Type-theoretic Approach to the Shimming Problem in Scientific Workflows

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Abstract—When composing Web services into scientific workflows, users often face the so-called shimming problem when connecting two related but incompatible components. The problem is addressed by inserting a special kind of adaptors, called shims, that perform appropriate data transformations to resolve data type inconsistencies. However, existing shimming techniques provide limited automation and burden users with having to define ontological mappings, generate data transformations, and even manually write shimming code. In addition, these approaches insert many visible shims that clutter workflow design and distract user’s attention from functional components of the workflow. To address these issues, we 1) reduce the shimming problem to a runtime coercion problem in the theory of type systems, 2) propose a scientific workflow model and define the notion of well-typed workflows, 3) develop an algorithm to typecheck workflows, 4) design a function that inserts “invisible shims”, or runtime coercions into workflows, thereby solving the shimming problem for any well-typed workflow, 5) implement our automated shimming technique, including all the proposed algorithms, lambda calculus, type system, and translation function in our VIEW system and present two case studies to validate our approach.

Index Terms—shim; shimming problem; web service mediation; scientific workflows

1 INTRODUCTION

Web Service composition plays a key role in the fields of services computing [1, 2, 3, 4, 5] and scientific workflows [6, 7, 8, 9]. Oftentimes composing autonomous third-party Web services into workflows requires using intermediate components, called shims, to mediate syntactic and semantic incompatibilities between different heterogeneous components.

Consider a workflow $W_s$ in Fig. 1 comprised of two Web services $WS_1$ and $WS_2$. $WS_1$ expects an XML document that differs from that returned by $WS_2$. Particularly, $WS_2$ expects an XML document with three child elements, rather than four, and the $\text{concentr}$ element should be of type Double rather than Float. Besides, $\text{concentr}$ element should be the last element under $\text{data}$ rather than the second one. To resolve this incompatibility (shown as a dashed line in Fig. 1) and ensure successful workflow execution, we need to obtain and insert the shim that will perform appropriate data transformation.

Determining where the shim is needed, obtaining appropriate shim and inserting it is known as the shimming problem, whose significance is widely recognized by the Web Service community [10, 11, 12, 13, 14, 15]. Existing approaches to the shimming problem have the following limitations.

First, existing techniques are not automated and burden users by requiring them to generate transformation scripts, define mappings to and from domain ontologies, and even write shimming code [13, 16, 17]. We believe these requirements are difficult and make workflow design counterproductive for non-technical users.

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**Fig. 1. Sample Workflow $W_s$.**
Second, current approaches produce cluttered workflows with many visible shims that distract users from main workflow components that perform useful work. Furthermore, recent workflow studies [18, 19] show that the percentage of shim components in workflows registered in myExperiment portal (www.myexperiment.org) has grown from 30% in 2009 [18] to 38% in 2012 [19]. These numbers indicate that such explicit shimming tends to make workflows even messier over time, which further diminishes the usefulness of these techniques.

Third, many shimming techniques only apply under a particular set of circumstances that are hard to guarantee or even predict. Some approaches (e.g., [13, 16, 20, 21]) apply only when all the right shims are supplied by Web Service providers and are properly annotated beforehand, and/or when required shims can be generated by automated agents (e.g., XQuery-based shims [21]), which cannot be guaranteed for any practical class of workflows. Such uncertainty makes these techniques unreliable in the eyes of end users (domain scientists) who need assurance that their workflows will run.

Finally, while these efforts resolve structural differences between complex types of Web services [13, 16, 20], they cannot mediate simple types, such as Int or Double.

To address these issues, we propose a fully automated technique that, given a workflow creates and inserts suitable shims. Inserted shims transform data appropriately allowing successful workflow execution. Specifically, we:

1. reduce the shimming problem to a runtime coercion problem in the theory of type systems,
2. propose a scientific workflow model and define the notion of well-typed workflows,
3. develop an algorithm to translate workflows into equivalent lambda expressions,
4. develop an algorithm to typecheck workflow expressions,
5. design a function that inserts “invisible shims” (coercions) into workflows, thereby solving the shimming problem for any well-typed workflow,
6. implement our automated shimming technique and present two case studies to validate the proposed approach to mediate Web services.

To our best knowledge, this work is the first one to reduce the shimming problem to the coercion problem and to propose a fully automated solution with no human involvement. Moreover, our technique frees workflow design from visible shims by dynamically inserting transparent coercions in workflows during execution time (implicit shimming). The proposed solution automatically mediates both structural data types, such as complex types of Web service inputs/outputs as well as primitive data types, such as Int and Double.

2 Scientific Workflow Model

Scientific workflows consist of one or more computational components connected to each other and possibly to some input data products. Each of these components can be viewed as a black box with well defined input and output ports. Each component is also a workflow, either primitive or composite. Primitive workflows are bound to executable components, such as Web services, scripts, or high performance computing (HPC) services and are viewed as atomic blocks. Composite workflows consist of multiple building blocks connected via data channels. Each of the building blocks can be either a workflow or a data product. We now formalize our scientific workflow model.

Definition 2.1 (Port). A port is a pair \((id, type)\) consisting of a unique identifier and a data type associated with this port. We denote input and output ports as \(ip_i:T_i\) and \(op_j:T_j\), respectively, where \(ip_i\) and \(op_j\) are identifiers, and \(T_i\) and \(T_j\) are port types.

Definition 2.2 (Data Product). A data product is a triple \((id, value, type)\) consisting of a unique identifier, a value, and a type associated with this data product. We denote each data product as \(dp_i:T_i\), where \(dp_i\) is the identifier, and \(T_i\) is the type of the data product.

Given a workflow \(W\), and the set of its constituent workflows \(W^*\), we use \(W_p\) to denote port \(p_i\) of \(W\) (be it input or output port) and \(W.W^*_p.IP\) (\(W.W^*_p.OP\)) to represent the union of sets of input (output) ports of all constituent workflows of \(W\). Whenever it is clear from the context we omit the leading “\(W\)”. Formally,

\[ W.W^*_p.IP = \{ip_i \mid ip_i \in W_p.IP, W_i \in W^*\} \]
\[ W.W^*_p.OP = \{op_j \mid op_j \in W_p.OP, W_i \in W^*\} \]

Definition 2.3 (Scientific workflow). A scientific workflow \(W\) is a 9-tuple \((id, IP, OP, W^*, DP, DC_{in}, DC_{out}, DC_{mid}, DC_{ldp})\), where

