Loci rule, the main control thread needs to be unblocked and continue the subsequent work. There needs to be a mechanism to signal that all work threads are done. This is similar to a barrier design (only that the barrier does not need to be reusable since we have a separate main control thread that can perform any reset operation). A common approach is to use a global variable initialized to the total number of work threads. Each work thread will decrement the counter once it finishes

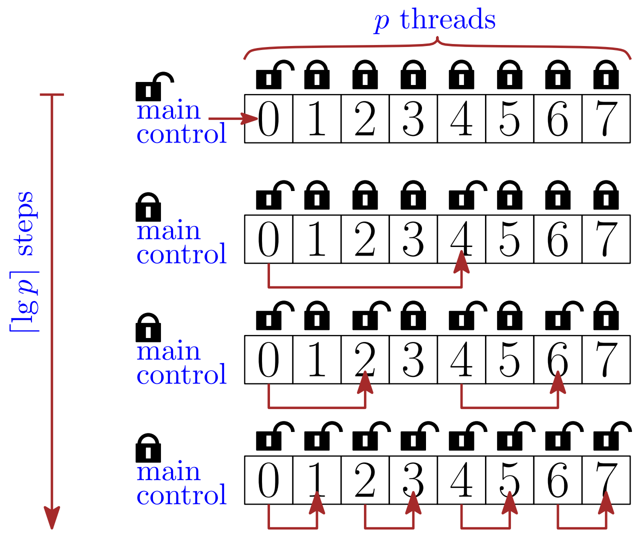


Figure 6: Thread starting mechanism

its work. Whoever decrements the counter down to zero will be responsible to unblock the main control thread. This scheme has the potential disadvantage of causing high memory contention at the location of the counter variable.

We have used a tree based distributed barrier design to put all work threads into suspension and unblock the main control thread. There are different ways to implement a tree based barrier. If we take the reverse process of the restart as suggested in Figure 6, then we would pair threads as in the left part of Figure 8 (the combining tree barrier). Each interior node will be responsible to check the status of its two children. When all children of a node are done (signaled via spin lock protected flags), the node then sends the signal upward the tree until the root node is activated, which then unblocks the main control thread.

Another way is to construct a static tree as suggested in the right part of Figure 8. It works almost the same than the left side tree. Each thread has at most two children and checks the status of them upon finishing its own work (also via spin lock protected flags). When the root node finds that all of its two children are done, it then unblocks the main control thread (since that means everyone is done). We have adopted this static tree based distributed barrier mechanism since it constructs a more compact tree with fewer locks and interactions. Since the work threads number is fixed, the thread manager can construct this static tree just once and reuse it in all subsequent computations (the procedure `build_term_tree()` in file `src/System/thread.cc` constructs such a tree). With all these synchronization mechanisms, each work thread will run the procedure as shown in Figure 7.

4.4 Multi-level partition

In order to deal with the complications of thread interactions within a Loci reduction computation (see section 4.5 for details), a multi-level data partitioning infrastructure was implemented in the Loci multithreading system. However this multi-level data partitioning and the associated scheduling policies in the Loci multithreading system may not be the best option available. We have indeed spent a lot of time trying to come up with different strategies to design thread scheduling for the Loci reduction rules. Currently we think there is a better way to schedule multithreaded reduction computations in Loci. Due to lack of time and infrastructure support, it was not implemented. Section 5.1 will discuss the main idea and what's needed to implement it. However the current multi-level partitioning based multithreaded reduction works reasonably well in the Loci system.

The basic idea of the multi-level partition is to extend the data partitions made for each MPI process

```
// full version in ThreadControl_pthread::thread_fun() in file src/System/thread.cc
void work_thread()
{ // block is an array of semaphores indexed by thread id
  // partner is an array of list indexed by thread id, it
  //    stores the restart partners for each thread as
  //    suggested in Figure 6
  // tree is an array of list indexed by thread id, it
  //    is the static tree barrier shown in the right part
  //    in Figure 8
  while(true) {
    wait(block[me]); // me represents the id of the calling thread
    for(p : partner[me])
      signal(p); // release all partner threads
    // perform thread work by executing the thread work unit explained in section 4.2
    // thread_work is a vector of ThreadedExecutionModule indexed by thread ID
    thread_work[me]->execute();
    // finishing ...
    for(c : tree[me]) {
      done = false;
      while(!done) { // check if child c is done
        spin_lock(c.lock);
        done = c.flag;
        spin_unlock(c.lock);
      }
      c.flag = true; // once child is done, reset its flag
      if(me.parent) { // has a parent node, change local flag
        spin_lock(me.lock);
        me.flag = true;
        spin_unlock(me.lock); // spin locks act as memory fence
      } else // must be the root node
        signal(main); // unblocks the main control thread
    }
  }
}
```

Figure 7: How a work thread functions

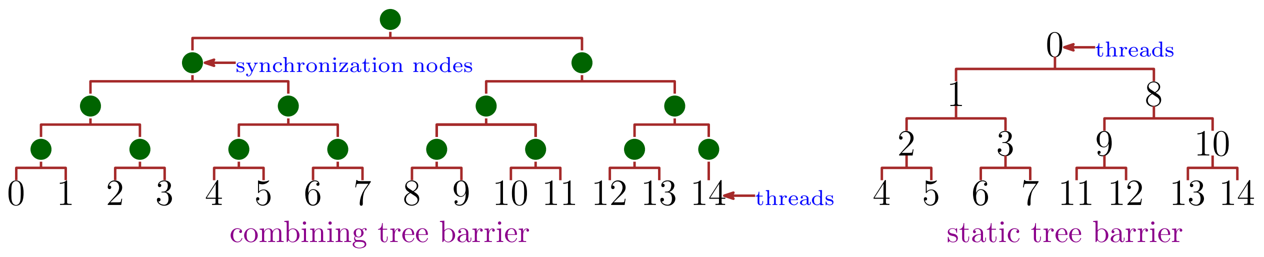


Figure 8: Tree based thread suspension

and further partition them for each work thread on an MPI process. Figure 9 shows an example of such partitioning. In this example, an input mesh is broken into three parts for a three-MPI process run. Each MPI process gets one piece of the input mesh (details such as ghost regions are omitted in this example). Furthermore each MPI process starts two threads. The light green colored region in Figure 9 shows an instance of the configuration on one of the MPI processes. The process owned data (in magenta) is further partitioned into two subparts. Each work thread gets one such part. Furthermore on each thread, the data is again partitioned into multiple smaller parts. Notice that the actual data is not being duplicated in such partitioning, only the data indices (i.e., the entities) are regrouped together.

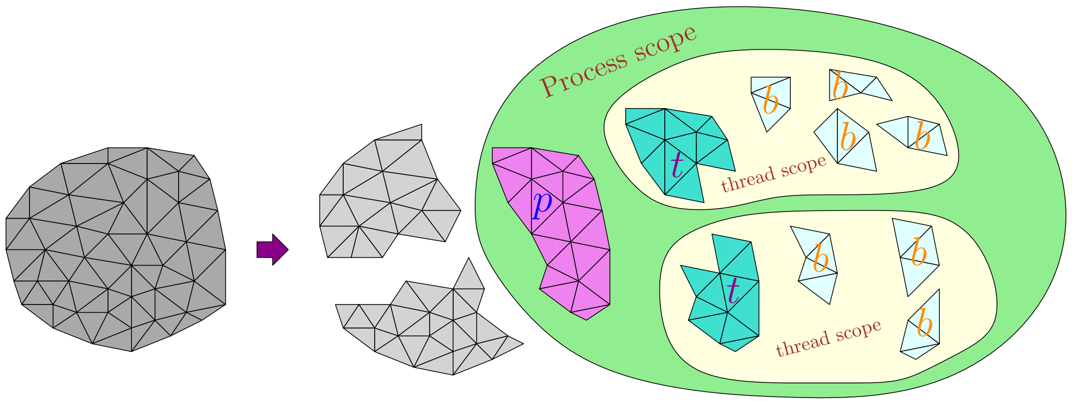


Figure 9: Multi-level partition overview

Essentially the entire process consists of a three-level partitioning and produces a triple "(p, t, b)" partitioning of the original input mesh. In this scheme p stands for the number of MPI processes, t stands for the number of work threads on each process, and b stands for the number of blocks on each thread. Thus, the initial mesh is first partitioned into p parts, then each of these p parts is partitioned into t parts, and each of the t part is again partitioned into b parts. As a result, each process owns one of the p parts. Each thread owns one of the t parts as well as all the b parts that form the single t part. Each of these partitions will try to balance the number of entities inside. They will also try to preserve data locality as much as possible. This means that all of the data that stay within a single such partition (no matter on the p, t, or b level) are close to each other with respect to the data access pattern in the application. However the actual partition strategy for each of the levels may be different from each other.

Parallelism is supported within the Loci framework on all of the (p, t, b) levels. The p level parallelism is generated by MPI calls and the t and b level parallelism are exclusive to threads. Some of the multithreaded computations will only have parallelism on the t level, while some of the threaded computations will have parallelism on the b level as well. Section 4.5 will give a detailed review. Below the b level, a single computation could decide to further partition the data to do special processing related to that particular computation. However there will be no thread level parallelism supported below the b level. Therefore any partition below the b level is solely managed by individual computation and is used for purposes other than generating parallelism.

Currently the p level partitioning strategy is handled by the Loci grid reader (using either a graph or a spatial based algorithm). The current t and b level partitioning are directly handled inside the thread controller object and are based on a spatial partitioning algorithm on a primary variable and topological affinity with tie-breaking. We use an abstract type `ThreadPartition` to define the interfaces that must be supported by any thread-level data partition implementation. Figure 10 shows the important portion of such an interface.

The interface `create_thread_domain()` is used to generate within an MPI process, all of the t and b partitions as discussed above. This interface is usually invoked by a concrete thread controller (the current `ThreadControl_pthread` calls this interface during its construction time, see file `src/System/thread.cc` for

```cpp
// in file "src/System/thread.h"
struct ThreadPartition {
  virtual void create_thread_domain(fact_db& facts) = 0;
  virtual std::vector<sequence> partition_by_domain(const sequence& s) const = 0;
  virtual std::vector<int> partition_by_blocks(int t, const sequence& s) const = 0;
  virtual sequence refine_seq_by_block(int t, int b, const sequence& s) const = 0;
};
```

Figure 10: Thread level partition interfaces

details). After calls to this interface, each MPI process should have a data structure containing information that assigns a given entity to a specific t and b partition.

