

DARPA ASKE TA2

Due September 17

1 Cover Sheet

Vanessa will put proposal into required template provided.

2 Summary Slide

Vanessa will insert Summary Slide

3 Discussion

Complex system analysis currently requires teams of domain experts, data scientists, mathematicians, and software engineers to support the entire life cycle of model-based inference. The models that result are often bespoke, lack generalizability, are not performable, and make it difficult to synthesize actionable knowledge and policies from their raw outputs. In this proposal we describe AMIDOL: the Agile Metamodel Inference using Domain-specific Ontological Languages, a project that aims to reduce the overhead associated with the model life cycle and enables domain experts and scientists to more easily build, maintain, and reason over models in robust and highly performable ways, and to respond rapidly to emerging crises in an agile and impactful way. AMIDOL is designed to support models in a number of scientific, physical, social, and hybrid domains by allowing domain experts to construct meta-models in a novel way, using visual domain specific ontological languages (VDSOLs). These VDSOLs utilize an underlying intermediate abstract representation to give formal meaning to the intuitive process diagrams scientists and domain experts normally create. AMIDOL’s abstract representations are executable, allowing AMIDOL’s inference engine to execute prognostic queries on reward models and communicate results to domain experts. AMIDOL binds results to the original ontologies providing more explainability when compared to conventional methods. We propose initial development of AMIDOL to address problems in the domain of epidemic outbreak and disease management, and to help coordinate policies and responses to these crises in real-time.

Figure 1 illustrates our three layer approach. The first, domain-specific ontological languages (VDSOLs), are visual formalisms used by domain experts and policy makers to construct scientific, economic, political, or other models, and to modify and maintain these models easily over time. Each VDSOL can be customized for a given domain and consists of formal objects which represent nouns and verbs found in the complex system of interest. Models built in a VDSOL are then compiled to the next layer, the abstract functional interface (AFI). The final layer is built to perform machine-assisted inference on a model.

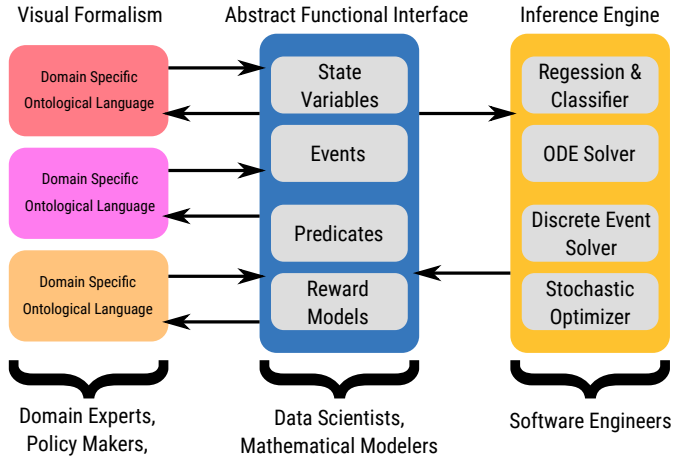


Figure 1: AMIDOL architecture.

Results from this layer are communicated using the AFI to associate outcomes of reward models with the states and actions on which they depend. The AFI binds these results to objects in the VDSOL to communicate results in a domain-specific and contextually informative way.

AMIDOL provides benefits for scientists, policy makers, and practitioners by enabling them to construct and modify robust, performable, and executable models of complex systems with minimal effort, and relating raw statistical and numerical outputs to concrete nouns and verbs represented in our visual formalism. AMIDOL helps highlight causal relationships, comparative analysis, counter-factuals, and aid in planning, risk assessment, and outcome avoidance.

The project consists of two phases over 18 months at a baseline cost to the government of \$XXX. By the end of the program we expect AMIDOL to provide novel mechanisms for machine assisted inference which closes current gaps for domain experts traditionally filled by teams of expert software engineers, data scientists, and mathematicians. We expect AMIDOL to provide a performable system capable of addressing prognostic queries within real-time bounds and to provide an environment enabling rapid response to emerging disasters and threats.

2 Goals and Impact

Our proposed work for AMIDOL consists of four core elements, each of which advances the state-of-the-art of machine-assisted inference and improves the ability of domain experts to efficiently and effectively derive new knowledge from models of systems. We propose AMIDOL to enhance the capabilities of domain experts working with complex computational models of physical, biological, sociological, engineered or hybrid systems. AMIDOL is designed to work as a symbiotic system which works with the domain expert to automatically generate executable models from VDSOLs, provide meaningful results, and explainable outcomes when dealing with crises and real-time events.

