

MytilX: A Scalable HPC+AI Framework for Marine Bacterial Contamination Forecasting in Mussel Farming

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Invited talk

High Performance Computing in Modelling and Simulation (HPCMS)

Abstract. Ensuring food safety in bivalve mollusc aquaculture requires timely and accurate predictions of microbiological contamination levels in coastal farming areas. In this talk, we present MytilX, a scalable, integrated High-Performance Computing and Artificial Intelligence framework developed at the University of Naples "Parthenope" to model and forecast bacterial contamination — specifically *Escherichia coli* — in mussel (*Mytilus galloprovincialis*) farming areas along the Campania coastline (Italy).

The system couples three state-of-the-art numerical models: the Weather Research and Forecasting (WRF) model for atmospheric dynamics, the Regional Ocean Modeling System (ROMS) for sea current simulation, and WaComM++, an open-source C++ Lagrangian transport-and-diffusion model for passive tracers, designed for hierarchical and heterogeneous HPC execution. The resulting particle concentration time series serve as input features to AIQUAM++, an ensemble-based AI module that performs time series classification across four contamination severity classes (from Class 0: <67 MPN/100g to Class 3: >4600 MPN/100g). The ensemble integrates multiple deep learning and machine learning architectures (including Transformer, Informer, DLinear, CNN, and KNN) using a weighted majority-voting strategy to exploit the complementary strengths of the individual models.

We discuss the scientific workflow orchestration via the DAGonStar engine, the data management pipeline (TALCO), and the HPC resource requirements for scaling the model from regional to national coverage. Preliminary results from the Campania coast demonstrate the feasibility of the approach, and we outline a roadmap to extend the methodology to other Italian coastal regions and marine species. The talk highlights key challenges in coupling physical simulation with AI inference at scale, and reflects on the broader potential of the HPC+AI paradigm for environmental monitoring and public health protection.

Short bio. Raffaele Montella is an Associate Professor with tenure in Computer Science at the Department of Science and Technologies (DiST), University of Naples "Parthenope" (UNP), Italy. His main research topics and scientific production are focused on tools for high-performance computing, cloud computing, and GPUs with applications in the field of computational environmental science (multi-dimensional geo-referenced big data, distributed computing for modeling, and scientific workflows

and science gateways), leveraging on his experiences in embedded, mobile, wearable, pervasive computing, and Internet of Things. He leads the design and development of GVirtuS (General-purpose Virtualization Service), enabling the execution of CUDA kernels on mobile and embedded devices. He leads a long-standing research effort founded by the Regione Campania, Veterinary Sector, which involves research projects and scientific contracts to model the mytilus farming system using high-performance computing-based coupled simulations to predict and assess mussel farm food quality and mitigate human gastric disease. The methodology developed leverages numerical simulation and Artificial Intelligence technologies to predict mussel contamination with pollutants. He is the Director of the High-Performance Scientific Computing SmartLab (HPSC-SmartLab), bringing together theoretical and practical knowledge from scientists in computer science, scientific computing, applied mathematics, bioinformatics, and computational environmental science, leveraging the best of these research fields to accelerate science and technology. He is the Chief of Technical Operations (CTO) and co-director of the Center for Marine and Atmosphere Monitoring and Modeling (CMMMA), leading the design and management of the HPC infrastructure. In this context, he designed a methodology for gathering coastal marine data through crowd-sourcing for environmental protection, development, and management, leveraging a distributed sensor network carried by leisure yachts. He is the founder and curator of the Museum of Computational Architectures (MArC) at the University of Naples "Parthenope". He heads the UNP node, the CINI National Laboratory, "HPC: Key Technologies and Tools". He leads the AWS Academy at the University of Naples' "Parthenope" initiative, providing full immersive cloud computing classes to undergraduates, master's, and Ph.D. students from diverse academic curricula. He teaches various computer science courses, primarily bachelor's and master's degrees in computing architectures, web technologies, and cloud computing. He pioneered innovative teaching methodologies focusing on various forms of gamification in computer programming education. He holds the Italian National Academic Qualifications as a Full Professor of Computer Science (01/B1, INFO/01-A) and of Computer Engineering (09/H1, 09/IINF-05).

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