A minimally invasive model data passing interface for integrating legacy environmental system models

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Abstract

This paper presents an approach to model integration utilizing the Model Data Passing Interface (MODPI). The approach provides fine-grained, multidirectional feedbacks between legacy environmental system models through read and write access to relevant model data during simulation using a bidirectional, event-based, publish-subscribe system. MODPI only requires commented directives in the original code and an XML linkage file with an optional custom data conversion module. Automated code generation, compilation, and execution reduce the programming burden on the modeler. Case study results indicated that MODPI required less code modifications within each model code base both before and after automated code generation, outperforming a baseline subroutine approach. Performance overhead for MODPI was minimal for the use case, offering speedup in some cases through parallel execution. MODPI is much less invasive than other techniques, encouraging adoption by the modeling community and improving maintainability and reusability of integrated model code.

Keywords: Framework invasiveness, Integrated Assessment and Modeling,

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1 Data and Software Availability

2 Software developed for the purposes of this paper are open-source and
3 publicly available. The implementation of MODPI presented in the paper is
4 found at <https://bitbucket.org/adozier/fortmodpi> (2.1 MB), and the
5 implementation of events is found at <https://bitbucket.org/adozier/forteevents> (11 KB). A summary of the packages is found at [https://www.
6 erams.com/resources/Platform/MaaS/Model_Integration](https://www.erams.com/resources/Platform/MaaS/Model_Integration). This software
7 requires an implementation of the Message Passing Interface (MPI) or Ze-
8 roMQ. Models (3 MB), performance test results (370 kB), a shell script that
9 reproduces the results (2 kB) in this paper are found at [https://erams.
10 com/resources/Platform/MaaS/Model_Integration](https://erams.com/resources/Platform/MaaS/Model_Integration).
11

12 1. Introduction

13 Model integration frameworks, or environmental modeling frameworks,
14 allow a plug-and-play methodology in connecting submodels of an environ-
15 mental system to enhance model representation of the overall system. How-
16 ever, framework invasiveness restricts reuse and maintenance of framework-
17 dependent models (Donatelli and Rizzoli, 2008; Lloyd et al., 2011). Thus, in-
18 stead of using the frameworks, many environmental system model developers
19 incorporate transplanted, and often outdated, submodels of other disciplines
20 into their codes (Laniak et al., 2013). Although modeling frameworks have
21 been used to integrate such models across disciplines, model developers often
22 maintain the model code base separate from its support of the framework.

23 Lloyd et al. (2011) defines framework invasiveness as “the quantity of
24 dependencies between model code and a modeling framework”. Modeling
25 frameworks that aim at minimizing imposed dependencies on a legacy model
26 improve maintainability and reuse (Lloyd et al., 2011). Historically, modeling
27 frameworks that attempt to be less invasive have focused on coarse-grained
28 interaction between “components” or submodels of a larger model (Donatelli
29 and Rizzoli, 2008; Lloyd et al., 2011). Finer-grained feedback schemes that
30 exchange data from within a component or submodel have previously taken
31 more invasive approaches or require extensive computer programming exper-
32 tise (Becker and Schuttrumpf, 2011). We argue that the amount of work
33 required within a legacy model for integration with another model or sup-
34 port of a framework interface is another obstacle to framework adoption.
35 Thus, we define invasiveness here to be the dependencies within each model
36 on either the integration platform or other models, and the amount of work
37 required within each model for integration or implementation of a framework
38 interface.

39 Attempts to incorporate multidirectional feedback between legacy models
40 include iterative, subroutine, and inter-process communication approaches
41 that are discussed in detail in the next section. To remain minimally in-
42 vasive, inter-process communication techniques are the most promising ap-
43 proaches as demonstrated by Becker and Schuttrumpf (2011) in making a
44 closed-source model compliant with the OpenMI standard (Moore and Tin-
45 dall, 2005) within a timestep loop. Inter-process communication techniques
46 have previously required too much programming knowledge for most model-
47 ers. Thus, there still remains a need for a minimally invasive, fine-grained,

48 generic model integration interface that does not require such extensive pro-
49 gramming expertise (Laniak et al., 2013).

50 The goal of developing the Model Data Passing Interface (MODPI) is to
51 facilitate and abstract the legacy model integration process to reduce frame-
52 work invasiveness while minimizing programming knowledge requirements.
53 Objectives of this study include:

- 54 1. Develop an abstracted interface for minimally invasive model integra-
55 tion that simplifies complex interactions between legacy models and
56 modeling platforms of disparate disciplines,
- 57 2. Automate code generation of MODPI-compatible wrappers for legacy
58 models to support ease-of-use, and
- 59 3. Evaluate invasiveness and performance of MODPI as compared to other
60 approaches.

61 To accomplish these objectives, a publish-subscribe concept is combined with
62 inter-process communication to provide external processes read and write ac-
63 cess to any relevant state variable within a legacy model during its execution.
64 A framework is built that automates wrapper generation, and a case study
65 serves to benchmark MODPI against another common approach to the same
66 problem.

67 **2. Background and Related Work**

68 Many researchers have previously addressed specific model integration
69 challenges, and some have even developed generic interfaces for model inte-
70 gration. However, no generic interface exists for fine-grained, multidirectional

71 feedbacks that preserves the individuality and maintainability of legacy mod-
72 els. Implementing interfaces for existing frameworks requires significant work
73 within the model, and often requires addition of code dependencies on the
74 framework.

75 This section identifies previous studies that have integrated legacy mod-
76 els to support fine-grained, multidirectional feedbacks, which is the primary
77 functional requirement for the integration studies we summarize here. Fine-
78 grained feedbacks refer to linkages of internal (and relevant) data or calcula-
79 tions between multiple models that cannot be represented by one model as
80 a whole, but are required to represent a particular process more accurately.
81 Multidirectional feedbacks refer to data or calculations within one model that
82 depend on another model and vice versa. When the need for such feedbacks
83 between models arises, there are various implementation considerations such
84 as 1) implicit versus explicit numerical solution techniques, 2) passing data
85 via subroutines or put/get calls, 3) hardware mechanism for communication,
86 and 4) single or multiple executable approaches (Valcke et al., 2012). The fol-
87 lowing framework design targets for MODPI are used to qualitatively assess
88 the different approaches:

- 89 1. Minimally invasive
- 90 2. Minimal interface requirements
- 91 3. Interoperable across languages and platforms
- 92 4. Links closed-source models
- 93 5. Reconciles data structure differences
- 94 6. Performance overhead is minimal

95 Interoperability and data structure reconciliation are functional requirements

96 for specific model integration tasks, which also may be true for linking closed-
97 source models and performance overhead in some cases, but not for a generic
98 model integration interface.

99 Framework design targets are prioritized to make the interface more ac-
100 ceptable to a diverse modeling community that individually maintains or uses
101 large legacy models. We argue that the first two targets, invasive changes
102 within a model code base and difficult or extensive interface requirements,
103 represent the largest factors that inhibit maintenance and reuse of integrated
104 modeling systems (Lloyd et al., 2011). The design target for minimal inter-
105 face requirements is aimed at reducing the amount of programming work
106 and knowledge required to be able to implement MODPI for a model. Since
107 modelers are often limited by an unfamiliarity with advanced programming
108 techniques to improve interoperability or link closed-source models, minimiz-
109 ing difficult code changes and refactoring requirements may provide a path
110 to encourage adoption and reuse of model integration frameworks. Ensuring
111 interoperability of languages, platforms, and linkages with closed-source
112 models would also broaden the applicability of an integration platform within
113 an increasingly diverse community of modelers (Laniak et al., 2013).

114 2.1. *Implicit versus Explicit Approaches*

115 Both implicit and explicit solution approaches have advantages and disad-
116 vantages. Although solving equations explicitly may intuitively seem numer-
117 ically faster, implicit approaches may utilize assumptions to solve much more
118 efficiently without sacrificing too much accuracy (Balaji, 2012). Within hy-
119 drology, several approaches based on successive approximations allow models
120 to be run separately, maintaining model individuality in partial fulfillment

121 of Target 1 (Fredericks et al., 1998; Ibanez et al., 2014). Lagrangian relax-
122 ation techniques are systematic implicit numerical methods that allow for
123 parallel execution of submodels Dozier (2012). Because implicit approaches
124 utilize original forms of equations, model individuality may be more easily
125 attained than explicit approaches addressing Targets 1, 3, 4 and 5. However,
126 most explicit solutions can improve geophysical model integration through
127 guaranteeing numerical solutions for feasible inputs (Dozier, 2012; Balaji,
128 2012).

129 *2.2. Subroutines versus Producer-Consumer Approaches*

130 In model integration, data can be passed through subroutine arguments
131 or through an exchanging mechanism such as a buffer that handles producers
132 and consumers through put/get calls (i.e., publishers and subscribers). These
133 are distinguished from hardware communication mechanisms because both
134 subroutine arguments and buffers could potentially utilize memory, hard disk,
135 or network communications, although there are typical implementations.