The interfaces `partition_by_domain()` and `partition_by_blocks()` split a given context according to the t and b partitions respectively. These two interfaces are primarily used to split a process-level context into thread-level context. Section 4.5 uses these interfaces to implement multithreaded scheduling of different Loci rules.

The interface `refine_seq_by_block()` generates an accurate context given a t and b partition index and a rough context. It is needed because a rule context may only span part of a block. For example, a thread may contain three b level blocks, each containing several entities: $b_0 = [1, 10]$, $b_1 = [11, 20]$, $b_2 = [21, 30]$ (the entire domain for the thread is therefore $[1, 30]$). A particular rule context may be $[5, 25]$ for example. Then such a context will span blocks b_0, b_1, and b_2 on this thread. Such block-level information is needed during scheduling phase. But such a context only spans part of b_0 ($[5, 10]$) and b_2 ($[21, 25]$). The interface `refine_seq_by_block()` is used to narrow a given context down to the range of an individual block at the b level. Section 4.5.3 gives examples of how it is used in the current code to schedule reduction rules.

Currently we use a concrete partitioner `ThreadPartition_simple` to implement the thread-level partitioning interfaces. This partitioner partitions the cells first in a mesh and then associates nodes and faces to the cell partitions. The cells in the mesh are initially split equally into p parts (p is the desired partition size). The split on cells is arbitrary by using a simple equal size cut on the cells set (however if cells are already grouped according to their spatial locations, then simple cuts will preserve the existing locality). For face and nodes partition, we use topology association in the current implementation. If all the neighboring cells of a particular face (or node) all belong to the same partition, then that face is also assigned to the same partition. If neighboring cells belong to different partitions, then the face (or node) sits on the partition boundary. For any partition boundary face (or node), we check to see the current size of all the partitions involved and assigns the face (or node) to the partition with the smallest size. The code contained in procedure `ThreadPartition_simple::partition_topology()` in file `src/System/thread.cc` implements this topology based partition algorithm. The source code is well commented and should be clear to follow. Such a topology based partition preserves much of the mesh locality and should improve cache performance in general. Potential drawbacks of this partition scheme include: 1) such a partition is entirely based on a specific mesh topology, it is not general enough to handle dramatically different types of input data. 2) the runtime performance may be slow as the current implementation is not heavily optimized and includes many constructions and queries of map based data-structures that can be fairly slow.

The code within `ThreadPartition_simple::create_thread_domain()` in file `src/System/thread.cc` uses the above topology partition procedure to generate the t and b level partition data-structures for all the work threads on any MPI process. Assuming an MPI process wants to generate t work threads and each work thread will need to have b blocks, then we will use the `partition_topology()` procedure to generate $t * b$ partitions. Each work thread will then take b of such partitions as its whole domain, which consists of b individual blocks. The actual source code is more complicated since it needs to handle various edge cases. The source code is however well commented and should be clear to follow.

4.5 Individual rule computation scheduling

The present Loci framework supports five major categories of computations and we discuss here the multithreading strategies for each of the computation category. The five computation categories are:

1. Pointwise computation, which is a straightforward calculation applied to a set of entities (the context). No entity interaction is expected in the output. For example, if we have a computation kernel k and a context of entities [e_1,e_2,e_3,e_4,e_5], then applying the pointwise computation pattern will give us the result: [$k(e_1)$,$k(e_2)$,$k(e_3)$,$k(e_4)$,$k(e_5)$].

2. Global reduction computation, which reduces a set of values to a single value. An example would be: suppose we have a list of numbers as [1,2,3,4,5,6,7,8,9] and an associative operator "+." Reducing the list means performing 1+2+3+4+5+6+7+8+9 and then obtaining the final value 55.

3. Local reduction (also known as partial reduction), which reduces a set of values to another set of values by using mapping associations. For example, suppose we have a list of numbers [1,2,3,4,5] and an associative operator "+." In addition, we also have a map that maps each number in the list to a location: [1→a, 2→b, 3→a, 4→a, 5→b]. And then when we apply the reduction through the map, we will get [a:1+3+4=8, b:2+5=7].

4. Chomping computation. It is not a different type of computation strictly, but rather a way of performing certain computations. By chomping, we group a set of direct computations (usually just pointwise and local reductions) and apply special transformation so that only a small piece of information is calculated at once for all the grouped computations. The primary benefit of chomping is to improve cache performance as well as to lower the peak memory consumption.

5. Recursive computation. This is also not a different type of computation by itself. Recursion in Loci does not happen at the computation phase, but rather happens within the Loci scheduling process itself. The specification of the recursive computation usually directs the Loci framework to deduce all necessary context information so that an actual computation will be applied to all entities that can receive the computation.

We present chomping and recursion as separate computation categories mainly from a perspective of Loci scheduling (for multithreading). Loci also supports several types of other minor computations such as the singleton and blackbox computations. These types of computations do not merit from multithreading and therefore we will not discuss them further. Thread parallelism happens at the t partition level for pointwise, global reduction, and recursive computations, while b partition level thread parallelism occur for local reduction and chomping computation.

4.5.1 Pointwise computation

A pointwise computation is a simple mapping of a computation kernel to a set of receiving entities. Therefore the multithreaded schedule is simple: we partition the receiving entities according to the t level partition information (by using the interface `partition_by_domain()` in `ThreadPartition` type, see section 4.4 for this type) and distribute each such resulting partition to a work thread. Figure 11 is an outline of the main code behind the multithreaded pointwise rule scheduling. The class `Threaded_execute_rule` plays the role of a Loci `execute_modules` as discussed in section 4.2. The class `ExecuteThreaded_pointwise` is a concrete implementation of the `ThreadedExecutionModules` that is specialized for the pointwise computations. The implementation for multithreaded pointwise rule scheduling is quite simple. The constructor of `Threaded_execute_rule` splits the pointwise rule context for all work threads (by using the interface `partition_by_domain()` discussed in section 4.4). It then uses the split contexts to create all work thread units (`ThreadedExecute_pointwise` objects). The `execute()` method in `Threaded_execute_rule` simply restarts all work threads (using the `restart()` interface in the thread controller, see section 4.1 for details) and then suspends the main control thread (using the `wait_threads()` interface, see section 4.1).

Line 12 and 15 in Figure 11 calls any sequential code before starting all work threads to run in parallel. Section 4.6 discusses the details further. The thread work unit class `ExecuteThreaded_pointwise` simply delegates all work to an underlying sequential Loci `execute_modules` with a new context. The sequential execution module is created in line 5 in Figure 11 in class `Threaded_execute_rule` and is passed to the thread work unit class `ExecuteThreaded_pointwise`. It is a normal execution module used to handle pointwise computations in the non-threaded code. This setup, including a multithreaded version of Loci `execute_modules` (`Threaded_execute_rule` in this case), a thread work unit `ThreadedExecutionModule` (`ThreadedExecute_pointwise` in this case), and an underlying normal execution module (`execute_rule` in this case) is a recurring scheme used throughout all other multithreaded rule scheduling.

```
 1 // code for multithreaded pointwise schedule, in file src/System/thread.h
 2 class Threaded_execute_rule: public execute_modules {
 3   Threaded_execute_rule(rule r, const sequence& s, fact_db& facts, sched_db& scheds):seq(s) {
 4     // exec_rule is a normal execute_modules for a pointwise rule
 5     exec_rule = new execute_rule(r, s, facts, scheds);
 6     int tnum = thread_control->num_threads();
 7     std::vector<sequence> partition = thread_control->partition_by_domain(seq);
 8     for(int i=0;i<tnum;++i)
 9       texec.push_back(new ExecuteThreaded_pointwise(partition[i], exec_rule));
10   }
11   void execute(fact_db& facts, sched_db& scheds) {
12     exec_rule->execute_prelude(seq);
13     thread_control->restart(texec);
14     thread_control->wait_threads();
15     exec_rule->execute_postlude(seq);
16   }
17   sequence seq; std::vector<ThreadedExecutionModule> texec;
18   executeP exec_rule; // the serial execution module corresponding to r
19 };
20 class ExecuteThreaded_pointwise: public ThreadedExecutionModule {
21   ExecuteThreaded_pointwise(const sequence& s, executeP er):seq(s), exec_rule(er) {}
22   void execute(fact_db& facts, sched_db& scheds) {
23     // we will just delegate the execution to the underlying
24     // sequential execute_modules with a refined new context
25     exec_rule->execute_kernel(seq);
26   }
27   sequence seq; executeP exec_rule;
28 };
```

Figure 11: Multithreaded pointwise computation scheduling

4.5.2 Global reduction computation

A global reduction computation usually starts out as a pointwise computation and then performs a total reduction on the pointwise result to produce a single value. A multithreaded schedule is thus similar to the pointwise schedule, except in the end, we would perform an additional concurrent reduction. The reduction strategy is to utilize a combining tree barrier discussed in section 4.3 and Figure 8. Each thread is assigned a list of partners and monitors their progress. Once a parter has done with its computation, the thread then combines its own result with the partner's result. The implementation uses the same two-class design approach shown in the pointwise implementation in the previous section. In the file `thread.h`, the class `Threaded_execute_param_reduction` is a subtype of `execute_modules` and is responsible to partition the rule context and create thread work units. The class `ExecuteThreaded_param_reduction` is a subtype of `ThreadedExecutionModule` and carries the actual work in each work thread. The class `Threaded_execute_param_reduction` also allocates a vector of `storeRepP` to be used by the work threads to store partial reduction results (one vector slot per work thread). Each `ExecuteThreaded_param_reduction` executed on a work thread is responsible to initialize its own slot using the unit value.

```
 1 // full version in file thread.h
 2 class Threaded_execute_param_reduction: public execute_modules {
 3   std::vector<ThreadedExecutionModule> texec; // thread work units
 4   std::vector<storeRepP> partial; // partial reduction results (one per work thread)
 5   // synchronization signals for the reduction,
 6   // SYNC is a user defined type representing the needed data structure
 7   std::vector<SYNC> sync;
 8   void execute(fact_db& facts, sched_db& scheds) {
 9     thread_control->restart(texec);
10     thread_control->wait_threads();
11     sync[root] = false; // all finished, resetting the sync signal for the root work thread
12     // "target" is the storeRepP to the reduction result in "facts"
13     target->copy(partial[root], target->domain());
14   }
15 };
16 class ExecuteThreaded_param_reduction: public ThreadedExecutionModule {
17   std::vector<int> partners; // reduction partners, see Figure 6 in section 4.3
18   void execute(fact_db& facts, sched_db& scheds) {
19     partial[me]->fast_copy(target, EMPTY); // me is the ID of the calling work thread
20     // exec_rule is the underlying normal execute_modules for the reduction
21     exec_rule->execute_kernel(seq);
22     for(size_t i=0; i<partners.size();++i) {
23       int p = partner[i];
24       bool done = false;
25       while(!done) {
26         spin_lock(sync[p]); // checking partner status
27         done = sync[p];
28         spin_unlock(sync[p]);
29       }
30       sync[p] = false; // partner finished, resetting partner status
31       ⊕(partial[me], partial[p]); // ⊕ is the reduction operator
32     }
33     spin_lock(sync[me]);
34     sync[me] = true; // setting self status
35     spin_unlock(sync[me]);
36   }
37 };
```

Figure 12: Global reduction with threads

Figure 12 gives an overview of the important steps. The variable `partial` in line 4 stores the reduction results in each work thread (one work thread per slot). In the `execute()` method in `Threaded_execute_param_reduction`, a structure used for work thread synchronization is maintained (the `sync` variable in line 7). Each work thread will set it to `true` when it finishes its reduction work (line 34).

