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AMIDOL Milestone 13 and 14 Report

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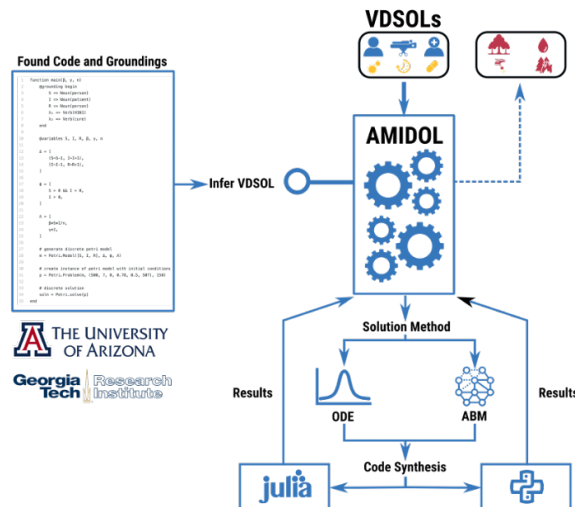## Contents

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Figure 1: AMIDOL Architecture

1. Introduction

Our advancements to AMIDOL have focused on preparing for the upcoming live demo, final code release, and expanding AMIDOL's use of VDSOLs, model composition interface, and the generation of a new "AMIDOL as a Service" (AaaS) API designed to allow other modeling tools to make use of AMIDOL's IR, transformation, and code synthesis capabilities. We have released the next version of AMIDOL at its github site (`https://github.com/GaloisInc/AMIDOL/`) under the BSD 3-Clause "New" or "Revised" License.

Figure 1 shows the current state of the AMIDOL framework. AMIDOL functions as an integrated prototype with the work of our colleagues at GTRI and their SemanticModels.jl development, and Automates from our colleagues at the University of Arizona. AMIDOL currently supports multiple VDSOLs, both graphical and textual, a universal IR, a code synthesis engine capable of generating solutions targeting both ODE solution and Agent-Based Methods (ABMs) in both Python and Julia.

Part I

Milestone 13

2. Recent Extensions to the AMIDOL Framework

The UI for comparing results of multiple models has been extended to support a rich language for combining traces. This is particularly useful for constructing derived measures without needing to re-run a given model. For instance, this might be used in a situation where an epidemiological model tracks multiple strains of a virus separately,

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but the hospital data only keeps aggregate data. Another similar case is when the scientist doing modelling is trying to quickly line up peaks of infected populations from model result and real world data. Our language contains primitives, such as shift, which simplify this sort of transformation.

A completely new VDSOL that is designed to take a system of differential equations written in LaTeX format has been added. The idea behind this new language is to simplify the work of going from a model written in an academic paper to an AMIDOL model. Scientists can enter LaTeX equations, constants, and initial conditions in a text box. Beside this input, they get a real-time LaTeX preview of their equations. From there, the model is compiled into the AMIDOL IR so that it can be executed and compared to results from other models (which may have been designed in completely different VDSOLs).

Finally, we are in the process of experimenting with model composition in the backend, with the goal of finding a minimal intuitive language for combining models. To this end, we've been refining our existing state-sharing composition operators and have started to experiment with other techniques revolving around substitution. Most of these changes are still not exposed to end users in the UI, as we are still developing appropriate primitives for model composition.

2.1. VDSOLs for Mathematical Languages

AMIDOL has been extended to include a VDSOL which compiles and translates a system of LaTeXequations into the AMIDOL IR. The VDSOL renders LaTeX equations using KaTeX, a fast browser-based Javascript library designed for this purpose. Once a user submits a system of differential equations, the backend tries to parse each line as a differential equation, initial condition, or constant. This step is complicated by the fact that the LaTeX source for equations can sometimes be interpreted in multiple ways (for instance: is '\frac{psi}{2}' the variable 'psi' divided by two, or the product of 'p', 's', 'i', and '0.5'). To solve this ambiguity, we require that implied multiplication include at least a space to separate the factors (eg. 'p s i' vs 'psi'), assuming identifiers without spaces are atomic. The final step is to convert the system of differential equations into an AMIDOL model, represented in the IR. This is fairly straightforward: variables given as derivitives with respect to time in the equations turn into states and the right-hand side of the equations turns into events and their associated rates. Positive and negative rates are matched to infer output predicates.

