

Lithuanian Computational Multi-physics Competence Centre



Mission

The Lithuanian Computational Multi-physics Competence Centre advances cutting-edge multi-physics research and innovation by supporting academia and industry with state-of-the-art computational expertise. We foster collaboration, translate science into impact, and educate the next generation of scientists and engineers to tackle complex real-world challenges.

Leadership

- **Lead:** Prof. em. Bernhard Peters, Chief Research Fellow
- **Consultant:** Prof. em. Rimantas Kačianauskas

Expertise

The Lithuanian Computational Multi-Physics Competence Centre at Vilnius Tech serves as a national hub for advanced computational modelling and simulation. Building on strong foundations in engineering, applied mathematics, and high-performance computing, the Centre brings together expertise in **discrete–continuum coupling, multi-scale modelling, and large-scale simulations** to address complex physical systems that cannot be captured by single-physics approaches alone.

By combining leading multi-physics platforms such as **XDEM** and **COMSOL Multiphysics**, the Centre supports the simulation and analysis of interacting physical phenomena across particles, fluids, structures, and fields. Our activities span fundamental research, applied industrial problem-solving, and advanced education, enabling accurate prediction, optimization, and virtual prototyping of real-world systems.

Core Multi-Physics Expertise

The Centre supports a wide range of multi-physics capabilities, including:

- Coupled **particle–fluid–structure** simulations for complex granular and particulate systems
- Integration of **CFD, FEM, and DEM** for fully resolved multi-physics environments
- Reactive particle systems involving **heat transfer, mass transfer, and chemical reactions**
- Thermo-mechanical interactions in particulate and porous media
- Multi-phase flow and particle transport in industrial and energy systems
- Electro-thermal and electro-chemical coupling in materials and devices
- Bio-process and environmental system modelling involving coupled biological and physical phenomena
- Large-scale and high-fidelity simulations for process optimization and design

- Digital twins and virtual prototyping of complex engineering systems
- Cross-scale modelling linking micro-scale particle behaviour to macro-scale system performance

Impact

For Research, the Centre enables high-impact, interdisciplinary studies by providing advanced modelling capabilities that push beyond conventional simulation boundaries and support international collaboration.

For Industry, it delivers predictive simulation tools that reduce development time, lower experimental costs, and support innovation in energy, manufacturing, materials, and environmental technologies.

For Education, the Centre trains the next generation of scientists and engineers in state-of-the-art multi-physics simulation, equipping them with skills essential for modern research and industry-driven problem solving.

Together, these activities position the Multi-Physics Competence Centre at Vilnius Tech as a key contributor to scientific excellence, industrial competitiveness, and sustainable technological development.

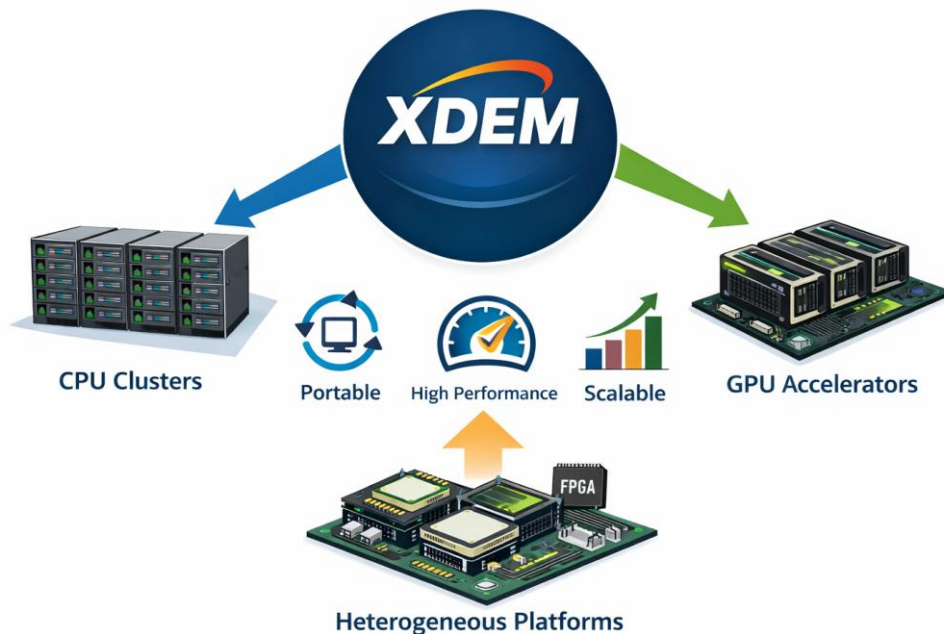
Extended Discrete Element Method (XDEM) Crossing the Exascale Threshold

