ORNL/TM-2023/3133

INTERSECT Architecture Specification: Use Case Design Patterns (Version 0.9)

Christian Engelmann and Suhas Somnath

September 30, 2023

Approved for public release.
Distribution is unlimited.

OAK RIDGE National Laboratory

ORNL IS MANAGED BY UT-BATTELLE LLC FOR THE US DEPARTMENT OF ENERGY

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

ORNL/TM-2023/3133

Laboratory Directed Research and Development Program
Self-Driven Experiments for Science/Interconnected Science Ecosystem (INTERSECT) Initiative

INTERSECT Architecture Specification: Use Case Design Patterns (Version 0.9)

Christian Engelmann and Suhas Somnath

September 30, 2023

Prepared by
OAK RIDGE NATIONAL LABORATORY
Oak Ridge, TN 37831-6283
managed by
UT-Battelle LLC
for the
US DEPARTMENT OF ENERGY
under contract DE-AC05-00OR22725

CONTENTS

LIST OF FIGURES v
LIST OF TABLES vii
GLOSSARY ix
ACKNOWLEDGEMENTS xi
ABSTRACT xiii
REVISION RECORD xv
1. INTRODUCTION 1
2. TERMINOLOGY AND CONCEPTS 4
3. DESIGN PATTERNS FOR SCIENCE USE CASES 6
3.1 INTRODUCTION TO DESIGN PATTERNS 6
3.2 ANATOMY OF A SCIENCE USE CASE DESIGN PATTERN 7
3.3 FORMAT OF A SCIENCE USE CASE DESIGN PATTERN 8
4. CLASSIFICATION OF SCIENCE USE CASE DESIGN PATTERNS 10
4.1 STRATEGIC PATTERNS 11
4.2 ARCHITECTURAL PATTERNS 11
5. CATALOG OF SCIENCE USE CASE DESIGN PATTERNS 13
5.1 STRATEGIC PATTERNS 13
5.1.1 Experiment Control 13
5.1.2 Experiment Steering 15
5.1.3 Design of Experiments 17
5.1.4 Multi-Experiment Work ow 20
5.2 ARCHITECTURAL PATTERNS 23
5.2.1 Local Experiment Control 23
5.2.2 Distributed Experiment Control 25
5.2.3 Local Experiment Steering 28
5.2.4 Distributed Experiment Steering 31
5.2.5 Local Design of Experiments 34
5.2.6 Distributed Design of Experiments 37
5.2.7 Local Multi-Experiment Work ow 40
5.2.8 Distributed Multi-Experiment Work ow 43
6. BUILDING SOLUTIONS USING SCIENCE USE CASE DESIGN PATTERNS 46
6.1 A STEP-BY-STEP GUIDE 46
6.2 PATTERN COMPOSITIONS 47
7. CASE STUDIES 50
7.1 AUTOMATION FOR GRID INTERCONNECTED-LABORATORY EMULATION 50
7.2 AUTONOMOUS ADDITIVE MANUFACTURING 52
7.3 AUTONOMOUS CONTINUOUS FLOW REACTOR SYNTHESIS 55
7.4 AUTONOMOUS MICROSCOPY 59
7.5 AUTONOMOUS ROBOTIC CHEMISTRY LABORATORY 62
REFERENCES 66