1. \(id\) is a unique identifier,
2. \(IP = \{ip_0, ip_1, ..., ip_n\}\) is an ordered set of input ports,
3. \(OP = \{op_0, op_1, ..., op_m\}\) is an ordered set of output ports,
4. \( W^* = \{W_0, W_1, \ldots, W_p\} \) is a set of constituent workflows in \( W \). Each \( W_i \in W^* \) is another 9-tuple.
5. \( DP = [d_{p0}, d_{p1}, \ldots, d_{pk}] \) is a set of data products,
6. \( DC_{in}: IP \rightarrow W^* IP \) is an inverse-functional one-to-many mapping. \( DC_{in} \) is a set of ordered pairs:
   \[ DC_{in} = \{ (ip_i, ip_j) \mid ip_i \in IP, ip_j \in W_0.ip, W_j \in W^* \} \]
   That is, each pair in \( DC_{in} \) represents a data channel connecting an input port \( ip_i \in IP \) to an input port \( ip_j \) of some component \( W_j \in W^* \).
7. \( DC_{out}: W^*.OP \rightarrow OP \) is an inverse-functional one-to-many mapping. \( DC_{out} \) is a set of ordered pairs:
   \[ DC_{out} = \{ (op_i, op_j) \mid op_i \in W_0.OP, W_i \in W^*, op_j \in OP \} \]
   That is, each pair in \( DC_{out} \) represents a data channel connecting an output port \( op_i \) of some component \( W_i \in W^* \) to an output port \( op_j \in OP \).
8. \( DC_{mid}: W^*.OP \rightarrow W^*.IP \) is an inverse-functional one-to-many mapping. \( DC_{mid} \) is a set of ordered pairs:
   \[ DC_{mid} = \{ (op_i, ip_j) \mid op_i \in W_0.OP, ip_j \in W_0.ip, W_i \in W^* \} \]
   That is, each pair in \( DC_{mid} \) represents a data channel connecting an output port \( op_i \) to an input port \( ip_j \) of some component \( W_i \in W^* \).

To enhance readability, we provide a visual reference in Fig. 2. The figure shows seven representative workflows that we will refer to in this paper as \( W_a, W_b, W_c, W_d, W_e, W_f, \) and \( W_g \) respectively. These seven workflows use other workflows as their building blocks. Such constituent workflows are shown as blue boxes with their ids written inside each box. Ports appear as red pins pointing right (input) or left (output). Data products are shown as yellow boxes with their values placed inside (e.g., “true” in \( W_e \)) in Fig. 2. Because the order of input arguments of a workflow matters (e.g., Divide workflow in \( W_e \) in Fig. 2), we use ordered set \( IP \) to store a list of input ports. The term data channel refers to a wire, connecting a workflow port to a data product or another port. All entries from the set \( \{DC_{in} \cup DC_{mid} \cup DC_{out} \cup DC_{idp}\} \) are data channels.

Each workflow can be represented as a lambda expression. To simplify lambda expressions, we focus on workflows with a single output port. We are currently extending our approach to allow set \( OP \) with a cardinality greater than one. Our definition requires that every workflow and every data product has a unique id. For simplicity we also require that for any workflow \( W \), all ports of \( W \) and all ports of all workflows in \( W^* \) have unique ids.

We model workflow \( W_e \) in Fig. 2 as a 9-tuple, where \( id = "W_e", IP = \emptyset, OP = \{(op_0, Float), (op_1, Mean, Sqrt), \} \), \( DP = \{(d_{p0}, 3, Int), (d_{p1}, 5, Int), (d_{p2}, 4, Int)\}, DC_{in} = \emptyset, DC_{out} = \{(Sqrt, op_0), (Sqrt, ip_0)\}, DC_{mid} = \{(Mean, op_0), (Sqrt, ip_1)\}, DC_{idp} = \{(op_0, Mean, ip_0), (op_1, Mean, ip_0), (op_2, Mean, ip_0)\}, Workflow \( W_e \) on the other hand does not have concrete input data products connected to its inputs. We model it using 9-tuple with \( id = "W_e", IP = \{(ip_0, Int), (ip_1, Int), (ip_2, Int)\}, OP = \{(op_0, Double), W^* = \{Mean, Sqrt\}, DP = \emptyset, DC_{in} = \{(ip_0, Mean, ip_0), (ip_1, Mean, ip_0), (ip_2, Mean, ip_0)\}, DC_{out} = \{(Sqrt, op_0), (Sqrt, ip_0)\} \), \( DC_{mid} = \{(Mean, op_0), (Sqrt, ip_1)\}, DC_{idp} = \{\} \).

Definition 2.4 (Primitive workflow). A workflow \( W \) is primitive if and only if it has both input and output ports, and \( W \) has neither constituent components, nor data products, nor data channels. Formally, \( W \) is primitive iff \( W.IP \neq \emptyset \land W.OP \neq \emptyset \land W.W^* = W.DP = W.DC_{in} = W.DC_{out} = W.DC_{mid} = W.DC_{idp} = \emptyset \).

We use isPrimitive WF(W) to denote the above predicate.

Intuitively, primitive workflows is a black box with inputs and outputs and that represents an atomic component (e.g., a Web service). Workflows such as \( W_a, W_b, W_c \) Not, Increment, Decrement, Sqrt, Square, Mean, and Divide in Fig. 1 and Fig. 2 are primitive.

Definition 2.5 (Composite workflow). A workflow \( W \) is composite if and only if it contains at least one reusable component (i.e. \( W.W^* \neq \emptyset \)) connected to ports and/or data products. Formally, \( W \) is composite iff \( (W.IP \neq \emptyset \land W.OP \neq \emptyset \land W.W^* \neq \emptyset \land W.DP = W.DC_{in} = W.DC_{out} = W.DC_{mid} = W.DC_{idp} \neq \emptyset) \lor (W.W^* \neq \emptyset \land W.OP \neq \emptyset \land W.DP \neq \emptyset \land W.DC_{idp} \neq \emptyset \land W.DC_{mid} \neq \emptyset) \).

We use isComposite(W) to denote the above predicate. All seven workflows in Fig. 1 and Fig. 2 are composite.

Intuitively, reusable workflows are primitive or composite tasks that can be reused as building blocks of more complex workflows. They are not executable as at least some of their input ports are not bound. Workflows \( W_a, W_e, W_g \) in Fig. 2 are reusable. Workflow \( W_e \) is reused inside \( W \). Executable workflows, on the other hand have all input data needed to perform computation. Workflows \( W_a, W_b, W_d, \) and \( W_f \) in Fig. 1 and Fig. 2 are executable. Each executable workflow must contain at least one component and one data product connected to it. Thus, every executable workflow is composite. The opposite is not true, as composite workflow may be reusable (e.g., \( W_b \)), i.e. have input port(s) instead of concrete data product(s).

3 WorkFlow Expressions

We rely on simply typed lambda calculus [22] enriched with a set of primitive types as a formal framework to reason about the behavior of workflows. For example, expression “\( x: Int. Increment x \)” is a function, or abstraction, that takes one integer argument, and returns its value increased by 1. \( x \) is the abstraction name and “Increment \( x \)” is the expression of this abstraction. The expression “Increment 3” is an application, which evaluates to 4.

Definition 3.1 (Workflow expression). Given a workflow \( W \), its expression \( expr \) is a lambda expression that represents computation performed by \( W \). If \( W \) is reusable, \( expr \) is an abstraction. If \( W \) is executable, \( expr \) is an application.