136 Implementing a subroutine approach often entails decomposing submod-
137 els into smaller components: initialization, run or update, and finalization
138 (Argent, 2004). For example, the Basic Model Interface (BMI) specifies
139 `initialize` and `finalize` methods in addition to an `update` function that
140 is used to advance a model or component to the next timestep while data is
141 passed by name via interface subroutines between updates (Peckham et al.,
142 2013). Kim et al. (2008) integrated a surface water model (SWAT) with
143 a subsurface water model (MODFLOW) by splitting MODFLOW up into
144 its sub-components, calling the computational component of MODFLOW
145 within the groundwater module of SWAT, and compiling the models to-

146 together. In the case of the Object Modeling System (OMS), data is exchanged
147 between multiple models during their simulation through separate (and po-
148 tentially parallel) execution of model subcomponents based on data avail-
149 ability (David et al., 2013). OMS avoids framework dependence through
150 annotations and custom wrappers in partial fulfillment of Target 1, but re-
151 quires decomposing models into smaller components for fine-grained analysis
152 (Lloyd et al., 2011; David et al., 2013).

153 In most cases with put/get approaches, data has previously been passed
154 through specific inter-process communication (IPC) or framework dependen-
155 cies within the original model code base (Valcke et al., 2012; Armstrong
156 et al., 2009). Dozier (2012) showed that event constructs can be utilized
157 to decouple models from the integrated modeling system while using the
158 subroutine approach, which could be extended to the producer-consumer
159 approach. Although the Earth System Modeling Framework (ESMF), the
160 Common Component Architecture (CCA), and Bespoke Framework Genera-
161 tor (BFG2) primarily utilize subroutine-based data passing techniques, they
162 allow subcomponents to use producer-consumer types of data interactions
163 through shared memory or some form of IPC (Allan et al., 2006; Armstrong
164 et al., 1999, 2006; Collins et al., 2005; Hill et al., 2004; Larson et al., 2004;
165 Lefantzi et al., 2003; Armstrong et al., 2009; Valcke et al., 2012). In cases
166 where the framework removes required IPC dependencies from the model,
167 only coarse-grained interactions between model subcomponents are allowed,
168 requiring the model to be broken into smaller components for fine-grained
169 analysis (Hill et al., 2004; Collins et al., 2005).

170 2.3. *Hardware Communication Mechanisms*

171 Mechanisms for communicating data between models primarily include
172 memory, hard drives, and network communications. For typical hardware
173 speeds, Dean (2009) describes that in general a disk seek is 100,000 times
174 slower than a reference to main memory, and reading 1 MB from disk is
175 80 times slower than from memory. To communicate data through slower
176 hardware such as hard drives or network infrastructure may prove to have
177 unacceptable overhead, although most model integration tasks require little
178 data exchange compared to model computations. For example, automating
179 the model integration in the cases of Fredericks et al. (1998) and Ibanez et al.
180 (2014) would have little framework overhead regardless of hard drive reads
181 and writes because of extremely long model runtimes relative to the small
182 data passing requirements. In designing a framework, though, care should
183 be taken to minimize overhead because it may be applied to a large variety
184 of models with different runtimes and data passing requirements.

185 2.4. *Single versus Multiple Executable Approaches*

186 Single executable applications typically require language interoperability,
187 which has been enhanced through tools like Babel (Dahlgren et al., 2012) as
188 used by Peckham et al. (2013). IPC techniques are well-known multiprocess-
189 ing methods for establishing interoperability by being platform-, framework-
190 , and language-independent (Magnoni, 2015). As discussed in Section 2.2,
191 prior frameworks have either required models to implement IPC mechanisms
192 or major refactoring to break models into subcomponents for fine-grained in-
193 teractions in multiple executables, trading off invasiveness with the number
194 of interface requirements.

195 2.5. Discussion of Previous Work

196 With regard to Targets 1 and 2, when a model requires significantly refac-
197 toring for model integration purposes or dependencies on the integrated mod-
198 eling system (i.e., either other models or a model integration framework),
199 it often no longer retains individuality or separability from the framework.
200 That is, we argue that invasiveness and excessive interface requirements dis-
201 courage adoption, maintainability, and reusability of the integrated model
202 code base by splitting legacy models into two code bases, one that imple-
203 ments the interface and one that does not. These two model code bases can
204 sometimes be merged into one when interface requirements are minimally
205 invasive as in the case of BMI (Peckham et al., 2013).

206 Laniak et al. (2013) express a need for interoperability (Target 3) be-
207 tween different disciplinary models and between integrated environmental
208 modeling frameworks that are implemented with different programming lan-
209 guages, compilers, and platforms (Matott et al., 2009). IPC techniques ad-
210 dress this need for interoperability between models with varying architec-
211 tural, platform, or license dependencies, but has previously required invasive
212 approaches or required extensive programming expertise (Targets 1 and 2).
213 Compiling multiple models together into one executable requires models be
214 interoperable either directly, or at least utilize a language interoperability tool
215 such as Babel (Dahlgren et al., 2012). In our experience with re-implementing
216 the approach by Yuan et al. (2011) discussed in Section 5, interoperability
217 of original model code was also compromised when compiling legacy models
218 together because of conflicting compiler flags, and overlapping global vari-
219 able names or file handles. Also, maintaining the state of the submodel

220 between timestep advancements required additional debugging and refactor-
221 ing. Baart et al. (2014) improved interoperability of models implementing
222 the Basic Modeling Interface (BMI) through an IPC technique.

223 Although component-based modeling may be easier to understand and
224 program, Target 4 with regard to linking closed-source models prohibits ex-
225 cessive refactoring of model code, which would need to be done by the model
226 developer. Dozier (2012) showed that event constructs can be utilized to de-
227 couple model codes, maintain model individuality, and allow plug-and-play
228 with different models, even closed-source models. Becker and Schuttrumpf
229 (2011) improved interoperability (Target 3) of this approach by implement-
230 ing the Open Modelling Interface (OpenMI) standard (Moore and Tindall,
231 2005) for a closed-source model through event constructs and remote proce-
232 dure calls. However, the extent to which a geophysical scientist is capable
233 of programming IPC in a similar manner is extremely limited, consequently
234 negatively impacting its potential acceptance in the broader modeling com-
235 munity.

236 Data structures need to be reconciled when compiling models together
237 or performing inter-process communication, but are facilitated by input and
238 output file formats when passing data via the hard drive (Target 5). Although
239 exchanging data via subroutines is one of the most utilized approaches for
240 fine-grained integration, legacy model developers do not often maintain sup-
241 port of model integration interfaces, thus downplaying advantages of plug-
242 and-play model integration (Donatelli and Rizzoli, 2008; Lloyd et al., 2011).

243 Performance overhead (Target 6) must be taken into consideration espe-
244 cially in cases when data must be passed between models at a fine-grained

245 resolution in time or space relative to the number of computations performed
246 by each model. Hard drives and networks communicate data between mod-
247 els more slowly than main memory, but overhead may be minimal when
248 computations outweigh data exchange requirements.

249 *2.6. A New Interface*

250 A generic interface for decoupling computations and disciplinary models
251 using IPC (to address interoperability, Target 3) without requiring extensive
252 legacy code refactoring (Target 1, 2, and 4) or unacceptable performance
253 overhead (Target 6) while generically allowing for data structure reconcili-
254 ation (Target 5) still remains to be developed. MODPI is introduced here
255 to address this need by attempting to satisfy each of the framework design
256 targets through use of an event-based publish-subscribe system with a mes-
257 sage broker (Salas, 2012). Although there are still limitations to the use of
258 MODPI and required work on the part of the modeler, MODPI represents a
259 significant advancement towards satisfying each of the framework design tar-
260 gets. Fig. 1 displays a schematic of the form of model integration presented
261 by MODPI.

262 Section 3 describes the interface, its components, requirements, and op-
263 tional features. Section 4 describes the implementation of the MODPI inte-
264 gration platform and choice of IPC mechanism for interoperability purposes.
265 Section 5 illustrates the use of MODPI with a case study application linking
266 two legacy models, DayCent and HYDRUS. Section 6 summarizes the re-
267 sults of the case study by presenting measures of required code modifications
268 and performance of the integrated modeling system. Section 7 presents dis-
269 cussions of benefits, limitations, advantages, and disadvantages of MODPI

Figure 1: Selected implementation of MODPI links model coupling equations either implicitly or explicitly, and passes data through publisher-subscriber interactions across separate processes. Depending on the inter-process communication mechanism and machine setup, data can be passed through either hard disk, shared memory, or network communications.

270 and its use for further different studies. Section 8 concludes with a discus-
 271 sion about the benefits of MODPI, its design considerations, and results of
 272 the case study application, while Section 9 presents potential future work to
 273 improve this study and future implementations of MODPI.