**When physics meets millions of cores,
scale is no longer a limit.**

At the Lithuanian Computational Multi-physics Competence Centre, we advance hardware-independent software development for XDEM, enabling high-performance simulations across CPUs and GPUs without compromising accuracy, scalability, or maintainability. This approach ensures that cutting-edge multi-physics models remain portable, future-proof, and ready to exploit evolving computing architectures.

By designing XDEM with architecture-agnostic algorithms and performance-portable programming strategies, the same simulation code efficiently runs on traditional CPU clusters, modern GPU-accelerated systems, and emerging heterogeneous platforms. This eliminates costly rewrites, accelerates innovation, and maximizes return on high-performance computing investments for both academia and industry.

The result is a robust and flexible simulation framework capable of tackling industrial-scale problems—from particle-resolved reactive flows to fully coupled multi-physics systems—while seamlessly adapting to the fastest available hardware. This work underpins sustainable software ecosystems and empowers the next generation of computational scientists to focus on physics, not platforms.



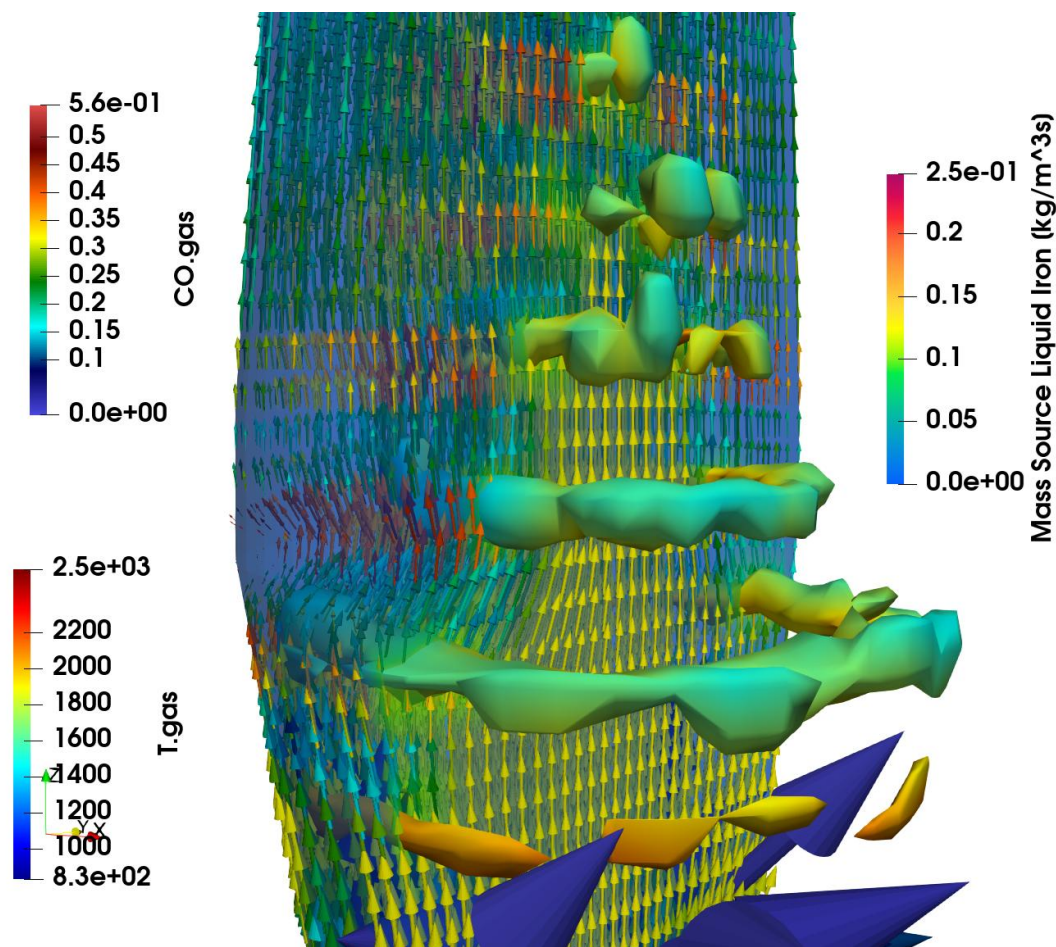
Contact: Prof. em. Bernhard Peters (bernhard-josef.peters@vilniustech.lt), Prof Dr Arnas Kačeniauskas (arnas.kaceniauskas@vilniustech.lt)