Visual Domain Specific Ontological Languages: AMIDOL will include a formal ontological language which describes systems as formal objects classified as either a noun or a verb [CG00]. Nouns define the state space, and verbs define transitions in the state space serving as a formal toolbox of interchangeable components. These VDSOLs will enable domain experts to build models of complex systems which are easier to maintain, validate, and verify, and avoid common pitfalls of monolithic and hand-coded implementations. VDSOLs can be designed specific to a domain and provide a visual formalism which allows domain experts to interact with process and ontological models in an intuitive fashion, providing revolutionary improvements to the ability of domain experts to rapidly test models against data, validate models, and calibrate them to improve accuracy and eliminate bias.

Intermediate Representation as an Abstract Functional Interface: Each VDSOL is implemented in a state-level AFI. Current diagrams used to represent complex systems relate to executable models only informally. Any change to the diagram must also be made separately by hand in the executable model, leading to inconsistencies and errors. Additionally, solution methods have no way to tie results and outcomes to these diagrams impairing the ability of domain experts to leverage their results. AMIDOL's AFI provides an intermediate representation backed by a formal and verified implementation of state variables, actions which alter state variables, input predicates which allow enabling conditions and state dependent rates for actions, and output predicates which define the resulting change in state variables after an action occurs. The AFI provides hooks for the inference engine to interact with these formal components in order to solve reward models which define metrics over state variables and actions. The results of the solver are then translated back through the AFI where they are bound to objects in the VDSOL to provide contextual meaning, and allow for comparative analysis and hypothesis testing using the visual formalism. The AFI will allow AMIDOL to achieve orders of magnitude improvement in terms of speed and accuracy of implementation and solution when compared to hand-coded and bespoke models. The AFI will support any system that can be represented as a state-transition diagram of either a discrete state, or continuous state, system.

Machine-Assisted Inference Engine: AMIDOL couples the AFI with a robust set of solvers in its inference engine. Avoiding the pitfalls of hand-coded models, the AFI provides a solver agnostic way of coupling executable semantics with complex models. The inference engine allows the application of appropriate solution techniques to solve both rate rewards and impulse rewards [CITE], allowing domain experts to execute a wide variety of prognostic queries. Monolithic models are often difficult to optimize and provide poor performance, and unknown quality of results. By using a common inference engine which has been optimized for performance, and for which sensitivity metrics, correctness measures, and validation can be easily defined, AMIDOL provides a more rigorous framework for prognostic queries and the performability necessary to respond to crises in real-time. Initial solvers will include ODE/PDE solution, regression, classification, and clustering analysis, followed shortly by the solution of

CTMC, DTMC, and discrete event simulations of the AFI to provide additional forecasting capabilities.

Usable and Explainable Results: We provide a mechanism for connecting the results of machine-assisted inference to our VDSOLs, allowing the results of our inference engine to be communicated in a domain specific way. The inference engine uses the AFI to recall the state variables and actions used to define a given reward variable, and then traces these to objects in the VDSOL. We will build on these connections and relations by additionally allowing domain experts to define rewards related to variations of a given model, enabling comparative analysis, and prognostic queries which relate to conditional forecasting, or comparative analysis. These results and outcomes can be viewed over a number of experiments, and are stored in a results database over which planning analysis for optimality, risk identification, and outcome avoidance can be executed. This aspect of the work helps domain experts extract knowledge from the results of machine learning and model analysis, providing not only raw results, but contextual information, and allows them to explore the results within the frame of reference of the models they have built, identifying bottlenecks and hazards, and giving the practitioners more agility when responding to real-time events and crises. Domain experts will be able to frequently update results, test new hypotheses, and leverage machine generated queries and results to extract scientific knowledge.

The four components described above combine to substantially advance the state-of-the-art, decreasing the effort required to build and maintain complex models, enables domain experts to be more independent of the support of machine-learning and mathematical modeling specialists, ensures robust and performable solution of the models over metrics of interest, and decreases the effort involved in interpreting the results of these solutions into actionable knowledge. AMIDOL embeds the results of first-wave algorithms (rule-based expert systems) into the provided AFI, couples them with second-wave algorithms (statistical learning) implemented in our inference engine, and enables contextual adaptation, abstraction, and explainability through the VDSOLs and inter-layer connections to provide a third wave approach for machine-assisted inference.

