Facundo Molina

Assistant Professor
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Research Statement: my main research interests are in the area of Software Testing and Analysis and the use of Artificial Intelligence for Software Engineering (AI4SE), with the goal of improving software reliability and quality.

Employment History

2025 - Present — **Assistant Professor** - *Complutense University of Madrid*, Madrid, Spain.
As an Assistant Professor, I conduct research on software testing and analysis and AI4SE. Key projects I currently work are:
- *Documentation-guided fuzzing:* use of Large Langugage Models (LLMs) to extract input constraints from documentation, and then use these constraints to perform constraint-aware fuzzing.
- *Metamorphic testing for AI models:* automated inference of metamorphic relations targeting AI models with the goal of identifying weaknesses in these models.
- *ASCEND:* industry project coordinated by Boeing Aerospace Spain SLU and ANZEN Aerospace Engineering SL, where I work with the IMDEA Software Institute implementing formal verification-based techniques for model-based safety analyses.

Additionally, I am currently teaching programming courses such as Programming Technology and Programming II for Computer Science and Data Science degrees.

2022 2025 — **Postdoctoral Researcher** - *IMDEA Software Institute*, Madrid, Spain.
I worked on software testing and analysis, which included developing and implementing novel program analysis techniques, and disseminating our research on top tier software engineering conferences and journals. The main projects I participated are:
- *State Field Coverage:* definition and implementation of a novel metric for oracle quality, based on a coverage criterion focused on object state (field values).
- *FixCheck:* patch correctness assessment improvement based on random testing and Large Language Models (LLMs). A tool is implemented using Java, Python, Docker and also using Hugging Face and llama.cpp for supporting LLMs.
- *MemoRIA:* automated inference of metamorphic oracles combining grammar-based fuzzing, dynamic analysis and SAT-based analysis. A prototype is implemented using Java and Python, and using Randoop for the dynamic analysis and Alloy for the SAT-based analysis.
- *PLI:* symbolic execution for programs that manipulate complex heap-allocated data. A prototype is implemented in Java on top of the Symbolic PathFinder engine.

2017 - 2022 — **Ph.D. Student** - *FaMaF, University of Córdoba*, Argentina.
My PhD was focused on developing techniques for the *automated generation of test oracles* using search-based and learning-based techniques (evolutionary algorithms and neural nets). My advisor was Prof. Nazareno Aguirre and my dissertation is available in the UNC digital repository. The main contributions of my thesis are:
- *SpecFuzzer:* automated inference of test oracles in the form of class specifications using grammar-based fuzzing. A tool is implemented using Java and Python, and built on top of the Daikon dynamic invariant detector.
- *EvoSpex:* search-based inference of postconditions of Java methods using genetic algorithms. A tool is implemented in Java using the JGAP library.
- *NNInvs:* data structure object classification using artificial neural networks. One prototype is implemented using Java and Python, relying on the scikit-learn library. A second prototype is developed (to be used in the context of symbolic execution) using the Keras deep learning library.

2014 - 2022 **Teaching Assistant** - *Department of Computer Science, University of Río Cuarto*, Argentina.
I was a Teaching assistant different courses of a Computer Science degree, including Computability and Complexity, Distributed and Outsourced Software Engineering, and Introduction to Programming. My teaching duties involved being in charge of practical classes where students had to solve assignments. Before graduating in 2017, I was a Student teaching assistant in courses such as Data Structures and Algorithms, Algorithms Design Techniques, Programming Paradigms and System Design and Analysis where I helped other teacher assistants.

2015 - 2019 **Software Engineer** - *SMF Consulting S.L.*
Java Software Developer providing solutions to different customers based on an ERP platform. During this time I worked with different teams implementing backend solutions in Java (CRUD operations, API definitions, and integrations with other platforms), maintaining a PostgreSQL database, extending and improving a frontend for retail operations using JavaScript, and performing DevOps taks managing AWS and Vultr servers.