Digital Twin of a Blast Furnace

The Lithuanian Computational Multi-physics Competence Centre has developed a high-fidelity digital twin of a blast furnace using the XDEM platform, pushing the boundaries of industrial-scale multi-physics simulation. This digital twin captures the complex interplay between granular solids, reactive flows, heat transfer, and chemical transformations that govern blast furnace performance—across scales ranging from individual particles to the full reactor.

By coupling discrete element modelling with fluid dynamics and thermochemical processes, the model provides unprecedented insight into burden descent, gas distribution, reaction kinetics, and energy efficiency. The digital twin enables virtual experimentation under real operating conditions, supporting process optimization, emission reduction, and safer, more sustainable ironmaking.

Beyond industrial innovation, the blast furnace digital twin serves as a powerful research and educational platform, showcasing how advanced computational multi-physics can translate fundamental science into actionable engineering solutions.

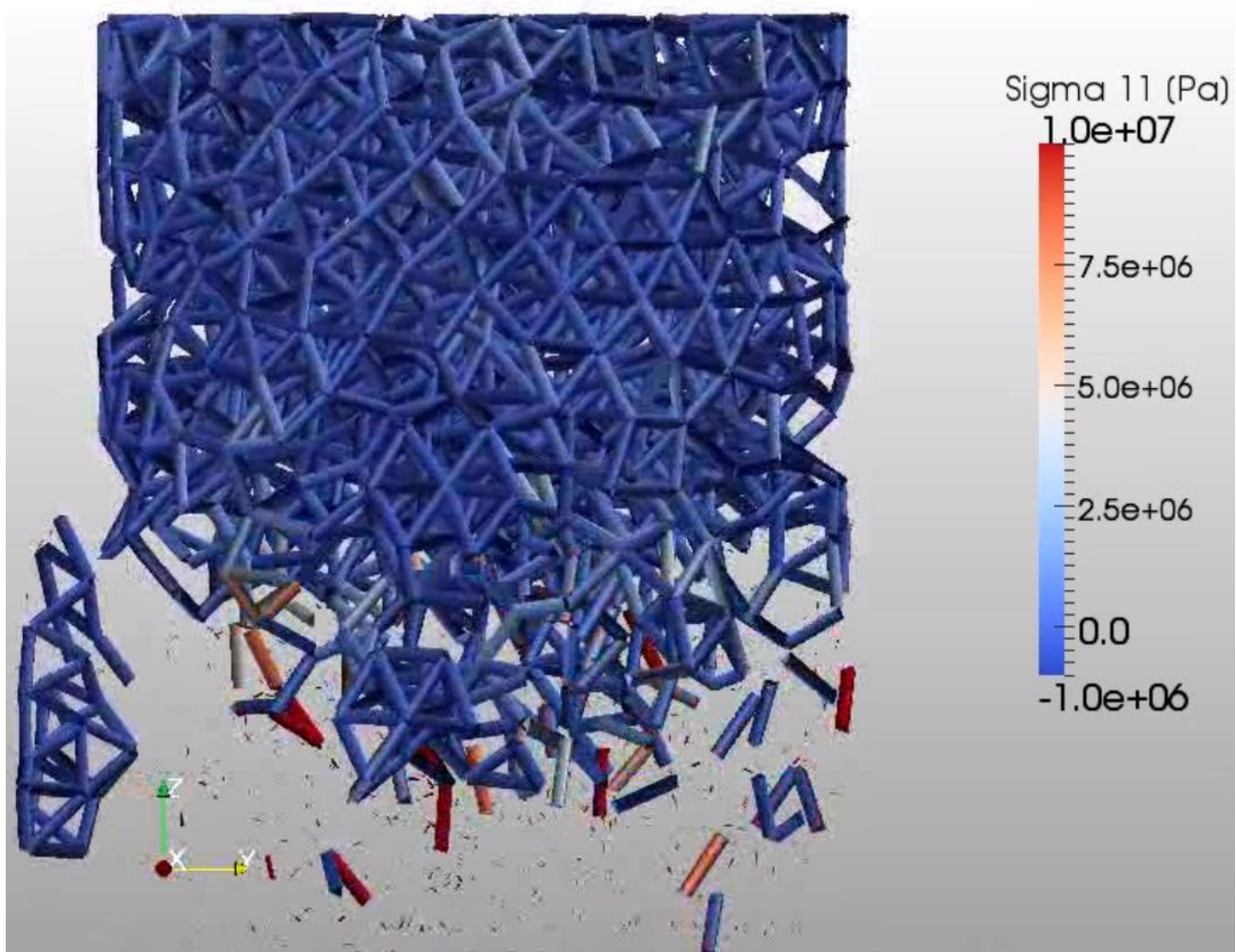


Shape and location of the cohesive zone represented by an iso-surface of the mass transfer rate of molten iron from the iron-bearing particles to the liquid phase of the Euler solver in a vertical slice through the centre of the blast furnace. In addition, the gas temperature and velocity in conjunction with ore particle layers with its surface temperature are depicted in a reduced particle size for better visibility.

Contact: Prof. em. Bernhard Peters (bernhard-josef.peters@vilniustech.lt)

Analysis of mechanical properties of Soil

