Taverna, reloaded

Paolo Missier[1], Stian Soiland-Reyes[1], Stuart Owen[1], Wei Tan[2], Alexandra Nenadic[1], Ian Dunlop[1], Alan Williams[1], Tom Oinn[3], and Carole Goble[1]

[1] School of Computer Science, The University of Manchester, UK
[2] Mathematics and Computer Science Division, Argonne National Laboratory, Argonne., IL., USA
[3] European Bioinformatics Institute, UK

Abstract. The Taverna workflow management system is an open source project with a history of widespread adoption within multiple experimental science communities, and a long-term ambition of effectively supporting the evolving need of those communities for complex, data-intensive, service-based experimental pipelines. This paper describes how the recently overhauled technical architecture of Taverna addresses issues of efficiency, scalability, and extensibility, and presents performance results based on a collection of synthetic workflows, as well as a concrete case study involving a production workflow in the area of cancer research.

1 Introduction

Taverna [10] is a workflow language and computational model designed to support the automation of complex, service-based and data-intensive processes. Although Taverna has been successfully applied in domains as diverse as bioinformatics, astronomy, medical research, and music, it is perhaps best known for its application to the Life Sciences [6, 15], where it has been used to support experimental investigation into a variety of research areas, including gene and protein sequence and structure annotation, proteomics, microarray analysis, text mining, systems biology, and more. The first version, launched in 2004 [18], has enjoyed broad adoption over the years[4], owing in part to a fairly intuitive model for service composition, and to a growing number (in the order of tens of thousands) of available services, mostly community-provided and free to use, and to Taverna's ability to invoke ad hoc scripts and Java object methods.

Taverna combines a dataflow model of computation [14], whereby a workflow consists of a set of processors (representing software components such as Web Services) that are connected through data dependencies links, with a functional model that accounts for collection-oriented processing. This hybrid model is designed to strike a balance between expressivity and simplicity, with the ultimate goal of empowering users, who may have only a rudimentary understanding of programming, to assemble complex workflows. While the model and its theoretical underpinnings [23] have remained largely stable over the years, the evolving requirements of e-science applications have recently prompted a radical re-design of the architecture, which we will refer to as "Taverna 2" (T2 for short) to distinguish it from the previous version, T1.x.

This paper presents the salient features of the new architecture, which has two main goals. Firstly, to improve the scalability of workflow execution, both in terms of data volume and execution times, over its predecessor. Secondly, to provide third-party developers with clear configuration points for performance tuning, and with extensibility points for adding new high-level constructs,

[4] In 2008 there were over 4000 active users of Taverna, a year-on-year increase of 43%. Currently it stands at more than 57,000 downloads total, running at 40 downloads/day.

such as a while-loop, to the dataflow model, in order to facilitate workflow design in paradigmatic scenarios. More specifically, the following architectural requirements have inspired the design of the T2 architecture:

Parallelism. Models of computation that combine dataflow and functional models are known to facilitate parallel execution [13], making the exploitation of the parallelism provided implicitly by the workflow specification a realistic goal. Potential parallelism can be found both amongst processors (*inter-processor*), by statically determining data dependencies amongst processors in the dataflow graph, as well as amongst multiple invocations of the same processors (*intra-processor* data parallelism), i.e., on individual elements of an input collection.

Configurability. Each processor may have different operational requirements, for example regarding its tolerance to transient error conditions in the underlying service invocation. Thus, it should be possible to fine-tune the behaviour of each processor independently from that of the others.

Openness. It should be possible for third party contributors to extend the functionality of the execution model in a principled way. For example, interacting with asynchronous services that require periodic polling to check on result availability, does not fit the data-driven model well. While in T1.x the model can be "stretched" to simulate polling processors, T2 accommodates this requirement by implementing a limited form of while-loop construct by exploiting a generic extensibility mechanism, called the *dispatch stack*.

Separation of data and process spaces. For data-centric computing to scale to arbitrary data volumes, the data space should be managed separately from the process space, and, whenever possible, data should be passed from one processor to the next by reference rather than by value.

This paper describes how the design principles listed above have been translated into a coherent architectural design for T2, and presents performance results for the current implementation.

1.1 Related work

Workflow modelling for data-intensive scientific applications is, of course, not new. One of the recognized challenges of scientific workflow management systems is to provide abstract modelling constructs that are then automatically instantiated as an orchestration of concrete tasks that execute on an sunderlying parallel architecture [4, 9]. This is the approach taken for example by the Pegasus system [5] and exemplified in the CyberShake case study [3], with the goal of decoupling the logical specification of the workflow from the pool of resources required to execute it. In this paradigm, resources are allocated by the scheduler incrementally and dynamically. In a similar fashion, Chimera [7] provides a dedicated language (VDL) for the partial specification of logical workflows. A complementary, bottom up approach, is to start with a job management system, like Condotr, and then provide users with a model for building complex workflows from a pool of individual jobs [1]. Another example of concrete and well-known mechanism used for the specification of complex dataflows is *shell pipes*, proposed in [26]. Finally, an interesting development [27] of the Kepler workflow manager is its integration with Hadoop[5], an open-source implementation of

[5] `http://hadoop.apache.org/`.

the MapReduce pattern [2]. Thanks to this integration, Kepler users are able to specify MapReduce problems at a high level, leaving the details of its realization through the Hadoop API to the workflow manager.

While the Taverna workflow manager shares some of the goals of abstraction and dataflow-based parallelism, the majority of the workflows designed by its traditional user base, for the most part in the bioinformatics domain, are rather more data-intensive than compute-intensive. Typically, Taverna workflows perform some form of "on-the-fly data integraton" on large collections of data values retrieved from a variety of databases through their Web service interfaces, exposed as Taverna processors. In this setting, each of the available parallel threads tends to carry a potentially large data item, while involving very small amount of computation. Also, its execution is bound to that of some underlying remote service, making an explicit mapping of Taverna threads to a parallel architecture less of a priority. Naturally, therefore, the emphasis in T2 has been on efficient data management, by separating the data space from the process space as much as possible, and on developer-facing features such as well-defined extensibility points. In turn, these translate into a simplification of the workflow design and testing phase, as well as access to large collection of third party services in specific application domains.