Each work thread will also query all its reduction partners' status when it needed to combine results from its partners (line 27). After a work thread combines one of its partner's result, it will also reset that partner's status (line 30). The main control thread is responsible to reset the status of the root work thread (line 11). The main control thread is also responsible to transfer the reduction result to the original variable in the `fact_db` (line 13). Line 19 is used to initialize each of the work thread's partial reduction storage to the unit reduction value. Note the `fast_copy()` method is a newly added method in the container hierarchy to address existing Loci thread synchronization problems (see section 5.2 for additional comments on this issue and other related issues).

4.5.3 Local reduction

The main complication in scheduling local reduction with threads is the increased interaction among all the work threads. Recall a global reduction is a set to a single value reduction, while a local (or partial) reduction is a set to another set of value reduction. When we partition the input set of a global reduction computation, there will be *no* interactions among all these subsets. The reduction in the global reduction computation is therefore a separate step after the computation. Therefore the thread scheduling only has to consider thread interactions in the reduction step and even then it is relatively straightforward by using a synchronization strategy presented in section 4.3.

In contrast, a local reduction maps from a set of values to another set of values. The previous example given in the opening of section 4.5 maps [1,2,3,4,5] to a set [a,b] through the map [1→a, 2→b, 3→a, 4→a, 5→b]. In a normal sequential execution, the reduction steps are typically embedded inside the computation steps. For example, when we sequentially run through the input set [1,2,3,4,5], the output set will look like: [a:1,b], [a:1, b:2], [a:1+3, b:2], [a:1+3+4, b:2], and [a:1+3+4, b:2+5] in successive steps. As can be seen, the reduction "+" is applied to the output set partially in each step (hence the name partial reduction).

From a concurrent point of view, this complicates the scheduling process because the reduction and computation are now tangled together. It therefore introduces race conditions as multiple threads attempt to read/write to the same set variable. For example, if we partition the input [1,2,3,4,5] into [1,2,3] and [4,5] and schedule two threads each handling one of the subsets. Then the first step on thread one might look like this: [a:1, b] and the first step on thread two may look like this: [a:4, b]. It can be seen that both threads may attempt to write to the location "a" at the same time, causing a race condition.

There are multiple strategies to schedule a local reduction on multiple threads. One way is to partition the input set according to the mapped locations and in this way, each subset is completely independent of each other and will just behave like a conventional global reduction. For example, reusing the above example, we could partition the input set [1,2,3,4,5] into [1,3,4] and [2,5]. In this way [1,3,4] entries will all be mapped to location "a" and entries in [2,5] will all be mapped to location "b." If we partition the set like this, then each subset ([1,3,4] or [2,5]) acts just as a smaller global reduction and there will be no interferences. However this strategy limits the available concurrency to the number of locations in the target set. Notice, we must use work thread number *exactly* equal to the number of target set locations to benefit from this strategy. Fewer or more threads will not have a clean and race condition free schedule. This is rather limiting. Further, the sizes of the subsets may be drastically different from each other and cause load balancing problems. It is possible to be a bit more sophisticated to group target locations to better utilize available concurrency. In general it may be difficult to do so. The reduction maps in reality may become far more complex than the simple example presented here and we may need to partition both the input sets and reduction map to benefit from this strategy.[2]

Previously we have used graph coloring and replication based approaches to schedule local reduction on multiple work threads. They have been shown to have several drawbacks in previous tests and evaluations and we have thus abandoned these two approaches. However for the sake of completeness (e.g. when examining previous versions of Loci thread codes), we have included a brief discussion of these two approaches. The discussions are only at a high level and do not attempt to explain the actual code used in previous versions. They only serve to document the overall approach and ideas.

[2]Section 5.1 discusses a more general and better solution to schedule multithreaded local reduction.

A replication based scheduling approach essentially replicates the target set on each work thread and then performs a final global reduction on the replicated target sets in the final step. For example, still using the previous example, if we partition the input set into three subsets: [1,3],[4,5],[2] and schedule each subset onto a thread (for a three work threads total). Then on each thread, we replicate the target set: [a1,b1] on thread one, [a2,b2] on thread two, and [a3,b3] on thread three. Since the replicated target sets are independent of each other, no race condition could happen. Finally, we perform a reduction like this: [a:a1+a2+a3, b:b1+b2+b3]. It can be seen that each of the target location calculation amounts to a single global reduction step and the technique presented in section 4.5.2 can be used. The main drawback of this approach is that it does not scale well. The replication of target set means that memory requirement is proportional to the number of work threads and that the final global reduction step may also add overhead.

The graph coloring approach assigns colors to each location in the input set such that the locations with the same color can safely be scheduled concurrently without the fear of race condition. For example, for the previous example input set [1,2,3,4,5], we could assign colors like this: [1→🟥, 2→🟥, 3→🟩, 4→🟦, 5→🟩]. There are three colors and therefore we have three input subsets: [1,2](🟥), [3,5](🟩), and [4](🟦). Each of these subsets can be safely scheduled onto any number of threads. For example, subset [1,2](🟥) can be scheduled on thread one (handling [1]) and thread two (handling [2]). Since [1→a] and [2→b], there will be no race conditions. However it does require that we synchronize the threads between the colors (such that a single color is fully computed on all threads before moving on to the next available color). Colors are typically assigned by modelling the interactions among the input locations using a directed graph and then run the graph through a heuristic search algorithm. In reality, we have found the coloring approach does not work very well. The memory required to store the location color information is high and the performance is also hindered by the synchronization requirements between different colors.

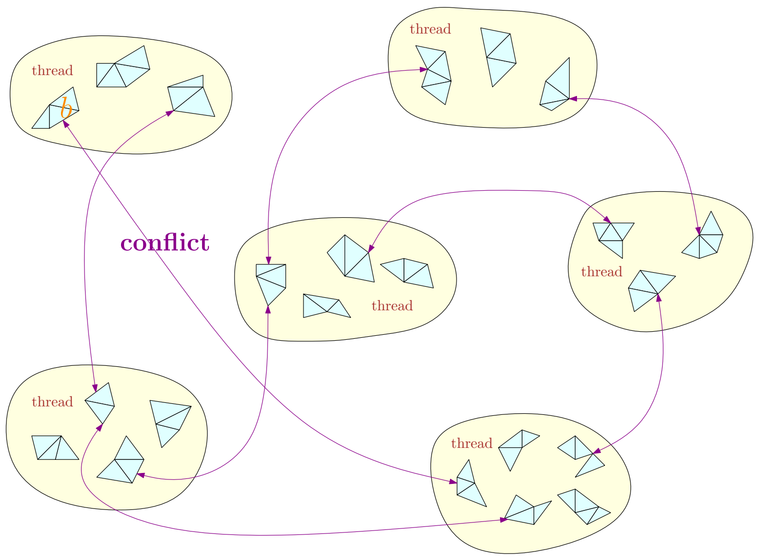


Figure 13: Conflicts graph based on block interaction

The current code uses the multi-level partition information to generate a conflict graph and then schedule the local reduction according to the conflict graph by using a composite conflict lock. We call this the "conflict-based" approach. We use the *b* level partition (see section 4.4 for details on multi-level partition and the meaning of different levels) to overcome the limits on concurrency and high memory requirements in the previous strategies. Recall that the *b* level partition is a much finer grain partition occurred within each work thread and that each such partition also preserves the data locality. Local reduction is scheduled on each work thread for each of the *b* partition a work thread owns. The execution flow within a single *b* partition is the same as it would be executed in sequential. Different *b* partitions on different work threads may present race conditions during the local reduction computation. However since each work thread will have many *b* partition blocks and each block holds its data locality, the possible chance for a data race is practically small. For the possible race conditions, we pre-compute a data race map (the conflict graph) between the possible *b* blocks on each thread first during the scheduling phase. At runtime, each thread checks if a *b* block to be computed is in conflict with any of the current work threads. If not, then the selected *b* block is committed to be computed. If conflict does exist (which should be rare), then the *b* block is put off and another *b* block is selected and repeats the previous process. Figure 13 gives an illustration of the conflicts graph concept based on the *b* partition. The arrows in the graph indicate that the connected *b* blocks on either end are in conflict and should not be scheduled at the same time.