274 3. The Model Data Passing Interface

275 MODPI provides read and write access to any relevant variable by name
 276 within a legacy model during simulation without legacy code refactoring
 277 through use of event constructs and an automated IPC message broker.
 278 MODPI formalizes, adapts, and expands the approach used by Becker and
 279 Schuttrumpf (2011) to generically and automatically apply IPC to any model,
 280 open-source or closed-source. A legacy model must implement the following
 281 elements to become MODPI-compatible:

Figure 2: Schematic of a wrapper program for a sample model that implements the Model Data Passing Interface (MODPI) using its three interface functions `get_event`, `get_var`, and `run_subscriber`, and runs the MODPI-compatible sample model after initializing and before finalizing.

- 282 1. Legacy model as a library with MODPI directives as code comments
- 283 2. Generated wrapper program with optional customization
- 284 3. XML linkage file

285 These essential elements of MODPI are discussed in the following three sub-
 286 sections and shown in Fig. 2 for a sample model. The *MODPI integration*
 287 *platform* refers to a controller that automates code generation (for event
 288 constructs and wrapper programs) and runs the integrated modeling system.
 289 The component that exchanges data between models during simulation using
 290 IPC is called the *MODPI Broker*.

291 3.1. Legacy Model as a Library with MODPI Directives

292 A legacy model that implements MODPI must be accessible to the MODPI
 293 integration platform as a library, and must contain MODPI directives. Prior

294 to compilation, the MODPI integration platform requires MODPI directives
 295 to generate the event constructs, but during compilation and runtime, it
 296 requires the actual event constructs to access model data. Thus, MODPI
 297 allows for the capability of wrapping closed-source models when generated
 298 event constructs are kept within the pre-compiled libraries delivered to model
 299 users, after which MODPI directives are no longer required to stay in the
 300 source code. The requirements for MODPI compatibility are very minimal
 301 changes to a legacy model code base. The model does not need to be decom-
 302 posed into initialization, body, and finalization subcomponents, but remains
 303 entirely intact. The hardest legacy models to refactor into multiple compo-
 304 nents are poorly modularized codes that utilize a lot of global data. These
 305 very common, yet poorly modularized models provide good use cases for
 306 MODPI since localized model data requires additional event data constructs
 307 where global data does not. Although being able to access both local and
 308 global data within a model allows MODPI flexibility, the model developer
 309 (in the case of closed-source models) or the one integrating models (in either
 310 closed-source or open-source models) should still take care to encapsulate or
 311 hide data from the model integration interface that should remain “private”
 312 in accordance with good practice. Local data is hidden from MODPI by
 313 not providing it as event data. Global data is hidden at compilation by not
 314 exporting certain variables to the library.

315 Directives have the following syntax directly after a comment mark (“!”
 316 in FORTRAN or “//” in C) to add an import statement and to invoke an
 317 event, respectively:

```

318 !MODPI$ use
319 !MODPI$ event <event_name>(<type> <intent> <variable_name>[<size>], ...)
```

MODPI directives are placed within the legacy model code as code comments to support automatic generation of event, or callback, constructs to allow any number of subscribers to access local or global data at various points during model execution. Automatic generation of event constructs from directives is a functional requirement for integration platforms implementing the Model Data Passing Interface to simplify programming responsibilities for the modeler, and to render MODPI less invasive. Automation is especially useful in low-level languages such as FORTRAN and C due to the lack of language-supported event constructs. Event constructs may remain in the model without affecting its normal execution either apart from or within MODPI linkages.

Using MODPI directives, the automated event generator determines where to place `use` or `import` statements, when to fire events, and the data to provide as event data. If all variables declared locally are to be added as event data, the keyword `all locals` is used in addition to any variable names used. Types are declared using either C or FORTRAN data type syntax (e.g., `int` and `integer` are interchangeable). If the event invocation lies within a C source file, the type should include an asterisk symbol (“*”) when a variable is declared as a pointer within the surrounding context. Intent of event data is an optional parameter that is declared using the following FORTRAN syntax:

1. `intent(in)`: variable is passed by value
2. `intent(inout)`: variable is passed by reference (or as a pointer)
3. `intent(out)`: variable is an output parameter only

Intent is used primarily to ensure that parameter types are passed by value

345 when declared as a constant, instead of being passed as a pointer, the de-
346 fault in FORTRAN. If a variable is an array, its dimensions are specified
347 using square brackets after the variable name similar to a C declaration,
348 and includes constant numbers or other variable names. The modeler tasked
349 with implementing MODPI for a model will want to ensure that data that
350 is meant to be read-only should be passed as value with `intent(in)`.

351 The entire MODPI-compatible model is called as a subroutine within the
352 compiled library. The model must not exit in a nonstandard manner (e.g.,
353 through using the `stop` keyword in FORTRAN) because the IPC mecha-
354 nism needs to be finalized. An optional consideration for making a model
355 compatible with MODPI is to ensure that any redundant calculations are
356 switched off. As in the case study in Section 5, a detailed, physically-based
357 model replaces the soil-water submodel of the biogeochemical model, which
358 is switched off to avoid calculations that are overridden anyways.

359 *3.2. Generated Wrapper Program with Optional Customization*

360 A wrapper program implements MODPI for a legacy model by using the
361 legacy model as a library. The MODPI integration platform generates the
362 wrapper program in addition to the event constructs given MODPI direc-
363 tives, the XML linkage file, and an optional custom, user-written module.
364 Any custom actions written in the module are not overwritten when code
365 generation is performed, but are rather subscribed to events in the model
366 based on subscriptions within the XML linkage file. The wrapper program
367 implements through interface functions, initializes and finalizes MODPI, and

368 runs the legacy model.¹ Fig. 2 shows each component and control flow of a
369 wrapper program.

370 When initializing, the MODPI Broker first obtains user-specified model
371 connection information from the XML linkage file. Then, it subscribes event
372 handlers to event constructs, and initializes the IPC mechanism. After ex-
373 ecuting the model, the MODPI Broker finalizes the IPC mechanism. The
374 wrapper program informs the MODPI Broker when to initialize and finalize
375 by performing the following three tasks consecutively:

- 376 1. Initialize MODPI by executing `modpi_init`
- 377 2. Run the model by executing its main subroutine
- 378 3. Finalize MODPI by executing `modpi_finalize`

379 The wrapper program also implements three interface functions:

- 380 1. `get_event`: retrieves events within the model
- 381 2. `get_var`: retrieves data within the model
- 382 3. `run_subscriber`: executes custom subscribers to the model

383 These three functions allow the MODPI Integration Platform to retrieve
384 model events and data, and to run custom subscribers during runtime based
385 on specifications within the XML linkage file described in the next section.

386 Custom subscribers perform any calculations necessary to convert and
387 manipulate data for any connection with another model (or modeling sys-
388 tem) without requiring code changes to the original legacy code base. Dur-
389 ing runtime, the MODPI Broker automatically subscribes any custom data

¹A detailed discussion of each interface function and other attributes of wrapper pro-
grams is found at https://bitbucket.org/adozier/fortmodpi/wiki/wrapper_detail

390 converter to events specified by the XML linkage file, allowing the modeler
391 to easily toggle specific data conversions. Additionally, custom subscribers
392 are compiled into the wrapper program for a model, not into the model
393 itself, thus decoupling model integration customization from the model to
394 aid maintainability of the integrated modeling system with future updates
395 to the model code base. Still, custom subscriber modules must be updated
396 when there is a change in names or locations of events and event data in
397 addition to when a data structure is altered. When custom subscribers are
398 changed, the automated code generator needs to be executed again to gener-
399 ate a `run_subscriber` routine that runs new custom subscribers. Although
400 custom data conversions might require more maintenance than if the MODPI
401 Integration Platform performed generic data conversions, MODPI remains
402 minimally invasive because it does not require certain data structures within
403 MODPI-compatible model code bases. Since customized model integration
404 actions are performed outside of the model library through events and event
405 data, there are minimal maintenance requirements compared to approaches
406 that add framework dependencies to the model code.

407 *3.3. XML Linkage File*

408 An XML file specifies data to exchange between MODPI-compatible mod-
409 els. Its structure provides the list of connected models, the data that is to be
410 exchanged, the data conversions that are to take place, and the intermediate
411 data required for data conversions. When building the XML file, a mod-
412 eler must be able to understand that data can be passed from one model to
413 another during its execution, but is not required to know how to program
414 message passing into any code.

415 At runtime, the MODPI Broker requires the XML file to be named
416 “modpi.xml” and found in the working directories for each of the models.
417 Prior to runtime, the MODPI integration platform copies and renames the
418 original XML file into each of the working directories automatically. The
419 XML file path is not passed to MODPI as a command line argument so
420 that some legacy models do not attempt parsing the file path incorrectly,
421 as MODPI is designed to be minimally invasive. Examples and detailed
422 descriptions of the XML file are found in the repository.²

423 4. The MODPI Integration Platform

424 This section describes the MODPI integration platform developed and
425 used in this paper. Fig. 3 displays the steps required to implement MODPI
426 for any model, where preliminary model changes and MODPI directives allow
427 a wrapper program to be generated. Linkage to another model is provided
428 through the MODPI XML linkage file. MODPI is highly interoperable be-
429 tween programming languages and platforms, being tested in FORTRAN,
430 C, and C++, and preliminarily tested in Java and MATLAB script on both
431 Ubuntu and Windows operating systems. MODPI has also been tested to
432 straddle different virtual machines, different physical machines, and Ubuntu
433 and Windows operating systems, running one model in Ubuntu and the other
434 in Windows.