1.2 Paper organization

The rest of the paper is organised as follows. The execution model is presented in Sec. 3; the dispatch stack model used for processor execution control is described in Sec. 3.1, its application to the design of the while-loop operator is described in Sec. 5, and the separation of data and process spaces is discussed in Sec. 4. Performance results are presented in Sec. 6, followed by the description of a concrete case study from the caGrid project, in Sec. 7.

2 Workflow model

We begin by briefly summarizing the Taverna computational model. While a full account is beyond the scope of this paper, the formal semantics for T1.x and T2 has been independently described in [23] and [21], respectively[6].

2.1 Dataflow specification

A Taverna workflow is specified by a directed graph where nodes, called *processors*, represent software components, typically Web Services or local scripts. A processor node consumes data that arrives on its *input ports* and produces data on its *output ports*. Each arc in the graph connects a pair of ports, and denotes a data dependency from the output port of the *source* processor to the input port of the *sink* processor. Additionally, *control links* can be placed between a source and a sink processor, to denote that the latter can only be executed after the former has produced all its output.

An example of a Taverna workflow for bioinformatics appears in Fig. 1 (the workflow is published on the `myExperiment` website[7]). The workflow accepts one or more input collections of gene IDs, and for each such list, on output port `paths_per_gene` it produces a list of metabolic pathway IDs,

[6] The two papers follow different approaches to formally define essentially the same semantics.
[7] `http://www.myexperiment.org/workflows/778`

obtained from the KEGG pathway database[8], which involve each of the genes in the list. In this model, data items are either of a simple type (string, number, etc.), or are lists of items, nested to arbitrary levels. For example, list [[`mmu:26416, mmu:34212 `],[`mmu:328788`]] is a valid input for the example workflow.

Conceptually, a workflow computation proceeds by pushing data through the directed data links from one processor to all of its successors, starting with the items that are presented on the workflow inputs. A processor is ready to execute when all of its inputs ports are populated with a data item. A processor's execution consists of the invocation of an associated *activity*, for example a Web Service or a local script, and produces new data items on its output ports. These are then propagated along the outgoing arcs.

Importantly, an activity *can itself be a workflow*, i.e., an entire workflow can be associated to any individual processor. This makes the Taverna model closed under activity composition, i.e., a workflow is a composition of activities, and can be an activity itself. This dual nature of workflows results in a structurally recursive model where a collection of elementary activities forms the baseline layer. This has two main benefits: firstly, it can be used to support control constructs from traditional programming languages, such as a while-loop, which operate on a "body of code"; here the body is encapsulated within a sub-workflow. And secondly, it allows for the dynamic specification of workflows, by allowing the late binding of activities to processors, a feature that was found to be useful in certain contexts [8], and which opens the way for service discovery to occur at workflow execution time.

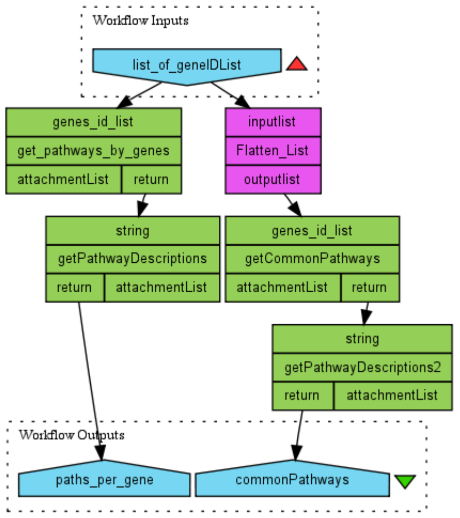


Fig. 1. Taverna workflow for metabolic pathways lookup

[8] `http://www.genome.jp/kegg/pathway.html`

2.2 List data types

The handling of input lists by processors in Taverna is based upon the declared depth associated to each input port. The depth denotes the level of nesting of the expected input, where an atomic input has depth = 0. For example, the list [['red', 'blue'], ['fox', 'parrot']] has depth 2. For processors that represent Web service operation invocations, the declared depth is determined automatically. Consider for example a KEGG Web service whose WSDL interface specification includes operation `getPathwayDescriptions`, with a single input parameter `string`[9], which accepts a string. When the operation invocation is added to the workflow of Fig. 1, typically using the *Taverna workbench* (the visual environment used for workflow composition), a processor with the same name as the operation, and one port of depth 0, are automatically generated.

During execution, the actual value that arrives on the port may have a different nesting level than expected. If the preceding processor `get_pathway_by_genes` produces a simple list (of depth 1) of pathway IDs, for example, there is a mismatch between the declared and the *offered* list depth on the port. In this case, list processing in Taverna is reminiscent of a functional computational model: the mismatch of 1 between declared and offered depths causes the engine to iteratively invoke the processor over each element of the list. In each such invocation, the port is bound to an atomic value, as expected by the underlying service invocation. The results of each invocation are then collected into a new output list. In our example, since each invocation generates a list of descriptions for an input pathway ID, the final value on the `return` port is a list of lists, of depth 2.

Iterations over collections have been formally described in terms of higher-order functions [13], and a complete account of the Taverna *implicit iteration* model can be found in [21][10]. The implicit list iteration semantics provides intra-processor parallelism, because the list elements that are being iterated upon are independent from each other, and thus multiple processor instances that operate on those elements one at a time can potentially proceed in parallel (assuming they generate no side effects). Furthermore, implicit iterations may propagate through a *sequence* of iterating processors. For example, if `getPathwayDescriptions`, which expects a string, is presented with a list produced by the preceding processor, the computation again unfolds into multiple processor instances.

As we explain in the next section, the runtime architecture of Taverna is designed to exploit both intra-processor parallelism, as well as the inter-processor parallelism that is implicit in the dataflow processing model.

3 Workflow processing model and architecture

We now describe the suite of architectural solutions adopted to realize each of the principles enunciated in the introduction. The overview architectural diagram is shown in Fig. 2.

A workflow specification is compiled into a multi-threaded object model (implemented in Java), where processors are represented by objects, and data transfers from output to input ports of downstream processor objects are realized using local method invocations between objects. One or more activities are associated to each processor. These activities may consist of entire sub-workflows, in addition to executable software components. While data-driven computation in T1.x relies on a centralized workflow enactment system, in T2 there is no need for a central controller: as each

[9] This is the name chosen by KEGG for this parameter.

[10] The full model described in [21] accounts for multiple mismatches on more than one input port. This level of detail does not add much to our architectural discussion and is omitted.

