1.1	**Proposal type**	Master thesis project
1.2	**Name**	Integrative Multi-Scale Computational Modeling of Burn Wound Acute Phase Response: A Mechanistic-Omics Approach with Surrogate Model speedup
1.3	**Description**	The activation of the complement system after burn injury is an essential component of the inflammatory response and mediates various immune reactions. This project presents a comprehensive multiscale computational framework that simulates the acute inflammatory phase during the first 18 days after burn injury through mechanistic modeling enhanced by omics data integration and surrogate model acceleration. **Objectives:** • Develop Agent-Based Multi-scale modeling with omics data integration using the Glazier-Graner-Hogeweg (GGH) model to simulate inflammatory agents behavior[2] • Integrate three distinct temporal and spatial scales: molecular-level omics dynamics, cellular-level agent interactions, and tissue-level spatial diffusion patterns[1] • Implement neural network-based surrogate models to approximate computationally expensive molecular dynamics simulations while maintaining biological fidelity[3] **References:** [1] John W Keyloun et al. "Early transcriptomic response to burn injury: severe burns are associated with immune pathway shutdown". In: *Journal of Burn Care & Research* 43.2 (2022), pp. 306–314. [2] H Ibrahim Korkmaz et al. "An in silico modeling approach to understanding the dynamics of the post-burn immune response". In: *Frontiers in Immunology* 15 (2024), p. 1303776. [3] Ioannis Papapanagiotou et al. "From simulations to surrogates: Neural networks enhancing burn wound healing predictions". In: *Journal of Computational Science* (2025), p. 102593.
1.4	**Work environment**	Research will be conducted within a computational biology research group specializing in burn injury modeling. The team combines expertise in agent-based modeling, bioinformatics, omics data integration, and neural network development. Access to established frameworks for mechanistic understanding of complement-mediated acute phase responses. The available resources include high-performance computing facilities and comprehensive biological databases. Active participation in research publication contributes to thesis grade evaluation.
1.5	**Expectations**	• Programming proficiency (Python for data analysis and modeling) • Understanding of agent-based modeling principles • Neural network and machine learning fundamentals • Bioinformatics data processing capabilities • Multi-scale modeling approaches • Ability to integrate mechanistic simulations with high-dimensional biological data • Strong analytical and problem-solving skills
1.6	**Research Tags**	computational biology, burn injury modeling, agent-based modeling, omics integration, surrogate models, neural networks, inflammation, complement system, acute phase response, multi-scale modeling
1.7	**Programmes**	Computational Science (joint degree UvA/VU)
1.8	**Contact**	Roland V. Bumbuc (r.v.bumbuc@uva.nl)