We now present our translateWorkflow function outlined in Algorithm 1, that given a workflow \( W \), translates it into an equivalent lambda expression which performs the same computations and produces the same result as \( W \). We assume that workflow diagrams are drawn horizontally with data flowing from left to right (see Fig. 1, 2). Given a workflow \( W \), our translateWorkflow algorithm translates components in \( W \) into lambda functions,
Algorithm 1. Translating workflows into lambda expressions

1: function translateWorkflow
2: input: workflow W
3: output: lambda expression for W
4: if isPrimitiveWF(W) /* If W is primitive, return its id */ then return Wid
5: else
6: /* Otherwise, W is composite (reusable or executable), translate it recursively into lambda expression: */
7: First, find component in W.W* that performs the very last computational step (componentProducingFinalRes): *
8: let outputPortsOfDCmid be an empty set
9: for each ((wv, op), (wv, ip)) ∈ WDCα do
10: add ip to outputPortsOfDCmid
11: end for
12: for each W ∈ W.W* do
13: if W.OP ≡ OutputPortsOfDCmid
14: then componentProducingFinalRes = W
15: end if
16: end for
17: /* Build the list of expressions that serve as arguments for componentProducingFinalRes: */
18: listOfArguments = ""
19: for each (id, type) ∈ componentProducingFinalRes.IP do
20: listOfArguments += getinputExpression(W, componentProducingFinalRes, id) + ""
21: end for
22: if W is reusable ||W.DCα| > 0
23: /* translate it into lambda abstraction: */
24: then
25: listOfNames = ""
26: for each (id, type) ∈ W.IP do
27: listOfNames += ""λ"" + id + ";" + type + ";".
28: end for
29: return ""λ"" + listOfNames + translateWorkflow(componentProducingFinalRes) + "" + listOfArguments + ")"
30: else
31: /* W is executable, thus translate it into a lambda application: */
32: return translateWorkflow(componentProducingFinalRes) + "" + listOfArguments;
33: end if
34: end if
35: end function

and builds an expression whose structure corresponds to composition of components in W. Each connection between two components becomes a lambda application.

We accomodate composite nested inside each other to arbitrary degree via recursive calls to translateWorkflow function that translates all sub-workflows at each level of nesting (depth-wise translation). We translate arbitrary workflow compositions within the same level of nesting (flat compositions) by recursively calling getinputExpression function outlined in Algorithm 2, that iterates over and translates all the connected components by backtracking along the data channels from right to left (breadth-wise translation). Thus, our two algorithms together cover the full range of possible workflow structures. We now provide a walk-through example by translating of Wd into an equivalent lambda expression.

Example 3.2 (Translating workflow Wd into an equivalent lambda expression). Consider a workflow Wd in Fig. 2. When the function translateWorkflow(Wd) is called, it first checks whether Wd is primitive, and because it is not, the else clause is executed (lines 5-34). translateWorkflow first determines that the component producing final result of the entire workflow Wd is Sqrt and stores it in the componentProducingFinalRes variable (line 14). Next, because Sqrt has a single input, for loop in lines 19-21 executes once, calling the function getinputExpression(Wd, Sqrt, ip), whose output (“Mean dp0 dp1 dp2”) is stored into a string listOfArguments. Next, translateWorkflow checks whether Wd is reusable (line 22), and because it is not it returns the application of workflow expression for Sqrt component to the list of arguments obtained earlier (line 32). Since Sqrt is a primitive workflow, translateWorkflow(Sqrt) returns its name “Sqrt”. Thus, the final result of the translation is “Sqrt (Mean dp0 dp1 dp2)”.

Example 3.3 (lambda expressions for workflows Wα, Wβ, Wγ, Wδ, Wε). We provide lambda expressions obtained by calling our translateWorkflow algorithm on each workflow in Fig. 1, 2:

Wd : WS1 (WS1 dp0) Wd : Increment (Not dp0) Wd : λx:Bool. Increment (Not x) Wd : λx:Bool. Increment (Not x0) dp0 Wd : Sqrt (Mean dp0 dp1 dp2) Wd : λx:Real. Int. λx1:Real. λx2:Real. (Sqrt (Mean x0 x1 x2)) Wd : Divide (Increment (Square dp0)) (Decrement (Square dp0)) Wd : λx:Real. Divide (Increment (Square x0)) (Decrement (Square x0))

Note that executable workflows (Wα, Wδ, Wd, Wε) are translated into lambda applications, whereas reusable ones (Wβ, Wγ) into lambda abstractions. Ports are translated into variables, e.g. port ip appears as x0 in the corresponding expression. We require that the workflow expression is flat, i.e. constituent components’ ids are replaced with their translations (see expression for Wd). Thus, a workflow expression only contains port variables, names of primitive workflows, and data products.

4 Type System For Scientific Workflows

For interoperability, we adopt the type system defined in the XML Schema language specification [23]. This allows us to mediate WSDL-based Web services since their input and output types are described in WSDL documents according to the XSD format. While our approach can accommodate all types defined in [23], in this paper we focus on the set of types that are most relevant to the scientific workflow domain.

T ::= TPRM | Txsd | T → T

TPRM ::= String | Decimal | Integer | NonPositiveInteger | NegativeInteger | NonNegativeInteger | UnsignedLong | UnsignedInt | UnsignedShort | UnsignedByte | Double | PositiveInteger | Float | Long | Int | Short | Byte | Bool

Txsd ::= { e : TPRM } | { e : Txsd | e → Txsd }

In our approach we allow primitive types (TPRM), XSD types (Txsd), and arrow types (T → T). A primitive type, such as Int or Boolean describes an atomic value. An XSD Type consists of an element name e and either a primitive type or an ordered set of other XSD.

Example 4.1 (XSD Type). Consider an XML document dψδ shown in Fig. 3 (top left)1. We denote its XSD type as

1 Although the two documents in Fig. 3 do not come from the scientific workflow domain, we use them in the paper to improve readability.

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The type $T_{\text{phd}}$ describes a set of XML documents with the root element gradStudent that has at least three children named major, gpa and dissertTitle of types String, Float and String respectively. Type $T_{\text{grad}}$ on the other hand is less demanding as it requires only two child elements (major and gpa). Because $T_{\text{phd}}$ is more specific, documents described by it form a subset of documents described by $T_{\text{grad}}$ as shown in Fig. 3. Thus, it is safe to pass an argument of type $T_{\text{phd}}$ to a workflow expecting an input of type $T_{\text{grad}}$ since it will contain all the data needed by this workflow plus some extra, which can be ignored.

More generally, an XSD type $S$ is a subtype of another XSD type $T$ (denoted $S < T$), if $S$’s children form a superset of $T$’s children. Besides, if for each pair of corresponding children of $S$ and $T$, $c_{i}$ and $c_{j}$, $c_{i} < c_{j}$ is true, then $S < T$ still holds. For example, if $T_{\text{grad}}$-gpa was of type Decimal, $T_{\text{phd}} < T_{\text{grad}}$ would still be true since Float $< $ Decimal.

Such view of subtyping, based on the subset semantics, is called the principle of safe substitution. Workflows $W_{a}$, $W_{b}$, $W_{c}$, and $W_{d}$, in Fig. 1, 2 are composed by this principle.