LIST OF FIGURES

1-1 The INTERSECT autonomous robotic chemistry laboratory operates using analysis of experimental data for the design of experiments. 1
1-2 The INTERSECT ecosystem vision connects instruments with edge and center computing resources. 2
1-3 The INTERSECT Architecture project in the context of Oak Ridge National Laboratory (ORNL)'s Self-driven Experiments for Scienti c Interconnected Science Ecosystem (INTERSECT) Initiative. 3
3-1 Science use case anatomy as experiment loop control problem and as multi-experiment work ow loop control problem 8
4-1 Classi cation of the science use case design patterns 10
5-1 Experiment Control strategic pattern components and control/data ow 13
5-2 Experiment Steering strategic pattern components and control/data ow 15
5-3 Design of Experiments strategic pattern components and control/data ow 17
5-4 Multi-Experiment Work ow strategic pattern components and control/data ow (using multiple experiments with Experiment Control strategic patterns in this example) 21
5-5 Example of a Multi-Experiment Work ow strategic pattern directed acyclic graph 21
5-6 Local Experiment Control architectural pattern components and control/data ow 24
5-7 Distributed Experiment Control architectural pattern components and control/data ow . . . 26
5-8 Local Experiment Steering architectural pattern components and control/data ow 29
5-9 Distributed Experiment Steering architectural pattern components and control/data ow . . . 32
5-10 Local Design of Experiments architectural pattern components and control/data ow 35
5-11 Distributed Design of Experiments architectural pattern components and control/data ow . 38
5-12 Local Multi-Experiment Work ow architectural pattern components and control/data ow (using multiple local experiments with Local or Distributed Experiment Control architectural patterns in this example) 41
5-13 Example of a Local Multi-Experiment Work ow architectural pattern directed acyclic graph 41
5-14 Distributed Multi-Experiment Work ow architectural pattern components and control/data ow (using multiple local and remote experiments with Local or Distributed Experiment Control architectural patterns in this example) 44
5-15 Example of a Distributed Multi-Experiment Work ow architectural pattern directed acyclic graph 44
6-1 Example: Components and control/data ow of Experiment Steering and Design of Experiments strategic pattern composition 48
6-2 Example: Components and control/data ow of Local Experiment Steering and Distributed Design of Experiments architectural pattern composition 49
7-1 The Automation for Grid Interconnected-Laboratory Emulation use case 50
7-2 Experiment Steering strategic pattern for the Automation for Grid Interconnected-Laboratory Emulation (AGILE) science use case 51
7-3 Local Experiment Steering architectural pattern for the AGILE science use case 51
7-4 The INTERSECT additive manufacturing system performs 3D metal printing with in-situ observations and thermo-mechanical simulations to build “born quali ed” structures. 52
7-5 Experiment Steering and Design of Experiments strategic patterns for the additive manufacturing (AM) science use case 53

7-6 Distributed Experiment Steering and Distributed Design of Experiments strategic patterns for the AM science use case 54
7-7 An autonomous continuous ow reactor synthesis science use case 55
7-8 Design of Experiments strategic pattern for the Autonomous Continuous Flow Reactor Synthesis (AutoFlowS) science use case 56
7-9 Design of Experiments strategic pattern for the AutoFlowS science use case, using the Multi-Experiment Work ow strategic pattern. 57
7-10 Local Design of Experiments architectural pattern for the AutoFlowS science use case . . . 57
7-11 Local Design of Experiments architectural pattern for the AutoFlowS science use case, using the Local Multi-Experiment Work ow architectural pattern 58
7-12 An autonomous microscopy science use case 59
7-13 Experiment Steering strategic pattern for the autonomous microscopy science use case . . . 60
7-14 Distributed Experiment Steering architectural pattern for the autonomous microscopy science use case 61
7-15 The INTERSECT autonomous robotic chemistry laboratory operates using analysis of experimental data for the design of experiments. 62
7-16 Design of Experiments strategic pattern for the autonomous robotic chemistry laboratory (ACL) science use case 63
7-17 Design of Experiments strategic pattern for the ACL science use case, using the Multi-Experiment Work ow strategic pattern. 63
7-18 Local Design of Experiments architectural pattern for the ACL science use case 64
7-19 Local Design of Experiments architectural pattern for the ACL science use case, using the Local Multi-Experiment Work ow architectural pattern 65

LIST OF TABLES

4-1 Feature comparison and relationships of the science use case strategic patterns 12
4-2 Relationships of the science use case strategic and architectural patterns 12