3 Technical Plan

Overview

AMIDOL addresses the problem of machine-assisted inference with two high-level goals: 1) improving the ability of domain experts to build and maintain models and 2) improving the explainability and agility of the results of machine-inference. Our techniques for achieving these goals incorporate abstract functional representations, intermediate languages, and semantic knowledge representation and binding in graph structures into traditional machine learning and model solution techniques.

Scientific Domain: We will to evaluate AMIDOL using the scientific domain of epidemics management and outbreak response. The domain is well supported with a rich body of open source models, freely available high quality data for validation, and benchmarking without extensive data cleaning, and is well documented in the literature. Specifically we propose to focus on modeling the outbreaks and management of the H5N1 strain of influenza [Cha02], and to cross validate our results with a vaccine effectiveness model of H3N2 influenza treatments [skowronski2017interi; Sko+14; Fla+15].

For H5N1 we will form queries and hypotheses in the form of configurations of the model specified in the VDSOL, building representations of various management protocols from the literature [arper2009seasonal]. Using models of the H5N1 outbreak of the early 1990s [Kan+14]

and its eventual treatment [Ari+08] we will answer questions and run diagnostics of various management plans that were proposed, evaluating outcomes with reward variables derived from formal risk models constructed for these events [Din+06].

For the purposes of cross validation, and to build evidence for the generalizability of AMIDOL we will also study the H3N2 vaccine effectiveness models generated when it was found modern vaccination procedures have been less effective [skowronski2017interi; Sko+14; Fla+15]. While these models are epidemiological, they present different models and data as well as user stories which will help us to prove out AMIDOL. We propose to focus on treatment models of H3N2 [Nor+01], including strategies of repeated vaccine application [McL+14], the serial vaccine hypothesis [Sko+17], and the intra-season vaccination model [Fer+17]. We will show comparative analysis of the various strategies and model outcome avoidance and risk by employing a cost-benefit model determined by the CDC [Bri+00].

These domain models have relevance to DARPA given both their relevance to real-time planning and incident response, and their application to treating outbreaks and managing the health of individuals deployed overseas, and models of biological weapon impact and countermeasures. The methods developed for AMIDOL do not assume a specific domain, and the proposed AFI is generalizable and designed to inter-operate with any domain.

Building and Maintaining Models

When modeling complex systems, domain experts often find capability gaps between themselves, data scientists, and mathematicians when attempting to construct models with predictive value and practical utility. Modeling formalisms are often arcane, individual models bespoke with little to no reusability, with large amounts of effort spent building, validating, verifying, and maintaining models. AMIDOL’s goal is to allow scientists to derive insights from models of complex systems by providing a Visual Domain Specific Ontological Language (VDSOL) to naturally represent knowledge about complex systems, as well as hypothesis and prognostic queries about these systems.

Visual Domain Specific Ontological Languages: VDSOLs are built on top of visual formalisms, taking their cue from attempts by other scientists to give meaning to the semi-formal drawings produced by domain scientists [Car05]. While previous work has succeeded in bespoke modeling languages which allow executable diagrams within a given domain [FH07], little attention has been given to the task of generalizing these methods to provide a common framework for machine-assisted inference.

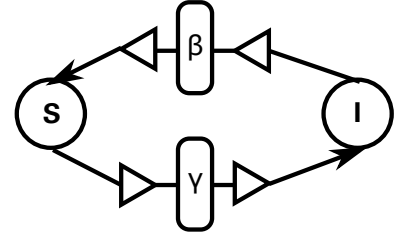
VDSOLs consist of nouns and verbs representing objects and the relationships between objects. As a running example, consider the simple epidemiological infection model presented in Figure 2. The ODEs presented in Figure 3a show the classical SIS model [AM92]. In order to implement this model in AMIDOL domain experts would build the model from a toolkit of visual objects representing common nouns and verbs in the system. In this case they might

$$\begin{aligned}\frac{dS}{dt} &= -\frac{\beta SI}{N} + \gamma I \quad (1) \\ \frac{dI}{dt} &= \frac{\beta SI}{N} - \gamma I \quad (2)\end{aligned}$$

(a) SIS Model ODE Representation



(b) SIS Model VDSOL Representation



(c) SIS Model AFI Representation

Figure 2: Example of VDSOL, AFI, and ODE representation of a SIS infection model. The inference engine in this case would implement a solver for the formal version of the model in (b).

be working from a broader VDSOL for infectious diseases, and choose to use a noun for susceptible patients, and a noun for infected patients, and connect them with verbs for infection and recovery. We represent the result of this modeling process in the visual formalism shown in Figure 2b. While the VDSOL has an underlying binary representation, AMIDOL will allow domain experts to build the VDSOL visually, in a similar manner to that used for generalized modeling environments [Cou+06] but with domain specific context and representation.