435 The subsections below describe concepts and features of three components
436 of the MODPI integration platform:

²The XML file definition is found at <https://bitbucket.org/adozier/fortmodpi/wiki/xml>

Figure 3: A flow chart displaying steps to implement MODPI for a generic model. A MODPI wrapper code generator within the MODPI integration platform called “modpi_generate.py” automates the generation of events, event data, and MODPI interface functions. Gray elements highlight the generated components of the integrated modeling system.

- 437 1. Event constructs
- 438 2. The MODPI Broker
- 439 3. The automated code generator

440 Two generic libraries, one for event constructs and one for the MODPI inte-
441 gration platform, are used within this paper to demonstrate implementation
442 of MODPI. Concrete code references and detailed descriptions for the XML
443 linkage file, event constructs, wrapper programs, automatic code generation
444 and execution, and tutorials on using the MODPI integration platform can
445 be found at the online MODPI repository.³

446 *4.1. Event Constructs*

447 The term “events” instead of “callbacks” is used here because the MODPI
448 integration platform utilizes new object-oriented features of the Fortran 2003
449 standard. Events refer to a class of objects that run any number of subscribed
450 subroutines to allow for customization without changing the control flow of
451 the original code or adding many logic statements. Event invocations are
452 placed in locations within the code of a model or component where something
453 of interest happens or is about to happen.

454 Subscribers are subroutines that handle an event to perform customized
455 calculations with model data at the location of the event during model exe-
456 cution. When invoked, an event executes each subscribing subroutine while
457 passing data associated with the event as an argument. When no subscribers

³The open-source and publicly available repositories for the implementation of events and the MODPI integration platform is found at <https://bitbucket.org/adozier/forteevents> and <https://bitbucket.org/adozier/fortmodpi>, respectively.

Figure 4: Schematic of a sample model that adds the numbers 1 through 10, and a wrapper that subscribes to the event within the data. This subscriber simply negates the addition within the sample model.

458 exist, the firing method of the event simply exits, consequently leaving the
 459 original flow of the model unchanged.

460 Fig. 4 illustrates events and subscribers for a sample model that adds
 461 the numbers one through ten. The wrapper subscribes to events within the
 462 sample model, and thus has access to local data that the event provides in
 463 addition to any globally exported variables within the library. In this sample
 464 case, the subscriber negates the calculations made by the sample model prior
 465 to the calculations being performed. If the sample model is executed by itself,
 466 it runs normally without needing recompilation.

467 Events add value to MODPI by decoupling the model from the integration
 468 platform while still allowing access to model state, whether local or global,
 469 during execution. To be MODPI-compatible, a model needs to fire events
 470 during its simulation, and its source code remains closed if desired when the
 471 model is compiled as a library and appropriate variables are exported. The

472 legacy model code base is executed and maintained separately from its sup-
473 port of any specific integration with another model and separate from the
474 integration platform. Other approaches, such as compiling models together
475 or implementing an invasive model integration framework, create two sepa-
476 rate code bases that need to be individually maintained in order to keep the
477 integration intact with future versions of the model, whereas MODPI allows
478 merging these two branches of code into one, reducing maintenance require-
479 ments. We argue that the use of events in MODPI will result in a higher
480 probability of framework adoption by the broader modeling community be-
481 cause events reduce framework invasiveness by preserving model control flow
482 and individuality.

483 A user of MODPI is not required to manually implement events within the
484 legacy model, because the interface only requires MODPI directives within
485 the comments of the legacy model code base. The MODPI integration plat-
486 form then automatically generates the event constructs within the legacy
487 model, without loss of generality since the event constructs are very generic
488 structures. However, so that the reader understands the event construct, this
489 section defines events and subscribers to reinforce why they render MODPI
490 less invasive.

491 *4.2. The MODPI Broker*

492 The MODPI integration platform performs data exchange between mod-
493 els through a construct called the MODPI Broker, which uses IPC to ex-
494 change data between MODPI-compatible models and also automatically sub-
495 scribes custom data converters to events within the models. The modeler
496 looking to implement MODPI for a legacy model does not need to build the

MODPI Broker. Fig. 3 displays steps required to implement MODPI for a generic model, and distinguishes automated steps. This section discusses the features, functionality, and dependencies of the various MODPI Broker components.

The MODPI Broker developed for use in this paper is implemented in FORTRAN, which is currently the most commonly used language for legacy geophysical models. This broker implementation effectively links models built in FORTRAN, C, or C++. It utilizes either the Message Passing Interface, MPI (The MPI Forum, 1993), or ZeroMQ (Hintjens, 2013) as the selected forms of IPC since they are well-developed standards, have widespread community support, and have proved to be very interoperable approaches. Interaction schemes implemented in this version of the broker are `MPI_Send` and `MPI_Recv` (and similar calls for ZeroMQ) with limited broadcasting support. Due to the dependency of the MODPI Broker on MPI, the number of times a variable is sent from one model must be matched with the number of times a variable is received in the other model, and vice versa. Thus, if timestep loops encompass events where MODPI exchanges data, the number of timesteps must be equivalent across models. Otherwise, execution will hang at the end of the simulation.

Fig. 5 illustrates the connection between the MODPI Broker, a MODPI-compatible model, and the wrapper program. The MODPI Broker subscribes to events retrieved by `get_event` and performs message passing between other models running as separate processes to exchange data retrieved through the `get_var` subroutine. The broker automatically subscribes and executes custom data converters to events within the model using the user-

Figure 5: A MODPI wrapper for a sample model to illustrate how the MODPI Broker connects models through the use of the interface functions `get_var`, `get_event`, and `run_subscriber` and IPC.

522 supplied `run_subscriber` subroutine. The implementation and interfaces
523 for these subroutines are discussed in more detail in the online repository.⁴

524 4.3. Automated Code Generation, Compilation, and Execution

525 MODPI requires that events, event data, and necessary wrapper compo-
526 nents be automatically generated from MODPI directives within the com-
527 ments of the source code. Section 3.1 describes the syntax and usage of the
528 MODPI directives, which render MODPI less invasive and potentially eas-
529 ier to use by novice programmers. To automatically implement MODPI for
530 a MODPI-compatible model, the modeler places MODPI directives within
531 comments of the original legacy model code, writes any necessary custom

⁴See footnote 3

532 data converters, potentially creates an XML linkage file to declare interme-
533 diate variables, and runs the automatic generation tool. Code generation
534 and automated compilation is performed for each model separately or for all
535 models in the integrated modeling system simultaneously.

536 Automatic detection of model source files, custom data converters, and li-
537 brary directories is achieved through use of the recommended directory struc-
538 ture shown in Fig. 6. After automated code generation, MODPI directives
539 within the original model source code are replaced with import statements
540 and calls to subroutines that fire events. A generated events module declares
541 event constructs and associated event data, and is compiled into the original
542 model source code. The generated wrapper program discussed in Section 3.2
543 includes the custom data converter and two other files that implement the
544 three interface functions, initializes the MODPI Broker, runs the model, and
545 finalizes the MODPI Broker.

546 Closed-source models are provided as a library, without original source
547 files. If customization of the generated MODPI-compatible wrapper program
548 is desired, the generated events module should be provided to users of the
549 model. In the case study discussed in Section 5, DayCent acts as a closed-
550 source model to demonstrate an implementation of MODPI for closed-source
551 models.

552 The code generator automatically attempts to compile the generated
553 wrapper program and associated model. Automated code compilation is
554 meant for models and wrapper programs written in any combination of FOR-
555 TRAN, C, or C++. Compiled libraries, modules, and executable files are
556 automatically placed in their respective directory locations according to the

Figure 6: Directory structure and naming conventions for automated MODPI wrapper generation. White elements are user-supplied, gray elements are generated.

557 directory structure shown in Fig. 6.

558 Additional features of the code generator include options to remove all
559 generated code, and perform automated execution of the integrated modeling
560 system. Automated execution sets up and starts the MPI job in a fashion
561 consistent with the model communication definitions found within the XML
562 linkage file. The repository documentation discusses specific file locations,
563 requirements and tools used for automatic code generation and execution of
564 MODPI-compatible modeling systems.