2.2. Definition of Derived Measures

The AMIDOL comparison UI has been updated to support a richer mathematical language for derived measures: In order to implement this, we've moved the work of combining data traces from the UI to the backend. The language for describing derived measures supports translations, linear distortions, component-wise arithmetic, as well as a limited, but expanding, set of built-in functions. The backend contains a parser for this language as well as an interpreter.
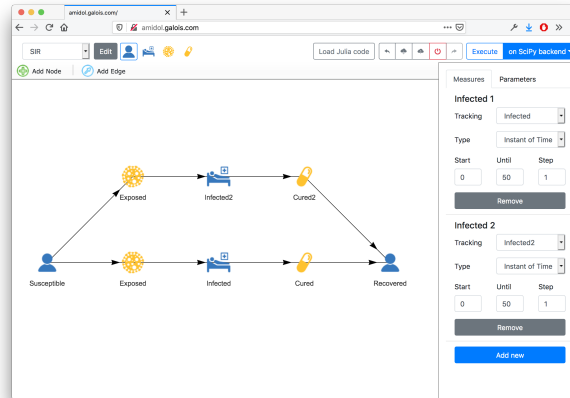
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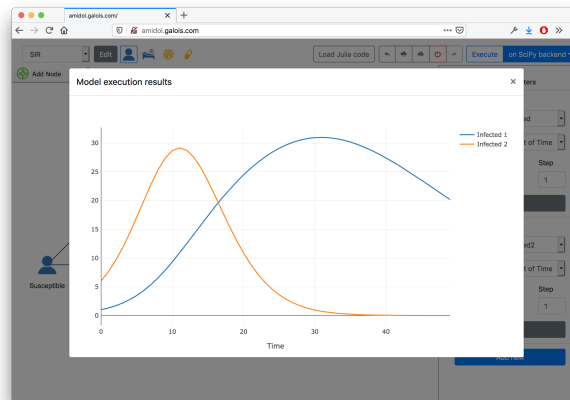Figure 2: SIIR Example Model

Figure 3: Comparison of model infection results.

3.   AMIDOL Demo Instructions

3.1.   AMIDOL Comparison UI

The following tutorial is designed to better explain the new AMIDOL comparison UI.

1. Download a simple SIIR model file from `https://raw.githubusercontent.com/GaloisInc/AMIDOL/master/examples/SIIR.json`

2. Starting at the main page (`http://amidol.galois.com`) click on the cloud-arrow-up button and, when prompted for a file, select the SIIR.json file that was just downloaded. You should see the model in Figure 2

3. Since this model comes with two measures already defined, it is ready to be executed immediately. Press on "Execute" in the top right corner of the page. The results will be similar to those shown in Figure 3.

4. Now, navigate to the model comparison page (`http://amidol.galois.com/compare.`
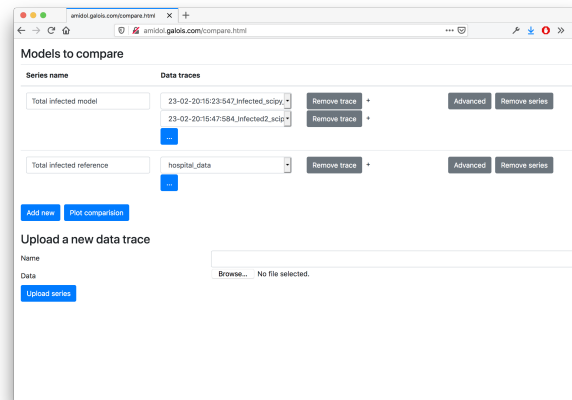
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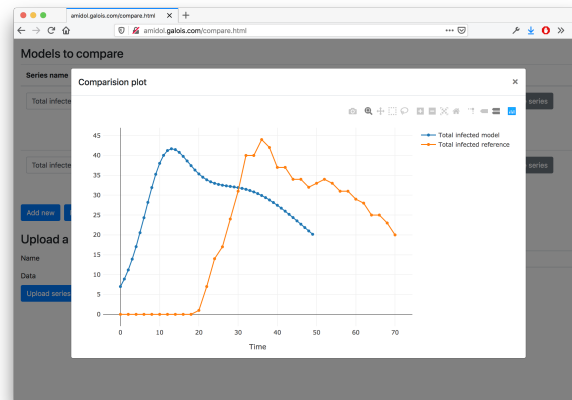Figure 4: AMIDOL Compare Model Page
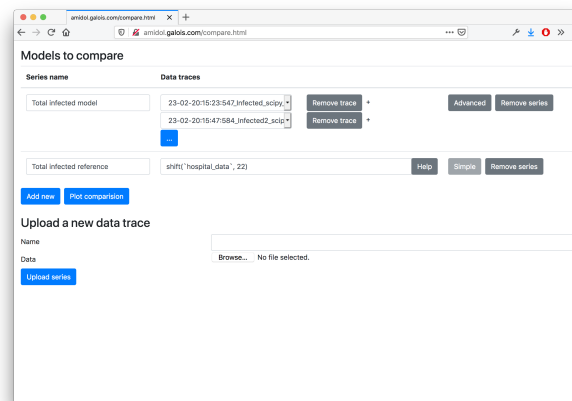

