Thank you for registering for the 3rd EuMINe General Meeting.

We have successfully received your registration.
Location: King Ferdinand Amphitheater, USAMV, (Calea Mănăștur no.11) Cluj-Napoca.
Date: 07 - 10 July 2026.

Name	Lorand Gabriel Parajdi
Affiliation	Babeş–Bolyai University
Role / position	PostDoc / Academic
Affiliated in an Inclusiveness Target Country (ITC)	Yes
Already participant in the EuMINe COST Action CA22143:	No
EuMINe Working Group Membership:	WG2: Cooperative Development of Materials Informatics Approaches, WG3: Training and Capacity Building, WG5: Dissemination and Communication
You already contacted EuMINe WG leaders/co-leaders about your contribution: (please, note that reimbursement to participants who contacted WG leaders and co-leaders about their contribution to WG work and deliverables will be prioritised)	No
Please briefly describe your contributions to the EuMINe Working Groups (WGs), deliverables, and your potential input to the collaborative and interactive sessions during the meeting (max 2000 characters).	My research focuses on polymer informatics, machine learning, molecular dynamics simulations, and scientific software development for polymer property prediction. I contributed to the development of the AdaptDelivery platform, an online computational framework integrating

molecular dynamics simulations, machine learning models, and interactive web-based visualization tools for predicting structural polymer properties such as the radius of gyration (Rg) and solvent-accessible surface area (SASA).

My contributions include the development of machine learning workflows, implementation of artificial neural network models, integration of computational simulations with predictive frameworks, scientific visualization and web-platform deployment using Python, Flask, PyTorch, Plotly.js, and 3Dmol.js. I also contributed to the development of distributed computational workflows for NAMD molecular dynamics simulations and to the design of scalable data-driven prediction pipelines.

Within the EuMINe COST Action, I am interested in contributing particularly to WG2 (materials informatics and computational approaches), WG3 (training and capacity building) and WG5 (dissemination and communication). I would be interested in collaborative activities related to machine learning for materials science, data-driven prediction frameworks, reproducible computational workflows, scientific web platforms and AI-assisted modeling approaches.

I also look forward to participating in collaborative discussions and interactive sessions activities focused on computational materials science, polymer informatics and interdisciplinary machine learning applications.

Contribution:	Oral
Abstract Title	AdaptDelivery: An Informatics Platform for Polymer Structure–Property Prediction
Authors [FirstName LastName] and Affiliation [Full address]	Lorand Gabriel Parajdi[1 2], Istvan Toth[2], Alex-Adrian Farcas[2], Zsuzsanna Balint[2], Alexandru Kiraly[4] and Alexandra Farcas[2 3] [1] Department of Mathematics, Babeș-Bolyai University, 1 Mihail Kogălniceanu Street, 400084 Cluj-Napoca, Romania [2] National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat Street, 400293 Cluj-Napoca, Romania [3] Department of Physics and Chemistry, Technical University of Cluj-Napoca, 400641 Cluj-Napoca, Romania [4] Department of Computer Science, Babeș-Bolyai University, 400084 Cluj-Napoca, Romania
Keywords [insert up to 7 keywords]	Polymer Informatics; Machine Learning; Molecular Dynamics Simulations; Artificial Neural Networks; Polymer Property Prediction; Scientific Visualization; Computational Materials Science
Abstract [Write the main text here]	Polymers are highly versatile materials with broad applications in materials science, biotechnology, and drug delivery. However, predicting their structural properties remains challenging due to their chemical complexity and conformational diversity. In this work, we present AdaptDelivery, a polymer informatics platform integrating molecular dynamics simulations, machine learning models and

	interactive web-based visualization for rapid prediction of key structural descriptors. The framework combines simulation-derived datasets with artificial neural networks to establish structure–property relationships across diverse synthetic and natural polymers. The resulting models are deployed within the online platform AdaptDelivery, enabling real-time prediction, interactive visualization and user-driven exploration of polymer systems. Ongoing developments focus on expanding the supported polymer space and incorporating additional physicochemical properties for broader applications in computational materials science and polymer informatics.
Acknowledgments [Write any acknowledgments here.]	This work was supported through the project no. 61TE, code PN-IV-P2-2.1-TE-2023-0300.

Best regards,
EuMINe Organizing Committee