There are several steps needed to implement such a scheduling policy and we discuss the operational overview of each of them. The first such task is to build a conflict graph for all the *b* partitions involved. This task actually is similar to the graph coloring approach discussed previously, except that the granularity is much coarser in this case. If we reuse the previous example and if we partition the input set into three *b* blocks: [1,2], [3,4], and [5]. Then according to the original reduction map: [1→a, 2→b, 3→a, 4→a, 5→b], we can map each *b* blocks to a set of output locations: [1,2]→[a,b], [3,4]→[a], and [5]→[b]. Using a doubly nested loop (with quadratic complexity), we can establish the conflicts between the three *b* blocks: [1,2] $\nparallel$ ([3,4],[5]), [3,4] $\nparallel$ ([1,2]), and [5] $\nparallel$ ([1,2]). For example, [1,2] $\nparallel$ ([3,4],[5]) means that the *b* block [1,2] can be computed as long as [3,4] and [5] are *not* currently being computed. In such a small example, the conflicts are dominating and this limits the amount of concurrency. In reality, with large input size, the conflicts are much more sparse. Section 6 contains a brief discuss of the effectiveness of the current *b*-level partition in terms of avoiding conflicts.

```
// full code in ThreadPartition_simple::generate_conflict_lock in file src/System/thread.cc
void create_conflict_graph(sequence context) {
  // context is the total context for a local reduction rule.
  std::vector<BlockID> blocks_id = partition_by_blocks(context);
  std::map<BlockID,entitySet> blocks_target;
  for(i=0; i<blocks_id.size(); ++i) {
    BlockID b = blocks_id[i];
    blocks_target[b] = vmap_target_exist(blocks[b]);// computes target entity set for block b
  }
  std::map<BlockID,std::vector<BlockID>> conflict_graph;
  for(t=blocks_target.begin(); t!=blocks_target.end(); ++t) {
    std::vector<BlockID> conflict_blocks;
    entitySet self_target = t->second; // target set of block t
    for(t2=blocks_target.begin(); t2!=blocks_target.end(); ++t2) {
      entitySet other_target = t2->second; // targetset of block t2
      if(self_target & other_target != EMPTY)
        conflict_blocks.push_back(t2.first);
    }
    sort(conflict_blocks.begin(), conflict_blocks.end(), BlockID.cmp());
    conflict_graph[t.first] = conflict_blocks;
  }
}
```

Figure 14: Conflict graph creation

In the current implementation, the conflict graph is built according to the original reduction maps ([1→a, 2→b, 3→a, 4→a, 5→b] in our example). This gives the most precise conflicts on all *b* blocks with the cost of needing to look into all output locations (which can be huge and when participating in multiple set operations, this can be costly). Figure 14 presents a somewhat high level sketch of the code. Some of the details have been simplified or omitted so that the code can be shown in this document. The type `BlockID` in line 4 is an abstraction of the structure used to encode a block's identity on any work thread. In practice, it is a two dimensional index with the first index being the work thread id and the second index being the block id within that particular work thread. The `partition_by_blocks()` method in line 4 breaks a given rule context into different blocks. It is defined in the thread partitioner `ThreadPartition` interface presented in section 4.4. The resulting blocks from the given context are then stored in a variable (the `blocks_id` variable in line 4). For each of these resulting blocks, we use the Loci function `vmap_target_exist()` to find out the output set through the maps defined in the local reduction rule. After this step, we then use a doubly loop to check if any of these output sets would intersect with any other ones. If so, then the two involved blocks would be in a conflict. This is a potentially expensive step since the time complexity is quadratic (proportional to the square of total blocks involved). Also note that we sort all blocks in conflict to a particular block according to a global order on the type `BlockID` (in line 19). The reason for this sorting step is ensure the conflict lists for all of the blocks are in the same order, which is very important for the `ReductionLock` operations described below.

As discussed, the present implementation suffers from a costly time complexity, particularly when run with a large number of blocks. Also such conflict graph is built for each of the local reduction rules involved in a Loci program. This could result in a considerable amount of total scheduling overhead. There are several ways to reduce this cost. In the future, we could have Loci pre-built reduction maps according to the multi-level partition. The original reduction map in the local reduction rule can be regarded as operating on the *p*-level. If we have a reduction map customized for the *b*-level (e.g., by coalescing the output locations), then the cost of computing the conflict graph will be much lower. In return, we get a less precise conflict graph. However in practice, this reduced conflicts precision may not be an issue due to large number of *b*-level parallelism available. Also in a typical Loci program, we could have a large number of local reduction rules but a small number of local reduction patterns. For example, several local reduction rules could share the pattern `A->B`. In the present code, each rule will always recompute the conflict graph. In the future, if sufficient infrastructure is in place, we could summarize the local reduction patterns from all of the local reduction rules. Then the conflict graph can be built based on the reduction patterns and be shared among all relevant rules.

Once we have the conflict graph, we will need to build a mechanism to check if an about-to-be scheduled *b* block is in conflict with any currently executing blocks. We do so by implementing a custom lock (it is called the `ReductionLock` defined in file `src/System/thread.h` with implementation in file `src/System/thread.cc`). Each of the *b* blocks in the system is assigned a primitive pthread spin lock that supports the "`try_lock`" query (i.e., returns `false` if the lock is already held by another thread, returns `true` and obtains the lock otherwise). Before a *b* block is to be scheduled for execution, it will need to acquire all the primitive locks correspond to all other conflicting *b* blocks. If any of such acquisition has failed, then the *b* block is put back and another one is selected. The scheduling finishes when all blocks have been successfully scheduled. A very important step in this design is that we agree on a global order on all of the *b* blocks and then always acquire the primitive locks according to such an order (see line 19 in Figure 14). This is essential to avoid deadlocks. Figure 15 presents a high-level overview of this design.

With the conflicts graph and the conflicts resolution mechanism, we can then implement the thread scheduling for local reduction on the *b* partition level. The main setup is again the same as other types of rules discussed previously. In file `src/System/thread.h`, the class `ExecuteThreaded_local_reduction` is a `ThreadExecutionModule` and is responsible to schedule and execute individual blocks. The class `Threaded_execute_local_reduction` is a `execute_modules` and is responsible to partition the context, generate the conflict graph, setup the reduction lock, and then generate and start all needed `ExecuteThreaded_local_reduction`. The general flow of control is similar to other discussed rule types. So we will not show its code. Figure 16 shows the main code for block scheduling using the previously developed utilities in the class `ExecuteThreaded_local_reduction`.

Figure 16 presents the main flow of the `execute()` method in the thread work unit class `ExecuteThreaded_local_reduction`. It maintains two lists of blocks, one for the blocks to be scheduled and the other for blocks that have been scheduled. If a block successfully acquires its reduction lock, then

```
// in file src/System/thread.h and src/System/thread.cc
class ReductionLock {
  void release(BlockIDIter begin, BlockIDIter end) {
    for(i=begin; i!=end; ++i)
      spin_locks[*i].unlock(); // spin_locks stores a pthread spin lock for every block
  }
  bool acquire(BlockID b) {
    std::vector<BlockID> conflicts = conflict_graph[b];
    for(c=conflicts.begin(); c!=conflicts.end(); ++c)
      if(!c->try_lock())
        release(conflicts.begin(), c);
        return false;
    return true;
  }
  void release(BlockID b) {
    std::vector<BlockID> conflicts = conflict_graph[b];
    release(conflicts.begin(), conflicts.end());
  }
};
```

Figure 15: Reduction lock design

it is scheduled to be executed on that work thread and then is put in the finished list. Otherwise if a block fails to acquire its reduction lock, it is skipped and another one (if available) is picked. The entire process ends when the to be scheduled list is empty. Finally the method swaps the two lists to prepare for the next run. Note in line 13, the method `refine_seq_by_block` from the interface `ThreadPartition` is called (see section 4.4 for detail). Its purpose is to get an accurate execution context within the chosen block. We could instead pre-compute all such precise contexts and store them. However since some of these contexts will likely become very scattered, the storage requirements for them is likely to be high. We have therefore chosen to dynamically compute them each time as the cost of such computation seems to be negligible (according to several benchmark tests conducted in the past). As discussed all current Loci scheduling do not feature dynamic workload balancing support. A possible improvement for this code would be to develop a distributed block migration scheme so that the *b* block lists on each work thread can be dynamically balanced at runtime to improve load balance issues. However developing such an infrastructure is a considerably more complex task and so far since our *b* partition also balances the block size and in our applications the computations on each entity is roughly equal, we have not had the need to dynamic balance the work load.

4.5.4 Chomping

The chomping computation can actually be categorized into two types: there are chomping computations that do not involve any local reduction computation and those that do. For chomping without local reduction, a normal *t*-level scheduling is adequate. However for chomping with local reduction, it is necessary to use the *b*-level scheduling discussed above in the local reduction section. The scheduling setup is therefore a bit different. In file `src/System/thread.h`, the class `Threaded_execute_chomp` (a subtype of `execute_modules`) is responsible to initialize relevant data structures and create and start the thread work units. The overall flow is similar to any previous rule type scheduling. The difference is that we now have two subtypes of `ThreadExecutionModule`: the class `ExecuteThreaded_chomp` is used to run chomping graphs that do not involve local reductions; and the class `ExecuteThreaded_block_chomp` is used to run chomping graphs that do have local reductions. `ExecuteThreaded_block_chomp` schedules blocks using a similar programming logic as the class `ExecuteThreaded_local_reduction` discussed in section 4.5.3. We also define a new type

```
// in file src/System/thread.h
class ExecuteThreaded_local_reduction: public ThreadedExecutionModule {
  std::list<BlockID> blocks; // total blocks to be scheduled by a work thread
  std::list<BlockID> done_blocks; // records all finished blocks
  ReductionLock& lock; // the reduction lock to be used for a reduction rule
  void execute(fact_db& facts, sched_db& scheds) {
    while(!blocks.empty()) {
      std::list<BlockID>::iterator candidate = blocks.begin();
      while(candidate != blocks.end()) {
        if(lock.acquire(*candidate)) {
          // successfully acquires the reduction lock for block candidate, schedule it
          // get an accurate execution context by narrowing it down with the selected block
          sequence block_seq = thread_control->refine_seq_by_block(*candidate, seq)
          exec_rule->execute_kernel(block_seq);
          lock->release(*candidate);
          // put the scheduled block to the finished list
          std::list<BlockID>::iterator r = candidate;
          ++candidate;
          done_blocks.splice(done_blocks.begin(), blocks, r);
        } else // failed to acquire the reduction lock, skip the current block first
          ++candidate;
      }
      // finally swap the block lists
      blocks.swap(done_blocks);
    }
  }
};
```

Figure 16: Thread scheduling for local reduction

`ChompBlock` to represent a thread partition block whose execution uses the chomping strategy. It internally delegates the real computations to a `ExecuteThreaded_chomp`. Therefore the purpose of the class `ExecuteThreaded_block_chomp` is to coordinate the scheduling of `ChompBlock`. The purpose of the class `ExecuteThreaded_chomp` is to perform chomping computation for a given context on work threads.