Figure 5: Total Infected Comparison

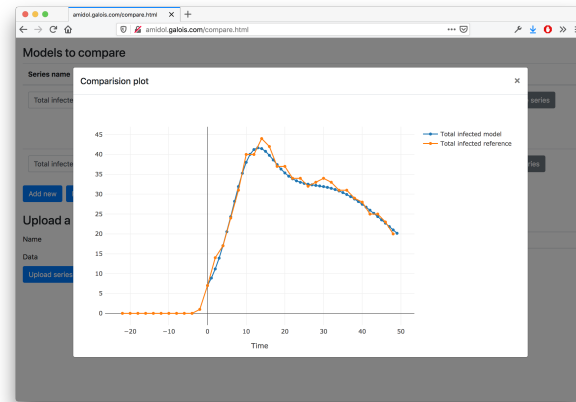Figure 6: Model Comparison Page with Shift Operator

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Figure 7: Shifted Results of Total Infection

`html`). Here we are going to compare the results of running our model to some hospital data.

5. Click on "Add new" and name the series "Total infected model".

6. Then, under data traces, click on the "..." button and add a trace that has a name that looks like "⟨date⟩_Infected_scipy_⟨counter⟩".

7. Click on the "..." button again and add a trace that has a name that looks like "⟨date⟩_Infected2_scipy_⟨counter⟩".

8. Now, we are going to upload to artificial data that is meant to simulate aggregate infection rates that a hospital might collect. In particular, the data is shifted in time compared to the model. Under "Upload a new data trace", enter "hospital_data" for "Name" and choose this file for data: `https://raw.githubusercontent.com/ GaloisInc/AMIDOL/master/examples/reference-data/SIIR_infection_rates_shifted. json`. Then, click "Upload series".

9. Next, click on "Add new" again and name the series "Total infected reference".

10. Then, under data traces, click on the "..." button and add the data trace you just uploaded: "hospital_data".

11. If we click "Plot comparison", we can see that the reference and hospital data match up, but they are offset in the time axis, as in Figure 5.

12. Exit the plot. Now, click on "Advanced" on the row of "Total infected reference" and paste into the textbox that appears "shift('hospital_data', 22)". This is going to dynamically adjust the "hospital_data" trace to start 22 time units earlier. See Figure 6

13. Now, when we click "Plot comparison", the infected populations over time match up. The results should match Figure 7.
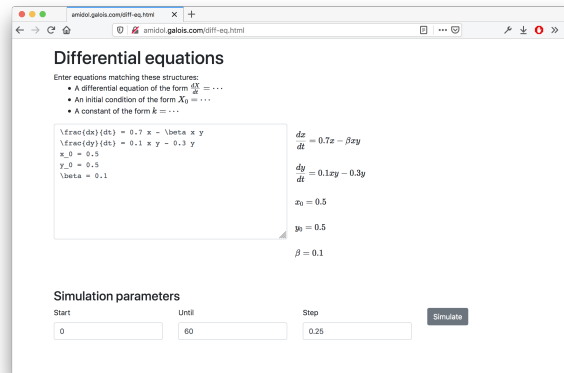
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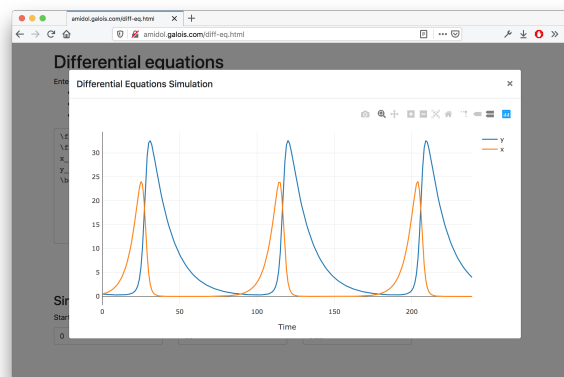Figure 8: AMIDOL LaTeX Differential Equations Editor

Figure 9: Example Output of a model created in the new Differential Equations Editor

14. The "Help" button to the right of the textbox shows you the other sorts of data trace transformation operations you can perform.

