Coercion Approach to the Shimming Problem in Scientific Workflows

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Abstract—**When designing 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 three algorithms to typecheck workflows by first translating them into equivalent lambda expressions, 4) design two functions that together insert "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 functions in our VIEW system and present a case study to validate the proposed approach.**

Keywords-shim; shimming problem; scientific workflows;

I. Introduction

Scientific workflows are becoming increasingly important to integrate, structure, and orchestrate a variety of heterogeneous services and applications into complex computational processes to enable and facilitate scientific discovery. Oftentimes, composing autonomous third-party services and applications into workflows requires using intermediate components, called *shims*, to mediate syntactic and semantic incompatibilities between different heterogeneous components.

Consider, a workflow W_a in Fig. 1 comprised of two web services – *Not* and *Increment.* Because the output of *Not* is a boolean value (true or false) while *Increment* is designed to process integer arguments, to execute the workflow we need to find and insert a shim that will resolve this incompatibility. Determining where the shim is needed, finding appropriate shim and inserting it is known as the shimming problem, whose significance has been widely recognized by the scientific workflow community [3-8]. 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 [10-11, 18]. We believe these requirements are difficult and make workflow design counterproductive for non-technical users.

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 [3, 20] show that the percentage of shim components in workflows registered in myExperiment portal (www.myexperiment.org) has grown from 30% in 2009 [20] to 38% in 2012 [3]. These numbers indicate that such *explicit shimming* tends to make workflows even messier overtime, 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., [9-12]) 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 [12]), 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, these efforts focus on shims for scientific data of a particular type, such as XML [10-12] or relational schemas [13], and cannot be generalized to handle all structured data types, let alone primitive types such as String or Double.

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 three algorithms to typecheck workflows by translating them into equivalent lambda expressions,
4. design two functions that together insert "invisible shims" (coercions) into workflows, thereby solving the shimming problem for any well-typed workflow,
5. implement our automated shimming technique and present a case study to validate the proposed approach.

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 does not insert shims in the workflow design, but instead performs *implicit shimming* by dynamically injecting coercions during workflow execution. While this paper focuses on primitive types, such as *Int* and *Float*, our general approach equally applies to structured data types as we explain in Section 6.

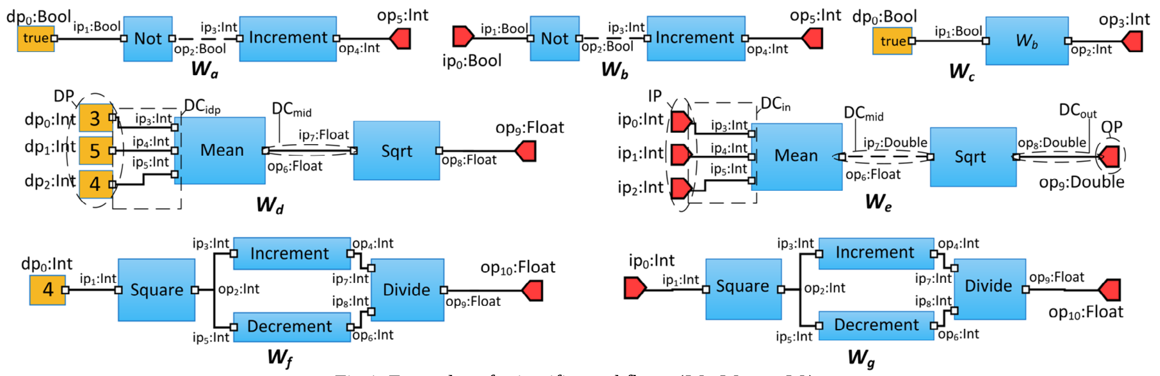


Fig 1. Examples of scientific workflows (W_a, W_b, …, W_g).

II. 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*. Every component is itself another workflow, either *primitive* or *composite*. *Primitive workflows* are bound to executable components, such as web services, scripts, or high performance computing (HPC) services and can be viewed as atomic entities. *Composite workflows* consist of multiple building blocks connected to one another via *data channels*. Each of these building blocks can be either a workflow or a data product. In the following we formalize the scientific workflow model used in this paper.

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 $W.p_j$ to denote port p_j of W (be it input or output port) and $W.W^*.IP$ ($W.W^*.OP$) 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,

$$W^*.IP = \{ip_i \mid ip_i \in W_j.IP,\ W_j \in W^*\}$$
$$W^*.OP = \{op_k \mid op_k \in W_l.OP,\ W_l \in W^*\}$$

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_{idp}), where

1. id is a unique identifier,
2. $IP = \{ip_0, ip_1, \ldots, ip_n\}$ is an ordered set of input ports,
3. $OP = \{op_0, op_1, \ldots, op_m\}$ is ordered set of output ports,
4. $W^* = \{W_0, W_1, \ldots, W_p\}$ is a set of constituent workflows used in W. Each $W_i \in W^*$ is another 9-tuple,
5. $DP = \{dp_0, dp_1, \ldots, dp_q\}$ is a set of data products,
6. $DC_{in} : IP \rightarrow W^* \times W^*.IP$ is an inverse-functional one-to-many mapping. DC_{in} is a set of ordered pairs:

$$DC_{in} \subseteq \{(ip_i, (W_j, ip_k)) \mid ip_i \in IP,\ W_j \in W^*,\ ip_k \in W_j.IP\}$$

That is, each pair in DC_{in} represents a data channel connecting input port $ip_i \in IP$ to an input port ip_k of some component $W_j \in W^*$.