The Multi-Physics Competence Centre at Vilnius Tech provides advanced analysis of **soil properties through tri-axial testing of granular materials** to support geotechnical engineering and infrastructure development. This activity focuses on evaluating key soil characteristics such as shear strength, stiffness, deformation behaviour, and failure response under representative stress conditions. Treating soil as a granular material enables realistic assessment of load-bearing capacity and stability relevant to foundations, embankments, slopes, and earth-retaining structures. The outcomes support **design validation, risk reduction, and performance-based engineering**, offering industry-relevant insights for construction, transportation, and civil infrastructure projects. Through this work, the Centre strengthens its role as a partner for industry in delivering reliable data and advanced analysis for safe, efficient, and sustainable geotechnical solutions.



Contact: Assoc Prof Dr Ona Lukoševičienė (ona.lukoseviciene@vilniustech.lt), Assoc Prof Dr Urtė Radvilaite (urte.radvilaite@vilniustech.lt), Assoc Prof Dr Sergejus Borodinas (sergejus.borodinas@vilniustech.lt), Prof. em. Bernhard Peters (bernhard-josef.peters@vilniustech.lt)

Separation Efficiency of a Cyclone

The Multi-Physics Competence Centre at Vilnius Tech conducts advanced analysis to support the **development of cyclone separators** with enhanced separation quality. This activity focuses on understanding and predicting the coupled fluid dynamics and particle behaviour that govern particle capture and efficiency under realistic operating conditions. By leveraging multi-physics modelling, the Centre evaluates the influence of design parameters, flow patterns, and particle properties on separation performance. The insights gained support the optimization of cyclone geometry and operating strategies to achieve higher efficiency, lower pressure drop, and improved reliability. This work contributes to the design of more effective particulate control systems for industrial processes, energy production, and environmental protection applications.