Abstract Functional Interfaces: VDSOLs in AMIDOL are provided meaning through the use of formal semantics using a state-level AFI. The AFI provides an abstract notion of state variables, actions, input and output predicates, and reward models which implements these abstractions in the form of template classes, a technique borrowed from the practice of generic programming [MDS09]. Objects in the VDSOL parameterize the components of the AFI providing a pipeline for code generation using these templates, an approach common to multi-level modeling [San99] approaches. The AFI itself is implemented in the manner of a labeled-transition system similar to a Petri-net [Mur89] or stochastic activity networks [SM00]. Allowing the state variables to take on real number values allows us to express continuous systems in a manner similar to fluid Petri-nets [TK93]. The current values of all state variables represents the state of the model, input predicates define action enabling conditions, and allow for state variable dependent rates, and output predicates define the changes to state variables when a given action occurs.

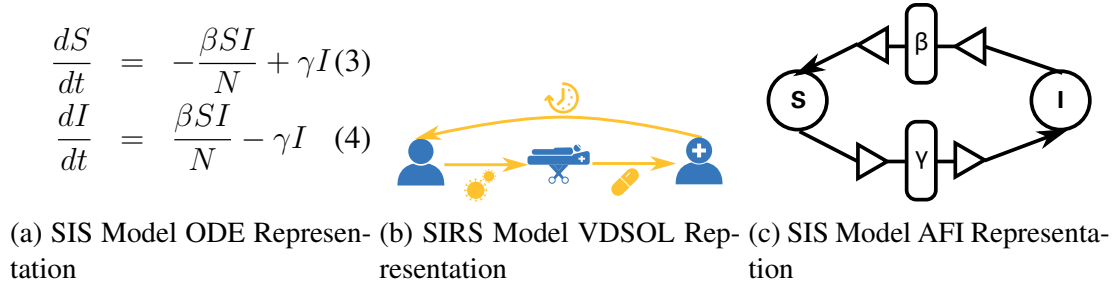


Figure 3: Example of VDSOL, AFI, and ODE representation of a SIRS infection model. The inference engine in this case would implement a solver for the formal version of the model in (b).

Because all objects in a given VDSOL are implemented in the AFI, and have corresponding representations it is possible for domain experts to test hypotheses and examine alternative configurations by changing components and building model variations. Figure 4 demonstrates how one might build differing versions of a single object in our SIS model to test a hypothesis. Here we have two versions of the susceptible, but healthy, patient population. The top variant uses the same object as 2b, while the bottom variant has vital dynamics included which account for birth and death. The AFI implementation of the vital dynamics variant includes up to two shared variables, indicated by "?" in the figure which will be parameterized by the modeler when the object is included, to allow the birth process that is part of this object to account for the total population. When connected in the VDSOL, the user will be prompted to indicate these shared variables, which should be set to I for the SIS model, or I and R for the SIRS model in Figure 3 to represent births of susceptible but healthy individuals at any stage of disease progression. Practitioners can then construct two different models by swapping out a few objects in the model to test the hypothesis as to the sensitivity of the model to different assumptions. Figure 3 shows an example with an expanded set of classes for individuals in the model, including a "recovered" step where individuals have been cured of the disease and are conferred temporary immunity against reinfection.