3.2. AMIDOL Differential Equation VDSOL

The following instructions explore the new Differential Equations editor implemented in AMIDOL.

1. Navigate the differential equations page editor at `http://amidol.galois.com/diff-eq.html`. Here, we can enter in raw differential equations.

2. For instance a simple Lokta Volterra model, enter the following equations, verbatim, as in Figure 8:

- $$\text{\textbackslash frac \{dx\}\{dt\} = 0.7 x - \textbackslash beta x y}$$

- $$\text{\textbackslash frac \{dy\}\{dt\} = 0.1 x y - 0.3 y}$$

- $$\text{x\_0 = 0.5}$$

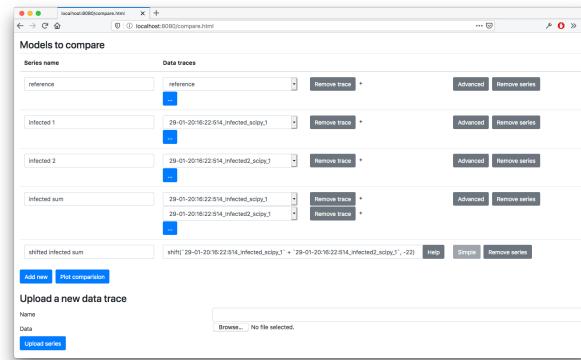|galois|

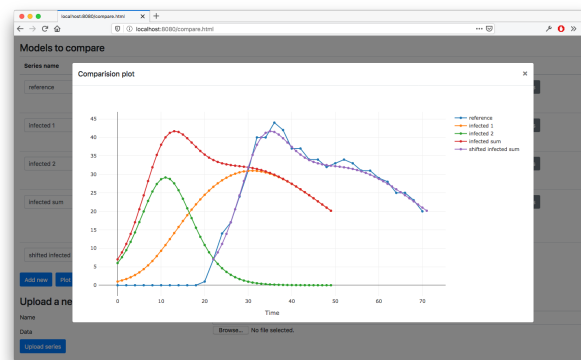Figure 10: New AMIDOL Model Comparison

Figure 11: New AMIDOL Model Comparison Results Visualization

y_0 = 0.5
\beta = 0.1

3. Then, click "Simulate" to see the results of the model running, resulting in the graph shown in Figure 9.

4. AMIDOL Performance for Real-World Systems and Processes

In order to characterize AMIDOL's current performance, we executed the benchmarks documented below, measuring over four models, the time to compile the VDSOL to the AMIDOL IR, the time to translate a Julia AST into a VDSOL (including the time required to search for groundings in the SNOMED ontology), the time to compile the IR to both Python and Julia backends, and the execution times of both backends.

We additionally measured the lines of code generated for each model in both Python and Julia by the AMIDOL code synthesis portion of the compiler. The results are provided below.
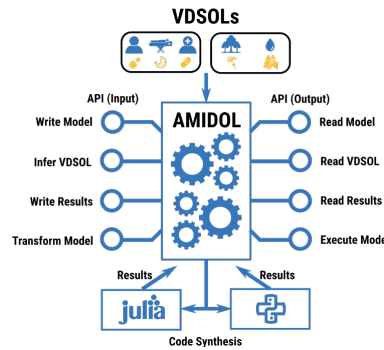
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Figure 12: AMIDOL as a Service

	Model	SIR	SIIR	Predator-Prey	SIR with vital dynamics
Time	Graph VDSOL to IR compilation	1.7ms	1.7ms	1.1ms	1.6ms
	Julia to Graph VDSOL (including ontology grounding search)	1.8s - 6s	2.1s - 6s	n / a	n / a
	IR compilation to Python backend	190ms	160ms	30ms	160ms
	IR compilation to Julia backend	24ms	25ms	15ms	52ms
	Execution of Python backend output	2.5s	2.4s	1.1s	2.5s
	Execution of Julia backend output	9.8s	12s	7.5s	7.0s
Lines of Code	Python backend output	40	45	39	47
	Julia backend output	44	62	51	60

Overall these times demonstrate performance comparable to, or faster than, hand-developed scientific models, with much faster and less error prone development cycles.

Part II

Milestone 14

5. Final Prototype Development

As part of the final prototype development of AMIDOL, we have worked to both expand the number and types of different VDSOLs supported by AMIDOL; implemented a model composition system that results in a model algebra, capable of composing models serially, in parallel, and substitutionally, even across different VDSOLs; and expanded AMIDOL's ability to operate as a service for external applications.