Experimental setup for investigating cyclone efficiency

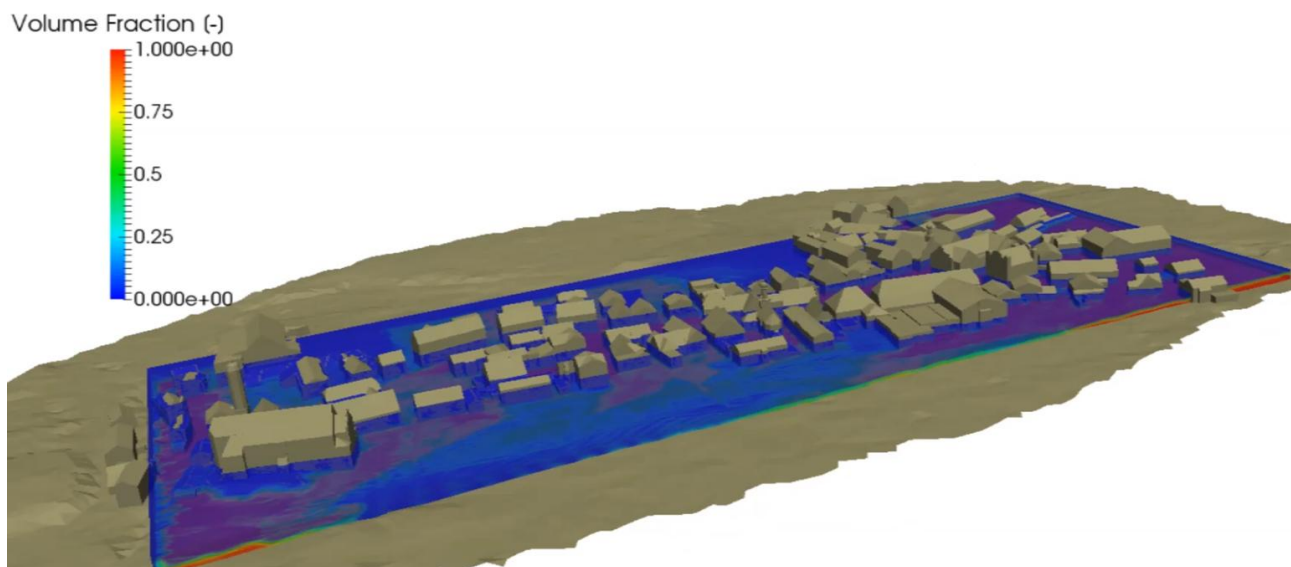
Contact: Dr Aleksandras Chlebnikovas (aleksandras.chlebnikovas@vilniustech.lt), Tautvydas Juknevičius (tautvydas.juknevicius@vilniustech.lt), Prof. em. Bernhard Peters (bernhard-josef.peters@vilniustech.lt)

Integrating Building Information Modelling (BIM) and Geophysical Topology into Multi-physics Analysis

Integrating Building Information Modelling (BIM) and Geophysical Topology into Multi-physics Analysis is a research and innovation project developed within the Multi-physics Competence Centre of Vilnius Tech. The project aims to bridge the gap between digital building design and the complex physical behaviour of the ground and surrounding environment by tightly integrating BIM data with geophysical and topological information.

By combining BIM with advanced multi-physics modelling—covering structural, geotechnical, thermal, and fluid-flow processes—the project enables more realistic and data-driven simulations of buildings and infrastructure systems. This integrated approach supports improved decision-making throughout the entire lifecycle of a structure, from early design and site assessment to construction and long-term performance analysis.

The project contributes to more resilient, sustainable, and efficient built environments by enhancing predictive accuracy, reducing uncertainty, and fostering interoperability between engineering disciplines and simulation tools.



Contact: Assoc Prof Dr Daiva Makutėnienė (daiva.makuteniene@vilniustech.lt), Prof. em. Bernhard Peters (bernhard-josef.peters@vilniustech.lt)

One Roof, Many Futures: Multi-Physics Optimisation of Urban Roof-scapes

The Multi-Physics Competence Centre at Vilnius Tech focuses on one of the most pressing spatial conflicts in sustainable cities: how to optimally use rooftops to meet competing environmental goals. Urban roofs represent a limited and valuable resource that can either host photovoltaic (PV) systems for renewable energy generation or green roofs that enhance air quality, thermal comfort, storm-water retention, and urban biodiversity. In most cases, these two solutions are mutually exclusive—once a roof is allocated, it cannot serve both functions at full efficiency.

