Computational Science as a driver of discovery for a sustainable society

Draft action agenda 2027-2030

The National Agenda for Computational Science NL laid the foundation for a shared national vision on the role of Computational Science in research and innovation. This Action Agenda builds on that work by translating the agenda into concrete priorities and actions for 2026–2029. It marks the transition from strategic orientation to implementation, with the aim of strengthening the Netherlands' position in Computational Science and maximising its contribution to science, innovation, and society.

Scientific discovery is undergoing an impactful digital transformation. Traditional, sequential and largely offline research workflows are increasingly giving way to automated, integrated and computation-driven approaches. In this context, Computational Science has become a central driver of discovery: explaining complex phenomena, accelerating hypothesis generation and testing, informing experiments and enabling more adaptive and reliable innovation across domains such as health, sustainability, defence and advanced manufacturing.

To remain internationally competitive and to address major societal challenges, the Netherlands must strengthen its position in computational methods, intelligent workflows and cross-sector connectivity. This action agenda therefore proposes three strategic priorities: leadership in methods, modelling and technology; acceleration of scientific discovery through advanced workflows; and ecosystem building through stronger national connectivity.

LEADERSHIP IN METHODS, MODELLING, AND TECHNOLOGY.

Computational Science spans many disciplines, but these share a common methodological basis in modelling, simulation, computing and machine learning. To address fundamental questions in domains such as health, sustainability and defence, Computational Science NL focuses on five cross-cutting areas: multiscale modelling and simulation, data-driven methods, ultra-fast simulation through machine learning, uncertainty quantification and energy-efficient computing.

Positioning Computational Science NL at the forefront of scientific and technological innovation requires a strong national profile through vision documents, position papers and strategic consortia, as well as deeper engagement with industry. It also requires investment in the tools, techniques and computational infrastructures that enable researchers to benefit fully from automation and intelligent systems. In parallel, the community should provide leadership on best practices, reproducibility and the responsible use of AI/ML in scientific computing, in close collaboration with SURF and other HPC and AI infrastructure providers. A forward-looking perspective on next-generation computing technologies, including GPU-based systems, specialised hardware and quantum acceleration, should form an integral part of this effort.

To support this priority, Computational Science NL will publish one to two national position papers yearly, establish three national method-oriented consortia in key areas such as multiscale modelling, ML surrogates and uncertainty quantification, develop a formal collaboration framework with SURF and relevant infrastructure partners, and organise a national roadmap workshop on next-generation computing.

ACCELERATING SCIENTIFIC DISCOVERY THROUGH ADVANCED SCIENTIFIC WORKFLOWS.

The future of scientific discovery is fundamentally hybrid. It combines physics-based modelling, AI-enhanced surrogate models, multiscale simulation, experimental feedback loops and embedded uncertainty quantification. Continuous integrated efforts of fundamental scientific understanding with data-driven acceleration can drive more efficient, reliable and adaptive discovery processes, with scientific reasoning grounded in disciplinary expertise. As such,