7. $DC_{out} : W^* \times W^*.OP \rightarrow OP$ is an inverse-functional one-to-many mapping. DC_{out} is a set of ordered pairs:

$DC_{out} \subseteq \{((W_i, op_j), op_k) \mid W_i \in W^*,\ op_j \in W_i.OP,\ op_k \in OP\}$. That is, each pair in DC_{out} represents a data channel connecting output port op_j of some component $W_i \in W^*$ to an output port $op_k \in OP$.

8. $DC_{mid} : W^* \times W^*.OP \rightarrow W^* \times W^*.IP$ is an inverse-functional one-to-many mapping. DC_{mid} is a set of ordered pairs: $DC_{mid} \subseteq \{((W_i, op_j), (W_k, ip_n)) \mid W_i, W_k \in W^*,\ op_j \in W_i.OP,\ ip_n \in W_k.IP\}$. That is, each pair in DC_{mid} represents a data channel connecting an output port op_j of some component $W_i \in W^*$ with an input port ip_n of some other component $W_k \in W^*$.

9. $DC_{idp} : DP \rightarrow W^* \times W^*.IP$ is an inverse-functional one-to-many mapping. DC_{idp} is a set of ordered pairs:

$DC_{idp} \subseteq \{(dp_i, (W_j, ip_k)) \mid dp_i \in DP,\ W_j \in W^*,\ ip_k \in W_j.IP\}$. That is, each pair in DC_{idp} represents a data channel that connects a data product $dp_i \in DP$ to the input port ip_k of some component $W_j \in W^*$.

Fig. 1 shows seven workflows that we will reference 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 port) or left (output port). Finally, data products are visualized as yellow boxes with their values placed inside (e.g., "true" in W_a in Fig. 1).

Because the order of input arguments of a workflow matters (e.g., *Divide* workflow in W_f in Fig. 1), we use *ordered* set IP to store a list of input ports. We use the term *data channel* to refer to any entity from the set $\{DC_{in} \cup DC_{mid} \cup DC_{out} \cup DC_{idp}\}$.

As we show in later sections, a workflow is 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_d in Fig. 1 as a 9-tuple, where id = *"W_d", IP* = Ø, *OP* ={op_9, *Float*}, *W** = {*Mean*, *Sqrt*}, *DP* = {(dp_0, 3, *Int*), (dp_1, 5, *Int*), (dp_2, 4, *Int*)}, $DC_{in} = DC_{out}$ = Ø, DC_{mid} = {((*Mean*, op_6), (*Sqrt*, ip_7))}, DC_{idp} = {(dp_0, (*Mean*, ip_3)), (dp_1, (*Mean*, ip_4)), (dp_2, (*Mean*, ip_5))}. 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_9, *Double*)}, *W** = {*Mean*, *Sqrt*}, *DP* = Ø, DC_{in} = {(ip_0, (*Mean*, ip_3)), (ip_1, (*Mean*, ip_4)), (ip_2, (*Mean*, ip_5))}, DC_{out} = {((*Sqrt*, op_8), op_9)}, DC_{mid} = {((*Mean*, op_6), (*Sqrt*, ip_7))}, DC_{idp} = Ø.

Definition 2.4 (Primitive workflow). A workflow *W* is primitive if and only if it has both input ports and output ports, and *W* has neither constituent components, nor data products, nor data channels. Formally, *W* is primitive iff

$W.IP \neq \varnothing \wedge W.OP \neq \varnothing \wedge W.W^* = W.DP = W.DC_{in} = W.DC_{out} = W.DC_{mid} = W.DC_{idp} = \varnothing$.

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

Intuitively, primitive workflow is a black box with inputs and outputs that represents an atomic component such as web service. Primitive workflows are used by other workflows as building blocks. Workflows such as *Not*, *Increment*, *Decrement*, *Sqrt*, *Square*, *Mean*, and *Divide* in Fig. 1 are examples of primitive workflows.

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** ≠ Ø) connected to ports and/or data products. Formally, *W* is composite iff

$(W.W^* \neq \varnothing \wedge W.IP \neq \varnothing \wedge W.OP \neq \varnothing \wedge W.DC_{in} \neq \varnothing \wedge W.DC_{out} \neq \varnothing) \vee (W.W^* \neq \varnothing \wedge W.OP \neq \varnothing \wedge W.DP \neq \varnothing \wedge W.DC_{idp} \neq \varnothing)$

We use *isComposite(W)* to denote the above predicate. All workflows W_a, W_b, …, W_g in Fig. 1 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_b, W_e and W_g in Fig 1 are reusable. Workflow W_b is reused inside W_c. Executable workflows, on the other hand have all input data needed to perform computation. Workflows W_a, W_c, W_d, and W_f in Fig. 1 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).

III. Workflow Expressions

We rely on simply typed lambda calculus [2] enriched with a set of primitive types as a formal framework to reason about the behavior of workflows. For example, expression "*λx*:*Int*. *Increment x*" is a function, or *abstraction*, that takes one argument of type *Int*, 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, and if *W* is executable, *expr* is an application.