The size of the chomp is calculated in the class `Threaded_execute_chomp`. The current implementation still uses the approach previously used in the sequential version of chomping. It evaluates the size of a single entity on all involved variables in the chomping graph and then calculates the chomping size by computing the ratio of the assumed data cache size and this single entity chomping variable size. However this may not be the optimal and in the future, it may be worthwhile to investigate and test the effects of different chomping size to determine what works the best. In the multithreaded schedule, all work threads need to allocate temporary storage space for all the chomping variables. On current architectures, threads do not usually have their own separate cache. Caches are usually shared among several threads (compute cores). Therefore we probably should reduce the chomping size accordingly to try to fit the chomping variable allocation on all work threads into the shared cache. The implementation of chomping also deals with several other low level details. The source code contains extensive comments that should also be consulted.

4.5.5 Recursive computation

Recursive computation in Loci is the simplest form of computation. As discussed, it is not recursive computation that happen at runtime. Rather the recursion happens at the Loci scheduling phase. A recursive computation specification is a particular way of letting the Loci scheduler to try to deduce all the available entities that can be applied to a computation. During the runtime schedule, there is no explicit recursion happening. Normally a computation has a straight computation context and the Loci scheduler is able to construct it in one pass. In a recursive rule specification, its computation context is iteratively computed because the target of the computation might be used to feedback into the inputs again (which might lead to more entities being computed). Thus the Loci scheduler needs to iterate the scheduling on this computation such that the computation context reaches a fixed point. Internally the Loci scheduler generates a list of schedules for a single recursive computation such that in each step in the list, there will be no dependency between the inputs and outputs.

For example, a recursive computation may initially output the set [3,4] from an input set [1,2], however because one of the outputs is also used as an input, the [3,4] set generated in the first output should be fed back to the computation again, and this time it generates [5], which is again a new set. If we input set [5] to the computation, we will discover that nothing new is being generated, and then we are done. Therefore the output should be the set [3,4,5]. However this output cannot be obtained from a single step since [5] depends on [3,4] being available. Therefore Loci generates a list of two individual computation schedules for this single recursive computation. The first one computes [3,4]←[1,2], and the second schedule computes [5]←[1,2,3,4]. Each of the two computation is just another normal non-recursive Loci computation and therefore can be scheduled for threads according to the previous strategies discussed. There are no specific new types that deals with recursive Loci rules for threads. Everything is handled as a patch to the method `create_execution_schedule()` in the class `recurse_compiler` in the file `src/System/comp_recurse.cc`.

4.6 Rule kernel interface

One significant change we have made to the Loci internal is to redesign the rule infrastructure so that the computation is divided cleanly in multiple phases. Previously all rule implementations in the Loci framework carry a single "`compute(seq)`" method that applies the computation kernel to all supplied entities in the context (`seq`). However the `compute()` method sometimes also carries out other non-kernel related tasks (e.g., global variable change, memory manipulation etc.). Doing so complicates thread scheduling because the `compute()` method includes both data parallel and serial tasks. Figure 17 illustrates such a design.

```
// simplified view of the previous Loci rule specification
rule(targets ← source) {
  compute(es) { // "es" is the Loci deduced context for the rule
    targets.resize(); // there may be non-concurrent part present
    for(e : es) kernel(e); // this is the data-parallel kernel call
  }
}
```

Figure 17: Previous Loci rule interface

In our new rule interface design, the data parallel kernel section is clearly separated from other potential non-concurrent part. Figure 18 presents an overview of the new interfaces. Essentially this interface distinguishes the computation at entity- and collection-level. Computations applied at the entity-level (the kernel) has transparent data parallelism and can be scheduled independently, while collection-level computation do not in general have any kinds of data parallelism. With this new rule interface, the thread scheduler can work more effectively.

Please refer to Figure 1 to find out the relevant source code files that contain implementation related to this functionality (those files marked in the "threading/non-threading rule kernel interface" category). The associated Loci pre-processor syntax has also been updated to reflect this newly designed rule interface. Figure 19 provides a template of rule computation specification. The "`prelude()`" and "`postlude()`" parts in the specification are meant for collection-level computations. Anything that is intended to be applied

```
// simplified view of the new rule interface specification
rule(targets ← source) { // "es" is the Loci deduced context for the rule
  prelude(es) {/* perform any task before applying the kernel */}
  compute(es) { // this is the data parallel kernel call
    for(e : es) kernel(e);}
  postlude(es) {/* perform any task after applying the kernel */}
}
```

Figure 18: New Loci rule interface

to collections should be placed in these two sections. The `prelude()` part is scheduled before the kernel-level computation and the `postlude()` part is schedule after the kernel-level computation. Example tasks that may go into these parts may include resizing a container's internal size and I/O operations etc. If not explicitly specified, the `prelude()` and `postlude()` sections will default to empty, which means no operation. The kernel compute part must be specified in a rule definition though. Overall this new interface enables better thread scheduling decisions. But it does require the users to become aware of the difference between entity- and collection-level computations (i.e., those computations that can benefit from side-effects free data parallel scheduling). Line 12 and 15 in Figure 11 in Section 4.5.1 contain examples of how such a new rule specification interface is typically used in the thread scheduler.

```
// Loci pre-processor definition for a generic rule type
$rule rule_type(...),
  prelude {/* this is the prelude part, defaults to empty */},
  postlude {/* this is the postlude part, defaults to empty */}
  {/* this is the kernel part, must be provided */}
```

Figure 19: New Loci pre-processor rule interface

4.7 Convenience functions

We have also added the "`$[once]`" and the "`$[atomic]`" directives to the Loci pre-processor syntax. `$[once]` supports events that should have a single occurrence in a parallel environment (but it is not important to specify where in the parallel and concurrent environment the event occurs). `$[atomic]` groups all operations within its own block and treat them as a single indivisible operation.

Consider the example presented in Figure 20. The rule specified may be scheduled and executed in any environment, e.g., a sequential run, a pure MPI-based parallel execution, a pure thread-based concurrent execution, or a hybrid MPI/thread environment. Without the "`$[once]`" directive and its block scope, the output statement may be executed multiple times in a parallel or concurrent environment and we will see (possibly garbled) multiple identical output messages. With the `$[once]` directive, the output message will only occur once (but we do not care who in the environment actually executes the output statement).

```
$rule singleton(...) {
  $[once] {cout<<"execution started\n";}
  // other parts
}
```

Figure 20: `$[once]` example

Internally the "$[once]" directly is implemented as a condition switch. The global function is_leading_execution() defined in file src/System/thread.cc provides true/false answers to any calling process/thread whether it is the pre-agreed execution unit for the $[once] directive. The ThreadControl interface (in file src/System/thread.h) provides a is_leading_thread() interface to determine among all the threads on an MPI process, which one is the leading thread. The function is_leading_execution() defines a representative execution path in an execution environment according to the following rules:

1. In a serial execution, the calling execution is the representative execution path.
2. In a multi-process program, the process with MPI rank zero is the representative execution path.
3. In a multithreaded program, the main thread and the first work thread are the representative path (in the current design, the main and work threads never overlap in execution, so this should not cause any problems).
4. In a hybrid multi-process and multithreaded program, the main thread and the first work thread on the MPI rank zero process is the representative execution path.

Figure 21 presents an example use of the $[atomic] directive. The intention of the operation defined in the rule is to display the value of a variable to the standard output stream "cout." If executed in parallel using threads and without the $[atomic] directive, then the output may become garbled since the output code is not atomic. The atomic directive thus ensures everything within its block scope is indivisible and as a result, we will be able to see meaningful output from the computation. In the file src/System/thread.cc, two functions global_atomic_region_begin() and global_atomic_region_end() are provided and the $[atomic] is translated to enclose its block within these two functions. The ThreadControl interface also provides the atomic_begin() and atomic_end() methods that ensures atomicity of the code in-between by using a global pthread spin lock to guard them. Note that the $[atomic] directive currently only works for the multithreaded environment. It does not work in a hybrid MPI/thread environment.

```
$rule pointwise(var...) {
  $[atomic] {cout<<"variable value = "<<$var;}
  // other parts
}
```

Figure 21: $[atomic] example

I/O operations are perhaps the most common use of such feature. However one should not overuse such atomic regions in the code. Since the semantics of a rule's per entity computation (those defined inside the "compute" method) is inherently parallel (i.e., can be scheduled in any order), putting an atomic region inside a rule greatly limits the performance potential. Ideally one should not use an atomic region in a rule and this feature is generally provided for debugging purpose for a user. There may be better (but much more complicated) ways to implement I/O operations in a parallel section. Since our code normally does not perform routine I/O operations within a rule, we did not invest time to optimize the implementation. Loci already has APIs in place for special purpose I/O operations. The "$[atomic]" notation also supports operations other than I/O.

5 Issues and future improvements

Some of the previous sections have mentioned a few issues and possible updates in the current code implementation. This section will discuss some of the important ones in detail. Maintenance and future developments of the Loci multithreading system should pay attention to the discussions presented in this section.

5.1 Synchronization free local reduction scheduling

So far the biggest possible improvement in the current multithreading design would be to use a different (and better) strategy to schedule the local reduction rule on threads. In the past, we have struggled a lot on this issue as it is one of the most complicated designs in the multithreading system and the design had great impact on the performance not only for the local reduction computations, but also the rest of the Loci scheduling system. The initial designs using graph coloring (see section 4.5.3) was not satisfying due to poor performance and high memory cost. It was later switched to the multi-level partition and the conflicts based dynamic scheduling (see section 4.4 and 4.5.3). This scheme works considerably better than the previous designs. It however has its own problems.

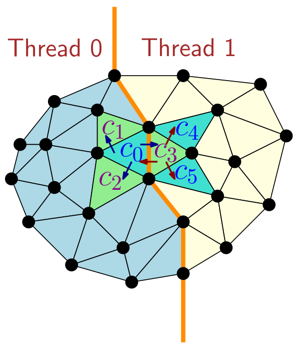
1. The conflicts based local reduction scheduling still has significant thread synchronization embedded at runtime. This is the only place in the current Loci multithreading system where runtime work thread coordination is needed[3]. Although in general the number of conflicts is generally small (see section 6), it nevertheless exists and is ultimately dependent on the Loci program specification. The existence of such thread coordination requirements is the primary reason why the local reduction is difficult to schedule efficiently.