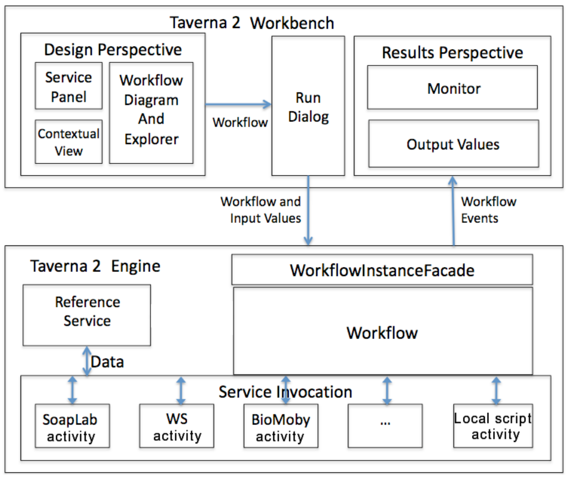


Fig. 2. Overview block diagram of Taverna 2 architecture

processor is mapped to an object, it independently starts its own execution, in a separate thread, as soon as all of its (connected) input ports are populated with a data item, and it autonomously transfers its output along the arcs upon completion. Although execution is decentralized, a `facade` pattern is used to provide external components, notably the monitor and result presentation components in Fig. 2, with a single point of contact (a different facade is used for each workflow run). The monitor listens to various events emitted by the processors, which are translated into visual information on the progress of execution.

3.1 The dispatch stack

A processor's execution culminates with the invocation of one of its associated activities. In doing so, however, a number of additional functionalities are involved, which collectively define a configurable and extensible runtime behaviour. These functionalities provide configurable quality of service management, and are implemented as separate components which are organized according to the *interceptor* design pattern. We use the terms *layers* and *stack* to denote the components and the pattern, respectively, as this resembles the behaviour of a protocol stack, as shown in Fig. 3(a). The following standard layers (in the order they are presented) are defined for each processor:

Parallelise: this ensures that, when iterations over lists are involved, independent concurrent threads are created to process each list element;

Error Bounce: is responsible for immediately terminating an execution when any of the inputs are in an error state. This protects the underlying activities from being invoked on invalid input;

Failover: detects the failure of an activity associated to the processor, and is responsible for selecting an alternate activity, if available (recall that activities can be added and removed dynamically);

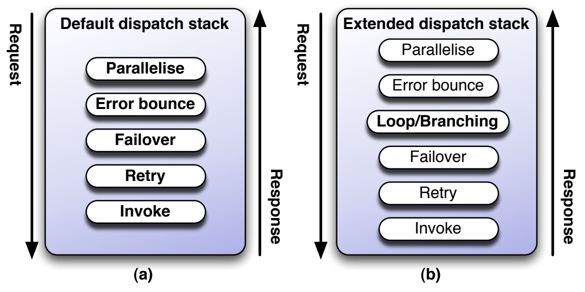


Fig. 3. Processor dispatch stack

Retry: provides tolerance to transient errors in the underlying activity, by repeatedly attempting the same invocation for a configurable number of times.

The stack is activated by a request message to the processor, consisting of the data on the input ports. The message is pushed down the stack, where each layer performs its function and, if needed, forwards a new version of the request to the next layer. At the bottom of the stack, the *Invoke* layer performs the actual invocation of an activity; in the case of a Web Service invocation, for instance, this layer is a Web Service client that maps the incoming request to a SOAP message, and manages the interaction with the service. The result is mapped to a response message, which finds its way back up along the stack, where it is intercepted by each layer, possibly transformed, and forwarded. Ultimately, the processor invocation terminates and the response is forwarded to downstream processors along the data links.

3.2 Configurability and extensibility

In this architecture, a private instance of the dispatch stack is associated to each processor, making it configurable independently of the others. Also, the interceptor pattern naturally allows new layers to be added to the standard stack shown in Fig. 3(a)[11]. Useful additional layers that are already available as part of the current release include the *while-loop* layer, shown in Fig. 3(b) and described in more detail in Sec. 5, as well a *Provenance layer*, designed to generate audit events from the processor's execution as a basis for collecting workflow provenance [17].

Layers are typically added and configured as part of the workflow design activity, but users need not be aware of the stack architecture. For example, the Taverna workbench has a new option that allows users to qualify any processor as a "while loop processor", and to specify the corresponding elements, i.e., the loop exit condition and the body of the loop. The body in particular can be an elementary activity, or an entire sub-workflow (which, as explained in Sec. 2, is itself an activity). The workbench then maps this specification to a local stack configuration where the activity associated to the processor is precisely the body of the loop, and where a while-loop layer is added and configured with an automatically generated script for testing the exit condition.

Configuration parameters for the standard layers could potentially be similarly exposed through advanced settings in the workbench[12]. These include the number of allowed retries in the *Retry* layer,

[11] Layers are Java classes that implement a particular interface.
[12] Currently, however, these settings can only be modified through a Java workflow management API.

the time delay between retries (needed to avoid flooding a Web Service with requests), as well as the maximum number of concurrent threads available for intra-processor parallelism, used by the *Parallelise* layer. Configuring the list of activities associated to a processor is especially important, as these typically represent alternative deployments of functionally equivalent services, which the *Failover* layer will try in succession in response to failures in service invocations.

Note also that a processor's behaviour is also affected by the relative position of the layers in the stack (the *Invoke* layer, however, is always at the bottom of the stack). By switching the positions of the *Retry* and *Failover* layers, for example, one obtains a processor that goes through the list of alternate services, trying each of them only once, but then iterates over the entire list a preset number of times.

3.3 Adding support for specific service types

We mentioned earlier that Taverna processors can be automatically generated in response to the user's request to add a Web service invocation to a workflow, by analysing the WSDL interface specification for the service. In some cases, however, interacting with the service requires the client to support an extended protocol beyond standard SOAP. The caGrid services [25], for example, support state preservation across invocations, through the Web Services Resource Framework[13], and furthermore, their clients must provide security credentials prior to accessing the service. In order to seamlessly interface with such services, Taverna provides a plugin architecture whereby third party service providers can extend the workflow manager's functionality through a Service Provider Interface (SPI), in order to support services with specific requirements. The SPI generalises Taverna's standard service discovery and automated client generation method, by letting providers implement specific service discovery methods, as well as client generation code that is dedicated to the specific services.