GLOSSARY

ACL autonomous robotic chemistry laboratory. v, vi, xv, 1, 18, 22, 36, 39, 42, 45, 62–65
AGILE Automation for Grid Interconnected-Laboratory Emulation. v, 50, 51
AI arti cial intelligence. xiii, 1, 2, 5, 7, 10, 16, 19, 36, 39, 46, 62
AM additive manufacturing. v, vi, 52–54
AutoFlowS Autonomous Continuous Flow Reactor Synthesis. vi, xv, 29, 55–58
CNMS Center for Nanophase Materials Sciences. 59
CPU central processing unit. 59
DAG directed acyclic graph. 20, 41, 44
DFT density functional theory. 59
DoDAF DoD Architecture Framework. 6
DOE U. S. Department of Energy. 1
ESSenergy storage system. 50
EV electric vehicle. 50
GPGPU general-purpose computing graphics processing unit. 59
GRID-C Grid Research Integration and Deployment Center. 50, 51
GUI graphical user interface. 32, 47, 48, 60
HMI human-machine interface. 33, 60
HPC high-performance computing. xiii, 7, 59
INTERSECT Self-driven Experiments for Scientific Interconnected Science Ecosystem. v, xiii, 2, 3, 6
IR infra-red. 52
MD molecular dynamics. 59
NAS network attached storage. 48
OO object-oriented. 7
OODA observe, orient, decide, and act. 5, 28, 29, 31, 32, 34, 35, 37, 38
OPL Our Pattern Language. 7
ORNL Oak Ridge National Laboratory. v, 2, 3, 6, 52, 59
PE power electronics. 50, 51
PID proportional–integral–derivative. 10, 16
PV photovoltaic. 50
SME subject matter expert. 18, 53, 55, 62
SNSSpallation Neutron Source. 45, 52
SoSsystem of systems. 2, 6
STEM scanning transmission electron microscopy. 16, 32, 33, 59, 60
TBB Thread Building Blocks. 7

ACKNOWLEDGEMENTS

Research sponsored by the Laboratory Directed Research and Development Program of Oak Ridge National Laboratory, managed by UT-Battelle, LLC, for the U. S. Department of Energy.

ABSTRACT

Connecting scientific instruments and robot-controlled laboratories with computing and data resources at the edge, the Cloud or the high-performance computing (HPC) center enables autonomous experiments, self-driving laboratories, smart manufacturing, and artificial intelligence (AI)-driven design, discovery and evaluation. The Self-driven Experiments for Scientific Discovery / Interconnected Science Ecosystem (INTERSECT) Open Architecture enables science breakthroughs using intelligent networked systems, instruments and facilities with a federated hardware/software architecture for the laboratory of the future. It relies on a novel approach, consisting of (1) science use case design patterns, (2) a system of systems architecture, and (3) a microservice architecture. This document introduces the science use case design patterns of the INTERSECT Architecture. It describes the overall background, the involved terminology and concepts, and the pattern format and classification. It further details the 12 defined patterns and provides insight into building solutions from these patterns. The document also describes the application of these patterns in the context of several INTERSECT autonomous laboratories. The target audience are computer, computational, instrument and domain science experts working in the field of autonomous experiments.

REVISION RECORD

Version	Date	Description
0.9	09/30/2023	Internal draft and review release with the following changes: ˆ Edits from the EuroPLoP paper review, improving readability and consistency ˆ Improved abstract and introduction ˆ Added autonomous additive manufacturing use case
0.8	06/30/2023	Internal draft and review release with the following changes: ˆ Edits from the EuroPLoP paper review, improving readability and consistency ˆ Improved graphics with color scheme ˆ Added autonomous microscopy use case ˆ Added autonomous robotic chemistry laboratory (ACL) use case ˆ Added Autonomous Continuous Flow Reactor Synthesis (AutoFlowS) use case
0.7	03/31/2023	Internal draft release with the following changes: ˆ Added Local and Distributed Multi-Experiment Work ow architectural patterns
0.6	31/12/2022	Internal draft release with the following changes: ˆ Changed naming scheme for architectural patterns from Remote ... to Distributed ... ˆ Improved the autonomous microscopy section
0.5	09/30/2022	Public release with the following changes: ˆ Further clari ed terminology in pattern component diagrams (using “Test”) ˆ Added section about design pattern compositions ˆ Removed sections for INTERSECT case studies from public release due to lack of maturity
0.4	06/30/2022	Internal draft release with the following changes: ˆ Added experiment result to terminology and pattern description diagrams ˆ Added optional post-processing of raw experiment result to all architectural patterns ˆ Clari ed language about remote components in architectural patterns ˆ Added legend about data/control paths to diagrams in architectural patterns ˆ Added a section for building solutions using science use case design patterns ˆ Added sections for INTERSECT case studies
0.3	04/04/2022	Internal draft release with the following changes: ˆ Clari ed terminology and concepts ˆ Improved science use case design pattern introduction ˆ Extended science use case design pattern format by clarifying existing pattern properties and adding new pattern properties ˆ Reorganized science use case design pattern classi cation ˆ Added 2 architectural patterns (local and remote experiment control) ˆ Signi cantly extended the descriptions of all patterns in the catalog, added new pattern property descriptions and improved pattern component diagrams
0.2	01/06/2022	Internal draft release
0.1	12/31/2021	Initial, unpublished draft