In this paper, we 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*. For simplicity we assume that workflow diagrams are displayed horizontally with data flowing from left to right (see Fig. 1). Given a workflow *W*, our *translateWorkflow* algorithm translates all components in *W* into lambda functions, and builds an expression whose structure corresponds to composition of components in *W*. Each connection between two components becomes an application in the equivalent lambda expression.

We accommodate composite workflows (containing sub-workflows) nested inside each other to arbitrary degree by making recursive calls to *translateWorkflow* function that translates all sub-workflows at each level of nesting (depth-wise translation). We also accommodate arbitrary workflow compositions within the same level of nesting (flat compositions) by recursively calling our *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 compositions. We now provide a walk-through example of how a workflow W_d is translated into an equivalent lambda expression.

Example 3.2 (Translating workflow W_d into an equivalent lambda expression). Consider a workflow W_d in Fig. 1. When the function *translateWorkflow*(W_d) is called, it first checks whether W_d is primitive, and because it is not, the **else** clause is executed (lines 7-35). *translateWorkflow* first determines that the component producing final result of the entire workflow W_d is *Sqrt* and stores it in the *componentProducingFinalRes* variable (line 16). Next, because *Sqrt* has a single input, for loop in lines 21-23 executes once, calling the function *getInputExpression*(W_d, *Sqrt*, ip_7), whose output "(*Mean* dp_0 dp_1 dp_2)" is stored into a string *listOfArguments*. Next, *translateWorkflow* checks whether W_d is reusable (line 24), and because it is not it returns the application of workflow expression for *Sqrt* component to the list of arguments obtained earlier (line 34). Since *Sqrt* is a primitive workflow, *translateWorkflow*(*Sqrt*) returns its name "*Sqrt*". Thus, the final result of the translation is "*Sqrt* (*Mean* dp_0 dp_1 dp_2)".

Example 3.3 (lambda expressions for workflows W_a, W_b, …, W_g). We provide lambda expressions obtained by calling our *translateWorkflow* algorithm on each workflow in Fig. 1:

W_a : *Increment* (*Not* dp_0)

W_b : *λ*x_0:*Bool*. *Increment* (*Not* x_0)

W_c : W_b dp_0 = (*λ*x_0:*Bool*. *Increment* (*Not* x_0)) dp_0

W_d : *Sqrt* (*Mean* dp_0 dp_1 dp_2)

W_e : *λ*x_0:*Int*. *λ*x_1:*Int*. *λ*x_2:*Int*. (*Sqrt* (*Mean* x_0 x_1 x_2))

W_f : *Divide* (*Increment* (*Square* dp_0)) (*Decrement* (*Square* dp_0))

W_g : *λ*x_0:*Int*. *Divide* (*Increment* (*Square* x_0)) (*Decrement* (*Square* x_0))

Algorithm 1. Translating workflows to lambda expressions

```
function translateWorkflow
input: workflow $W$
output: lambda expression for $W$
if $isPrimitive(W)$
  /* If $W$ is primitive, return its $id$ */
  then return $W.id$
else
  /* Otherwise, $W$ is composite (reusable or executable), translate it recursively into lambda expression: */
  /* First, find component in $W.W^*$ that performs the very last computational step ($componentProducingFinalRes$): */
  let $OutputPortsOfDCmid$ be an empty set
  for each $((w_j, op_j), (w_k, ip_l)) \in W.DC_{mid}$ do
    add $op_j$ to $OutputPortsOfDCmid$
  end for
  for each $W' \in W.W^*$ do
    if $W'.OP \not\subset OutputPortsOfDCmid$
      then $componentProducingFinalRes = W'$
    end if
  end for
  /* Build the list of expressions that serve as arguments for $componentProducingFinalRes$:*/
  $listOfArguments$ = “”
  for each $(id_i, type_i) \in componentProducingFinalRes.IP$ do
    $listOfArguments$ += getInputExpression($W$, $componentProducingFinalRes$, $id_i$) + “ “
  end for
  if $W$ is reusable      //$|W.DC_{in} > 0|$
    /* translate it into lambda abstraction: */
    then
    $listOfNames$ = “”
    for each $(id_i, type_i) \in W.IP$ do
      $listOfNames$ += “$\lambda x$” + $id_i$ + “:” + $type_i$ + “. ”
    end for
    return “(” + $listOfNames$ +
          translateWorkflow($componentProducingFinalRes$)
          + “ ” + $listOfArguments$ + “)”
  else
    /* $W$ is executable, thus translate it into a lambda application: */
    return translateWorkflow($componentProducingFinalRes$)
           + “ ” + $listOfArguments$;
  end if
end if
end function
```

Note that executable workflows (W_a, W_c, W_d, W_f) are translated into lambda applications, whereas reusable ones (W_b, W_e, W_g) into lambda abstractions. Ports are translated into variables, e.g. port ip_0 appears as x_0 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 W_c above). Thus, a workflow expression only contains port variables, names of primitive workflows, and data products.

IV. Type System for Scientific Workflows

For interoperability, we adopt the type system defined in the XML Schema language specification [1]. While our approach can accommodate all types defined in [1], due to the space limit, in this paper we focus on the following types, which are most relevant to the scientific workflow domain.

