Bialystok University of Technology

Doctoral School

COURSE DESCRIPTION CARD

Course name	Numerical Methods and Machine Learning in Material Processing II				
Course type	Optional	**Course code**	SDPB0135	**ECTS credits**	2
Forms and number of hours	Lecture: 20 h	**Scientific discipline**	Mechanical Engineering		
Course objectives	The objective of the course is to extend the competences acquired in Part I towards coupled multiphysics models of material processing and physics-informed, uncertainty-aware machine learning, so that the PhD student can build, calibrate, verify and validate simulation-based and hybrid (physics + data) process models, use them for process design and digital-twin applications, and design AI systems that automate and verify simulation workflows.				
Course content	The course continues Numerical Methods and Machine Learning in Material Processing I and assumes its completion. (1) Coupled thermo-chemo-mechanical models of material processing: cure kinetics of thermosets and photopolymers (autocatalytic Kamal-Sourour type models), heat transfer with reaction exotherm, evolution of process-induced residual stresses and distortion in composites and additively manufactured parts. (2) Solution strategies for coupled problems: monolithic and staggered schemes, stability, stiff kinetics, adaptive time-step control. (3) Verification and validation: method of manufactured solutions, mesh and time-step convergence (Richardson extrapolation, grid convergence index), closure of energy and mass balances, validation metrics against experiment. (4) Inverse problems and parameter identification: least-squares and Bayesian calibration of material and kinetic parameters from DSC, rheometry and thermography data; identifiability and parameter correlation. (5) Uncertainty quantification: sampling designs, Monte Carlo, polynomial chaos, global sensitivity analysis (Sobol indices). (6) Surrogate and reduced-order models: Gaussian process regression, proper orthogonal decomposition, neural operators (DeepONet, Fourier neural operator). (7) Physics-informed machine learning: physics-informed neural networks for forward and inverse problems, embedding of conservation laws and constitutive constraints, limits of applicability. (8) Bayesian optimisation and surrogate-based design of process windows. (9) Digital twins of manufacturing processes: data assimilation, in-situ monitoring, online model updating. (10) Building AI systems for simulation: LLM-based agents orchestrating geometry, meshing, solver set-up, run monitoring and post-processing through deterministic solver APIs (e.g. PyAnsys, open-source FEM/CFD libraries); tool calling with schema-validated input and output; retrieval-augmented generation over solver documentation and literature; the principle that the model proposes and a deterministic layer verifies (dry runs, unit and range checks, balance checks) before any solver start; human approval gates for costly runs; reproducibility (pinned versions, random seeds, full audit trail) and statistical evaluation of agent reliability. The project is an individual hybrid model of a selected material process: a verified and validated numerical model and a calibrated surrogate with				

	quantified uncertainty, optionally embedded in an AI-agent workflow that automates its set-up, execution and verification.		
Teaching methods	Multimedia presentation, problem-based lecture, case studies with solver and ML scripts, live demonstration of AI-agent simulation workflows, individual project		
Assessment method	Exam and defence of the individual project		
Symbol of learning outcome	**Learning outcomes**	**Reference to the learning outcomes for the field of study for the 8th level of Polish Qualification Framework (PRK)**	**Methods of assessing the learning outcomes**
LO1	The PhD student will formulate and solve coupled thermo-chemo-mechanical models of material processing and verify them (mesh and time-step convergence, balance closure).	SD_W1, SD_W2	Passing the lecture and project
LO2	The PhD student will identify material and process parameters from experimental data and quantify the uncertainty and sensitivity of model predictions.	SD_U1	Passing the lecture and project
LO3	The PhD student will build and critically validate physics-informed and surrogate ML models and apply them to process optimisation and digital twins.	SD_U1	Passing the lecture and project
LO4	The PhD student will design an AI-agent system that automates a simulation workflow and enforces deterministic verification of its solver input and results.	SD_W2, SD_U1	Passing the lecture and project

Student workload (in hours)	
Lecture, project	0 / 20 / 0 / 0 / 0
Consultations	5
The unassisted student work	15
Implementation of project tasks and preparation for and participation in exams/tests	30

Total	70
ECTS credits	3
Basic references	1. Oberkampf, W. L., & Roy, C. J. (2010). Verification and Validation in Scientific Computing. Cambridge University Press. ISBN: 978-0521113601. 2. Brunton, S. L., & Kutz, J. N. (2019). Data-Driven Science and Engineering: Machine Learning, Dynamical Systems, and Control. Cambridge University Press. ISBN: 978-1108422093. 3. Rasmussen, C. E., & Williams, C. K. I. (2006). *Gaussian Processes for Machine Learning*. MIT Press. ISBN: 978-0262182539.
Supplementary references	1. Zienkiewicz, O. C., Taylor, R. L., & Zhu, J. Z. (2013). The Finite Element Method: Its Basis and Fundamentals (7th ed.). Butterworth-Heinemann. ISBN: 978-1856176330. 2. Advani, S. G., & Sozer, E. M. (2010). Process Modeling in Composites Manufacturing (2nd ed.). CRC Press. ISBN: 978-1420090819. 3. Raissi, M., Perdikaris, P., & Karniadakis, G. E. (2019). Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. Journal of Computational Physics, 378, 686-707. doi: 10.1016/j.jcp.2018.10.045. 4. Karniadakis, G. E., Kevrekidis, I. G., Lu, L., Perdikaris, P., Wang, S., & Yang, L. (2021). Physics-informed machine learning. Nature Reviews Physics, 3(6), 422-440. doi: 10.1038/s42254-021-00314-5. 5. Saltelli, A., Ratto, M., Andres, T., Campolongo, F., Cariboni, J., Gatelli, D., Saisana, M., & Tarantola, S. (2008). Global Sensitivity Analysis: The Primer. Wiley. ISBN: 978-0470059975. 6. Lewis, P., Perez, E., Piktus, A., Petroni, F., Karpukhin, V., Goyal, N., Küttler, H., Lewis, M., Yih, W., Rocktäschel, T., Riedel, S., & Kiela, D. (2020). Retrieval-augmented generation for knowledge-intensive NLP tasks. Advances in Neural Information Processing Systems, 33, 9459-9474. 7. Yao, S., Zhao, J., Yu, D., Du, N., Shafran, I., Narasimhan, K., & Cao, Y. (2023). ReAct: Synergizing reasoning and acting in language models. International Conference on Learning Representations (ICLR 2023).
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