Education

2017 - 2022 **Ph.D., Computer Science**
Dissertation: Techniques based on Learning and Search for Specification Inference.
Faculty of Mathematics, Astronomy, Physics and Computing - FaMaF
University of Córdoba - Argentina

2012 - 2017 **Computer Science Licenciate**
(5-year + thesis undergraduate program of study)
Department of Computer Science - FCEFQyN
University of Río Cuarto - Argentina
Thesis project: Automatic Learning of Relational Specifications using Evolutionary Computation.
Average score: 9.43 out of 10

2012 - 2014 **B.S. in Computer Science**
Department of Computer Science - FCEFQyN
University of Río Cuarto - Argentina
Thesis project: Project in the course of Distributed and Outsourced Software Engineering.
Average score: 9.33 out of 10

Publications

July 2024 **Abstraction-Aware Inference of Metamorphic Relations**
Agustín Nolasco, Facundo Molina, Renzo Degiovanni, Alessandra Gorla, Diego Garbervetsky, Mike Papadakis, Sebastian Uchitel, Nazareno Aguirre and Marcelo F. Frias.
ACM Conference on the Foundations of Software Engineering, FSE 2024, Porto de Galinhas, Brazil, July 15 - 19, 2024. [doi]

May 2024 **Improving Patch Correctness Analysis via Random Testing and Large Language Models**
Facundo Molina, Juan Manuel Copia and Alessandra Gorla.
To appear in the 17th IEEE International Conference on Software Testing, Verification and Validation, ICST 2024, Toronto, Canada, May 27 - 31, 2024. [pdf]

October 2023 **Enabling Efficient Assertion Inference**
Aayush Garg, Renzo Degiovanni, Facundo Molina, Maxime Cordy, Nazareno Aguirre, Mike Papadakis, and Yves Le Traon.
IEEE 34th International Symposium on Software Reliability Engineering, ISSRE 2023, Florence, Italy, October 9 - 12, 2023. [doi]

October 2023 **Precise Lazy Initialization for Programs with Complex Heap Inputs**
Juan Manuel Copia, Facundo Molina, Nazareno Aguirre, Marcelo F. Frias, Alessandra Gorla, and Pablo Ponzio.
IEEE 34th International Symposium on Software Reliability Engineering, ISSRE 2023, Florence, Italy, October 9 - 12, 2023. [doi]

September 2023 **SpecFuzzer: A Tool for Inferring Class Specifications via Grammar Based Fuzzing** - Facundo Molina, Nazareno Aguirre and Marcelo d'Amorim
IEEE/ACM 38th International Conference on Automated Software Engineering, ASE 2023, Luxembourg, September 11 - 15, 2023. [doi]

July 2023 **EvoSpex: A Search-based Tool for Postcondition Inference**
Facundo Molina, Pablo Ponzio, Nazareno Aguirre and Marcelo F. Frias.
ACM SIGSOFT 32nd International Symposium on Software Testing and Analysis, ISSTA 2023, Seattle, USA, July 17 - 21, 2023. [doi]

April 2023 **Efficient Bounded Exhaustive Input Generation from Program APIs**
Mariano Politano, Valeria Bengolea, Facundo Molina, Marcelo F. Frias, Nazareno Aguirre, and Pablo Ponzio.
26th International Conference on Fundamental Approaches to Software Engineering, FASE 2023, Paris, France, April 22 - 27, 2023. [doi]

November 2022 **Learning to Prune Infeasible Paths in Generalized Symbolic Execution**
Facundo Molina, Pablo Ponzio, Nazareno Aguirre and Marcelo F. Frias.
IEEE 33rd International Symposium on Software Reliability Engineering, ISSRE 2022, Charlotte, NC, USA, October 31 - Nov. 3, 2022. [doi]

May 2022 **Fuzzing Class Specifications**
Facundo Molina, Marcelo d'Amorim and Nazareno Aguirre.
Proceedings of the 44th ACM/IEEE International Conference on Software Engineering, ICSE 2022, Pittsburgh, USA, May 22-27, 2022. [doi]

May 2021 **EvoSpex: An Evolutionary Algorithm for Learning Postconditions**
Facundo Molina, Pablo Ponzio, Nazareno Aguirre and Marcelo F. Frias.
Proceedings of the 43rd ACM/IEEE International Conference on Software Engineering, ICSE 2021, Madrid, Spain, May 23-29, 2021. [doi]