Algorithm 2. Algorithm for obtaining lambda expressions representing inputs at certain workflow ports

```
function getInputExpression
input: workflow $W$, constituent component $c$, input port $ip_m$
output: lambda expression that serves as input argument of port $W.id$.
/* first, if there is a data product $dp_i$ in $W.DP$ connected to port $ip_m$, return $dp_i.id$ of that data product: */
for each $(dp_i, (w_j, ip_k)) \in W.DC_{idp}$ do
  if $w_j.id = c.id$ and $ip_k.id = ip_m.id$
    then return $dp_i.value$
  end if
end for
/* if there is an input port $ip_j$ in $W.IP$ connected to port $ip_m$, return variable named “$x$” + $ip_j.id$ */
for each $(ip_j, (w_k, ip_l)) \in W.DC_{in}$ do
  if $w_k.id = c.id$ and $ip_l.id = ip_m.id$
    then return “$x$” + $ip_j.id$
  end if
end for
/* if there is another constituent workflow $w_i$ whose output is connected to $ip_m$, construct the list of input arguments (expressions) of $w_i$ and return application of these arguments to $w_i$: */
$listOfArguments$ = “”
for each $((w_i, op_j), (w_k, ip_l)) \in W.DC_{mid}$ do
  if $w_k.id = c.id$ and $ip_l.id = ip_m.id$ then
    for $ip_q \in w_i.IP$ do
      $listOfArguments$ += getInputExpression($W$, $w_i$, $ip_q$) + “ ”
    end for
    return “(” + translateWorkflow($w_i$) + “ ” +
           $listOfArguments$ + “)”
  end if
end for
return “error - cannot obtain input expression”
end function
```

T ::= *String* | *Decimal* | *Integer* | *NonPositiveInteger* | *NegativeInteger* | *NonNegativeInteger* | *UnsignedLong* | *UnsignedInt* | *UnsignedShort* | *UnsignedByte* | *Double* | *PositiveInteger* | *Float* | *Long* | *Int* | *Short* | *Byte* | *Bool* | $T \rightarrow T$

The type constructor $\rightarrow$ is right-associative. i.e. the expression $T_1 \rightarrow T_2 \rightarrow T_3$ is equivalent with $T_1 \rightarrow (T_2 \rightarrow T_3)$. This type constructor is useful in defining types of reusable workflows. For example, the workflow W_b has type *Bool→Int*, because it expects boolean value as input and produces integer value as output. Workflow W_e has the type *Int→Int→Int→Double*. The type of an executable workflow is simply the type of its output, e.g., type of W_a is *Int*.

We now introduce the notion of subtyping which is based on the fact that some types are more descriptive than others. For example, any value described by type *Int* can also be described by *Decimal*. That is, the set of values associated with the type *Int* is a subset of values associated with the type *Decimal*, or, in other words, *Decimal* is a more descriptive type than *Int*. Therefore, it is safe to pass integer argument to a workflow expecting a decimal number as input. Such view of subtyping, based on the *subset semantics*, is also called the *principle of safe substitution*. Workflows W_a, W_b, and W_c in Fig. 1 are composed by this principle.

We formalize the subtype relation as a set of inference rules used to derive statements of the form $T_i <: T_j$, pronounced “ T_i is a subtype of T_j ”, or “ T_j is a supertype of

$$\mathsf{T} <: \mathsf{T} \quad \text{(S-REFL)} \qquad \frac{\mathsf{T_i} <: \mathsf{T_j} \quad \mathsf{T_j} <: \mathsf{T_k}}{\mathsf{T_i} <: \mathsf{T_k}} \quad \text{(S-TRANS)} \qquad \{\mathsf{l_i}{:}\mathsf{T_i}^{\,i\,\in\,1\ldots n+k}\} <: \{\mathsf{l_i}{:}\mathsf{T_i}^{\,i\,\in\,1\ldots n}\} \quad \text{(S-R)}$$

$$\left.\begin{array}{l}\mathsf{Bool} <: \mathsf{Int}\\ \mathsf{Int} <: \mathsf{Long}\\ \mathsf{Long} <: \mathsf{Decimal}\\ \mathsf{Long} <: \mathsf{Integer}\end{array}\right. \quad \text{(S-PRIM)}$$

Fig. 2. Subtyping inference rules.

T_i", or " T_j subsumes T_i", where T_i and T_j are two types. As shown in Fig. 2, the first two rules (S-REFL, and S-TRANS) state that the subtype relation is reflexive and transitive. They are then followed by an incomplete set of rules for primitive data types (collectively labeled S-Prim) derived from the hierarchy presented in [1]. As *Bool* type is less descriptive than *Int* (*true* and *false* can be mapped to 1 and 0, a subset of *Int*), we consider *Bool* to be a subtype of *Int*. We also include the rule for records (S-R), which is a structured type. A record is a labeled n-tuple that has a type, e.g. r_1 = {a:1, b:true, c: 2.25} is a 3-fields record, whose type is t_1 = {*a*:*Int*, *b*:*Bool*, *c*:*Float*}. We denote an n-fields record and its type as $\{l_i{=}v_i\}{:}\{l_i{:}T_i\}$, $i \in 1\ldots n$ where l_i, v_i and T_i denote labels, values and types respectively. Given two record types T_1 and T_2, T_1 is subtype of T_2 if all T_1's fields form a superset of T_2's fields. For example, t_1 is a subtype of {*a*:*Int*, *b*:*Bool*}. Indeed, it is safe to pass a record r_1 where a record of type {*a*:*Int*, *b*:*Bool*} is expected, since r_1 provides all necessary information (and even some extra) needed by the workflow.