565 **5. Case Study Application Linking DayCent and HYDRUS-1D**

566 To investigate invasiveness of MODPI, DayCent (Parton et al., 1998) and
567 HYDRUS-1D (Simunek et al., 2008) are integrated using both MODPI and
568 a previous approach where models were compiled into one executable and
569 HYDRUS is called as a subroutine within DayCent (labeled the “subroutine
570 approach” or “SUB”). DayCent provides daily simulation of biogeochemical
571 fluxes using one-dimensional representation of vegetation, atmosphere, or-
572 ganic decomposition, and water movement through the soil (Parton et al.,
573 2001). DayCent and HYDRUS-1D have been previously linked using the
574 subroutine approach to analyze the added benefit of improved soil-water dy-
575 namics, because HYDRUS-1D provides necessary physically-based modeling
576 of soil water content at fine time and spatial scales (Yuan et al., 2011). This
577 linkage serves as a benchmark to compare the MODPI approach.

578 The subroutine approach is used to call the finite element solver within
579 HYDRUS-1D as a subroutine within DayCent. Yuan et al. (2011) pro-
580 vided code for the implementation of the subroutine approach for DayCent-

581 HYDRUS. Since DayCent and HYDRUS are compiled together, code bases
582 of the integrated models are dependent on each other, and no longer stand
583 as individual models. Additional changes to the code are difficult to sepa-
584 rate from the integrated DayCent-HYDRUS modeling system. The original
585 linkage combined an earlier version of DayCent with an earlier version of
586 HYDRUS (Yuan et al., 2011). For our investigation, we utilized the cur-
587 rent versions of DayCent and HYDRUS to integrate the models using the
588 same approach and data conversion code. The updated linkage required
589 nontrivial adaptation of the code to carefully preserve HYDRUS model state
590 between daily timestep updates within DayCent. These characteristics and
591 requirements demonstrate the difficulties of maintaining individual legacy
592 model code to support integration with another model using the subroutine
593 approach.

594 The second approach integrates the models using MODPI. DayCent and
595 HYDRUS are minimally changed to compile as libraries. Original data con-
596 version between DayCent and HYDRUS provided by Yuan et al. (2011) is
597 preserved and supplied to the DayCent-HYDRUS model as a custom sub-
598 scriber. By placing conversions within the wrapper program through cus-
599 tom subscribers, modifications to the DayCent library are avoided. MODPI
600 directives are added to the original source files, and the MODPI wrapper
601 code generator creates event constructs and event data within each model.
602 The MODPI-compatible DayCent and HYDRUS executable files still exe-
603 cute independently, just as before MODPI integration. A wrapper program
604 implements the MODPI interface for each model. The only dependency for
605 MODPI-compatible DayCent and HYDRUS is the event library discussed in

606 Section 4.1.

607 Fig. 7 illustrates the evolution of the DayCent model code base to make
608 it compatible with MODPI. HYDRUS underwent a similar process. A con-
609 nection between DayCent and HYDRUS using MODPI is achieved through
610 the following three steps:

- 611 1. Minimal code modifications include creating a new program entry point,
612 removing nonstandard model exits using the keyword `stop`, and refac-
613 toring code specific to the Windows operating system to compile and
614 run HYDRUS on Linux using GNU compilers.⁵ Two MODPI directives
615 are added to DayCent, and five to HYDRUS, in locations where the
616 most desirable model states for linkage are achieved.
- 617 2. A single XML linkage file is built to provide specific information on
618 data exchanges between the models.
- 619 3. Model events and a wrapper program are generated using the auto-
620 mated code generator.

621 The XML linkage file, events, and wrapper program for the DayCent-HYDRUS
622 integrated model are found in the MODPI open-source repository.⁶ The link
623 between DayCent and HYDRUS achieved through MODPI was intuitive be-
624 cause it provides access to model state at specific locations within the code.
625 Unlike the subroutine approach, the MODPI-connected DayCent-HYDRUS
626 did not require special consideration to preserve model state, because model

⁵Code for DayCent is available by email. Code for HYDRUS-1D is available in the repository <https://bitbucket.org/adozier/fortmodpi>.

⁶See footnote 3

Figure 7: A flow chart displaying the evolution of DayCent from its original code base (left), to the MODPI-ready code (middle), to the full MODPI-compatible code (right). The MODPI integration platform generates events and event data that are placed into DayCent. Gray elements highlight incremental changes made within the legacy model code base.

627 state is internally preserved in HYDRUS when running as its own process
 628 without an adapted control flow.

629 Fig. 8 displays the flow of data for the DayCent-HYDRUS connection and
 630 the events at which custom data converters are subscribed to each model.
 631 At runtime, the wrapper programs for DayCent and HYDRUS are started
 632 as two separate processes, running in parallel. MODPI enables the models
 633 to exchange data using MPI over the network, or shared memory if both
 634 processes are running on one machine.

635 Within a DayCent-HYDRUS simulation, MODPI sends precipitation (`pptsoil`),

636 potential evaporation (`bserate`), potential transpiration (`bstrate`), and root
637 depth (`tadep`) from DayCent to HYDRUS prior to calculating soil water
638 flux within HYDRUS. Since HYDRUS has an adaptable timestep but Day-
639 Cent has a daily timestep, output data from HYDRUS is summarized at a
640 daily timestep within the subroutine `OnOutput_handler`, in which the event
641 `OnCumQdlyCalc` fires every day. Within the XML linkage file, the summarized
642 daily output data are sent back to DayCent from the `OnCumQdlyCalc` event,
643 not directly from the `OnOutput` event, which fires at a sub-daily timestep.
644 The number of layers `n`, the depth of each layer `x`, an array `cumqdly` con-
645 taining actual evaporation, transpiration, drainage, and runoff data, flux of
646 water between soil layers `vnacc`, and soil water content of each layer `thnew`
647 are received by DayCent at the event `OnSWCalc`. After arriving, the variables
648 are converted within the custom subscriber `convert_SWCalcs` and used to
649 update model state of DayCent. Other custom subscribers set variables or
650 flags that aid linkage between DayCent and HYDRUS to improve console
651 output readability.

652 6. Results

653 DayCent-HYDRUS serves as a case study to benchmark the MODPI in-
654 tegration platform presented in this paper.⁷ This section quantifies invasive-
655 ness and performance of MODPI in comparison with the subroutine (SUB)
656 approach.

⁷Case study model files for the DayCent-HYDRUS integrated model are found at the Environmental Risk Assessment Management System (eRAMS) Resource Center: https://erams.com/resources/Platform/MaaS/Model_Integration

Figure 8: Data flow between MODPI-connected DayCent-HYDRUS. Links to and from events represent subscriptions that are automatically attained by the MODPI integration platform. Gray elements are essential for MODPI to perform linkage between DayCent and HYDRUS. Custom subscriber modules and the list of data to exchange between models found in the XML file are manually constructed, but events are automatically generated from MODPI directives within the code.

657 *6.1. Code modifications*

658 The goal for developing MODPI is to reduce invasiveness of model integra-
659 tion tasks, thus necessitating use of metrics. Here, we quantify invasiveness
660 using five software metrics based on lines of code (LOC):

- 661 1. Code modifications within each model code base (IN-LOC)
- 662 2. Code additions outside of each model code base (OUT-LOC)
- 663 3. Directive additions within each model (DIR-LOC)
- 664 4. Generated lines of code within the model (GEN-IN-LOC)
- 665 5. Generated lines of code outside of the model (GEN-OUT-LOC)

666 The first (IN-LOC) attempts to quantify the amount of work performed
667 within each model code base, and serves as a surrogate measure for the
668 amount of effort that would be required to maintain the integrated modeling
669 system with changing versions of the original code base. The rest of the
670 measures are specific to the coupled modeling system implementing MODPI
671 in the case study. The second (OUT-LOC) attempts to measure the amount
672 of work required to maintain the integrated model only when events or vari-
673 ables within the original model code base are renamed or moved. The third
674 (DIR-LOC) attempts to quantify the amount of work performed to imple-
675 ment syntactically correct MODPI directives within the model code base,
676 although there is no dependency of MODPI within the model through the
677 use of directives since the directives are placed within the comments and not
678 in code.

679 Finally, the GEN-IN-LOC and GEN-OUT-LOC metrics attempt to iden-
680 tify the amount of generated code that benefits abstraction and interoperabil-
681 ity of model integration through inter-process communication. GEN-IN-LOC

682 quantifies the number of lines of code to invoke events within the model, and
683 is equal to 1 when global data is retrieved at an event and greater than 1 when
684 using local data, which populates the event data construct. GEN-OUT-LOC
685 quantifies the lines of code generated for the model wrapper that implements
686 the Model Data Passing Interface for the model, but is compiled separately
687 from the model code base.

688 The first three measures are better when lower assuming the same level
689 of difficult, elegant code writing between each model integration technique.
690 The fourth and fifth measures depend on modeler preference because they
691 add value to the integrated modeling system but are additional lines of code
692 not readily understood by the modeler. Therefore, GEN-IN-LOC and GEN-
693 OUT-LOC are provided here for evaluation by the reader.