A discovery method for services of a certain type, for example caGrid, enables workflow designers to find services of that type, from locations that are known to the provider, and to add them to the local Taverna service registry. Once the services are visible, they can be added to workflows as normal. This, however, triggers the generation of client code that is specific for the service type. In the case of caGrid, the generated code supports the exchange of security credentials required by the service as part of its initial handshake. Additionally, the SPI implementor may provide a provider-specific configuration UI that integrates with Taverna's visual workbench. For caGrid, such a UI is used to obtain the security access credential from users, either at design or at execution time. The caGrid Taverna plugin is described in [22].

The plugin functionality is a vital component of Taverna's open architecture, providing a way to accommodate third party contributions, for example the Biomoby and Rshell plugins, which were developed by external contributors but are now shipped as part of the core Taverna distribution.

3.4 Parallelism and pipelining

Inter-processor parallelism, which is available for processors that have no data dependency amongst them, is achieved by letting those processors begin execution in a new thread as soon as they receive their input data. Since a request is pushed down the stack only when data is present on all the input ports, this criterion is sufficient to ensure that data-independent processors can always execute

[13] `http://www.globus.org/wsrf/`.

in parallel. The stack execution model also ensures intra-processor parallelism, by exploiting the implicit iteration on collections described in Sec. 2. To recall, when a list appears on a port where a simple type is expected, each element of the list is processed independently from the others. This is a case of SPMD parallel processing [11], where the same function is applied concurrently to multiple data elements, and potentially results in multiple independent pipelines (see also the "Multiple instances with a priori runtime knowledge" pattern described in [24]), and is achieved in T2 by having the *Parallelise* layer allocate one thread to each element in the input collection, with an appropriate setting for the max number of threads. Since this layer is at the top of the stack, this has the effect of activating the processor on multiple concurrent requests (which may succeed or fail independently of one another). The collection of all the corresponding responses is then collated into a new output list, which is forwarded to the next processor. Since the requests may be served at different speeds, the elements of the response collection may be produced in arbitrary order. The *Parallelise* layer deals with this by simply waiting for the last element to arrive, before emitting the entire output list, with its order preserved. Additionally, however, a chain of processors which both iterate on their inputs, say P1 and P2, provide an opportunity for pipelining, as follows. The *Parallelise* layer of P1 forwards each response element *as soon as it arrives*, without waiting for the others and regardless of its position in the collection. In P2, each such element is again independent of the rest of the list, so the *Parallelise* layer of P2 can consume it immediately as part of a new thread. When extended to a chain of iterating processors, this strategy results in multiple, parallel pipelines, where both intra- and inter-processor parallelism is maximized. Clearly, any processor that requires to see the entire input before starting its processing represents a serialization point in the pipeline.

This form of *superscalar* and *streaming* pipelining [19] provides the basis for efficiently supporting workflow processing over streams of data, i.e., sequences of discrete input elements of unbounded length that are continuously produced by a source. Biomart[14][20] is an example of a service that supplies its output in a streamed fashion.

4 The Data Manager

In T1.x, the data produced and consumed by services needs to be entirely loaded into the enactor's process space for as long as there are processors that need it, with the risk that large lists, or a few large data items (images, for example) would consume unbounded memory resources. In contrast, the T2 data architecture is based on the principle that data is only loaded into the execution process space on demand, when it is required by some processor's input port, and it is swapped out to a separate persistent storage when it is no longer needed. Thus, while the same data may be transferred back and forth from storage multiple times, the total amount of main memory required by an execution is bounded. The max memory footprint is determined by the size of each data item and the number of concurrent threads that require in-memory data at any given time. As shown in the use case presented in Sec. 7, the max number of active threads, a parameter that can be configured independently for each processor, can be used to control the total amount of memory required.

The separation of the data from the workflow execution space is achieved by registering all values that are produced during a computation with a new Data Manager (DM). The DM's main function is to index the values by assigning to them a unique data reference (a URI) and store them

[14] `www.biomart.org`.

into a database, from where a processor that requires the values as part of its input can retrieve them using the reference. As shown in Fig. 4, all requests to register a new value or retrieve a value are issued by activities (`A1` and `A2`) associated to processors (`P1` and `P2`), while the services themselves are oblivious to T2 data references.

Consider for example a dataflow consisting of two processors, with associated activities, where one output port of `P1` is connected to one input port of `P2`. The sequence diagram of Fig. 4 illustrates the operations that occur when some input data reaches `P1`. `ref0` is a reference to a piece of data that has been registered with the DM as a result of some prior service execution. Upon receiving this reference, `P1` pushes it down its dispatch stack until it reaches the `Invoke` layer, where `A1` is activated (this is summarized in Fig. 4 by the initial "invoke" call). Activities are responsible for obtaining the data values, e.g. `m1`, from the DM and for passing it to their associated service as part of its invocation (operation `S1.op(m0)`). Upon completion, `S1` produces value `m1`, which `A1` registers with the DM, obtaining a reference `ref1` for it. This reference is returned to `P1`, which pushes it to `P2` along their connecting arc, represented by the `receive` call. This new data event triggers `P2`'s execution, which culminates in `A2`'s invocation on input `ref1`. `A2` obtains the corresponding value `m1` from the DM, which becomes `S2`'s input. In this interaction, only the activities interact with the DM, thus acting as wrappers around the unaltered Web Services.