1. INTRODUCTION

The U. S. Department of Energy (DOE)'s Arti cial intelligence (AI) for Science report [23] outlines the need for intelligent systems, instruments, and facilities to enable science breakthroughs with autonomous experiments, self-driving laboratories, smart manufacturing, and AI-driven design, discovery and evaluation [29]. The DOE's Computational Facilities Research Workshop report [1] identi es intelligent systems/facilities as a challenge with enabling automation and reducing human-in-the-loop needs as a cross-cutting theme.

Autonomous experiments, self-driving laboratories and smart manufacturing employ machine-in-the-loop intelligence for decision-making. Human-in-the-loop needs are reduced by an autonomous online control that collects experiment data, analyzes it, and takes appropriate operational actions to steer an ongoing or plan a next experiment. It may be assisted by an AI that is trained online and/or offline with archived data and/or with synthetic data created by a digital twin. Analysis and decision making may also rely on rule-based approaches, causal or physics-based models, and advanced statistical methods. Human interaction for experiment planning, observation and steering is performed through appropriate human-machine interfaces.

For example, both the rate and output of traditional materials synthesis and discovery are currently too slow and too small to e ciently provide needed advances. An autonomous robotic chemistry laboratory (ACL) (Figure 1-1) can operate 24/7 with high precision to greatly accelerate materials discovery and innovation. It relies on the design of a laboratory utilizing robotic and autonomous tools for the manipulation of laboratory equipment and characterization tools. A robotic platform with three major components is used: a mobile base, a robotic arm, and software characterization tools including integration/feedback with AI.

Figure 1-1. The INTERSECT autonomous robotic chemistry laboratory operates 24/7 using analysis of experimental data for the design of experiments.

A federated hardware/software ecosystem (Figure 1-2) for connecting instruments with edge and center computing resources is needed that autonomously collects, transfers, stores, processes, curates, and archives scienti c data in common formats. It must be able to communicate with scienti c instruments and computing and data resources for orchestration and control across administrative domains, and with

humans for critical decisions and feedback. Standardized communication and programming interfaces are needed that leverage community and custom software for scientific instruments, automation, workflows and data transfer. Pluggability is required to permit quickly adaptable and deployable solutions, reuse of partial solutions for different use cases, and the use of digital twins, such as a virtual instrument, robot or experiment. This federated ecosystem needs to follow an open architecture standard to enable adoption.

Figure 1-2. The INTERSECT ecosystem vision connects instruments with edge and center computing resources.

Oak Ridge National Laboratory (ORNL)'s Self-driven Experiments for Scientific Interconnected Science Ecosystem (INTERSECT) architecture project (Figure 1-3), titled “An Open Federated Architecture for the Laboratory of the Future”, creates an open federated hardware/software architecture for the laboratory of the future using a novel system of systems (SoS) and microservice architecture approach, connecting scientific instruments, robot-controlled laboratories and edge/center computing/data resources to enable autonomous experiments, self-driving laboratories, smart manufacturing, and AI-driven design, discovery and evaluation.

The project describes science use cases as design patterns that identify and abstract the involved hardware/software components and their interactions in terms of control, work and data flow. It creates a SoS architecture of the federated hardware/software ecosystem that clarifies terms, architectural elements, the interactions between them and compliance. It further designs a federated microservice architecture, mapping science use case design patterns to the SoS architecture with loosely coupled microservices, standardized interfaces and multi programming language support. The primary deliverable of this project is an INTERSECT Open Architecture Specification, containing the science use case design pattern catalog, the federated SoS architecture specification and the federated microservice architecture specification.

This document introduces the science use case design patterns of the INTERSECT Open Architecture Specification. The basic template for a science use case design pattern is defined in a loop control problem paradigm. At the moment, there are two classes of science use case design patterns, based (1) on high-level solution methods using experiment control architecture features at a very coarse granularity and (2) on more specific solution methods using hardware and software architecture features at a finer granularity. The classification scheme itself is open for extension, such as for adding new patterns for each class or new