694 IN-LOC and DIR-LOC are invasive according to the definition in the in-
695 troduction, and OUT-LOC and GEN-OUT-LOC is not since they are code
696 additions outside of the original model code base. Attribution of invasive-
697 ness to GEN-IN-LOC is more subjective since some work is performed by the
698 modeler run the generator, which is a relatively cheap operation compared
699 to manually writing the code. MODPI outperforms SUB for code changes
700 within the model (IN-LOC plus DIR-LOC), but requires more changes out-
701 side of the model (OUT-LOC) in addition to generated lines of code (GEN-
702 IN-LOC and GEN-OUT-LOC).

703 Understand 3.1 (Scientific Toolworks, 2014) was used to quantify total
704 LOC for each model, which do not include comments or blank lines. Code
705 modifications within each model code base are identified as insertions and

706 deletions in the Mercurial version control system.⁸ For each changeset in the
707 Mercurial repository, all blank and commented lines were removed except for
708 MODPI directives to quantify DIR-LOC. Although utilizing insertions and
709 deletions through a version control system captures changed lines of code as
710 an additional work item not otherwise captured when counting total LOC,
711 changed lines of code are represented by both an inserted and deleted line of
712 code, and are thus double-counted.

713 Table 1 shows code modifications necessary to integrate DayCent and
714 HYDRUS for each approach. DayCent contains 236 source files with 23,057
715 LOC, and the original HYDRUS code base contains 9,034 LOC in 10 source
716 files. The baseline HYDRUS code base used in this analysis is a Linux-
717 compatible version with 8,995 LOC. The SUB approach required 123 (and
718 562) LOC modifications to the DayCent model (and the HYDRUS-1D model,
719 respectively) specific to the integrated modeling system. The MODPI ap-
720 proach required only 116 (and 204) LOC modifications within DayCent (and
721 HYDRUS-1D), 11 (and 21) of which are manual modifications while the rest
722 are generated. Total LOC modifications including the wrapper code to link
723 DayCent (and HYDRUS-1D) using MODPI were 354 (and 515) LOC, while
724 only a total of 87 (and 109) LOC were manually modified.

725 Five MODPI event directives and five import directives (10 DIR-LOC
726 total) are added to the HYDRUS code. Import directives are required in
727 FORTRAN for utilizing event constructs and subroutines found in modules.
728 However, the same requirement does not apply to events invoked through

⁸Mercurial documentation and software is found at <http://mercurial.selenic.com/>.

Table 1: Comparison of code modifications (insertions plus deletions) of lines of code (LOC) within DayCent and HYDRUS (Linux version) using the subroutine (SUB) and MODPI approaches to model integration.

Code Base	LOC	IN	OUT	DIR	GEN-IN	GEN-OUT	TOTAL
DayCent	23,057						
SUB	23,157	123	–	–	–	–	123
MODPI	23,399	11	74	2	103	164	354
HYDRUS-1D	8,995						
SUB	9,066	562	–	–	–	–	562
MODPI	9,455	21	78	10	173	233	515

729 subroutines from C source files, and thus only two MODPI event directives
730 and zero import directives (2 DIR-LOC total) are added to the DayCent
731 source code.

732 Yuan et al. (2011) provided 82 LOC that perform data conversion between
733 HYDRUS and DayCent for the SUB approach within the DayCent model
734 code, and is reported within the IN-LOC measure for DayCent. These LOC
735 were adapted slightly to convert data within the MODPI linkage using a
736 custom subscriber, and are therefore reported as OUT-LOC for DayCent
737 (74 LOC) because the changes remain outside the original model code base.
738 MODPI-compatible HYDRUS-1D incorporated 78 lines of converter code.

739 Filling event constructs with data and invoking them consume 103 and
740 173 LOC while generated wrapper codes include 164 and 233 LOC for Day-
741 Cent and HYDRUS-1D, respectively. These generated LOC represent 75%
742 and 79% of the 354 and 515 LOC changes for DayCent and HYDRUS-1D, re-
743 spectively. These LOC are provided to the modeler as value-added attributes

744 of MODPI, but they also represent code that is not readily understood by
745 the modeler.

746 Minimal IN-LOC modifications for MODPI-compatibility come from adding
747 flags to suppress redundant calculations and creating a new entry program
748 (main) routine that calls the original entry as a subroutine. Total LOC for
749 HYDRUS is based on a Linux version derived from the original Windows
750 version with minimal changes. IN-LOC modifications for HYDRUS-1D are
751 slightly disproportionate to the LOC within the SUB linkage (562 LOC)
752 because several hundred file handle constants were changed to be able to
753 compile HYDRUS-1D directly with DayCent.

754 All 123 (and 562) LOC modifications for the SUB approach in DayCent
755 (and HYDRUS-1D) are integration-specific and consequently invasive. The
756 MODPI approach does not require any integration-specific code changes
757 within a model rendering it less invasive. However, the modeler can pa-
758 rameterize the automatic code generator to insert integration-specific event
759 data to support a specific desired interface without effecting normal model
760 execution or control flow. To illustrate this, modifications to DayCent in-
761 clude 12 lines of generated code that declare and allocate intermediate event
762 data. This can be avoided by placing an event within the custom data con-
763 verter (i.e., `convert_SWCalcs` in Fig. 8) that directly receives data from
764 HYDRUS. To illustrate the minimally invasive potential for implementing
765 MODPI, generated modifications to HYDRUS contain 0 integration-specific
766 modifications.

767 *6.2. Performance characteristics*

768 Use of MPI in the MODPI integration platform provides an opportunity
769 to perform parallel processing on different CPUs and storage facilities, to
770 potentially speed up model execution. The DayCent-HYDRUS integrated
771 model, however, does not contain overlapping computations beyond initial-
772 ization and output file writing, leading to little potential for parallelization.
773 Consequently, network communication overhead may be an issue leading to
774 slow model execution. To address this issue, four different HYDRUS models
775 with differing discretizations of soil layers (50, 100, 300, and 1000) are used
776 to help diagnose performance issues from arbitrarily increasing the number
777 of computations between MPI network access. Computational overhead for
778 DayCent-HYDRUS is assessed by comparing runtimes between the MODPI-
779 connected integrated modeling system with those of the baseline subroutine
780 (SUB) approach. Although runtime combines both overhead due to MODPI
781 (and network communication) and time reduction due to parallelization, it
782 serves to compare the SUB and MODPI approaches, and is more readily
783 reproducible.

784 Tests are performed on a single SUN Blade x6270 server running Ubuntu
785 12.04 with two quad-core 2.8 GHz Intel Xeon processors each with hyper-
786 threading for a total of 16 logical cores. The servers offered 72 gigabytes
787 of random access memory (RAM), and 145 gigabytes hard disk storage on
788 a virtual local area network (VLAN) network connected with a 1 gigabit
789 switch.

790 Table 2 summarizes runtimes of 200 identical test runs for each computa-
791 tional scenario, and Fig. 9 displays associated runtime variability. Overhead

Figure 9: Normalized model runtimes of 200 identical simulations comparing the sub-routine (SUB) approach with MODPI on a single machine with four different HYDRUS model setups to arbitrarily increase computations between network access. Runtime is normalized by the mean runtime of the SUB approach for each HYDRUS model setup. Outliers are runtimes that occur outside of the 95% confidence interval assuming a normal distribution.

Table 2: Mean runtime (in seconds) for 200 DayCent-HYDRUS simulations when linked using both the subroutine (SUB) approach and MODPI. Four models were run with varying numbers of soil layers (50, 100, 300, and 1000) within HYDRUS to arbitrarily increase computation time between network access. Bold MODPI mean runtimes highlight statistically significant differences from the corresponding SUB mean runtime with a p-value < 0.01.

Integration Type	HYDRUS Layers			
	50	100	300	1000
SUB	2.374	5.791	43.79	75.53
MODPI	2.397	5.787	43.40	74.86

792 due to MPI network communication within MODPI-connected DayCent-
793 HYDRUS is minimal and is outweighed by benefits of parallelization for
794 more computationally expensive scenarios. Mean runtime for the MODPI-
795 connected model deviated from that of the SUB-connected model by -0.9% to
796 0.9%. MODPI outperforms SUB for computationally expensive models with
797 300 and 1000 soil layers. Additional performance analyses for MODPI found
798 in Appendix A demonstrate larger overhead in virtualized environments and
799 across machines, except in cases where there is little network communication
800 relative to the number of computations and when running in Amazon EC2
801 instances.

802 7. Discussion

803 Very few code modifications are required to implement MODPI for a
804 model compared to other model integration framework requirements for fine-
805 grained, multidirectional feedbacks that would generally require significant

806 refactoring of the legacy model code base. For the case study, although code
807 modifications remain very minimal for both the MODPI and SUB model
808 integration approaches, MODPI is less invasive for the following reasons:

- 809 1. Code changes are not specific to the linkage between DayCent and
810 HYDRUS
- 811 2. Code changes retain the control flow of the original code base
- 812 3. DayCent and HYDRUS are not compiled together, nor do they depend
813 on each other or even on MODPI after integration
- 814 4. Fewer code changes are required within each model using MODPI than
815 required by the SUB approach to model integration

816 By utilizing custom subscribers for external data manipulation and accessing
817 variables and events by name, wrapper programs support a plug-and-play
818 methodology for linking MODPI-compatible models or systems of models.
819 Customized calculations can be turned on and off within the XML linkage file
820 without having to recompile or generate model wrapper code again. Models
821 using MODPI still retain model individuality and can be run individually or
822 when connected to MODPI, and even run on separate operating systems and
823 frameworks. These are benefits that could not be afforded even if the SUB
824 approach was re-implemented with events to decouple the model code bases
825 from the integrated modeling system as performed by (Wible, 2014).