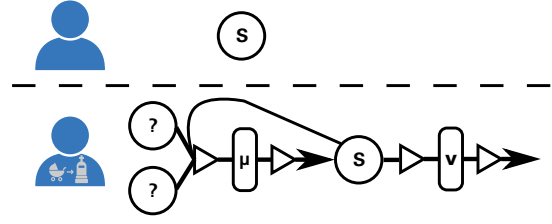
Machine-Assisted Inference Engine: Solution of the AFI in AMIDOL will support a rich set of prognostic queries using a machine-assisted inference engine. Included in the AFI is the ability to define reward models in the form of rate and impulse rewards [SM91]. Rate rewards are defined for discrete subsets of the values of state variables in the model, (e.g. average number of infected individuals, or the number of infected individuals at time t) and impulse rewards are defined on the basis of action occurrence (e.g. how many vaccinations were administered). This approach allows for a solver agnostic approach to metric definition. Users can select from a library of implemented solvers, applying the most appropriate and performable solver for each study. The inference engine will support classification, regression, conditional metrics on the basis of variable input predicates applied to actions in the AFI, counter-factual

identification by employing trace analysis [KT09], and methods such as bifurcation analysis [CCH06] to understand the phase space geometry of the output to explore comparative impact.

AMIDOL supports grouping models via a design of experiments interface. Statistically designed experiments help build a valid basis for developing a set of empirical models of the system being investigated, and allow the models model can be manipulated mathematically or graphically [DON84; EP78]. This approach allows users to represent alternative plans or hypotheses, and perform analysis for planning and policy analysis by assessing risk, optimality, and scoring experiments on the basis of avoidance criteria.

Improving Explainability

We propose to make our results more accessible to domain experts, when compared to the current state of the art, by utilizing the AFI not just for translation from the VDSOL into executable primitives with formal meaning, but also to communicate metrics and results back into the domain in question. Just as the AFI links nouns and verbs in the domain space to formal primitives and class implementations, reward variables on formal primitives can be communicated back into the domain on the basis of the relationships defined by the AFI and objects in the VDSOL. Outcomes from our inference engine will be represented as a property graph, connected to domain knowledge as represented by the ontology given by VDSOL object relations. Outcomes will be aligned as feature vectors and connected to elements in the AFI, and their corresponding objects in the VDSOL. Optional domain knowledge will be incorporated as structural types in the VDSOL, and used to help clarify outcomes from the AFI. Validated knowledge will be fed back into the system as domain knowledge and used to help strengthen the VDSOL's representation and encode new information derived from hypotheses tests allowing a repetitive feedback process of continuous refinement.



(a) Comparison of susceptible patients with and without vital dynamics.

$$\frac{dS}{dt} = \mu N + \frac{\beta SI}{N} + \xi R - \nu S$$

(b) ODE modification for vital statistics impacting susceptible patients.

Figure 4: Example of different building block versions for our healthy patients object in the VDSOL, one without vital dynamics (birth/death factors), one with, along with their AFI representations.

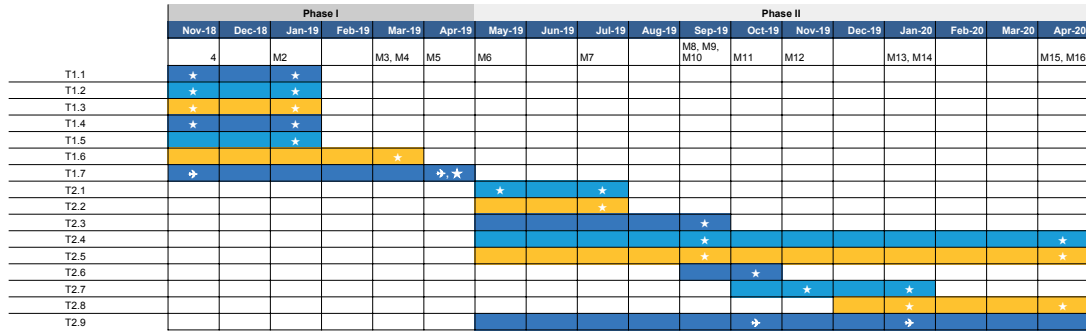


Figure 5: Gantt Chart.

4 Capabilities/Management Plan

The team will be led by Galois PI Dr. Eric Davis. Dr. Davis will lead a team of engineers at Galois' office in Portland. AMIDOL will be developed from an agile perspective to enable it to integrate with other TA performers where necessary, and ensure responsiveness to ASKE program goals. A project manager will assist by tracking engineering requirements and development schedules and helping to coordinate development efforts for TA2.

Our development will follow a model of continuous integration (CI). Code changes will undergo automatic checking and nightly build tests to catch defects and problems as early as possible. Test models and benchmarks will be assembled early in the process to ensure development efforts are providing accurate results in reasonable performance bounds, with a special focus on issues of model sensitivity and uncertainty quantification. These development practices are standard at Galois and have been successfully employed for a number of previous DARPA programs such as Transparent Computing and Brandeis.