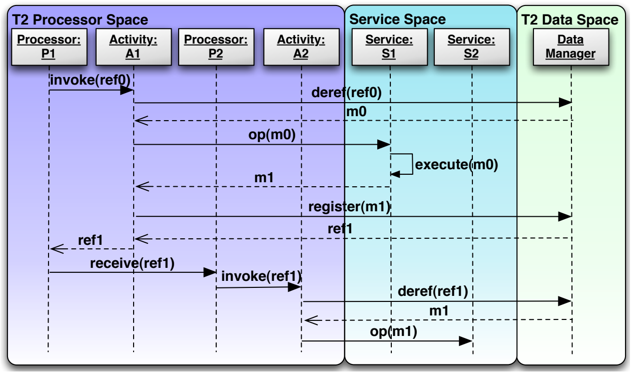


Fig. 4. Data Manager interactions

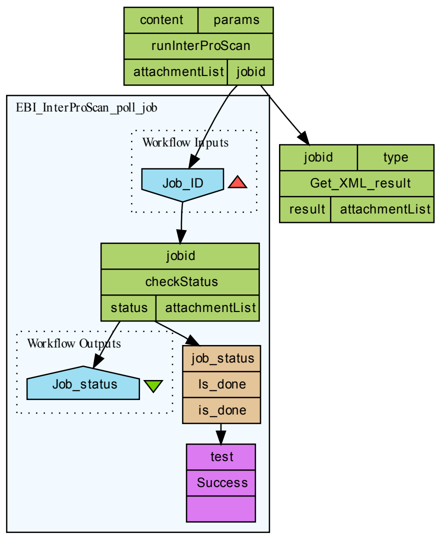
Thus, the sequence in Fig. 4 has the effect of "swapping out" data values as soon as they are produced (and the associated thread terminates). While most of these values still need to be transferred back to the process space when other activities need to consume them, as is the case for `A2` in the example, this now only happens on demand, and at a rate that is ultimately determined by the number of active threads in the workflow. This decoupling between data and their references removes the need to keep all data in memory at all times, and is particularly beneficial in the case of pipelined execution on a sequence of processors, where the number of active threads is configurable, as explained in the previous section.

Note also that, in data-intensive applications, it is increasingly common for services to store their output on dedicated data servers, which typically make it available through FTP or HTTP. In this case, the data values stored in the DM are references to the data, i.e., URLs, and the corresponding T2 data references simply map to these native references. Clearly, in this scenario the actual data is transferred directly from service to service, and never needs to be transferred into the workflow process space.

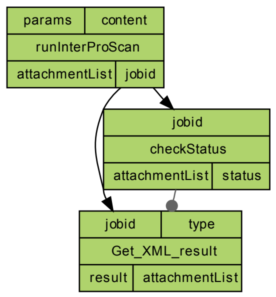
The DM is also capable of mapping across some of the native data reference types, for example by returning a file-URL as a handle to a file in a local filesystem. Of particular importance is the capability to register data files and return them as *streams*. T2 can exploit this capability to implement a further type of optimization whereby large data, such as XML documents or images, is *streamed* to a Web Service rather than being constructed as one large message, thus avoiding having to buffer the entire data into memory. This option relies on the ability to inject a stream of discrete data elements into a SOAP message as the message is being sent. While the streaming Web Service idea has been tested in the past (such a "Data Proxy" was implemented as an optional component of T1.x), the DM's ability to return data values as streams is a new opportunity for controlling the memory footprint of a workflow execution.

5 Control structures as model extension: the case of While-loop

Control constructs such as while-loop and if-then-else are not part of a pure dataflow model. In some cases, however, using an iteration control structure within a well-defined context solves paradigmatic design problems. We have implemented the loop structure as a new layer in the dispatch stack (see Sec. 3.1), to address the specific problem of interacting with asynchronous services, which accept a job request and expect the client to check for result availability at some later time.



(a) Loop construct in T1



(b) Equivalent T2 construct with looping processor

Fig. 5.

To appreciate the problem, consider the T1.x workflow in Fig. 5(a). The sub-workflow is an example of a pattern used to "simulate" an iteration structure: it tests whether a job submitted using `runInterProScan` has finished, by requesting a status report from the service. Processor `checkStatus` outputs the status report from the service; `Is_done` outputs `true` if and only if the status indicates that the result is available, and the `Success` processor fails its execution (and thus causes the entire sub-workflow to fail) if the value of the input is not `true`. This achieves the expected behaviour, because (i) the failed sub-worfklow will be re-tried (after a configurable time interval and for a set number of times), thus testing the service status again, and (ii) a control link (not shown in the figure) from the sub-workflow to `get_XML_Result` ensures that the result is only retrieved after the sub-workflow terminates successfully, i.e., the result is indeed available.

Compare this with the corresponding workflow pattern in T2 and shown in Fig. 5(b), where `runInterProScan` submits a job to the Interpro database, and `checkStatus` is a new *loop processor*. As explained in Sec. 3, the loop's functionality is specified using the T2 Workbench, and as a result the dispatch stack is configured so that (i) the activity associated to the processor is a Web Service call to get the job status from Interpro, (ii) a loop layer is added to the stack, and (iii) the test condition tested by the layer predicates on the value of the `status` port. When the iteration terminates, i.e., `status` = `true`, the control link (denoted by the dot on the sink end) enables the `Get_XML_result` processor, which also receives the job ID value it needs to retrieve the result, on the `jobId` port.

This example illustrates how the idea of an extensible dispatch stack promotes the principled implementation of new functionalities, in this case a control structure, which in turn provides workflow designers with natural patterns for addressing typical design problems.

6 Performance Evaluation

In this section we compare T2's execution times and memory usage with those of T1.x, under a variety of experimental conditions. Focusing on intra- and inter-parallelism, we have programmatically generated a test workflow for performance analysis. The workflow consists of a linear chain of processors, each of which is made to iterate over elements of an input list of varying size. This simple workflow is sufficient to test the effect of both intra-processor parallelism, i.e., concurrent processing of the list elements, and pipelining through the chain of processors, as explained in Sec. 3.4. We have used this workflow to assess the execution times and memory usage for both T1.x and T2, with varying length of the input list and sizes of the list elements (strings). All experiments were conducted using a Taverna workbench running on a Java 6 JVM on a PC with 2GB of RAM and 2.3GhZ dual core processor. The workflows and source code used for all measurement are publicly available[15]. All processors invoke the same *echo* remote Web service, deployed on a concurrent server on a dual core machine on the same local network.

The experiments support the intuition that, when the workflow is structured in a way that makes pipelining available, T2 exploits it effectively, at the cost of an increase in memory usage, while T1.x must rely solely on intra-processor parallelism. Furthermore, the T2 Data Manager with a database back-end (as opposed to an in-memory data model) make the engine scalable over large data inputs. In the rest of the section we analyse these results in detail.

Fig. 6 compares the T1.x memory usage with that of T2 in two Data Manager configurations, namely (a) using a database (embedded Derby) or (b) in-memory data (in the latter, intermediate

[15] Please visit `http://code.google.com/p/ws-menagerie/`.

values are kept in memory throughout the entire execution). For these measurements, the workflow iterates over a list of 1,000 strings, each 10,000 characters in length, using 1 thread for each processor. The charts illustrate the trade-off between overall parallelism and memory usage. In particular, configuration T2(a) provides a “safe” option in that it guarantees bounded memory usage, at the cost of increased execution time over the faster T2(b). The shorter execution time of T2 over T1.x is due to pipelining, which is not available in T1. In this case, although each processor runs a single thread, each processor in the chain is activated as soon as the previous processor has produced *one element* of the output list. Thus, up to 10 concurrent threads exist in the system, each requiring a string to be loaded into memory. In T1, however, setting the max number of threads to 1 results in a serial computation through the entire chain.