September 2020 **Applying Learning Techniques to Oracle Synthesis**
Facundo Molina
Doctoral Symposium, Proceedings of the 35th IEEE/ACM International Conference on Automated Software Engineering, ASE 2020, Australia, September 21-25, 2020. [doi]

July 2019 **An Evolutionary Approach to Translating Operational Specifications into Declarative Specifications** - Facundo Molina, César Cornejo, Renzo Degiovanni, Germán Regis, Pablo Castro, Nazareno Aguirre and Marcelo Frias
Science of Computer Programming, Volume 181, Pages 47-63, 2019. [doi]

May 2019 **Training Binary Classifiers as Data Structure Invariants**
Facundo Molina, Pablo Ponzio, Renzo Degiovanni, Germán Regis,

Nazareno Aguirre and Marcelo Frias
Proceedings of the 41th International Conference on Software Engineering, ICSE 2019, Montreal, Canada, May 25-31, 2019. [doi]

SEPTEMBER 2018 **A Genetic Algorithm for Goal-Conflict Identification**
Renzo Degiovanni, Facundo Molina, Germán Regis and Nazareno Aguirre
Proceedings of the 33rd ACM/IEEE International Conference on Automated Software Engineering, ASE 2018, Montpellier, France, September 3-7, 2018. [doi]

MAY 2018 **From Operational to Declarative Specifications using a Genetic Algorithm** - Facundo Molina, Renzo Degiovanni, Germán Regis, Pablo Castro, Nazareno Aguirre and Marcelo Frias
Proceedings of the 11th International Workshop on Search-Based Software Testing, SBST@ICSE 2018, Gothenburg, Sweden, May 28-29, 2018. [doi]

NOVEMBER 2016 **An Evolutionary Approach to Translate Operational Specifications into Declarative Specifications** - Facundo Molina, César Cornejo, Renzo Degiovanni, Germán Regis, Pablo Castro, Nazareno Aguirre and Marcelo Frias
Proceedings of the 19th Brazilian Symposium on Formal Methods SBMF 2016, Natal, Brazil, November 22-25, 2016. [doi]

PUBLIC TALKS

JULY 2024 **Abstraction-aware Inference of Metamorphic Relations**
Research track, FSE conference, Porto de Galinhas, Brazil.

MAY 2024 **Improving Patch Correctness Analysis via Random Testing and Large Language Models** - Research track, ICST conference, Toronto, Canada.

OCTOBER 2023 **Automated Generation of Test Oracles**
Invited speaker at the *Jornadas de Ciencias de la Computación*, JCC 2023, Rosario, Argentina.

SEPTEMBER 2023 **SpecFuzzer: A Tool for Inferring Class Specifications via Grammar-based Fuzzing** - Tool Demonstrations track, ASE conference, Luxembourg.

JULY 2023 **EvoSpex: A Search-based Tool for Postcondition Inference**
Tool Demonstrations track, ISSTA conference, Seattle, USA.

NOVEMBER 2022 **Learning to Prune Infeasible Paths in Generalized Symbolic Execution**
Research track, ISSRE conference, Charlotte, USA.

OCTOBER 2022 **Fuzzing Class Specifications** - Oral communication,
Simposio Argentino de Ingeniería de Software ASSE 2022 (virtual), Argentina.

MAY 2022 **Fuzzing Class Specifications** - Research track, ICSE conference, Pittsburgh, USA.

MARCH 2022 **EvoSpex: An Evolutionary Algorithm for Learning Postconditions**
Invited talk, Argentine Workshop on Fundamentals for the Automatic Analysis and Construction of Software FACAS 2022, La Falda, Argentina.

OCTOBER 2021 **EvoSpex: An Evolutionary Algorithm for Learning Postconditions**
Oral communication, Simposio Argentino de Ingeniería de Software ASSE 2021 (virtual), Argentina.

May 2021 **EvoSpex: An Evolutionary Algorithm for Learning Postconditions**
Research track, ICSE conference (virtual), Madrid, Spain.

September 2020 **Applying Learning Techniques to Oracle Synthesis**
Doctoral symposium, ASE conference (virtual), Melbourne, Australia.