826 There are advantages and disadvantages to using any model integration
827 framework. Many situations exist where MODPI is a preferable approach
828 to fine-grained model integration as discussed through the paper. However,
829 there are situations when MODPI is not the preferable approach. Here we
830 list situations on both sides of the spectrum starting with situations where

831 MODPI is a preferable approach:

- 832 1. Integrating closed-source models with hidden or difficult input file for-
833 mats
- 834 2. Performance overhead of input-output exchange between model runs is
835 unacceptable
- 836 3. Subprocess representation within a model needs to be modified or over-
837 ridden without changing the original model code
- 838 4. Poorly modularized legacy models that are otherwise difficult to inte-
839 grate
- 840 5. Integrating models across different operating systems or frameworks
- 841 6. Integrating models without a predetermined number of connections to
842 other models

843 Legacy models that are poorly modularized or that otherwise use a lot of
844 global variables, which is characteristic of arguably most legacy models, are
845 good use cases for MODPI because global variables grant MODPI easier
846 access to model data. In this case, MODPI minimizes required refactoring
847 for integration as compared to component-based frameworks, although care
848 must still be taken to incorporate the correct model data in the linkage, as ex-
849 pected when using any model integration framework. Model integration with
850 MODPI can also be performed across operating systems and has been shown
851 to effectively link models across an Ubuntu and Windows systems. Although
852 the current implementation of MODPI, the MODPI Integration Platform
853 presented in this paper, has only been preliminarily tested in higher-level lan-
854 guages such as MATLAB and Java, the concept of multilingual frameworks is
855 a well-known contribution of inter-process communication approaches. The

856 use of events allows MODPI to grant publish-subscribe type interactions to
857 models so that any number of subscribers (i.e., other models, visualizations,
858 or analysis packages) can listen to events being invoked within the publishing
859 model.

860 MODPI is not always the preferable approach to model integration due
861 to the specific use cases that MODPI was designed to address. The follow-
862 ing situations should prompt consideration before attempting to implement
863 MODPI:

- 864 1. There is no intention to maintain up-to-date versions of integrated mod-
865 els and model codes are already easily interoperable
- 866 2. There is no need for within-simulation data access and exchange, or
867 it is desirable to implement an iterative approach to obtain implicit
868 solutions to equations
- 869 3. There is little potential for parallel execution but computational speed
870 is high priority
- 871 4. The framework, language, or operating system is known not to support
872 the inter-process communication mechanism (the MODPI Integration
873 Platform currently supports both MPI and ZeroMQ)

874 If high performance is top priority for short jobs (less than 10 seconds),
875 MODPI can help speed computations through parallel processing when pos-
876 sible, especially in high performance computing environments with high-end
877 network hardware and proper configurations. Optimized configuration of a
878 virtual environment and of the selected form of inter-process communica-
879 tion can also significantly improve performance. If no or very little parallel
880 execution is possible for a specific model integration task, compiling mod-

881 els together (when possible) or utilizing events to decouple the models (still
882 within a single process) without overhead due to inter-process communica-
883 tion may be a preferable approach.

884 The MODPI integration platform potentially reduces the amount of pro-
885 gramming work and the required level of programming expertise for specific
886 model integration tasks through automated wrapper generation. However,
887 there are a few tasks to be performed by the modeler that must be taken
888 consideration. First, the modeler must conceptualize the model integration
889 task correctly regarding both semantics and logistics as must be performed
890 for integrating any model regardless of the framework or approach. Second,
891 linkage locations within each model must be identified based on where certain
892 data is available. Either events can be placed where the data is available, and
893 custom subscribers can track references to the data, or data handling within
894 the model is slightly refactored to provide certain data at a specific event.
895 Third, the modeler must have knowledge of either event constructs, which is
896 more probable with higher level languages, or the syntax of MODPI directives
897 and rely on the MODPI code generation process to make a model compatible
898 with MODPI. Fourth, nomenclature of the XML linkage files must be learned
899 for specifying the data to be passed between models. Fifth, debugging a par-
900 allel application with automatically generated code may prove to be more
901 difficult than sequential, manual approaches to model integration. Finally,
902 custom data conversions will likely need to be performed (and maintained)
903 by the modeler since MODPI does not currently require specific data struc-
904 tures within its interface. Aggregation and data conversion in space or time
905 must currently be performed by the modeler, but this may change in future

906 versions of MODPI. Benefits of custom data conversion includes flexibility,
907 applicability to a broader set of model integration tasks, and computational
908 speed addressed by removing potentially slower generic conversions.

909 One significant benefit is that MODPI can be used to integrate models
910 with closed-source models in a fine-grained manner. The closed-source model
911 developer must be willing to add events into the model, compile the model
912 as a library with exported and relevant model data, and provide the names
913 of events, event data, and other model data of interest to the modeler. In
914 this manner, the model can still be used for integration with other models
915 without having to share the source of the code or input file format. Closed-
916 source model developers in the environmental sciences would benefit from
917 this because they would not have to directly support interfaces of model
918 integration platforms, but could still attract users that want to integrate
919 the model with another. A finite set of interaction points within the closed-
920 source model can be provided to users that would allow for varying degrees of
921 granularity in integration and customization. This has been done in closed-
922 source models like MODSIM (Labadie, 2010; Dozier, 2012) and FEFLOW
923 (Becker and Schuttrumpf, 2011), for instance.

924 Potential users of MODPI include interdisciplinary researchers interested
925 in model integration for improving process representation in geophysical mod-
926 eling. Model developers for either open-source or closed-source models would
927 be interested in using event constructs because they decouple the model from
928 customized actions, other models, and model integration frameworks. Using
929 events, model developers can maintain one code base instead of different code
930 branches that implement interfaces for external integrated modeling systems.

931 Modelers and consultants that perform integrated analysis of environmental
932 systems may find MODPI a useful framework for minimizing programming
933 time while allowing for fine-grained feedbacks between models.

934 8. Conclusions

935 The case study application demonstrates that minimal code modifications
936 to a legacy model are required to implement MODPI for a model integration
937 task. Only 11 and 21 lines of code were manually modified within legacy
938 model code bases respectively, compared to 123 and 562 lines of manual
939 code modifications for a baseline approach. At runtime, MODPI-compatible
940 models incorporate 116 and 204 lines of code modifications, respectively,
941 including generated code and MODPI directives found in the comments.
942 Although the case study application required some user-written custom data
943 converters and a bit of MODPI-generated wrapper code, MODPI requires less
944 code changes in the original model code base than the baseline “subroutine”
945 approach.

946 Performance tests demonstrate that MODPI not only has minimal over-
947 head for the use case on a single machine, but provides speedup through
948 parallel execution of linked models. Further evaluation of performance re-
949 sults as described in Appendix A highlights worsening overhead when running
950 across two machines, except when little network communication is performed
951 relative to computations or when running in virtual machines in Amazon
952 EC2, depending on hardware, hypervisor, and virtual network setup. Mean
953 runtime of MODPI-connected models varies between -0.9% to 0.9% when
954 compared to that of the subroutine approach, representing a shift from min-

955 imal overhead to minimal speedup for a model integration scenario with few
956 overlapping computations.

957 Inter-process communication provides MODPI a large degree of interoper-
958 ability across languages, platforms, hardware, and license requirements,
959 although only fully implemented and tested in Ubuntu and Windows with
960 FORTRAN, C, and C++. Closed-source models can be linked with other
961 models using MODPI given that they come precompiled as a library with
962 events. Customization allows any data structure to be converted and ma-
963 nipulated outside of the original model code base through use of event sub-
964 scribers.

965 The design of MODPI attempts to address each of the six framework
966 design targets discussed in Section 2. MODPI performs fine-grained, mul-
967 tidirectional feedbacks while remaining less invasive than other approaches,
968 enhancing the maintainability and reusability of MODPI-integrated models.
969 MODPI does not require any framework component or integration-specific
970 code modification within the original model code base other than directives
971 within model code comments and event constructs at runtime.

972 The MODPI-compatible model contains event constructs that generically
973 provide read and write access to relevant data for model integration while
974 preserving original control flow. The MODPI integration platform delivers
975 most of these benefits by automated means, and therefore reduces modeler
976 programming time.

977 Maintenance is minimal, but MODPI still does require care in event lo-
978 cations and naming, data access encapsulation and naming, and correct data
979 conversion logic both within the wrapper program and the XML linkage file.

980 Although inter-process communication offers interoperability and speed up
981 through parallel execution, debugging a parallel program with automatically
982 generated code is potentially more difficult than sequential approaches.