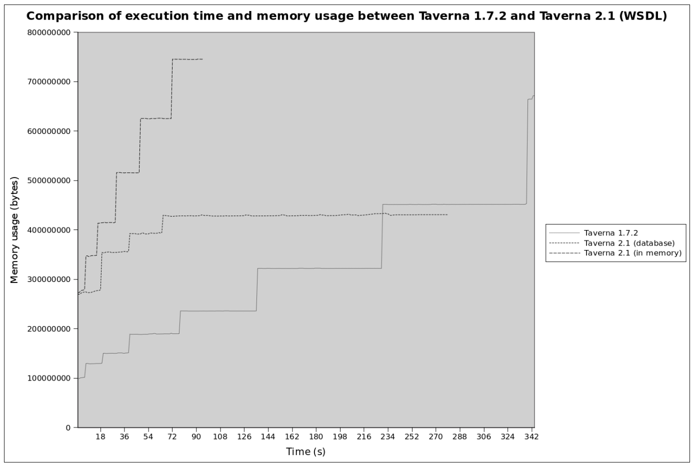


Fig. 6. Comparison of memory usage between T1.X and T2

Next, varying the max thread setting on each processor when comparing T1.x vs T2 reveals the impact of inter-processor parallelism, available only in T2, on overall memory usage and execution times. This is illustrated in Fig. 7, where the times are measured across different settings of the max number of threads. The plot for T2 suggests that, for this test workflow, this setting is not as critical as it is in T1.x. One reason is that, even with a small number of threads available for intra-processor parallelism, in T2 pipelining provides substantial inter-processor parallelism, resulting in lower overall execution times. A similar performance in T1.x requires 16 threads per processor or more.

At the same time, increasing the number of threads does not translate in a drastic memory increase. For T1.x, the difference between running on 1 thread per processor vs 16 is only 3.8% (Fig. 8), while for T2 (with a database back-end) it is 12% (Fig. 9)[16].

Finally, Fig. 10 confirms that the T2 Data Manager ensures bounded memory usage that scales well with the size of the input and intermediate values. Not only does memory allocation stabilizes

[16] In order to prevent the server becoming the bottleneck, in these experiments a random delay between 200 and 400ms was introduced in the echo service to reduce contention. Also, data values for these experiments are smaller, 1,000 char strings to reduce execution time in T1.x.

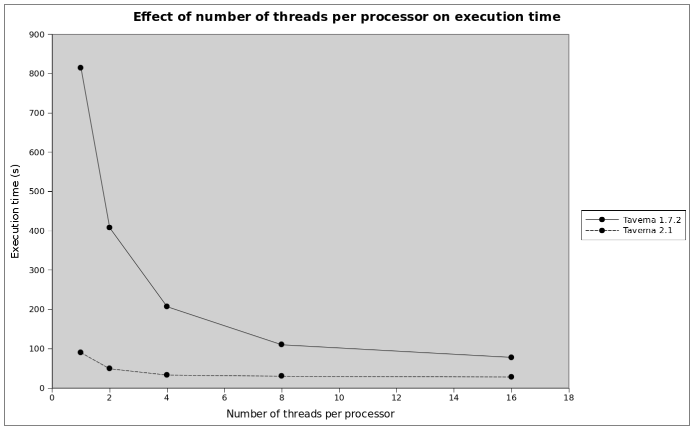
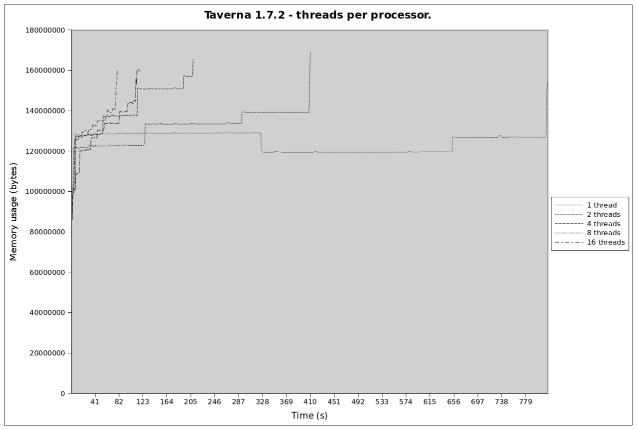
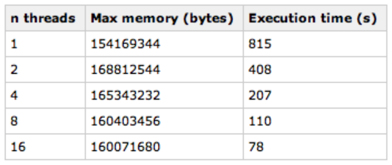


Fig. 7. Comparison of execution times between T1.X and T2 with varying thread limits





n threads	Max memory (bytes)	Execution time (s)
1	154169344	815
2	168812544	408
4	165343232	207
8	160403456	110
16	160071680	78

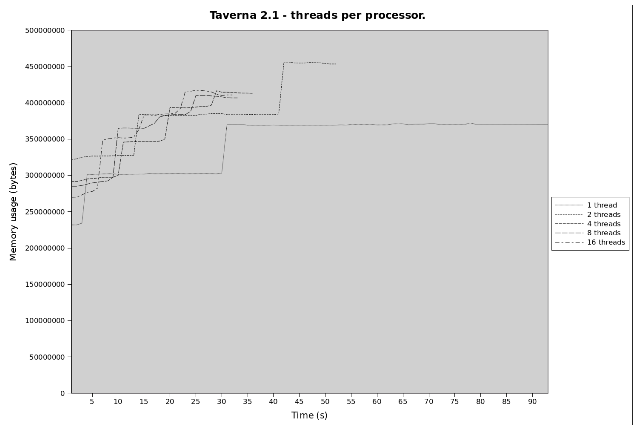
Fig. 8. T1.x memory usage for different "max thread" processor settings

as the execution progresses, but, importantly, this is true across a range of data sizes that vary by an order of magnitude.