We formalize the subtype relation as a set of inference rules used to derive statements of the form $S < T$, pronounced “$S$ is a subtype of $T$”, or “$T$ is a supertype of $S$”, or “$T$ subsumes $S$”, where $S$ and $T$ are two types. As shown in Fig. 4, the first two rules (S-Refl, and S-Trans) state that the subtype relation is reflexive and transitive. They are then followed by a set of rules for primitive data types (collectively labeled S-Prim) derived from the

$$S < T < U$$

(S-Refl)

$$S < U$$

(S-Trans)

{Byte, Short, Int, Long, Float, Double}

(S-Prim)

$$\text{int}$$

(S-XSD)

Fig. 4. Subtyping inference rules.

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$$S < T < U$$

(S-Refl)

$$S < U$$

(S-Trans)

{Byte, Short, Int, Long, Float, Double}

(S-Prim)

$$\text{int}$$

(S-XSD)

Fig. 4. Subtyping inference rules.
which is a superset of \( \text{Int} \) values discussed above, hence \( \text{Int} \subset \text{Long} \). We detail our subtyping and its rules in [24].

We also include a rule S-XSD that formalizes the intuitive notion of subtyping for XSD types. This rule can be used, for example to infer that the type \( T_{\text{phd}} \subset T_{\text{grad}} \) (Fig. 3).

**Definition 4.1 (Subtype relation).** A subtype relation is a binary relation between types, \( S \subset T \) that satisfies all instances of the inference rules in Fig. 4.

Thus, according to the Definition 4.1, the existence of the subtyping derivation concluding that \( S \subset T \) shows that \( S \subset T \) belongs to the subtype relation. We now show the use of the inference rules in Fig. 4 to infer subtyping.

**Example 4.2 (Subtyping derivation inferring \( T_{\text{phd}} \subset T_{\text{grad}} \)).** Fig. 5 (a) shows subtyping derivations concluding that the two types \( T_{\text{phd}} \) and \( T_{\text{grad}} \) in Fig. 3 belong to the subtype relation, i.e. \( T_{\text{phd}} \subset T_{\text{grad}} \). Each derivation step is labeled with the corresponding subtyping inference rule. In Fig. 5(a) we first note that the set \( \{ \text{major}: \text{String}, \text{gpa}: \text{Float} \} \) is a subset of \( \{ \text{major}: \text{String}, \text{gpa}: \text{Float}, \text{dissertTitle}: \text{String} \} \). We then show that \( \{ \text{major}: \text{String} \} \) is a subset of \( \{ \text{major}: \text{String}, \text{gpa}: \text{Float} \} \) using S-Refl rule. Similarly we show that \( \{ \text{gpa}: \text{Float} \} \) is a subset of \( \{ \text{gpa}: \text{Float} \} \).

In our rules \( \text{gradStudent}: \{ \text{major}: \text{String}, \text{gpa}: \text{Float}, \text{dissertTitle}: \text{String} \} \subset \{ \text{major}: \text{String}, \text{gpa}: \text{Float} \} \) based on the rule S-XSD as shown in Fig. 5(a). This derivation formalizes the intuition that if a workflow can handle XML documents describing graduate students it can certainly handle documents describing PhD students.

**Example 4.3 (Subtyping derivation inferring \( T_{1} \subset T_{2} \)).** Fig. 5(b) shows a subtyping derivation inferring that the two types \( T_{1} \) and \( T_{2} \) in Fig. 1 belong to the subtype relation, i.e. \( T_{1} \subset T_{2} \). As shown in the figure, here we use four statements to form a premise from which we derive that \( T_{1} \subset T_{2} \) according to the rule S-XSD.

In practice, the need arises to algorithmically determine whether for the two given types \( S \) and \( T \) the statement \( S \subset T \) is true. To this end, we now present a function that given two types \( S \) and \( T \) returns \( \text{true} \) if \( S \subset T \) and \( \text{false} \) otherwise. The function \( \text{subtype} \) is outlined in Algorithm 3. An XSD type \( T \) is a data structure containing element name \( e \) and an ordered set of children \( T.\text{children} \). If \( |T.\text{children}| > 1 \), then each element in \( T.\text{children} \) is another XSD type. If \( |T.\text{children}| = 1 \), then a single child \( T.\text{children}[0] \) is either a primitive type or an XSD type.

We assume the existence of several functions that are described as follows. The function \( \text{isPrimitive}(T) \) returns \( \text{true} \) if \( T \) is a primitive type and \( \text{false} \) otherwise. The function \( \text{isXSDType}(T) \) checks whether a given type is an XSD type. The function \( \text{findChildWithTheName(name, E)} \) returns an item \( c \) from the set of XSD types \( E \) such that \( c.e = \text{name} \).

Finally, the function \( \text{subtypePrim}(S, T) \) embodies rules S-Refl, S-Trans, and S-Prim by returning \( \text{true} \) if two given primitive types belong to the subtype relationship. For example, \( \text{subtypePrim} \) (\( \text{Int} \), \( \text{Float} \)) returns \( \text{true} \), whereas \( \text{subtypePrim} \) (\( \text{Float} \), \( \text{Int} \)) returns \( \text{false} \). As all four of these functions are trivial we omit their details for brevity.

**Example 4.4 (Determining that \( T_{\text{phd}} \subset T_{\text{grad}} \) using the subtype function).** When the function \( \text{subtype} \) (\( T_{\text{phd}} \), \( T_{\text{grad}} \)) is invoked, it first checks whether the two types are equal (line 4), and since \( T_{\text{phd}} \neq T_{\text{grad}} \) it proceeds to line 5 to check whether both types are primitive. Since both \( T_{\text{phd}} \) and \( T_{\text{grad}} \) are XSD types (i.e. not primitive) the algorithm enters the else if clause (lines 7-28). It first ensures that both element names are the same (\( \text{gradStudent} \)) (line 8). It then checks whether \( T_{\text{phd}} \) and \( T_{\text{grad}} \) are both simple types, i.e. they do not contain nested XSD types inside (lines 9-11). Since both \( T_{\text{phd}} \) and \( T_{\text{grad}} \) are complex types, the algorithm builds two sets of element names of children of both types (lines 16-22):

\[
\text{childrenNamesOfS} = \{ \text{major}, \text{gpa}, \text{dissertTopic} \}
\]
\[
\text{childrenNamesOfT} = \{ \text{major}, \text{gpa} \}
\]

It then checks whether the set \( \text{childrenNamesOfT} \) is a subset of \( \text{childrenNamesOfS} \) (line 19) and because it is, the algorithm iterates over every child in \( T.\text{children} \), finds corresponding child from \( S.\text{children} \) and checks whether they belong to the subtype relation (lines 20-25). If at least one pair of corresponding children did not satisfy the subtype relation, algorithm would return \( \text{false} \). For example, if \( T_{\text{phd}}, \text{gpa} \) was Decimal, the algorithm would detect it and return \( \text{false} \) since \( \text{gpa}: \text{Decimal} \) is not subtype of \( \text{gpa}: \text{Float} \) (lines 22-24). However, since every pair of respective children satisfies subtype relation, after iterating over each pair the algorithm returns \( \text{true} \) (line 26). Note that the algorithm would still return \( \text{true} \) if for example \( T_{\text{grad}}, \text{gpa} \) was of type Decimal since \( \text{gpa}: \text{Float} \subset \{ \text{gpa}: \text{Decimal} \} \).