May 2019 **Training Binary Classifiers as Data Structure Invariants**
Research track, ICSE conference, Montréal, Canada.

March 2019 **Learning Hybrid Invariants to Improve Symbolic Execution on Structurally Complex Inputs** - Invited talk, Argentine Workshop on Fundamentals for the Automatic Analysis and Construction of Software FACAS 2021, La Falda, Argentina.

September 2018 **A Genetic Algorithm for Goal-Conflict Identification**
Research track, ASE conference, Montpellier, France.

November 2016 **An Evolutionary Approach to Translate Operational Specifications into Declarative Specifications** - Research track, Brazilian Symposium on Formal Methods SBMF 2016, Natal, Brazil.

Research Prototypes

FixCheck FixCheck is a tool for improving patch correctness analyses in Java. It combines static analysis, random testing and LLMs to automatically generate tests that highlight and explain the potential incorrectness of a patch.
FixCheck is available at: https://github.com/facumolina/fixcheck

SpecFuzzer SpecFuzzer is a tool that automatically infers test oracles in the form of class specifications (postconditions, invariants), and works for Java classes. SpecFuzzer uses a fuzzer as a generator of candidate assertions; a dynamic invariant detector –Daikon– to filter out assertions invalidated by a test suite; and a mutation-based mechanism to cluster and rank assertions, so that similar constraints are grouped and then the stronger prioritized.
SpecFuzzer is available at: https://github.com/facumolina/specfuzzer

EvoSpex EvoSpex is a tool that, given a Java method, uses an evolutionary algorithm to produce a specification of the method's current behavior, in the form of postcondition assertions. EvoSpex implements a classic genetic algorithm that searches for a succinct postcondition that accepts the current method behavior, while rejecting any deviation from such behavior.
EvoSpex is available at: https://github.com/facumolina/evospex

PLI PLI is an efficient symbolic execution approach for programs that manipulate complex heap-allocated data structures with rich structural constraints. PLI works for Java, and allows preconditions to be specified as standard operational predicates for concrete structures, eliminating the need for additional specifications tailored to symbolic heaps.
PLI is available at: https://github.com/JuanmaCopia/spf-pli

Research Grants & Scholarships

2017 **Doctoral Scholarship**
5-year Scholarship granted by Argentina's National Scientific and Technical Research Council (CONICET) to fund doctoral students.

2016 **EVC-CIN Scholarship**
1-year Scolarship granted by the argentinian National Inter University Council (CIN) to encourage undergraduate students to pursue scientific vocations.

Participation in Funded Research Projects

11/2023-02/2024 **ANZEN: Model-based Safety Analysis through Formal Verification.**
This project is a collaboration between IMDEA and Anzen Aerospace Engineering, SL to explore the use of formal verification tools in the context of model-based safety analysis. I participate as part of the team from IMDEA Software.

09/2023-08/2027 **ESPADA: Efficient and Secure Data Protection Against Digital Attack.**
Project lead by Juan Caballero and Alessandra Gorla, granted by the spanish Ministerio de Ciencia e Innovación, co-funded by European Union ESF, EIE and NextGeneration funds. I participate as a member of the research team.

12/2022-11/2024 **PRODIGY: Asegurando la seguridad, escalabilidad y funcionalidad de los sistemas digitales de procedencia.**
Project lead by Juan Caballero y Pedro Moreno-Sánchez, granted by the spanish Ministerio de Ciencia e Innovación, and co-funded by European Union ESF, EIE and NextGeneration funds. I participate as a member of the research team.

Honors & Awards

2020 **Latin America PhD Award**
A research award for PhD students in computing related fields in their 3rd year or beyond at universities in Latin America, and granted by Microsoft Research.

2018 **Best Paper Award**
From Operational to Declarative Specifications using a Genetic Algorithm 11th International Workshop on Search-Based Software Testing, SBST 2018.

2016 **Best Paper Award**
An Evolutionary Approach to Translate Operational Specifications into Declarative Specifications, 19th Brazilian Symposium on Formal Methods, SBMF 2016.

2016 **University of Rio Cuarto flag bearer for a 1-year period**
Traditional honour in educational institutions in Argentina to the three top students in the institution.