7 Case study: performance of a caGrid workflow

Taverna is the workflow model of choice for the caGrid project [25], which provides a service-based infrastructure consisting of data and computation resources designed to assist in-silico scientific investigation in cancer research [12]. As a specific case study, in this section we compare the performance of T2 against T1.x using a caGrid production workflow[17] used to carry out cancer diagnosis based on microarray analysis [16]. The workflow begins by extracting hybridization data, obtained

[17] The workflow, not reproduced here due to space constraints, is available from the myExperiment web site, at `http://www.myexperiment.org/workflows/746`.



n threads	Max memory (bytes)	Execution time (s)
1	372375552	90
2	456052736	49
4	414695424	33
8	410411008	30
16	417431552	28

Fig. 9. T2 memory usage for different "max thread" processor settings

from samples that belong to two different lymphoma types, from a microarray database. The data is then normalized and used to learn a classification model for lymphoma type prediction, using the Support Vector Machine (SVM) and K-Nearest Neighbour (KNN) algorithms. The model can then be used to classify lymphoma types from an unknown microarray dataset.

Our observations confirm the insight provided by the results presented in the previous section, regarding the time/memory trade-off available in T2. Specifically, Fig. 11 shows similar execution times (380sec. for T1.x and 450sec for T2 with a similar total number of threads, 40 vs 47), but better memory management for T2. The main difference between the two execution models is that T2 resolves references to microarray datasets, each about 10MB in size, on demand, transferring them from disk to process space and flushing them after use. This makes better use of memory but involves additional disk transfers. The in-memory model of T1.x saves transfer time but results in unbound memory usage.

As a second experiment aimed at showing the effect of pipelining, we have monitored the execution time and memory usage under different settings of max threads per processor, for a portion of the same caGrid workflow consisting of a linear chain of processors (Fig. 12), which are made to iterate over an input list of 10 experiment IDs. The results, shown in Fig. 13, indicate a near-linear correlation between max-thread setting on the processors and execution time, up to 10 threads per processor. A higher number of threads would bring diminishing returns, however, since the amount of real concurrency available on the Java-based workflow engine is limited by the number of cores that the JVM can use (2, in this experiment), and at the same time those threads saturate the concurrent server where the Web services execute, making it a bottleneck.

8 Conclusions

We have presented the salient architectural features of the Taverna 2 workflow management system, which make it both more scalable and extensible than its predecessor. These features include, among others: (i) a runtime environment in which the available intra- and inter-processor parallelism that are implicit in the dataflow model are exposed as multiple execution threads; (ii) extensibility and configurability points based on the interceptor pattern; (iii) openness to thrid party service types,

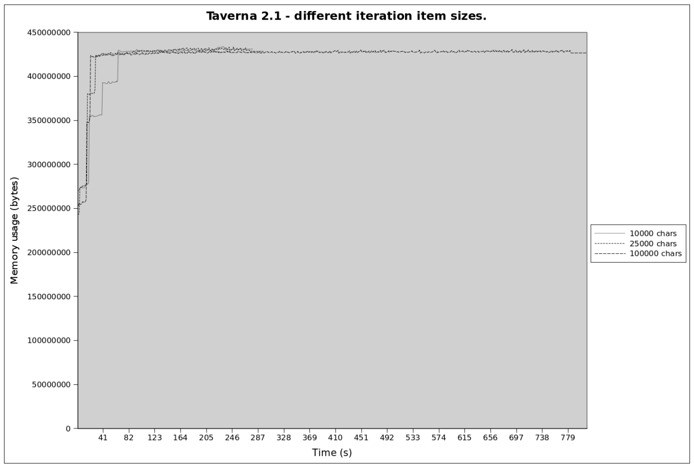


Fig. 10. Memory usage in T2 for different input strings lengths

based on a Service Provider Interface model, and (iv) a two-tier data architecture that separates the data space from the workflow enactment space. We have exploited the extensible dispatch stack by adding custom layers to add control constructs, such as a while-loop and if-then-else, to the workflow model.

Our performance results, measured on a suite of programmatically generated workflows that exhibit both processor iteration and pipelining, indicate that T2 with a database-based Data Manager offers good control of workflow execution memory while exhibiting competitive execution time. Furthermore, when pipelining can be exploited, the performance is not sensitive to the size of the thread pool available to each processor.

Finally, we have presented a concrete case study that highlights the memory usage / execution time trade-offs on a production workflow from the caGrid project.

References

1. Peter Couvares, Tevfik Kosar, Alain Roy, Jeff Weber, and Kent Wenger. *Workflows for e-Science*, chapter Workflow Management in Condor. Springer, 2007.
2. Jeffrey Dean and Sanjay Ghemawat. MapReduce: Simplified Data Processing on Large Clusters. In *OSDI*, pages 137–150, 2004.
3. Ewa Deelman, Scott Callaghan, Edward Field, Hunter Francoeur, Robert Graves, Nitin Gupta, Vipin Gupta, Thomas Jordan, Carl Kesselman, Philip Maechling, John Mehringer, Gaurang Mehta, David Okaya, Karan Vahi, and Li Zhao. Managing Large-Scale Workflow Execution from Resource Provisioning to Provenance Tracking: The CyberShake Example. In *e-Science*, page 14, 2006.
4. Ewa Deelman and Ann L Chervenak. Data Management Challenges of Data-Intensive Scientific Workflows. In *CCGRID*, pages 687–692, 2008.
5. Ewa Deelman, Gurmeet Singh, Mei-Hui Su, James Blythe, Yolanda Gil, Carl Kesselman, Gaurang Mehta, Karan Vahi, G Bruce Berriman, John Good, Anastasia C Laity, Joseph C Jacob, and Daniel S Katz. Pegasus: A framework for mapping complex scientific workflows onto distributed systems. *Scientific Programming*, 13(3):219–237, 2005.