Definition 4.1 (Subtype relation). A subtype relation is a binary relation between types, $T_i <: T_j$ that satisfies all instances of the inference rules in Fig. 2.

Due to the small number of primitive types, the algorithm to check whether $T_i <: T_j$ is true straightforward. We assume the function *subtype*(T_i, T_j) that returns true iff $T_i <: T_j$.

V. TYPECHECKING FOR 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 expression (*Increment* dp_0) has the type *Int*, assuming *Increment* expects integer argument and returns integer (formally, *Increment*:*Int*→*Int*) and dp_0 is *Int*. In other words, we can derive workflow type given a set of assumptions.

Typing derivation is done according to the following inference rules (see Fig. 3) for variables (T-VAR), abstractions (T-ABS), records (T-R), and applications (T-APP), as well as the rule for *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 [2], although modified to suit the scientific workflow domain and to ensure determinism of the typechecking algorithm presented later in this section.

$$\frac{\mathsf{x} : \mathsf{T} \in \Gamma}{\Gamma \vdash \mathsf{x} : \mathsf{T}} \quad \text{(T-VAR)}$$

$$\frac{\Gamma \cup \{\mathsf{x} : \mathsf{T_1}\} \vdash \mathsf{t} : \mathsf{T_2}}{\Gamma \vdash \lambda \mathsf{x} : \mathsf{T_1} \,.\, \mathsf{t} : \mathsf{T_1} \to \mathsf{T_2}} \quad \text{(T-ABS)}$$

$$\frac{\Gamma \vdash \mathsf{t_f} : \mathsf{T_{in}} \to \mathsf{T_{out}} \quad \Gamma \vdash \mathsf{t_{arg}} : \mathsf{T_{in}}}{\Gamma \vdash \mathsf{t_f}\ \mathsf{t_{arg}} : \mathsf{T_{out}}} \quad \text{(T-APP)}$$

$$\frac{\Gamma \vdash \mathsf{t_f} : \mathsf{T_{in}} \to \mathsf{T_{out}} \quad \Gamma \vdash \mathsf{t_{arg}} : \mathsf{T_{arg}} \quad \mathsf{T_{arg}} <: \mathsf{T_{in}}}{\Gamma \vdash \mathsf{t_f}\ \mathsf{t_{arg}} : \mathsf{T_{out}}} \quad \text{(T-APPS)}$$

$$\frac{\text{for each } \mathsf{i}\ \Gamma \vdash \mathsf{v_i} : \mathsf{T_i}}{\Gamma \vdash \{\mathsf{l_i}{=}\mathsf{v_i}^{\mathsf{i}\in 1\ldots n}\} : \{\mathsf{l_i}{:}\mathsf{T_i}^{\mathsf{i}\in 1\ldots n}\}} \quad \text{(T-R)}$$

Fig. 3. Workflow typing rules.

Here, variable *x* represents a *primitive object* such as primitive workflow, port or data product, *t*, t_{arg} and t_f are lambda expressions, and *T*, T_1, T_2, T_{in} and T_{out} denote types. Set $\Gamma = \{x_0{:}T_{p0}, x_1{:}T_{p1}, \ldots, x_n{:}T_{pn}\}$ is a *typing context*, i.e. a set of assumptions about primitive objects and their types. The first rule (T-VAR) states that variable *x* has the type assumed about it in Γ. The second rule (T-ABS) is used to derive types of expressions representing reusable workflows. It states that if the type of expression with *x* plugged in is T_2, then the type of abstraction, with the name *x* and expression *t* is $T_1 \to T_2$. The third rule (T-APP) is used to derive types of applications, which represent data channels in workflows. The next rule (T-APPS) is necessary to typecheck workflows with subtyping connections (shown dashed in Fig. 1). We call such compositions *workflows with subtyping*. The last rule is used to typecheck records. We show concrete type derivation that uses the above rules in Example 5.3.

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.

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. 3, and whose conclusion is $Z \vdash W : T$, where Z is a workflow context for *W*.

Example 5.3 (Typing derivation for workflow W_a). Consider the workflow W_a shown in Fig. 1. Its workflow expression is *Increment* (*Not* dp_0). W_a's workflow context Z is a set {*Increment*:*Int*→*Int*, *Not*:*Bool*→*Bool*, dp_0:*Bool*}. Typing derivation tree for this workflow is shown in Fig. 4. Each step is labeled with the corresponding 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*, dp_0:*Bool*} ⊢ *Increment* (*Not* dp_0) : *Int*, proves that *W* is well-typed.

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 expression. 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. 3 by stating it "from bottom to top". Note that for T-ABS we add variable-type pair for name *x*, which is given explicitly in the abstraction.

$$\dfrac{\dfrac{\text{Increment:Int} \to \text{Int} \;\in\; \Gamma}{\Gamma \vdash \text{Increment:Int} \to \text{Int}}\,\text{T-VAR} \qquad \dfrac{\dfrac{\dfrac{\text{Not:Bool} \to \text{Bool} \in \Gamma}{\Gamma \vdash \text{Not:Bool} \to \text{Bool}}\,\text{T-VAR} \quad \dfrac{\text{dp}_0\text{:Bool} \in \Gamma}{\Gamma \vdash \text{dp}_0\text{:Bool}}\,\text{T-VAR}}{(\text{Not dp}_0)\text{:Bool}}\,\text{T-APP} \quad \dfrac{}{\text{Bool} <: \text{Int}}\,\text{S-PRIM}}{\Gamma \vdash (\text{Increment (Not dp}_0))\text{:Int}}\,\text{T-APPS}$$

Fig. 4. Typing derivation for workflow W_a.