2. The multi-level partition introduces two levels of partition into the multithreading system. This not only means more processing time, it also means that the programming logic is much more complicated. Several special purpose new types had to be designed from scratch to deal with the complexity of introducing blocks into the system.

3. The conflicts graph creation could also become a bottleneck in the system. Section 4.5.3 mentioned that currently a quadratic time algorithm is used to create the graph and each local reduction rule recreates the conflict graph even though some of the reduction patterns can be the same between several rules. Improving these current issues is possible, but may not be simple and straightforward.

5.1.1 Arrow view and arrow partition

We have indeed developed a new proposal to schedule local reduction computation on multiple concurrent threads that is completely synchronization free and logically easier to reason about. We think that this proposal is feasible and actually if designed and implemented appropriately, will also expand the Loci framework's capability considerably. However due to the current Loci architecture design and implementation, this new proposal requires significant rework of the Loci architecture to realize. We will outline the main ideas first and then discuss several ways to approach the implementation and their challenges.



```
$rule apply(neighbor->target <- source) {
  for(int i=0; i<$neighbor.size(); ++i)
    $neighbor[i]->$target += $source / 3.;
}
```

Figure 22: Arrow view of local reduction

[3]Technically the global reduction rule also involves thread synchronization. However it is a straightforward and isolated step that is much easier to reason about and has standard and efficient implementation.

Figure 22 shows an example of a Loci local reduction rule (on the right side) and visualization of the computation on a small 2D mesh (on the left). The local reduction sums a value on each cell in the mesh to all of its neighboring cells. The small arrows in the figure represent the direction of data flow (the accumulation of values) from the source of the local reduction to the target of the local reduction. The thread that "owns" an arrow will need to read data from the site at the arrow's source and write data to the site at the arrow's destination. Whenever an arrow on a thread points to a site inside another thread's partition, then a potential synchronization problem arises. The reason why a particular local reduction scheduling scheme cannot avoid thread synchronization is because it cannot arrange all arrows on any thread to *not* pointing outside its own partition. This is true for all the schemes discussed so far (replication, graph coloring, and dynamic conflicts resolution). In fact, all other current numerical software we are aware of have this problem. The root cause that a particular scheme cannot contain arrow direction to be within a thread is because we always group arrows based on their origination. In the example shown in Figure 22, all previous scheduling policies group the three arrows pointing outward of cell c_0 together on thread zero, so is the case for cell c_3 on thread one. Under such a partition, thread synchronization is unavoidable. We have not seen any discussion of synchronization free local reduction multithread scheduling in the current literature.

However if the Loci framework could support these arrows as a fundamental computational and scheduling unit, then multithreaded local reduction can be easily scheduled synchronization free. We will just need to partition all of the arrows among the threads such that no arrow on any thread will be pointing outside of its partition. It is okay to have an arrow on a thread to come from another thread partition, i.e., the arrow's origination can be from another thread partition. This just amounts to read data from another thread partition, which is safe to do[4].

An arrow is equivalent to a single entry in a Loci map in the Loci framework. For example, if we have a Loci map m where $m[c_0] = c_1$, $m[c_0] = c_2$, and $m[c_0] = c3$, etc (this would be a `multiMap` in the Loci container type). Then each of these entry amounts to an arrow. Present Loci framework uses entity (i.e., c_0, c_1, and c_2 etc.) as the fundamental unit. Thus we can only compose and schedule computation on entities. For example, using the previous example, when we schedule computations related to map m, we can only supply entities like c_0, c_1, and c_3. When an entity such as c_0 is feed to a map (in this case a `multiMap`), then we will automatically get the image as a set of $[c_1, c_2, c_3]$, i.e., we will be forced to group the three arrows pointing outward of c_0 together. This is the reason why we cannot define and compose arrows in the Loci framework.

It is perhaps very powerful to make arrow the fundamental unit in composition and scheduling in the Loci framework instead of the entities (entities are merely abstraction for data locations). Arrows are an even fine grain and low level abstraction in computation compared to the entities. It provides an abstraction that is more elegant and composable. Under the arrow abstraction, maps are just collections of arrows. Computation which do not involve maps can be viewed as going through an identity map, which makes scheduling based on arrows universal (this is a special case, in which an arrow degenerates to be equivalent to an entity).

5.1.2 Ad hoc emulation of arrow partition

Properly implementing the arrow abstraction and its scheduling in the Loci framework is not an easy task. It is also a new concept and we perhaps do not have a full grasp of all its implications. Incorporating arrows in the Loci framework would certainly have a wide range of effects and applications. However if we only want to make scheduling multithreaded local reduction synchronization free, there is an ad hoc way of emulating arrows and its partition among threads.

In the left part of Figure 22, we illustrated a normal partition in Loci. Under such a partition, any cell in the mesh (an entity) is owned by a unique thread. For example, the cells $[c_0, c_1, c_2]$ are owned by thread zero and the cells $[c_3, c_4, c_5]$ are owned by thread one. The arrows are captured in a single map. Suppose we call such a map m. The part of m accessible on thread zero is called m_{t_0} and the part of m accessible

[4]So long as the arrows do not represent in-place update. However local reduction computation with in-place update is inherently non-deterministic, even in the sequential case. E.g., consider the Game of Life implementation.

on thread one is called m_{t_1}. Then thread zero will make use of the mapping $m_{t_0}[c_0] = c_1$, $m_{t_0}[c_0] = c_1$, $m_{t_0}[c_0] = c_2$ in its local reduction. And thread one will make use of the mapping $m_{t_1}[c_3] = c_0$, $m_{t_1}[c_3] = c_4$, and $m_{t_1}[c_3] = c_5$ in its local reduction computation. Since each thread has a single map and can only retrieve the entire image set of a single entity input, the schedule will have synchronization problems.

If instead we split the map m on each thread into two copies and spread it contents into these two copies, then we could emulate an arrow partition. For example, still using the previous example, we split m_{t_0} into $m^o_{t_0}$ and $m^*_{t_0}$ on thread zero, where $m^o_{t_0}[c_0] = c_1$, $m^o_{t_0}[c_0] = c_2$, and $m^*_{t_0}[c_3] = c_0$. And we also split m_{t_1} into $m^o_{t_1}$ and $m^*_{t_1}$ on thread one, where $m^o_{t_1}[c_3] = c_4$, $m^o_{t_1}[c_3] = c_5$, and $m^*_{t_1}[c_0] = c_3$. We can see that $m^o_{t_0} \cup m^o_{t_1} \cup m^*_{t_0} \cup m^*_{t_1} = m_{t_0} \cup m_{t_1} = m$. This effectively forms a partition of arrows by using multiple maps. Now when thread zero runs the local reduction through $m^o_{t_0}$ and $m^*_{t_0}$, and thread one runs the local reduction through $m^o_{t_1}$ and $m^*_{t_1}$ concurrently, there will be no interference and no synchronization will be needed. In practice we will merge $m^o_{t_0}$ and $m^*_{t_0}$ into a single map $m^b_{t_0}$ and similarly we merge $m^o_{t_1}$ and $m^*_{t_1}$ into $m^b_{t_1}$. Thus the map $m^b_{t_0} \cup m^b_{t_1}$ is equivalent to the original map m, and $m^b_{t_0}$ and $m^b_{t_1}$ form an reorder of the maps m_{t_0} and m_{t_1}. In this way, if the local reduction rule use the new maps $m^b_{t_0}$ and $m^b_{t_1}$ instead of the original maps m_{t_0} and m_{t_1} on corresponding threads, then we obtain a synchronization free multithreaded local reduction schedule. We can use map reordering on threads to emulate the effects of arrow partition.

Implementing such a scheme is however complicated as well in the present Loci framework. The complication comes from the limitation in the Loci framework to swap individual variable representation in a rule kernel. The current Loci rule `execute_modules` will need to use the interface `initialize()` in type `rule_impl` to setup a connection between the variables declared in a rule and storage spaces in the Loci `fact_db`. This step makes replacing a single (or a few) individual variable storages (perhaps generated locally and not in the `fact_db`) difficult. This is perhaps still doable with moderate refactoring of the current interface. However the Loci framework is unable to change the source code specified in a rule kernel as well, which makes replacing the original map with an enhanced reordered map impossible. Consider the example given in Figure 23. This reduction happens through a chain of maps and the source code in C++ encodes the reference of all the maps involved in the chain. When we generate a reordered map, we do not want to reorder all of the individual maps in chain. Instead we wanted to replace the chain `$m0->$m1->$m2` with a single reordered map, i.e., we would want to flatten the chain first and then reorder the flattened map. But we cannot change the C++ source code in the kernel to match up. The only feasible way in the current setup seems to have an intelligent Loci pre-processor that can generate new C++ source code.

```
$rule apply(m0->m1->m2->target <- source) {
  $m0->$m1->$m2->$target += $source / 3.;
}
// ...... corresponding C++ source code for the kernel
void calculate(Entity e) {
  target[m2[m1[m0[e]]]] += source[e] / 3.;
}
```

Figure 23: A general Loci reduction rule

5.2 Hidden synchronization

The current Loci framework uses a subscriber pattern in the storage hierarchy design. A storage allocation (`storeRep`) can be shared among different names (called the shell, e.g., a `store`) and the shells also maintain pointers to the underlying storage memory location for direct access. Whenever a storage allocation changes itself, it calls the interface `dispatch_notify()` to update the shell pointers (which defines the routine `notification()` as a callback). This mechanism is necessary to use a list to record who to send the notification in case it is needed. In a multithreading environment, such a subscriber list is shared among all the threads and will need to be guarded by a thread lock to prevent data corruption. This then creates a hidden thread synchronization cost. Since the Loci storage interface is ubiquitous in the system, this can be a concern for thread performance.