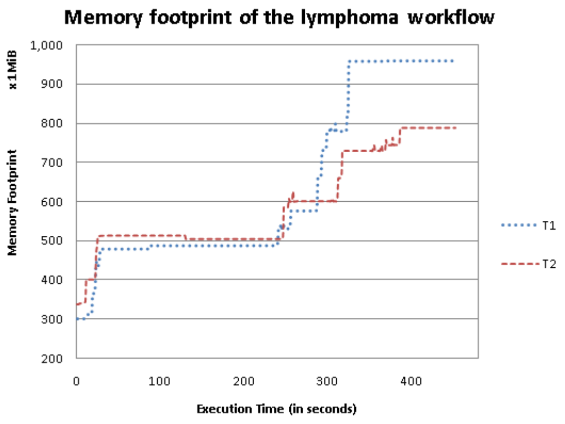


Fig. 11. Memory footprints for the lymphoma workflow in T1.X and T2

6. P. Fisher, C. Hedeler, K. Wolstencroft, H. Hulme, H. Noyes, S. Kemp, R. Stevens, and A. Brass. A systematic strategy for large-scale analysis of genotype phenotype correlations: identification of candidate genes involved in African trypanosomiasisafrican trypanosomiasis. *Nucleic Acids Research*, 35(16):5625–33, Aug 2007.
7. Ian T. Foster, Jens-S. Vöckler, Michael Wilde, and Yong Zhao. Chimera: Avirtual data system for representing, querying, and automating data derivation. In *SSDBM*, pages 37–46. IEEE Computer Society, 2002.
8. D. Georgakopoulos, H. Schuster, D. Baker, and A. Cichocki. Managing escalation of collaboration processes in crisis mitigation situations. In *Data Engineering, 2000. Proceedings. 16th International Conference on*, pages 45–56, 2000.
9. Y. Gil, E. Deelman, M. Ellisman, T. Fahringer, G. Fox, D. Gannon, C. Goble, M. Livny, L. Moreau, and J. Myers. Examining the challenges of scientific workflows. *Computer*, 40(12):24–32, Dec. 2007.
10. D. Hull, K. Wolstencroft, R. Stevens, C. A. Goble, M. R. Pocock, P. Li, and T. Oinn. Taverna: a tool for building and running workflows of services. *Nucleic Acids Research*, 34(Web-Server-Issue):729–732, 2006.
11. K. Hwang and F. A. Briggs. *Computer architecture and parallel processing.* McGraw-Hill, New York, 1986.
12. S Joel, K Tahsin, H Shannon, L Stephen, and O Scott Et al. e-Science, caGrid, and Translational Biomedical Research. *Computer*, 41:58–66, 2008.
13. E. A. Lee. Dataflow process networks. Memorandum UCB/ERL M94/53, UC Berkeley EECS Dept, 1994.
14. E. A. Lee and A. Sangiovanni-Vincentelli. Comparing models of computation. In *ICCAD '96: Proceedings of the 1996 IEEE/ACM international conference on Computer-aided design*, pages 234–241, Washington, DC, USA, 1996. IEEE Computer Society.
15. P. Li, J. Castrillo, G. Velarde, I. Wassink, S. Soiland-Reyes, S. Owen, D. Withers, T. Oinn, M. Pocock, C. Goble, S. Oliver, and D. Kell. Performing statistical analyses on quantitative data in taverna workflows: an example using R and maxdBrowse to identify differentially-expressed genes from microarray data. *BMC Bioinformatics*, 9(334), August 2008.
16. M. A. Shipp, K N Ross, P Tamayo, A P Weng, J L Kutok, and R C T Aguiar. Diffuse large B-cell lymphoma outcome prediction by gene-expression profiling and supervised machine learning. *Nature Medicine*, 8:68–74, 2002.
17. Paolo Missier, Norman Paton, and Khalid Belhajjame. Fine-grained and efficient lineage querying of collection-based workflow provenance. In *Procs. EDBT*, Lausanne, Switzerland, 2010.

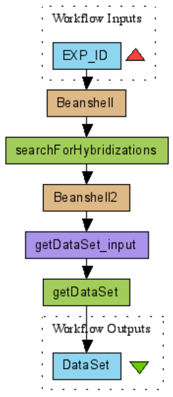


Fig. 12. Pipelined portion of the lymphoma workflow

thread pool size	**exec time (sec)**	**max memory (MB)**	**max thread count**
1	41	317	47
1	29	317	47
5	24	383	55
10	21	442	56

Fig. 13. Execution times and memory usage by thread pool size

18. T. Oinn, M. Addis, J. Ferris, D. Marvin, M. Senger, M. Greenwood, T. Carver, K. Glover, M. R. Pocock, A. l Wipat, and P. Li. Taverna: a tool for the composition and enactment of bioinformatics workflows. *Bioinformatics*, 20(17):3045–3054, 2004.
19. C. Pautasso and G. Alonso. Parallel computing patterns for grid workflows. In *Proc. of the HPDC2006 Workshop on Workflows in Support of Large-Scale Science (WORKS06)*, Paris, France, 2006.
20. D. Smedley, S. Haider, B. Ballester, R. Holland, D. London, G. Thorisson, and A. Kasprzyk. Biomart – biological queries made easy. *BMC Genomics*, 10(22), 2009.
21. Jacek Sroka, Jan Hidders, Paolo Missier, and Carole Goble. Formal semantics for the taverna 2 workflow model. *Journal of Computer and System Sciences*, 2009.
22. Wei Tan, Ravi Madduri, Kiran Keshav, Baris E. Suzek, Scott Oster, and Ian Foster. Orchestrating cagrid services in taverna. *The 2008 IEEE International Conference on Web Services (ICWS 2008),Beijing, China (Accepted)*, September 2008.
23. D. Turi, P. Missier, D. De Roure, C. Goble, and T. Oinn. Taverna Workflows: Syntax and Semantics. In *Proceedings of the 3rd e-Science conference*, Bangalore, India, December 2007.
24. Wil M. P. van der Aalst, Arthur H. M. ter Hofstede, Bartek Kiepuszewski, and Alistair P. Barros. Workflow patterns. *Distributed and Parallel Databases*, 14(1):5–51, 2003.
25. W. Tan I. Foster and R Madduri. Combining the Power of Taverna and caGrid: Scientific Workflows that Enable Web-Scale Collaboration. *IEEE Internet Computing*, 12:61–68, 2008.
26. Edward Walker, Weijia Xu, and Vinoth Chandar. Composing and executing parallel data-flow graphs with shell pipes. In *WORKS '09: Proceedings of the 4th Workshop on Workflows in Support of Large-Scale Science*, pages 1–10, New York, NY, USA, 2009. ACM.
27. Jianwu Wang, Daniel Crawl, and Ilkay Altintas. Kepler + Hadoop: a general architecture facilitating data-intensive applications in scientific workflow systems. In *WORKS '09: Proceedings of the 4th Workshop on Workflows in Support of Large-Scale Science*, pages 1–8, New York, NY, USA, 2009. ACM.