Lemma 5.4 (Generation lemma).

1. $\Gamma \vdash x{:}T \Rightarrow x{:}T \in \Gamma$ /* inverses T-VAR */
2. $\Gamma \vdash (\lambda x{:}T_1.\ t) : T \Rightarrow \exists T_1\ \exists T_2\ (\ T = T_1 \to T_2 \wedge (\Gamma \cup \{x{:}T_1\} \vdash t{:}T_2\ ))$ /* inverses T-ABS */
3. $\Gamma \vdash t_f\ t_{arg} : T \Rightarrow \exists T_{in}\ \exists T_{out}\ (\ (\Gamma \vdash t_f : T_{in} \to T\ ) \wedge ((\Gamma \vdash t_{arg}{:}T_{in}\ ) \wedge \exists T_1\ (\Gamma \vdash t_{arg}{:}T_1 \wedge T_1 <: T_{in}))\ )$ /* inverses T-APP and T-APPS*/

Proof: Part 1 - by contradiction. Assume $\Gamma \vdash x{:}T$, and $x{:}T \notin \Gamma$. Since $\Gamma \vdash x : T$, there must be a typing derivation satisfying inference rules in Fig. 3 with the conclusion $\Gamma \vdash x$: T. Rules T-ABS and T-APP and T-APPS cannot be used to derive the type of x, since neither of them deduces a type of primitive object. The rule T-VAR is also not applicable since $x{:}T \in \Gamma$ is false. Thus, there exists no derivation with the conclusion $\Gamma \vdash x : T$, and hence $\Gamma \vdash x : T$ cannot be true, which is a contradiction. Parts 2 and 3 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 3. Given a workflow W, it derives W's type from

Algorithm 3. Typechecking of scientific workflows

```
function typecheckWorkflow
input: workflow expression expr, context Γ
output: type of W
if expr is primitive object /* i.e. variable representing port,
primitive workflow or data product*/ then
  return Γ.getBinding(expr)
else if expr is Abstraction then
  let Γ ' = Γ
  Γ '.addBinding(expr.name, expr.nameType)
  typeOfExpr = typecheckWorkflow (expr.expression, Γ ')
  return expr.nameType → typeOfExpr
else if expr is Application then
  typeOfF = typecheckWorkflow(expr.f, Γ)
  typeOfN = typecheckWorkflow (expr.n, Γ)
  if typeOfF is of the form $T_0 \to T_1 \to \dots \to T_n$, where $n > 0$,
  then
    if subtype(typeOfN, $T_0$)
      then return $T_1 \to \dots \to T_n$
    else
      return “error: parameter type mismatch”
    end if
  else
    return “arrow type expected”
  end if
end if
end function
```

the primitive objects inside W according to the typing rules in Fig. 3. This function is a transcription of the generation lemma (Lemma 5.4) that performs backward reasoning on the inference rules. Each recursive call of *typecheckWorkflow* is made according to the corresponding entry of the generation lemma. We assume that 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, *abstraction*.name, *abstraction*.nameType and *abstraction*.expression return name, type of name variable and expression of the given abstraction respectively.

VI. AUTOMATIC COERCION IN WORKFLOWS

Our approach not only allows to determine workflow well-typedness, but also ensures the correct execution of well-typed workflows. Consider the workflow W_a shown in Fig. 1. Although the *Bool* type is a subtype of *Int*, 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 wrap data products 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 execution.

Thus, 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. In this paper, we use $C :: T_1 <: T_2$ to denote subtyping derivation tree whose conclusion is $T_1 <: T_2$. Similarly, we use $D :: \Gamma \vdash t{:}T$ to denote typing derivation whose conclusion is $\Gamma \vdash t{:}T$. Given a subtyping derivation $C :: T_1 <: T_2$, function *translateS*(C) returns a coercion (lambda expression) that converts data products of type T_1 into data products of type T_2. We denote function *translateS*(C) as [[C]] and define it in a case-by-case form:

$$\left[\!\left[\dfrac{}{\text{T} <: \text{T}}\,\text{S-REFL}\right]\!\right] = \lambda\text{x:T. x}$$

$$\left[\!\left[\dfrac{}{\text{Bool} <: \text{Int}}\,\text{S-PRIM}\right]\!\right] = \text{Bool2Int}$$

$$\left[\!\left[\dfrac{}{\text{Int} <: \text{Long}}\,\text{S-PRIM}\right]\!\right] = \text{Int2Long}$$

$$\vdots$$

$$\left[\!\left[\dfrac{}{\text{T}_\text{i} <: \text{T}_\text{j}}\,\text{S-PRIM}\right]\!\right] = \text{T}_\text{i}\text{2T}_\text{j} \quad \text{for each } \text{T}_\text{i} \text{ and } \text{T}_\text{j}\text{, such that } \text{T}_\text{i} <: \text{T}_\text{j}$$

$$\left[\!\left[\dfrac{}{\{\text{l}_\text{i}{:}\text{T}_\text{i}^{\;\text{i} \in 1\ldots\text{n+k}}\} <: \{\text{l}_\text{i}{:}\text{T}_\text{i}^{\;\text{i} \in 1\ldots\text{n}}\}}\,\text{S-R}\right]\!\right] = \lambda\text{r:}\{\text{l}_\text{i}{:}\text{T}_\text{i}^{\;\text{i} \in 1\ldots\text{n+k}}\}.\{\text{l}_\text{i}\text{=r.l}_\text{i}^{\;\text{i} \in 1\ldots\text{n}}\}$$