A general solution to this problem might be to use more effective atomic variables instead of mutual exclusion locks to guard the subscriber list (such as those atomic constructs supported in the c++11 standard). A better way is to redesign the storage hierarchy in Loci altogether to remove such hidden thread synchronization cost completely. Currently we have designed some special interfaces in the storage hierarchy to help mitigate this problem. A special copying routine `fast_copy()` has been added to the `storeRep` type. Currently only the `paramRepI` class implements this new interface. Other `storeRep` types delegate the implementation to the normal `copy()` routine. Some of the `storeRep` types, notably the `paramRepI`, will need to invoke the `dispatch_notify()` interface, which will cause thread locks to be acquired and released. While it may be the case that in the multithreading execution, there is only one or no subscriber in the list and only one thread will be accessing the list, having to acquire and release the locks may still cost a little performance. Instead the `fast_copy()` routine implemented in the `paramRepI` class skips the `dispatch_notify()` call. But it is then only safe to call the `fast_copy()` on a `paramRepI` only if it is not linked to any of the shell containers. This is the case in global reduction scheduling and so it is used (see line 19 in Figure 12 in section 4.5.2).

There are several other issues related to this general problem in the Loci framework that a developer needs to be aware of in a multithreading environment. The current implementation of the `entitySet` type uses a similar setup. It uses a "handle" type to share data via a counted pointer. This reference counted pointer is not protected for thread access though. And this will cause certain calls involve `entitySet` to fail in a multithreaded environment. An example would be that calling the `domain()` function on a shared container will likely to fail since the `entitySet` that represents the domain being returned by the call will be copied, which is not thread safe[5]. Another potential error would be to perform conversion between the `sequence` and the `entitySet` types. Currently converting to an `entitySet` from a `sequence` is thread safe, however, converting to a `sequence` type from an `entitySet` type is *not* thread safe due to the way the internal data sharing is implemented. Note however that we do not want to protect the underlying shared data in `entitySet` since doing so will possibly severely degrade thread performance because `entitySet` is the most important foundation in the current Loci implementation.

5.3 Thorny Loci abstractions and semantics

Currently some of the Loci abstractions and semantics are also causing inconvenience in several situations. These are probably manifestations of the design problems in the associated Loci abstractions and semantics. Future developments would need to consider improving or redesigning these and possibly other related abstractions and semantics.

The first inconvenience comes from the need to frequently convert between the `sequence` and `entitySet` types in the scheduler and during runtime execution of certain rule kernels. These two types are closely related (they share a large portion of underlying implementation), yet they are not entirely compatible (e.g., the "`-`" operator is only defined on `entitySet` and not on `sequence`). The current `compute()` interface in a `rule_impl` type takes a `sequence` to represent the execution context. While many operations on variables produce `entitySet` type as a result (such as the `domain()`, `image()`, and many set operations). The multithreading code does a lot of set manipulations and calculations. In many cases, we are forced to convert between the `sequence` and the `entitySet` types just so we can call the functions needed (e.g., converting an `entitySet` to a `sequence` so that we can use it as the context for a rule to compute). Doing these conversions (especially frequently) is not only costly (particularly when the `entitySet` contains a large number of segments), but it may also be thread unsafe (such as when converting from an `entitySet` to a `sequence`). In fact, if we change the rule context type to be `entitySet` instead of the current `sequence` type, then most of these conversion problems will go away. It is also more appropriate to use the `entitySet`

[5]This is a hard lesson learned from a seemingly innocent bug in the code, which took some time to understand and fix.

type as the general rule context type since a fundamental Loci rule semantics is referential transparency in a rule kernel. The rule kernel can be applied to any entity in its context regardless of order. Then it makes sense to use `entitySet` as the context type since it is just a collection of entities without order. While the purpose of `sequence` is to encode a total order of the entities collected. In the multithreading schedule, such transparent execution of the rule kernel is also the foundation of the data parallelism employed. Therefore we strongly suggest the rule context type be changed to `entitySet` from `sequence` in future revisions of the Loci framework. Doing so will likely produce more efficient code and enforce the Loci semantics assumptions.

In practice a Loci rule can have side-effects and there is no way to enforce side-effect free rule specifications in the Loci abstraction. Then to ensure the correctness of a schedule, certain procedures must always be (re)evaluated. An example comes from the implementation of chomping. When we run the chomping schedule, we will need to allocate small storage spaces for all those chomping variables. Ideally since these storage spaces are quite small (after all, they should fit inside a small cache), we could create them once and keep them for repeated reuse. However there is no guarantee that the variables involved in chomping would be the same type. It is possible that a rule can set different variable types during different invocation (e.g., by changing the vector size of a `storeVec`), thus invalidating the previously created chomping storage. Therefore to ensure complete correctness, every time before the chomping schedule runs, we have to query the `fact_db` for all chomping variables and recreate the temporary chomping storage again. In reality probably no current Loci rules will change a variable type in different execution time (indeed this is the assumption made in the older sequential chomping code so it only query the `fact_db` once). However there is no guarantee that this will not happen.

Another potential problem related to side-effects and execution orders also exists in the chomping schedule. As section 4.6 discussed, a rule now has three execution points, the `prelude()` and `postlude()` are now used to specify non-data parallel computations, and `compute()` is used to specify data parallel entity-level computations. A normal schedule of a rule would call `prelude()` first, followed by `compute()`, and then finally the `postlude()` interface. If a group of rules (e.g., `r0` and `r1`) is not run in chomping mode, then the order of their execution will be: `r0.prelude()`, `r0.compute()`, `r0.postlude()`, `r1.prelude()`, `r1.compute()`, `r1.postlude()`. However if the rule group is run in chomping mode, then they will effectively become a single execution unit, i.e., the chomping execution of `r0` and `r1` has to occur together. But the `prelude()` and `postlude()` cannot be chomped and have to be called outside of the chomping. The current setup uses this order: `r0.prelude()`, `r1.prelude()`, `chomping(r0,r1)`, `r0.postlude()`, `r1.postlude()`. This is a different order than the non-chomping run and if there are side-effects in any of these interface specifications, then the chomping and non-chomping execution results may be different. This is usually not a problem (and has not been a problem so far for all Loci applications). But again there is no guarantee offered by the Loci framework.

We can instead leave these semantics issues there and rely on the fact that probably no Loci rule specifications will break the current assumptions made in the code. However these do cause some unease and discomfort. Worse, they may be forgotten in the long run and if future application specifications do violate some of these assumptions, then weird bugs may appear and will be hard to understand, particularly if multiple of such assumptions are embedded in the Loci implementation and interact in some unpredictable and complex ways. Having clean, strict, and well behaved semantics is thus important.

6 Preliminary tests and assessments

For completeness purpose, we include a preliminary performance assessment of the multithreading system in this section. This is only a preliminary assessment based on a 2016 version of Loci. So it is just for reference only. The brief performance evaluation is carried on a simple "`euler`" program constructed using the Loci framework with various threading options enabled. Several moderately sized input grids are used. Experiments using eight processes/threads and less are conducted on a desktop workstation with 3.7GHz Intel Xeon E5-1630 CPU (four physical cores with eight hardware threads) and 32GB of memory. Experiments utilizing beyond eight processes/threads are performed on a Linux cluster whose single node consists of 2.8GHz Intel Xeon E5-2680 v2 CPU (ten physical cores with 20 hardware threads) and 64GB of memory.

The `euler` program is run in chomping and non-chomping modes. Table 1 shows the total and threaded computation of each rule type. It may seem strange why not all of the pointwise computations are threaded. This is mainly because some of the pointwise computations are inherently sequential (such as I/O processing) and some may contain non-safe operations for threads.

Table 1: Type of computations in the `euler` program

	pointwise	global reduction	local reduction	chomping	recursion
with chomping	25/37[1]	1/1	2/2	3/3	0/0
no chomping	38/50	2/2	6/6	0/0	0/0

[1] This denotes 25 computations are threaded out of a total 37. The same goes for the rest of the table.

Table 2 presents the wall timing results of the `euler` program execution with different parallel options. The execution is carried using a single process with eight working threads, two MPI processes each with four working threads, four MPI processes each with two working threads, and purely eight MPI processes. The two middle configurations represent a hybrid parallel execution and is the main intended use of the threading infrastructure (together with MPI parallelism). All measurements are in seconds. The execution timing is the total time taken to execute 100 iterations and does not include any Loci pre-processing time. In these measurements, each working thread uses a 25-block division. The numbers in the parentheses represent the slow down when compared to the eight MPI-process run (which represents the highest performance so far).

Table 2: Wall time of `euler` execution (small grid, 25 blocks per thread)

	8 threads	2 mpi 4 threads	4 mpi 2 threads	8 mpi
with chomping	114.2 (18.1%)	101.1 (4.6%)	99.4 (2.8%)	96.7
no chomping	145.2 (26.3%)	122.7 (6.7%)	119.5 (3.9%)	115.0

Table 3: Wall time of `euler` execution (large grid, 25 blocks per thread)

	8 threads	2 mpi 4 threads	4 mpi 2 threads	8 mpi
with chomping	447.1 (11.1%)	408.0 (1.3%)	405.1 (0.6%)	402.6
no chomping	564.3 (17.1%)	490.1 (1.7%)	495.1 (2.7%)	482.1

Table 3 shows the timing results of the same configuration as measured in Table 2, except that the program is run on a larger input grid (roughly four times larger). These results give an indication of the overall performance of the threads compared to the MPI run (as well as two hybrid runs).

The raw performance of threads (8-thread run) lags behind the raw MPI performance (8-mpi run) by somewhat between 10-25%. While any of the hybrid runs has a raw performance much closer to that of the raw MPI performance. It should be noted that these are results obtained from a thread implementation that has not been polished yet. Section 5 discusses several improvements that can be done.

However, given the assumption that the current thread implementation is correct, these results are actually fairly encouraging. First of all, the raw thread performance does not lag behind raw MPI performance by too much. Secondly, in a typical setting, we would like to have a hybrid run (e.g., mixing threads with MPI). The hybrid run results shown here are almost identical to the raw MPI performance.

Then one would ask what is the reason that the raw thread performance cannot compete with the raw MPI performance? This is a tough question to be fully explained. So far, our guess is this is due possibly to the following reasons:

1. As we have said, the current thread implementation is not yet fully optimized.

2. The 8-thread run essentially uses the sequential version of Loci schedule, which may not have the same level of optimization as a parallel MPI schedule. This means the base performance of a serial Loci schedule is worse than a MPI schedule.

3. Memory locality may also play a major role in determining the performance. In the 8-thread run, threads may be accessing non-local memory (meaning accessing memory locations on a different chip), thereby slowing down the performance.