### 5 Typechecking Scientific Workflows

To determine whether a given workflow can execute successfully, we need to check whether connections between its components are consistent, i.e. each component receives input data in the format it expects. The expected format is constrained by a type declared in component’s specification. We formalize such consistency of connections through the notion of workflow well-typedness. We check whether a workflow is well-typed by attempting to find its type.

Intuitively, we can derive the type of a workflow expression if we know the types of primitive workflows and data products involved in it. For example, it is easy to see that the expression \( \text{Increment} \) (\( d_{p0} \)) has the type \( \text{Int} \), assuming \( \text{Increment} \) expects integer argument and returns integer (formally, \( \text{Increment} : \text{Int} \rightarrow \text{Int} \) and \( d_{p0} \) is of type \( \text{Int} \)). In other words, we can derive workflow type given a set of assumptions.

Typing derivation is done according to a set of inference rules (Fig. 6) for variables (T-Var), abstractions (T-Abs), and applications (T-App), as well as the rule for \( \text{application with substitution} \) (T-Apps) that provides a bridge between typing and subtyping rules. Our inference rules for typing and subtyping are based on those from the classical theory of type systems [22], although modified to suit the scientific workflow domain and to ensure determinism of the typechecking algorithm presented later in this section. In our rules, variable \( x \) represents a primitive object, such as primitive workflow, port or data product, \( t_{u}, t_{a_1}, t_{a_2} \) are lambda expressions, and \( T, T_{1}, T_{2}, T_{in}, T_{out} \) denote types. Set \( \Gamma = \{ x_{1}: T_{1}, x_{2}: T_{2}, \ldots \} \).

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Algorithm 3: Algorithm for checking whether two given types belong to the subtype relation.  

1: function subtype(S, T)  
2: input: two types S and T.  
3: output: true if S < T, otherwise false  
4: // if the two types are equal, return true (S-Ref):  
5: if S = T then return true end if  
6: //S and T are primitive, call subtyping on prim. types (S-Prim):  
7: if isPrimitive(S) and isPrimitive(T) then  
8: return subtypePrim(S, T) end if  
9: else if (isXSDType(S) and isXSDType(T)) then  
10: return subtypeXSD(S, T) end if  
11: //First, both element names must be the same for S < T to be true  
12: for each child e of T.children  
13: let childNamesOfS, childNamesOfT be two empty sets  
14: end for  
15: for each child e of T.children  
16: childNamesOfS.add(e.name)  
17: add e.name to childNamesOfT  
18: end for  
19: //if child names in S must be a superset of those in T  
20: for each child e of T.children  
21: let childNamesOfS = findChildWithTheName(childOfT.e, S.children)  
22: if e.name not in childNamesOfS then return false end if  
23: end for  
24: return true  
25: end if  
26: end if  
27: end if  
28: return false  
29: end function

Definition 5.2 (Well-typed workflow). A workflow W is well-typed, or typable, if and only if for some T, there exists a typing derivation that satisfies all the inference rules in Fig. 6, and whose conclusion is Z -> W: T, where Z is a workflow context for W.

Example 5.3 (Typing derivation for workflow W₂). Consider the workflow W₂ shown in Fig. 2. Its workflow expression is Increment (Not dp₁). W₂’s workflow context Z is a set [Increment: Int → Int, Not: Bool → Bool, dp₁: Bool]. A typing derivation tree for this workflow is shown in Fig. 7.

Definition 5.1 (Workflow context). Given a workflow W, a workflow context Z is a set of all data products and primitive workflows used inside W (at all levels of nesting) and their respective types.

Each step here is labeled with the corresponding typing inference rule. Derivation holds for Γ = Z. According to Definition 5.2, existence of typing derivation with the conclusion [Increment: Int → Int, Not: Bool → Bool, dp₁: Bool] -> Increment (Not dp₁) : Int, proves that W is well-typed.

Example 5.4. (Typing derivation for workflow W₃). Consider a workflow W₃ in Fig. 1 whose workflow expression is WS₁ (WS₁ dp₁). Its workflow context Z is a set [WS₁: String → String], [T₁: String → String], dp₁: String), where T₁ = [data: [experiml: String, concentr: Float, degree: Int, model: [response: Double, hillSlope: Double]]], and

T₂ = [data: [degree: Int, model: [response: Double, concentr: Double]]].
Algorithm 4. Typechecking of scientific workflows
1: function typecheckWorkflow()
2: input: workflow expression expr, context Γ
3: output: type of W
4: if expr is primitive object /*GL1: expr is a variable representing port, primitive workflow or data product*/ then
5: return Γ.getBinding(expr)
6: else if expr is abstraction /*GL2 */ then
7: let Γ’ = Γ
8: Γ’.addBinding(expr.name, expr.nameNameType)
9: ofTypeExpr = typecheckWorkflow(expr.expression, Γ’)
10: return expr.nameType → ofTypeExpr
11: else if expr is application /*GL3 */ then
12: ofType = typecheckWorkflow(expr.f, Γ)
13: typeOFN = typecheckWorkflow(expr.n, Γ)
14: if typeOF is of the form T0 → T1 → ... → Tn where n > 0 then
15: if subtype(typeOFN, T0) then return T1 → ... → Tn
16: else return “error: parameter type mismatch”
17: end if
18: end if
19: return “error: type mismatch”
20: end if
21: return “arrow type expected”
22: end if
23: end if
24: end function

flow is well-typed, according to the Definition 5.2.

We now introduce the generation lemma that we use to
design our typechecking function. Generation lemma
captures three observations about how to typecheck a given
workflow. Each entry is read as “if workflow expression has
the type T, then its subexpressions must have types of these forms.” Each observation inverses the corresponding
rule in Fig. 6 by stating it “from bottom to top.” Note
that for T-Abs we add to the context variable-type pair for
name x, which is given explicitly in the abstraction.

Lemma 5.5 (Generation lemma).

1. GL1. Γ x:T ⇒ x:T ∈ Γ /* inverses T-Var */
2. GL2. Γ x:(x:T1, I) ⇒ ∃T2 ( T = T1 → T2 ∧ (Γ ∪ {x:T1} → t:T2) ) /* inverses T-Apps */
3. GL3. Γ t t a:Tout ⇒ ∃Tin ((Γ t t f : Tin → Tout) ∧ ((Γ t t arg Targ : Tin ) ∨ ∃T1 (Γ t t arg : Targ T1 < Tin ))) /* inverses T-Apps */

Proof: GL1 - by contradiction. Assume Γ x:T and x:T ∈ Γ. Since Γ x:T, there must be a typing derivation satisfying
inference rules in Fig. 6 with the conclusion Γ x:T. Rules T-Apps and T-App and T-Apps cannot be used to
derive the type of x, since neither of them deduces a type of a primitive object. The rule T-Var is also not applicable
since x:T ∈ Γ is false. Thus, there exists no derivation with the conclusion Γ x:T and hence Γ x:T cannot be true,
which is a contradiction. GL2 and GL3 can be proved similarly by contradiction.