The last case defines a function producing a record by extracting a subset of fields (1…n) from an input record. Given a typing derivation $D :: \Gamma \vdash t{:}T$, 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 one is used. Similarly, we define *translateT* by cases:

$$\left[\!\left[\dfrac{\text{x:T} \;\in\; \Gamma}{\Gamma\ \vdash \text{x:T}}\,\text{T-VAR}\right]\!\right] = \text{x}$$

$$\left[\!\!\left[\frac{D :: \Gamma \cup x{:}T_1 \ \vdash t{:}T_2}{\Gamma \ \vdash \lambda x{:}T_1.\ t : \ T_1 \to T_2}\text{T-ABS}\right]\!\!\right] = \lambda x{:}T_1.\ [\![D]\!]$$

$$\left[\!\!\left[\frac{D_f :: \Gamma \vdash t_f{:}T_{in} \to T_{out} \quad D_{arg} :: \Gamma \vdash t_{arg}{:}T_{in}}{\Gamma \ \vdash t_f \ t_{arg}{:}T_{out}}\text{T-APP}\right]\!\!\right] = [\![D_f]\!]\ [\![D_{arg}]\!]$$

$$\left[\!\!\left[\frac{D_f{::}\Gamma \vdash t_f{:}T_{in} \to T_{out} \quad D_{arg}{::}\Gamma \vdash t_{arg}{:}T_{arg} \quad C{::}T_{arg} <: T_{in}}{\Gamma \vdash t_f \ t_{arg}{:}T_{out}}\text{T-APPS}\right]\!\!\right] =$$
$$= [\![D_f]\!]\ ([\![C]\!]\ [\![D_{arg}]\!])$$

$$\left[\!\!\left[\frac{\text{for each i } D_i \ :: \ \Gamma \ \vdash v_i{:}T_i}{\Gamma \ \vdash \{l_i{=}v_i{}^{i\in 1\ldots n}\}{:}\{l_i{:}T_i{}^{i\in 1\ldots n}\}}\text{T-R}\right]\!\!\right] \ = \ \{l_i = [\![D_i]\!]^{i\in 1\ldots n}\}$$

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 (i.e. T-APPS rule) is used. In the last case, *translateT* translates typing derivation for records by recursively calling itself on typing derivations of individual fields.

Example 6.1 (Automatic coercion injection). Consider the workflow W_a in Fig. 1. To inject coercions into it, we call function *translateT* on its typing derivation shown in Fig. 4. The function evaluates as follows

$$\left[\!\!\left[\frac{D_f{::}\Gamma \vdash \text{Increm:Int}{\to}\text{Int} \quad D_{arg}{::}\Gamma \vdash (\text{Not dp}_0){:}\text{Bool} \quad C{::}\text{Bool}{<:}\ \text{Int}}{\Gamma \vdash \ (\text{Increm (Not dp}_0)) \ : \ \text{Int}}\text{T-APPS}\right]\!\!\right]$$

$$= \left[\!\!\left[\frac{\text{Increment:Int} \to \text{Int} \in \Gamma}{\Gamma \vdash \text{Increment:Int} \to \text{Int}}\text{T-VAR}\right]\!\!\right] \ \left(\left[\!\!\left[\frac{}{\text{Bool} <: \text{Int}}\text{S-PRIM}\right]\!\!\right]\right.$$

$$\left.\left[\!\!\left[\frac{D_f :: \Gamma \vdash \text{Not:Bool} \to \text{Bool} \quad D_{arg} :: \Gamma \vdash \text{dp}_0{:}\text{Bool}}{(\text{Not dp}_0){:}\text{Bool}}\text{T-APP}\right]\!\!\right] \right) =$$

$$= \text{Increment } (\textbf{Bool2Int} \ (\left[\!\!\left[\frac{\text{Not:Bool} \to \text{Bool} \in \Gamma}{\Gamma \vdash \text{Not:Bool} \to \text{Bool}}\text{T-VAR}\right]\!\!\right]$$

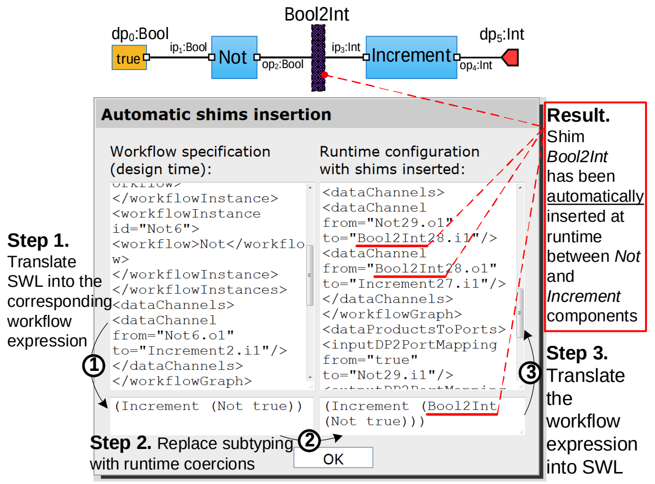
$$\left[\!\!\left[\frac{\text{dp}_0{:}\text{Bool} \in \Gamma}{\Gamma \vdash \text{dp}_0{:}\text{Bool}}\text{T-VAR}\right]\!\!\right])) = \text{Increment } (\textbf{Bool2Int} \ (\text{Not dp}_0))$$

The resulting expression contains coercion *Bool2Int* that converts boolean data products to integer data products. Note that coercion *Bool2Int* (implemented as a primitive workflow) is inserted dynamically at runtime and is transparent to the user.