Dr. Eric Davis is a Principal Scientist at Galois, where he performs research on data science, data engineering, and formal modeling. He conducted work on large-scale data-dependence modeling as part of an IBM Doctoral Fellowship which received the Best Paper Award from the Symposium for Reliable and Distributed Systems.

5 Task Description Document(TDD)

Phase I

Task 1.1: Definition of initial VDSOL for epidemic outbreak and response. Design VDSOL specification for initial domain based on published research, focus on models of H5N1 and H3N2 incidents and responses. **Milestones:** M1, M2.

Task 1.2: Design and development of initial AMIDOL Abstract Functional Interface. Specification of AFI primitives: state variables, actions, and predicates. **Milestones:** M2, M2.

Task 1.3: Initial AMIDOL machine-assisted inference engine development for prognostic queries on models defined in the VDSOL. **Milestones:** M1, M2.

Task 1.4: Investigation of epidemic response domain model. Implementation of Epidemic Response domain model for H5N1 and H3N2. Experiments on counter-factual analysis from models derived from these domains, and to build user stories on analysis, planning, and crisis response. **Milestones:** M1, M2.

Task 1.5: Definition of correctness, sensitivity, and uncertainty metrics. Communication of these results using the AFI to provide context in the ontology described by the VDSOL to improve practitioner understanding. **Milestones:** M2.

	Milestones	Month
M1	Report on initial architectures, algorithms, and approaches.	1
M2	Interim report describing prototype system.	3
M3	Initial code release.	5
M4	Phase I report.	5
M5	Milestone report on initial prototype, phase I development, and major challenges.	6
M6	Report on lessons learned, updated architectures, algorithms and approaches.	7
M7	Report describing initial results and proposing evaluation metrics.	9
M8	Interim code release.	11
M9	Scripted demonstration of system showing performance for real-world system.	11
M10	Milestone report on scripted demonstration prototype and initial performance benchmarks.	11
M11	Milestone report on progress towards live demo and final code release.	12
M12	Interim report quantifying system performance, comparing with alternative state-of the art approaches.	13
M13	Live demonstration of system showing performance for real-world system/process.	15
M14	Milestone report on final prototype development and remaining challenges.	15
M15	Final code release.	18
M16	Phase II Report.	18

Figure 6: Milestones.

Task 1.6: Prototype integration. Full initial prototype integrating tasks 1.1 - 1.5 ready for demonstration and initial code release. **Milestones:** M3, M4.

Task 1.7: Project integration, PI meetings, travel, project management, reporting. **Milestones:** M1, M4.

Phase II

Task 2.1: Integrate feedback from PI meeting and lessons learned from the initial prototype into the plan for maturing to the demo milestone **M13**. **Milestones:** M3, M4, M5, M6.

Task 2.2: Performance benchmarking of AMIDOL. Design and release of test models to stress performance, accuracy, and validation. Testing of the initial prototype and highlight of areas for improvement. **Milestones:** M7.

Task 2.3: Graph-based knowledge representation utilizing meta-model ontology. Development of rich outcome representation in the VDSOL ontologies and meta-models to improve explainability of the model for practitioners. **Milestones:** M8.

Task 2.4: Verification and validation of inference engine. Verification, and validation of back-end algorithms using benchmarks developed for 2.2 to find possible flaws in prototype implementation. Refinement of metrics developed in 1.5. **Milestones:** M8, M10, M15.

Task 2.5: Refinement of VDSOL, AFI, and Inference Engine. Based on lessons learned in task 2.1, and V&V efforts for 2.4, we will update the VDSOL, AFI, and inference engine implementations for the scripted demonstration of the new system for use in a real-world example of crises response to an emerging epidemic. **Milestones:** M9, M10, M15.

Task 2.6: We will extend the existing VDSOL to support additional models of epidemic and crises response to prepare for the live demonstration in month 15. **Milestones:** M11.

Task 2.7: User story and scenario development for live demo. **Milestones:** M12, M13.

Task 2.8: Final Integration and Testing of AMIDOL. **Milestones:** M14, M15, M16.

Task 2.9: Project integration, PI meetings, travel, project management, reporting. **Milestones:** M5, M11, M14, M15, M16.

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