In practice, to reason about workflow behavior we need a deterministic algorithm to derive the type of W. To this
end, we now present the typecheckWorkflow function outlined in Algorithm 4. Given a workflow W, it derives
W’s type from the primitive objects inside W according to the typing rules in Fig. 6. This function is a transcription
of the generation lemma (Lemma 5.5) that performs backward reasoning on the inference rules. Each recursive
call of typecheckWorkflow is made according to the corresponding entry (GLX) of the generation lemma. We
assume the methods Γ.getBinding(name) and Γ.addBinding(name, type) get the type of a given variable and add the
variable-type pair to the context Γ, respectively, abstracta-

name, type) and abstractation.expression return name, type of name variable and expression of the given abstraction,
respectively. application.a and application.f return function and argument of application.

6 Automatic Coercion in Workflows

Workflow well-typedness is a necessary but not sufficient
condition for the successful execution. In order to run
properly, workflows with subtyping need to have shims
at every subtyping connection to explicitly convert data.

Although the Bool type is a subtype of Int (e.g., in W1 in
Fig. 2), data products of these two types may have entirely
different physical representations in workflow manage-
ment systems. In particular, the workflow engine may
use two different classes BoolDP and IntDP to represent
data products holding values of types Bool and Int. If
neither of the two classes is a subclass of the other, casting
BoolDP to IntDP is impossible and hence using BoolDP in
place of IntDP will result in runtime error during workflow
run. To avoid such error, data products of type Bool
need to be explicitly converted or coerced to Int.

Similarly reasoning applies to XML data products. As
shown in Fig. 1, the dashed connection in workflow W1
links two ports whose types satisfy the subtype relation-
ship (T1 <: T2). However, sending d1 as input for W2 will
cause an error unless d1 transformed appropriately to

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6 Automatic Coercion in Workflows

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Although the Bool type is a subtype of Int (e.g., in W1 in Fig. 2), data products of these two types may have entirely different physical representations in workflow management systems. In particular, the workflow engine may use two different classes BoolDP and IntDP to represent data products holding values of types Bool and Int. If neither of the two classes is a subclass of the other, casting BoolDP to IntDP is impossible and hence using BoolDP in place of IntDP will result in runtime error during workflow run. To avoid such error, data products of type Bool need to be explicitly converted or coerced to Int.

Similar reasoning applies to XML data products. As shown in Fig. 1, the dashed connection in workflow W1 links two ports whose types satisfy the subtype relationship (T1 <: T2). However, sending d1 as input for W2 will cause an error unless d1 transformed appropriately to correspond to the input schema of W2. To ensure successful evaluation, we adopt the so-called coercion semantics for workflows, in which we replace subtyping with runtime coercions that change physical representation of data products to their target types. We express the coercion semantics for workflows as a function translateT that translates workflow expressions with subtyping into those without subtyping. We use C :: S <: T to denote subtyping derivation tree whose conclusion is S <: T. Similarly, D :: Γ t:t denotes typing derivation whose conclusion is Γ t:t. Given a subtyping derivation C :: S <: T, function translateS(C) returns a coercion (lambda expression) that converts data products of type S into those of type T. We denote function translateS(C) as [C] and define it in a case-by-case form:

$$\begin{align*}
[\lambda x:T \cdot x] & = \lambda x:T \cdot x \\
[\text{Bool} <: \text{Byte}] & = \text{Bool2Byte} \\
[\text{Int} <: \text{Long}] & = \text{Int2Long} \\
[S <: T] & = S2T \text{ for each } S \text{ and } T
\end{align*}$$
Note that in the case of T-AppS rule, translateT calls translateS(C) to retrieve appropriate coercion and insert it into the application where subsumption took place. Thus, while translateT is used for typing derivations (e.g., Fig. 7), translateS is used for subtyping derivations (e.g., Fig. 5a, b).

**Example 6.1 (Inserting a primitive coercion into the workflow \(W_a\) using the function translateT).** Consider the workflow expression Increment\((\text{Not}\ dp_0)\) which corresponds to the workflow \(W_a\) shown in Fig. 2. To inject co-er- rions into it, we call function translateT. The function takes the typing derivation tree shown in Fig. 7 as input and produces a workflow expression with coercion inserted as output. The function evaluates as follows

\[
\begin{align*}
D_1: \text{Gamma} & \rightarrow \text{Increment: Int} \rightarrow \text{Int} \ \\
C & \llbracket \text{Not} (\text{dp}_0) \rrbracket: \text{Bool} <: \text{Int} \\
D_2: \Gamma & \rightarrow \text{Not: Bool} \rightarrow \text{Bool} \ \\
\text{C} & \llbracket \text{Bool} <: \text{Int} \rrbracket
\end{align*}
\]

The translation begins from the last derivation step in Fig. 7 and progresses from bottom to top. Because the rule T-AppS was used at the final inference step, the last case applies from the definition of translateT yielding an application \([D_1]: \Gamma \rightarrow \text{Increment: Int} \rightarrow \text{Int}\) which \((\text{C} \llbracket \text{Bool} <: \text{Int} \rrbracket\) isPrimitive\((\text{S})\) with the coercion \(\llbracket \text{C} \rrbracket\) shown in Fig. 5(a).

Given a typing derivation \(D:: \Gamma : t : T\), function translateT\((D)\) produces an expression similar to \(t\) but in which subtyping is replaced with coercions. We also denote translateT\((D)\) as \([D]\). From the context, it will be clear which of the two functions is being used. Similarly, we define translateT by cases:

\[
\begin{align*}
&[\text{T-VAR}] = x \\
&[\text{T-ABS}] = \lambda x. T_1 \ [D] \\
&[\text{T-APPS}] = [D_1] \ [D_2]\end{align*}
\]

The first four cases describe how to translate subtyping derivations consisting of only one inference step, made using the rule S-Prim. The fifth case applies when S-Trans rule is used at the final step to infer subtype relationship between primitive types. The sixth case applies for derivation trees that use S-XSD rule and when isPrimitive\((S)\) is true. E.g., it applies for the derivation concluding \(\llbracket\text{concentr:Float}\rrbracket = \llbracket\text{concentr:Double}\rrbracket\). Last case applies for derivations whose last step is made using S-XSD rule and when isPrimitive\((S)\) is false, e.g., \(T_{\text{prim}} <: T_{\text{grad}}\) in Fig. 5(a).

The function \(\text{translateT}\) calls itself recursively on \(D_1\) and \(D_2\) and also calls translateS on \(C\). Since \(T\)-Var was used for the last inference step in \(D_1\), translateT\((D_1)\) returns Increment. In \(D_2\) on the other hand, T-App was used to make the last inference step and so the third case in translateT’s definition applies. Thus, translateT calls itself recursively on \(D_0:: \Gamma \rightarrow \text{Not: Bool} \rightarrow \text{Bool}\) and on \(D_2:: \Gamma \rightarrow \text{dp}_0: \text{Bool}\). In both calls the first case of translateT applies yielding \(\text{Not}\) and \(\text{dp}_0\) respectively. The call translateS\((C::\text{Bool}<:\text{Int})\) returns a coercion \(\text{Bool2Int}\) which corresponds to the fifth case in translateT’s definition since isPrimitive\((\text{Bool})\) is true. Thus the function translateT replaced subtyping in the typing derivation (i.e. \(\text{Bool} <: \text{Int}\)) with the coercion \(\text{Bool2Int}\) that converts \(\text{Bool}\) data products to \(\text{Int}\) data products. Coercion \(\text{Bool2Int}\) implemented as a primitive workflow is inserted dynamically at runtime and is transparent to the user.