VII. IMPLEMENTATION AND CASE STUDY

We now present the new version of our VIEW system [19], in which we implement our proposed workflow model, algorithms 1, 2, and 3, simply typed lambda calculus, and our translation functions *translateS* and *translateT*. We give a walk-through explanation of our automated shimming technique using workflow W_a in Fig. 1.

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 stored in a specification document written in our XML-based workflow language SWL. Fig. 5 displays the workflow W_a from earlier examples, and a screenshot of the VIEW system dialog window showing W_a's SWL (top left part of the dialog). The composed workflow is executed by pressing the "Run" button in the browser. First, using algorithms 1 and 2, our system translates workflow into typed lambda calculus with subtyping (bottom left section


Bool2Int
dp₀:Bool
true
ip₁:Bool
Not
op₂:Bool
ip₃:Int
Increment
op₄:Int
dp₅:Int
Automatic shims insertion
Workflow specification (design time):
Runtime configuration with shims inserted:
Result. Shim Bool2Int has been automatically inserted at runtime between Not and Increment components
Step 1. Translate SWL into the corresponding workflow expression
Step 2. Replace subtyping with runtime coercions
Step 3. Translate the workflow expression into SWL
1
2
3
OK

```
</workflowInstance>
<workflowInstance
id="Not6">
<workflow>Not</workflo
w>
</workflowInstance>
</workflowInstances>
<dataChannels>
<dataChannel
from="Not6.o1"
to="Increment2.i1"/>
</dataChannels>
</workflowGraph>
```

```
(Increment (Not true))
```

```
<dataChannels>
<dataChannel
from="Not29.o1"
to="Bool2Int28.i1"/>
<dataChannel
from="Bool2Int28.o1"
to="Increment27.i1"/>
</dataChannels>
</workflowGraph>
<dataProductsToPorts>
<inputDP2PortMapping
from="true"
to="Not29.i1"/>
```

```
(Increment (Bool2Int
(Not true)))
```

Fig. 5. Automatically inserting shims in scientific workflow using the VIEW system.

of the dialog in Fig. 5), and typechecks it using Algorithm 3. If the workflow is well-typed, using *translateS* and *translateT* functions, VIEW inserts coercions (primitive workflows performing type conversion) into the workflow expression by translating it into lambda calculus without subtyping. For example, coercion Bool2Int is inserted in the expression for W_a workflow (bottom right part of the dialog). Finally, the latter expression is translated back into a runtime version of SWL, which has necessary shims in it and is supplied to the workflow engine for execution.

Note that all these steps are fully automated and hidden from the user, who sees results of workflow execution upon pressing the "Run" button.

RELATED WORK

The significance of the shimming problem has been widely recognized by the scientific workflow community [3-8]. Much work to address shimming problem was focused on transforming XML documents whose elements are associated with domain models, (e.g., expressed using OWL) [10-12]. The common limitations of these approaches are: (1) they all focus on translating syntactically different XML documents, whereas other data types, including primitive, or structured types (e.g., record, relational schema) are not supported, (2) they all require services to be semantically annotated and hence they cannot compose arbitrary (not annotated) web services, let alone other kinds of executable components (e.g., scripts, local applications or HPC jobs).

Sellami et al. [9] 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. Ambite and Kapoor [13] present a planning approach to the shimming problem that focuses on relational data types and does not apply to primitive types or other non-relational structured types (e.g., record). Existing scientific workflow systems [14, 16, 17, 22] provide limited support to the shimming problem, i.e. shimming is 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 [4], we presented a primitive workflow model and a workflow specification language that allowed 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 [2] to represent workflows which is naturally suitable for dataflow modeling due to its functional characteristics [7]. While recognizing the importance of shims, [7] does not address the shimming problem. We formalize coercion in scientific workflows with typetheoretic rigor [2, 15]. Existing typechecking techniques apply in contexts other than scientific workflows, e.g., Hindley-Milner algorithm [21] requires typed prefix to typecheck expressions with polymorphic types (not used in our model) 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 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.

VIII. Conclusions and Future Work

In this paper, we first reduced the shimming problem to the runtime coercion problem from in theory of type systems. Secondly, we proposed a scientific workflow model and defined the notion of well-typed workflow. Thirdly, we developed three algorithms to typecheck workflows by first translating them into equivalent lambda expressions. Fourthly, we designed two functions that together insert "invisible shims", or runtime coercions in workflows, 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 a case study to validate the proposed approach. In the future, we plan to extend our technique to mediate structured data types such as relational schema, and to develop real-world scientific workflows relying on our implicit shimming approach.

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