Ultimately, one would wonder if the raw thread performance is ever possible to match (or even exceed) the raw MPI performance? It appears that this is unlikely (although we do not have proof). A pure MPI run inherently has more locality than a pure thread run. This will usually provide much tighter integration and have better performance gains. A pure thread run also suffers from frequent thread synchronizations and unpredictable system effects. For example, during the measurements of the above data, we have observed that a pure 8-mpi run will have a CPU utilization of 796% or more (as reported by the `top` program), while a pure 8-thread run has a varying CPU utilization of 700-790%, sometimes even dips below 600%. Although the CPU utilization is not an absolute performance indication (a program can be busy doing nothing useful), it is nevertheless a hint that the pure MPI run is more tightly coupled, while a pure thread run probably suffers from constant thread stalls due to synchronization and/or random system effects.

After our initial performance measurements on the desktop machine, we had a brief opportunity to conduct a measurement of the same `euler` program on a larger Linux cluster with up to 60 hardware threads. We performed a simple and brief measurements for a larger scale hybrid MPI/thread performance and compared the results to an equivalent pure MPI schedule. We have chosen to measure the performance using two MPI processes each with ten threads, four MPI processes each with ten threads, and then six MPI processes each with ten threads. We have chosen these combinations because on the Linux cluster, it appears to have two physical chips per node and each chip supports ten hardware threads at most. Running more than ten threads on a single process will likely to cause remote memory access, which would severely degrade the thread performance. Running ten threads within a single MPI process helps to let all the threads stay within a local hardware chip, which helps to improve the memory access cost. However we have not made any efforts to try to pin all threads generated from an MPI process to stay on a particular hardware core. Ensuring thread affinity may be important and should probably be investigated in the future.

Table 4: Wall time of `euler` execution (large grid, 10 blocks per thread) on Linux Cluster (with chomping)

	20mpi vs. 2mpi,10threads	40mpi vs. 4mpi,10threads	60mpi vs. 6mpi,threads
pure MPI	98.4	50.4	785.5
hybrid	107.9 (9.7%)	65.5 (30.0%)	1138.8 (45.0%)

Table 4 presents the results obtained on the Linux cluster. The `euler` program is run with chomping option enabled. The default option of ten *b* blocks per thread is also used. The timing results presented in the table are all in seconds. For the first two columns, an 100 iteration execution is used and a 2500 iteration execution is used for the last column measurement (otherwise the execution duration will become too short). The numbers in the parantheses indicate the slow down of the hybrid run compared to the pure MPI run. Table 4 suggests that the four-MPI/ten-thread and six-MPI/ten-thread hybrid execution incur much higher overhead as compared to the other (smaller scale) configurations. These results seem to suggest that the thread scheduling does not scale well (at least when compared to a pure MPI schedule). Currently, we have not made detailed investigations to the cause of this result. There could be several reasons for such a result. We have outlined above that the thread scheduling will naturally be less parallel than a pure MPI schedule. Another reason is that these measurements are essentially fixed problem size scaling tests. When we are at larger numbers of concurrency (e.g., 40 and 60 processes/threads), the per thread problem size may become very small indeed. And this would make the thread overhead become a dominating factor. In the future, it would be helpful to scale the measurement with a fixed per thread problem size. Another factor that may affect the performance is that when we use large number of threads, if dynamic thread migration occur, that may also cause thread performance degradation. As we have mentioned, currently we do not have any thread affinity options within Loci scheduling.

We will further examine the runtime performance by zooming in to two simple individual computations in the `euler` program. Examining these individual computations may help to reveal if there is any performance loss in a simple calculation. As these are simple straightforward calculation, we should not expect any performance differences in the various configurations.

Here we have selected two pointwise computations. The first one is denoted as "c_1" and corresponds to the following rule (note it does not involve any indirect memory access):

```
Q{n,rk+1}<-$rk{n,rk},Q{n,rk-1},Q{n,rk},Residual{n,rk},deltaT{n,rk}
```

The second pointwise computation is denoted as "c_2" and corresponds to the following Loci rule (note that it involves many indirect memory accesses):

```
gradv3d(u){n,rk}<-(lower{n,rk},upper{n,rk})->(cl{n,rk},cr{n,rk})->(u{n,rk},vol{n,rk}),
    (lower{n,rk},upper{n,rk})->area{n,rk},boundary_map{n,rk}->(area{n,rk},u_f{n,rk}),
    vol{n,rk},CONSTRAINT(geom_cells{n,rk},greensGradient{n,rk})
```

Table 5: Two computation timing within `euler` execution (large grid, 25 blocks per thread, with chomping)

	8 threads	2 mpi 4 threads	4 mpi 2 threads	8 mpi
c_1	11.0	9.9	11.3	11.2
c_2	57.3	58.1	55.2	57.1

Table 5 shows the measured execution time for these two pointwise computations under different thread and MPI configurations. The measurements are in seconds and represent the slowest time in a parallel run (e.g., the 8-mpi results are the maximum timing of these two computations on all of the 8 processes).

This result shows that there is virtually no difference in the performance of these computations under different parallel configurations. This is a good indication that the threads have no perceived overhead during the actual computation phase when there is no synchronization requirements. Previously we have reported that we have observed the computation performance of threads lags behind the raw MPI performance when there is indirect memory access involved. At that time, we cannot fully explain the reason. We have suspected that it was possible due to non-local memory access in threads caused by the indirect memory accesses. The data shown here does not seem to suggest this is an issue. It is possible that the use of multi-level thread partition strategy has helped to improve performance in this area.

Table 6: Stat info of `euler` execution with 8 threads and varying number of b thread blocks

b block number	5	10	25	50	75
total work units	40	80	200	400	600
max conflicts[1]	3	3	3	6	10
max non-local conflicts	1	1	1	2	4
20-iter wall time	88.5	87.1	88.5	87.4	87.2

[1] These conflicts numbers are obtained on a single chomping computation group that has 14 rules including 4 local reductions.

Next in Table 6 we show some of the statistical information regarding the thread partition strategy. One of the purposes of designing the thread partition strategy is to deal with thread synchronization requirements during the execution of certain types of computation (e.g., local reduction and chomping). The data presented in Table 6 show the effectiveness of our thread data partitioner and the effects of varying b block numbers on the schedule execution time.

The maximum conflicts numbers presented in Table 6 represent for any of the thread block, the maximum number of other blocks that are in conflicts (and thus requires synchronization). The non-local conflicts refers to related blocks that are owned by other threads (a block can be related to itself or other blocks that are owned by the same thread). In terms of synchronization cost, the non-local conflicts are the ones that really matter. From the data we can conclude that the current thread data partitioner is effective, i.e., the partition removes much of the block conflicts. When there are enough such work units presented in the system, each thread can almost become non stalled. Note these conflicts numbers are obtained by measuring the conflicts on a chomp computation group that has total 14 rules inside including four local reduction computations. This is a fairly large group with complex interactions in the target dependency. It is a good example to show the effectiveness of data locality among the blocks involved. Another note is that the blocking number does not seem to have significant impact on the execution time in this case. However the effectiveness of block conflicts resolution ultimately also depends on the way a Loci program is structured. If the Loci program intrincaly has a high number of block conflicts, then the thread partitioner cannot help.

Table 7: Loci pre-processing time of `euler` schedule (large grid, 25 blocks per thread)

	8 threads	2 mpi 4 threads	4 mpi 2 threads	8 mpi
with chomping	139.9	422.8	168.9	89.5
no chomping	141.0	422.1	168.8	89.6

Tables 2 and 3 only give the performance of the program execution. Table 7 shows one instance of the cost of the current Loci schedule when creating threads. Comparing to the pure MPI run, the threads schedule generation currently incurs some large overhead. Also note that the cost in the 2-MPI-4-Thread run is particularly large. We currently do not have an explanation for this. It is somewhat unusual that this occurs within a hybrid run where a pure thread and another hybrid run do not exhibit such anomalies.

When comparing to the pure MPI schedule cost, the thread schedule cost is going to be inherently higher since all thread related scheduling information will be generated in addition to those related to MPI. The current thread scheduling cost mainly involves two types of overhead: 1) the thread data partitioner, and 2) the scheduling of each individual computation that is threaded.

Although we have shown that the present thread partitioner is effective in producing locality aware partitions, it is nonetheless not optimized for speed. The scheduling of each thread computation can possibly also be improved as well. For example, as discussed in section 4.5.3, the b blocks conflicts graph creation is currently performed on a per computation basis, and uses a $O(n^2 * k)$ algorithm, where n is the total number of b blocks involved in a particular graph and k is the cost of all entity set manipulations involved. This is a straightforward naive algorithm that can be improved once we have a systematic multi-level mapping infrastructure established. Also such conflict resolution can potentially be performed on a per-pattern basis instead of per-computation basis, which would save a lot of processing time. Although this is an advanced processing technique that requires careful design.

Also in the present Loci schedule, a query will invoke two schedule executions, the first one is an internal schedule execution that generates all the dynamic constraints and mapping information etc. The current internal schedule does not actually benefit from threads, so it is excluded from multithreading schedule. However this implementation improvement was made after the measurements performed shown in Table 7. So the measurements in Table 7 include a redundant thread schedule (mainly the thread data partitioning is run twice). Right now, the performance of the Loci threads schedule generation should be better than the results indicated in Table 7.

Finally Table 8 shows the peak memory reached during the execution of the `euler` program on the larger grid under various configurations. These numbers were obtained by observing the `top` program's output during the program execution as we do not know any other reliable and accurate way to obtain real memory

Table 8: Peak memory consumption during `euler` execution (large grid, 25 blocks per thread)

	8 threads	2 mpi 4 threads	4 mpi 2 threads	8 mpi
with chomping	6.1g	8.2g	8.6g	8.9g
no chomping	7.3g	9.7g	9.9g	9.9g

consumption in an automated way.

It is very clear that in this respect, a pure thread run performs the best and uses significantly less amount of memory than a pure MPI run. This is one of the primary reasons why we are interested in threads. Although the table suggests that once MPI is mixed in, no matter how small amount, the peak memory starts to climb fairly quickly.

Finally as a reminder, this is only a very preliminary performance evaluation and should not be taken as the final performance characteristics of the Loci multithreading infrastructure. Future tuning and work can dramatically change the performance. Also simply using the bigger and far more complex Chem code can give very different conclusions even for the present code. We should conduct more extensive evaluations in the future.