**Example 6.2 (Inserting a composite coercion into the workflow \(W_u\) using the function translateT).** We now demonstrate how function translateT inserts coercion in the workflow expression WS1\((WS_1: dp_0)\) which corresponds to the workflow \(W_u\) shown in Fig. 1. translateT takes a typing derivation tree in Fig. 8 as input. The evaluation proceeds as follows

\[\text{translateT}\(\text{S}\rrbracket = \\text{translateS}\(\text{S}\rrbracket\]

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where \( \text{compositeCoercion}_{T_1,T_2} \) denotes the result of \( [[C :: T_1 <: T_2]] = \)

\[
\{ \text{degree: Int}, \text{model: \{ \text{response: Double, hillSlope: Double} \}}, \text{concenr: Float} \} \subseteq \\
\{ \text{experimentId: String, \text{concenr: Float, degree: Int, model: \{ \text{response: Double, hillSlope: Double} \}} \}
\]

\[
C_1 :: \{ \text{degree: Int} \} <:\ C_2 :: \{ \text{model: \{ \text{response: Double, hillSlope: Double} \}} \} <:\ C_3 :: \{ \text{concenr: Float} \}
\]

\[
\{ \text{data: \{ \text{experimentId: String, \text{concenr: Float, degree: Int, model: \{ \text{response: Double, hillSlope: Double} \}} \}} \} <:\ \{ \text{data: \{ \text{degree: Int, model: \{ \text{response: Double, hillSlope: Double} \}}, \text{concenr: Double} \}} \}
\]

\[
= (\lambda x. \text{compose (data} \\
\{ \text{degree: Int} \} <:\ \{ \text{degree: Int} \}) (\text{extract degree x}))
\]

\[
= (\lambda x. \text{compose (model} \\
\{ \text{response: Double} \} <:\ \{ \text{response: Double} \}) (\text{extract response x})) (\text{extract model x})
\]

\[
= (\lambda x. \text{compose (data} \\
\{ \text{concenr: Float} \} <:\ \{ \text{concenr: Float} \}) (\text{extract concenr x}))
\]

\[
= \text{compositeCoercion}_{T_1,T_2}
\]

as shown in Fig. 9, the function \( \text{translateS} \) calls itself recursively on derivations \( C_1 \), \( C_2 \) and \( C_3 \). Because S-Refl rule was used in \( C_1 \), \( [[C_1]] \) yields the identity function \( \lambda x. x \), which simply returns its argument. Thus application \( \lambda x. x \) (extract degree x) evaluates to (extract degree x). The translation process eventually yields a lambda expression, which we denote as \( \text{compositeCoercion}_{T_1,T_2} \) for convenience.

The role of \( \text{compositeCoercion}_{T_1,T_2} \) is to transform XML documents produced as the output of \( WS_1 \) into documents that will validate against the input XSD schema of \( WS_2 \) which will allow \( WS_2 \) to execute properly. This enables safe execution of the workflow \( W_s \). For example, when applied to the XML document \( d_1 \) in Fig. 1, this coercion extracts sub-elements of \( d_1 \), coerces them to the target types and composes the resulting elements into a new XML document of type \( T_2 \). The result is the document \( d_2 \).

\[
\text{concenr: Float}
\]

\[
U_i = \{ \text{experimentId: String, \text{concenr: Float, degree: Int, model: \{ \text{response: Double, hillSlope: Double} \}}}
\]

As shown in Fig. 9, the function \( \text{translateS} \) calls itself recursively on derivations \( C_1 \), \( C_2 \) and \( C_3 \). Because S-Refl rule was used in \( C_1 \), \( [[C_1]] \) yields the identity function \( \lambda x. x \), which simply returns its argument. Thus application \( \lambda x. x \) (extract degree x) evaluates to (extract degree x). The translation process eventually yields a lambda expression, which we denote as \( \text{compositeCoercion}_{T_1,T_2} \) for convenience.

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In particular, the coercion extracts \( \text{degree element leaving it unchanged since its type is identical to that of the corresponding element in the target type} \( T_2 \). It then extracts \( \text{model and response elements and creates a new} \)
ment that only contains response element, leaving out the hillSlope, which is not part of T2. The coercion also extracts element concentr, gets its simple content, converts it from Float to Double and wraps it back into <concentr> tags. Finally, the coercion builds data element out of the three previously obtained elements - degree, model, and concentr. The resulting XML element validates against WS2's input schema, and hence WS2 will now run without an error.

7 IMPLEMENTATION AND CASE STUDIES

We now present the new version of our VIEW system [25], in which we implement our automated shimming technique including the proposed workflow model, algorithms 1, 2, 3, and 4, simply typed lambda calculus, and our translation functions translates and translateT.

Our new version of VIEW is web-based, with no installation required. Scientists access VIEW through a browser and compose scientific workflows from Web services, scripts, local applications, etc. A workflow structure is captured and stored in a specification document written in our XML-based language SWL. A workflow is executed by pressing the “Run” button in the browser. Once the “Run” button is pressed, our system inserts shims and executes the workflow. To avoid cluttering the workflow and help scientists focus on its functional components, inserted shims are hidden from the user.

7.1 Primitive Shimming in Workflow W

Fig. 10 displays the workflow W, from earlier examples, and a screenshot of the VIEW system dialog window showing W's SWL (top left part of the dialog). Once the user has pressed the “Run” button the system uses Algorithm 1 (which calls Algorithm 2 as a subroutine), to translate the workflow into a typed lambda expression with subtyping (Step 1 in Fig. 10). It then typechecks W, using Algorithm 4. After VIEW ensures that W is well-typed, using the function translateT (which in turn uses translates) our system inserts coercions (workflows performing type conversion) into the workflow expression by translating it into lambda calculus without subtyping (Step 2 in Fig. 10). Particularly, subtyping Bool<Int is replaced with the corresponding coercion ~ Bool2Int. Finally, the obtained expression is translated into a runtime version of SWL (Step 3 in Fig. 10), which contains all the necessary shims. This runtime version of SWL is supplied to the workflow engine for execution.

Note that these three steps are fully automated and transparent to the user, who will see results of workflow execution upon pressing the “Run” button.