Supervised Students

2024 **Claudio Dosantos** - *Undergraduate student* - University of Río Cuarto, Argentina.
Claudio's thesis aims to analyze the effectiveness of regression testing when using different kind of oracles, such as unit assertions and contracts.

2024 **Ignacio Gonzalez** - *Undergraduate student* - University of Río Cuarto, Argentina.
Automated test generation tools play a crucial role on dynamic specification inference techniques. Ignacio's work aims at studying how different test generation approaches

affects the effectiveness of specification inference techniques.

2023 **Agustin Nolasco** - *Undergraduate student* - University of Río Cuarto, Argentina. Agustin's thesis presents a new technique for the inference of metamorphic oracles, based on runtime analysis, grammar-based fuzzing and SAT solving.

Academic Service

2024 Program committee at *International Conference on AI Foundation Models and Software Engineering (FORGE 2024)*. Reviewer at *IEEE Transactions on Software Engineering (TSE)*. Programm committee of the Industry track at *International Conference on Software Maintenance and Evolution (ICSME 2024)*. Artifact Evaluation committee at *International, Conference on Software Engineering (ICSE 2024), International Symposium on Software Testing and Analysis (ISSTA 2024)*.

2023 Program committee at *International Working Conference on Source Code Analysis and Manipulation (SCAM 2023)*. Reviewer at *IEEE Transactions on Software Engineering (TSE)*. Artifact Evaluation committee at *International Symposium on Software Testing and Analysis, (ISSTA 2023), Static Analysis Symposium (SAS 2023)*.

2022 Student volunteer at *International Conference on Software Engineering (ICSE 2022.)*

2021 Program committee at *International Workshop on Test Oracles (TORACLE 2021)*.
Student volunteer at *International Conference on Software Engineering (ICSE 2021.)*

2019 Student volunteer at *International Conference on Software Engineering (ICSE 2019.)*

2018 Student volunteer at *International Conference on Automated Software Engineering (ASE 2018)*.

2017 Student volunteer at *International Conference on Software Engineering (ICSE 2017.)*

Extracurricular Courses Taken

October 2019 **Neural Networks and Deep Learning** - Adjunct Professor Andrew Ng
Foundations of Deep Learning
An online non-credit course authorized by deeplearning.ai
Coursera

March 2019 **Introduction to Data Science in Python** - Christopher Brooks
Introduction to data manipulation and cleaning techniques using pandas
An online non-credit course authorized by University of Michigan
Coursera

August 2018 – November 2018 **Neural Networks** - Dr. Francisco Tamarit
Mathematical Foundations of Artificial Neural Networks
Postgraduate courses
University of Córdoba - Argentina

August 2017 – November 2017 **Text Mining** - Dr. Laura Alonso Alemany
Text Mining techniques applied to Natural Language Processing problems (Word similarity, Document clustering, Sense discrimination, Machine translation)
Postgraduate courses

University of Córdoba - Argentina

August 2017 – November 2017 **Information and its Demons** - Dr. Javier Blanco
Information Philosophy
Postgraduate courses
University of Río Cuarto - Argentina

February 2017 **Human Dynamics: Data, Networks and Modelling** - Dr. Márton Karsai
Summer School of Computer Science RIO 2017
University of Río Cuarto - Argentina

March 2016 – June 2016 **Software Testing** - Dr. Renzo Degiovanni
Main software testing techniques using state-of-the-art tools
Postgraduate courses
University of Río Cuarto - Argentina

February 2016 **Systematic Test Case Generation** - Prof. Sarfraz Khurshid
Summer School of Computer Science RIO 2016
University of Río Cuarto - Argentina

February 2016 **Symbolic Program Analysis** - Prof. Willem Visser
Summer School of Computer Science RIO 2016
University of Río Cuarto - Argentina

February 2015 **Description Logic Reasoning** - Dr. Anni-Yasmin Turhan
Summer School of Computer Science RIO 2015
University of Río Cuarto - Argentina

February 2015 **Fundamentals of Quantum Programming Languages** - Dr. Alejandro Díaz-Caro
Summer School of Computer Science RIO 2015
University of Río Cuarto - Argentina

Languages

Spanish: Mother tongue
English: Fluent