6. AMIDOL as a Service

We have worked to expose AMIDOL's capabilities to external applications via a number of RESTful end points in order to allow for AMIDOL to work not only as a stand-alone application with its own UI, but to accept workloads from external applications seeking to leverage AMIDOL as part of their own tool chain, or as part of a library.

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Figure 12 shows the general architecture of the AaaS framework, with input and output APIs, in roughly matched pairs based on their intended use. We discuss those APIs in more detail in the following sections.

6.1. Read/Write Model

The `Read/Write Model` API end points are designed to allow external applications to read and write models directly to AMIDOL's IR. This allows the import and export of models into AMIDOL for further API calls. To support this we have been exploring future work including a searchable model database, and the support of a query interface for finding models by their properties.

6.2. Infer/Read VDSOL

The `Infer/Read VDSOL` API end points are designed to import found code, generating an inferred VDSOL, or to read an existing VDSOL from AMIDOL. Imported code takes the form of Julia code, with grounding information supplied by AutoMATES. The Read end point allows for retrieval of VDSOLs already in AMIDOL's database. We have been exploring future work to also allow retrieval using a query system over VDSOL properties.

6.3. Read/Write Results

The `Read/Write Results` API end point is designed to allow external applications to read and write to the AMIDOL results database. AMIDOL is implementing a graph-based results database, supporting model comparison, and including mechanisms to index into the database to write data, traces, or external model results. This will allow users to access and compare measures generated by AMIDOL, and submit new data or measures for comparison. Measure indexing by outside applications is an open question. We need a clear definition of measure equivalence. What does it mean for two measures to be the same? At a basic level, they have the same sigma-algebraic structure, over borel sets that are proxies for the same space. We are exploring what this means in practice as part of our future work.

6.4. Transform/Execute Model

The `Transform/Execute Model` API end point allows external applications to compile and transform models in AMIDOL, including through model composition, and then execute compiled models.

7. Model Algebras and Transformations

In order to support the `Transform/Execute Model` API end point, and enable users to compose models generated in one, or multiple, VDSOLs, we have implemented a model algebra to allow for serial, parallel, and substitional model composition. Models in AMIDOL are composed via the process of **state sharing** a powerful primitive which unifies the values of states across models, joining them. While many unanswered questions exist on state sharing workflows for users, the current AMIDOL framework allows for parallel and serial composition using this mechanism.
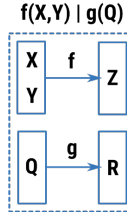
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$$f(X,Y) \mid g(Q)$$

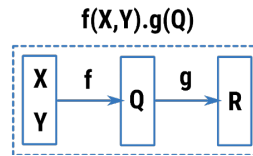Figure 13: Parallel Model Composition in AMIDOL

$$f(X,Y).g(Q)$$

Figure 14: Serial Model Composition in AMIDOL

Parallel composition is accomplished by sharing no state variables, resulting in the diagram shown in 13. This has the effect of taking the union of input and output objects of both morphisms, and treating the new parallel composition as a morphism between these unions. While seemingly simple, this construct allows for a richer set of serial compositions by altering the apparent input and output model signatures of the new composed models to potential match other models with which it can then be composed.

Serial composition, shown in Figure 14, is accomplished by taking the disjoint union of two open models in AMIDOL's IR, $P : X \rightarrow Y$, and $Q : Y \rightarrow Z$ resulting in $P + Q : X \rightarrow Z$, sharing all similar states in the objects Y belonging to P and Q.

Lastly, AMIDOL implements substititional composition using the double-push out rule shown in Figure 15, implementing the double-push out graph rewriting mechanism. Substitution of subgraphs (of events and states) with other compatible subgraphs provides a mechanism for quickly swapping out sub-models used in a bigger model (for instance: changing an SIR model into an SEIR one). The substitional transformation requires a user to give an example of the initial model, the model invariants, and the resulting new model to be obtained via substition. While semantically valid, it presents some possible issues as it is entirely possible for subgraph substitution to accidentally "break" some other part of the model. Consider the case of swapping an SIR sub-model for an SEIR sub-model: elsewhere in the larger model, uses of $S + I + R$ probably indicated "total population" and should be replaced with $S + I + E + R$. To address this issue
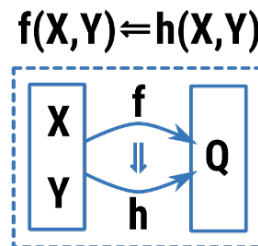
$$f(X,Y) \Leftarrow h(X,Y)$$

Figure 15: AMIDOL Architecture

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we are focusing our future work on providing a mechanism for building up symbolic expressions alleviating the pain of "refactoring" after substitution.