7.2 Composite Shimming in Workflow W

Workflow W in Fig. 1 comes from the biological domain. Scientists use VIEW to gain insight into the behavior of the marine worm Nereis succinea [26]. Biologists study the effect of the pheromone excreted by female worms on the reproduction process. They compose a workflow that calculates the number of successful worm matings given a set of parameters, including pheromone concentration, initial degree of male worm, and a worm model. The model includes parameters describing worm’s behavior, such as maximum response to pheromone and steepness of the dose-response relationships (hill slope). Scientists use Web service WS1 to retrieve a set of parameters and a worm model associated with a particular experiment. These data are fed into Web service WS2 that simulates the movement and interaction between worms according to the supplied input parameters and model. The output of WS2 is the number of successful worm matings, which is the final result of this workflow. However, to execute workflow W, the syntactic incompatibilities between WSDL interfaces of WS1 and WS2 must be resolved. We now demonstrate how our system accomplishes this by creating and inserting composite shim between WS1 and WS2. The coercion builds into translated into the runtime version of the SWL specification (Step 3). The coercion becomes a composite shim, as shown in Fig. 11. During workflow execution, this shim decomposes a document that comes out of WS1 (i.e. <data>... </data>) into smaller pieces, orders them to fit WS2’s input, converts them to the appropriate target types, and composes a new document out of the obtained elements. This new document validates against the input schema of WS2 allowing it to successfully compute the number of matings in a given experiment.

The inserted shim leaves out element “<hillSlope 3.8</hillSlope>”, which is not used by WS2. This reduces the size of the SOAP request sent to the server where WS2 is hosted by 9.3%. In other workflows, this portion may be much larger. Removing such unnecessary data from requests using our technique decreases the load on the network and on servers hosting Web services. Such efficient use of resources is especially important in workflows running in distributed environments.

The composite shim was generated solely based on the information in WSDL documents of WS1 and WS2. Our approach uses neither ontologies nor semantic annotations, nor does it require users to write shim scripts.

7.3 Mediating Web Services from myExperiment portal

Using our VIEW system, we have validated our technique with many workflows from myExperiment portal. Due to space limit, here we summarize results of our experiments with three WSDL-based Web services from myExperiment. Specifically, we have generated shims for the following three Web services: 1) eUtils by National Center for Biotechnology Information, 2) WSDbFetch by the European Bioinformatics Institute, and 3) InChiKeyToMol service by ChemSpider. These services
are used in various bioinformatics and chemistry workflows throughout myExperiment portal. Using the proposed technique our VIEW system was able to automatically generate shims to mediate interface differences of these Web services to allow connecting them to other services. The average shim generation times were 7.15, 10.2, and 4.4 ms for the three services, respectively.

8 RELATED WORK

Web Service composition plays a key role in the fields of services computing [1, 2, 3, 4, 5] and scientific workflows [6, 7, 8, 9]. The main challenge in the field of service composition is to mediate autonomous third-party Web services [10, 11, 12, 13]. Resolving interface incompatibilities between services by means of an intermediate component called shim is known as the shimming problem, widely recognized in the community [10, 11, 12, 13, 14, 15]. Another important research direction is mediating partially compatible Web services whose interaction patterns do not fit each other exactly [37].

Some researchers have developed techniques to resolve Web services protocol mismatches [10, 27, 28]. These mismatches occur when the permitted sets of messages and/or their order differ in the protocols of Web services that are connected together. While such techniques focus on reconciling behavioral differences between Web services, (e.g., differences in number and/or order of messages) our work focuses on resolving the interface differences (e.g., different types of inputs/outputs).

Another category of mediation techniques relies on semantic annotations in Web Services as well as domain models. For example, authors of [13, 16, 21] develop shims that transform XML documents whose elements are associated with semantic domain concepts, expressed in languages, such as OWL. Sellami et al. [20] address the shimming problem by using semantic annotations of Web services to find shims. Besides requiring composed Web services to be semantically annotated, this approach also expects Web service providers to supply all the necessary shims that are also annotated.

In contrast to [13, 16, 20, 21], our work focuses on the syntactic layer rather than the semantic layer, and relies solely on data types defined in WSDL schema. It applies regardless of whether semantic information was provided or not. Nonetheless, integrating our shimming technique would benefit the semantics-based solutions. Existing scientific workflow systems [29, 30, 31, 32] provide limited shimming capabilities i.e. shimming is either explicit or requires additional workflow configuration. None of the above approaches (1) guarantees an automated solution with no human involvement, (2) makes shims invisible in the workflow specification, (3) provides a solution for arbitrary workflow (even within some well-defined class), (4) applies to both primitive and structured types. Our approach addresses all four issues.

To address these issues, in [12], we present a primitive workflow model and a workflow specification language that allows hiding shims inside task specifications. This paper improves our earlier work by proposing an approach that determines where a shim needs to be placed in the workflow, and inserts appropriate coercion in the workflow expression. Specifically, we choose typed lambda calculus [22] to represent workflows which is naturally suitable for dataflow modeling due to its func-
tional characteristics [33]. While recognizing the importance of shims, [33] does not address the shimming problem. We formalize coercion in scientific workflows with type-theoretic rigor [22, 34]. Existing typechecking techniques apply in contexts other than scientific workflows, e.g., Hindley-Milner algorithm [35] requires typed prefix to typecheck expressions with polymorphic types (not used in workflows) and therefore cannot be directly applied to typecheck workflow expressions. We present a concrete fully algorithmic solution and demonstrate its application to the specific workflow type system with primitive and structured (XSD) types.

Reasoning about typing and subtyping could potentially be accomplished with other formalisms such as Datalog rules [38]. However, because Datalog is a declarative language, it might not be trivial to use for multi-step shimming procedures for converting objects to their target data types (e.g., 4 and 5 sequential steps in Fig. 11). Lambda calculus, on the other hand, allows to automatically generate multi-step coercion procedure given the two data types.

To our best knowledge, this work is the first one to reduce the shimming problem to the coercion problem and to propose a fully automated solution. This paper extends [36] with the following additional contributions:

1. We add support for Web services mediation by extending our type system with XSD types defined in WSDL and by introducing a subtype algorithm to check the subtype relationship between types (Algorithm 3).
2. We define four new functions \text{wrap}, \text{getContent}, \text{compose}, and \text{extract} to generate composite coercions for XML data products.
3. We extend the definition of function \text{translates} with two new cases to handle subtyping between Web service inputs/outputs.
4. We implement the proposed composite shimming technique for Web services in our VIEW system and add a case study that demonstrates how our VIEW system generates and inserts a composite shim to mediate two Web services from the biological domain.

9 CONCLUSIONS AND FUTURE WORK

In this paper, we first reduced the shimming problem to the runtime coercion problem in the theory of type systems. Second, we proposed a scientific workflow model and a notion of a well-typed workflow, and developed an algorithm to translate workflows into equivalent lambda expressions. Third, we developed an algorithm to typecheck scientific workflows. Fourth, we designed a function that inserts “invisible shims”, or runtime coercions that mediate Web services, thereby solving the shimming problem for any well-typed workflow. Finally, we implemented our automated shimming technique, including all the proposed algorithms, lambda calculus, type system, and translation functions in our VIEW system and presented two case studies to validate the proposed approach. Our technique is able to mediate well-typed workflows of arbitrary structure and complexity. In the future, we plan to develop more workflows to showcase our approach and use our shimming technique and to address the data variety challenge in Big Data. We also plan to explore how other approaches can be utilized to generate shims, including Datalog rules [38].

REFERENCES

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