983 **9. Future Work**

984 Future work and developments will improve implementation of the MODPI
985 Integration Platform to be more interoperable, generic, and widely applica-
986 ble. Full MODPI implementations in Java, MATLAB, Python, R, and .NET
987 languages will improve its assertion of interoperability. Although MODPI
988 has already been tested on Ubuntu and Windows operating systems (and
989 across both operating systems with one model on Ubuntu and one on Win-
990 dows), more cross-platform tests for other operating systems such as Mac,
991 Debian, BSD, HP-UX, Solaris, CentOS, and RHEL will increase its broader
992 applicability.

993 MODPI benefits technically from not specifying data structures in order
994 to allow model data to remain in its current structure to achieve minimal in-
995 vasiveness, but this complicates generic data transformations in space, time,
996 and across various data structures. Future research will focus on implement-
997 ing generic data transformations within the MODPI Integration Platform
998 followed by further advancements up the levels of conceptual interoperabil-
999 ity model (Wang et al., 2009). Other future work on MODPI can be to
1000 implement it as a proxy between the model and a more generic model in-
1001 tegration standard such as OpenMI or BMI for example, which will have a
1002 much broader impact on integrated modeling through use of open standards.

1003 Currently, MODPI does not detect potential deadlock situations, but

1004 could in the future. Since timesteps are a common feature of many legacy
1005 environmental models, MODPI could be improved to include a timestep-
1006 tracking feature that detects when time periods are out of sync so that models
1007 do not hang at the end of execution waiting for more IPC. Another area of
1008 future work is to utilize MODPI to link more than two models or models in
1009 more spatial dimensions, since the current case study performs analysis only
1010 in one spatial dimension. Use cases for models with significant amounts of
1011 computation to be run in parallel will improve analysis of potential speedup
1012 benefits of MODPI.

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1193 **A. Appendix: Additional Performance Results**

1194 Additional scenarios are assessed in this appendix to quantify potential
1195 computational overhead for a variety of machine setups. The DayCent-
1196 HYDRUS model was executed on two different physical machines labeled
1197 “PM1” and “PM2” for operating systems running on “bare metal”, and on
1198 two virtual machines labeled “VM1” and “VM2”. These scenarios are com-
1199 pared with the MODPI-connected system straddling both machines, with
1200 DayCent on Machine 1 and HYDRUS on Machine 2 (“Both PMs” for physi-
1201 cal machine cases, “Both VMs” for virtual machine cases). Due to increasing
1202 support for and usage of virtual machines in addition to interest in Modeling-
1203 as-a-Service within the cloud (David et al., 2014), tests are executed in both a
1204 private cloud environment and within Amazon Elastic Compute Cloud (Ama-
1205 zon EC2) cloud platform, which help to assess performance in the presence
1206 of network jitter.

1207 Machines in the private cloud environment are SUN Blade x6270 servers
1208 that run Eucalyptus 3.1 Infrastructure-as-a-Service (IaaS). Each machine

1209 has identical hardware with two quad-core 2.8 GHz Intel Xeon processors
1210 each with hyper-threading for a total of 16 logical cores, 72 gigabytes of
1211 random access memory (RAM), 145 gigabytes hard disk storage, and use a
1212 virtual local area network (VLAN) network connected with a 1 gigabit switch.
1213 Virtual machines execute on a XEN 4.1.2 hypervisor, have 8 logical cores,
1214 4 gigabytes RAM, and 30 gigabytes hard disk storage. The same network
1215 adapter is used for communication on both physical and virtual machine
1216 runs. For performance tests in Amazon EC2, we use the c3.xlarge virtual
1217 machine instances, which have one quad-core 2.8GHz Intel Xeon processor
1218 with 7.5 gigabytes of random access memory (RAM) and 40 gigabytes storage
1219 on a solid state drive. All machines in the analysis run Ubuntu 12.04 as the
1220 operating system.

1221 By default, Open MPI utilizes shared memory when running on the same
1222 machine, but a large variance in performance occurs due to internal tuning
1223 options within the shared memory modules of Open MPI. To address this
1224 issue, we conduct tests restricting message passing communication to the
1225 Transmission Control Protocol (TCP), which gives more consistent perfor-
1226 mance results, and supports direct comparison as all tests then use TCP
1227 inherently.

1228 Table A.1 displays mean runtime in seconds of 200 identical test runs for
1229 each model integration scenario, and Fig. A.1 summarizes runtime variability
1230 when comparing specific scenarios. Most observable differences in Table A.1
1231 are statistically significant according to t-tests because of the large sample
1232 size and small variance. Many differences are very minuscule when nor-
1233 malized against the subroutine method on Machine 1 (SUB-M1) except for

Table A.1: Mean runtime (in seconds) for 200 DayCent-HYDRUS test runs for both the subroutine integrated system (SUB) and the MODPI integrated system (MODPI) executed on both a physical and virtual machine in a private cloud (PM1 and VM1), in Amazon EC2 (Amazon VM1), and with DayCent on one machine and HYDRUS on another communicating over the network (Both PMs, Both VMs, and Amazon VMs). Four models were run with varying number of soil layers (50, 100, 300, and 1000) within HYDRUS to arbitrarily increase computation time between network access.

Integration Type	Machine	HYDRUS Layers			
		50	100	300	1000
SUB	PM1	2.4	5.8	43.8	75.5
	VM1	2.4	5.8	43.8	75.7
	Amazon VM1	2.1	5.1	38.5	66.1
MODPI	PM1	2.4	5.8	43.4	74.9
	VM1	2.4	5.9	44.5	76.7
	Amazon VM1	2.3	5.5	41.4	71.2
	Both PMs	2.9	6.3	44.2	75.7
	Both VMs	3.1	6.6	44.4	76.0
	Amazon VMs	2.7	5.6	38.4	65.6

1234 computationally inexpensive cases executed in the private cloud environment.

1235 As discussed in the Results section, overhead due to MPI network commu-
1236 nication when running on one machine within MODPI-connected DayCent-
1237 HYDRUS is minimal and is outweighed by benefits of parallelization for the
1238 more computationally expensive scenarios when running on a physical ma-
1239 chine. MPI network communication across machines in a private cloud has
1240 a much larger effect on runtime results. Increases in mean runtime when

Figure A.1: Boxplots of normalized model runtime of 200 identical simulations on a private cloud comparing (top) a MODPI execution on a single physical machine and across two machines, (middle) a MODPI execution on a single physical machine and a single virtual machine, and (bottom) a MODPI execution across two physical machines with that across two virtual machines. Runtime is normalized by the mean runtime of the case on the left of the panel for each HYDRUS model setup (see mean runtimes in Table A.1). Outliers are runtimes that occur outside of the 95% confidence interval assuming a normal distribution.

1241 using the MODPI method on both physical machines (MODPI-Both-PMs)
1242 range from 1.1% to 20.9% as compared to the MODPI method running on
1243 one physical machine (MODPI-PM1) as shown in the top of Fig. A.1, but
1244 absolute differences in mean runtimes is relatively the same across scenarios,
1245 ranging from 0.5 to 0.8 seconds.

1246 Overhead due to virtualization is minimal when on one machine, 0.1-0.5%
1247 more than baseline runtime for SUB scenarios and 2.0-2.5% more than base-
1248 line for MODPI scenarios. As shown in the middle component of Fig. A.1,
1249 much more variation in runtime occurs for MODPI-connected models when
1250 running on virtual machines. The cost of virtualization is more exaggerated
1251 when running across two machines, increasing runtime by 0.3-8.2% when
1252 compared to MODPI running across two physical machines (see the bot-
1253 tom component in Fig. A.1) and by 1.5-30.8% when compared to MODPI
1254 performance on a single physical machine.

1255 Performance results of scenarios executed within Amazon EC2 show a dif-
1256 ferent pattern as summarized in Table A.2. MODPI executing on one virtual
1257 machine has approximately the same relative slowdown when compared with
1258 the SUB approach of 8% regardless of the number of computations. This
1259 may likely indicate a computational bottleneck due to scheduling of tasks in
1260 the virtualized environment instead of a network bottleneck, which would be
1261 expected to have the same absolute overhead in runtime. Operating across
1262 machines, MODPI has a relatively higher cost for jobs with little computa-
1263 tional requirements with slowdown of 10.6-28.5%, but little overhead for jobs
1264 with high computational requirements with speedup of 0.3-0.9%.

Table A.2: Increases in runtime (%) for MODPI scenarios with two different machine setups within the private cloud and within Amazon EC2. The SUB-VM1 serves as the baseline scenario.

Platform	Machine	HYDRUS Layers			
		50	100	300	1000
Private cloud	VM1	2.5%	1.4%	1.5%	1.3%
	Both VMs	31.4%	12.5%	1.2%	0.4%
Amazon EC2	VM1	8.7%	7.9%	7.5%	7.6%
	Both VMs	28.5%	10.6%	-0.3%	-0.9%

Graphical abstract