To address this challenge, the Centre develops advanced multi-physics modelling and optimisation frameworks that integrate energy systems, structural mechanics, fluid dynamics, heat transfer, and environmental performance. By coupling solar irradiance models with building energy simulations, airflow and pollutant dispersion analyses, and structural constraints, the Centre evaluates how different roof-use strategies perform at building and district scales.

Rather than promoting a single solution, the Centre aims to support evidence-based decision-making. Its tools identify when photovoltaic roofs maximise climate impact through clean energy production, when green roofs provide greater benefits for air quality and urban resilience, and how hybrid or district-level strategies can balance these trade-offs across the city. In doing so, the Multi-Physics Competence Centre positions Vilnius Tech at the forefront of integrated, data-driven urban sustainability research.



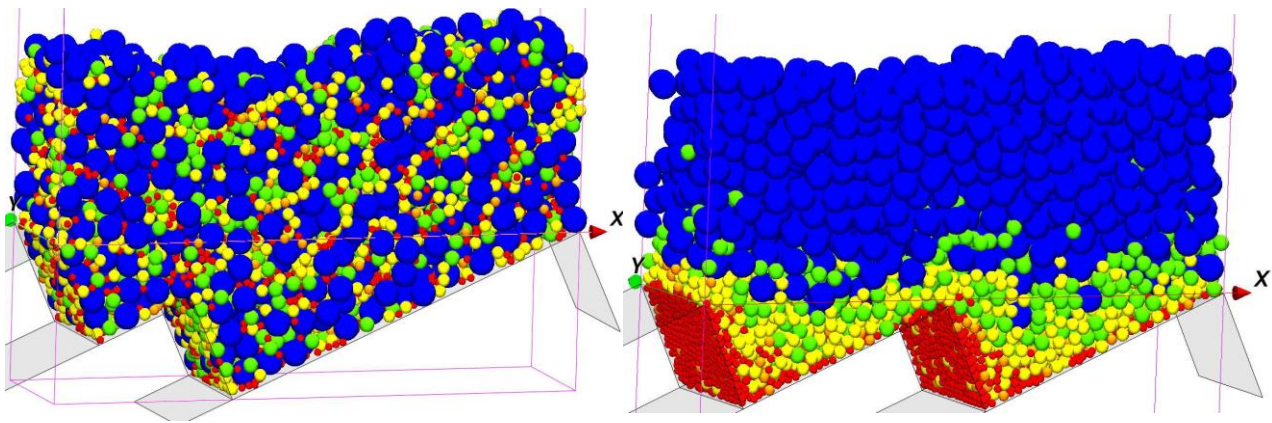
Interplay between renewable energy and air quality

Contact: Assoc Prof Dr Daiva Makutėnienė (daiva.makuteniene@vilniustech.lt), Prof Dr Jonas Gradauskas (jonas.gradauskas@vilniustech.lt), Prof. Vladimir Simic (vsima@sf.bg.ac.rs), Prof em. Bernhard Peters (bernhard-josef.peters@vilniustech.lt)

Segregation on a Forward Acting Grate

The Lithuanian Multi-Physics Competence Center, in close collaboration with the **Lithuanian Energy Institute**, is advancing state-of-the-art understanding of material segregation on forward-acting grates—a critical phenomenon in modern thermal conversion and energy systems. This initiative addresses one of the key challenges in grate-based technologies: the non-uniform distribution of particles that directly affects efficiency, emissions, and operational stability.

Our approach integrates **discrete element methods (DEM)**, enabling a high-fidelity description of particle motion, size and density segregation along the grate. This framework provides unprecedented insight into how operational parameters, fuel properties, and grate kinematics influence segregation dynamics in real operating conditions. The resulting digital tools and validated models support **design optimization, fuel flexibility, and predictive control strategies** for next-generation grate-based energy systems.

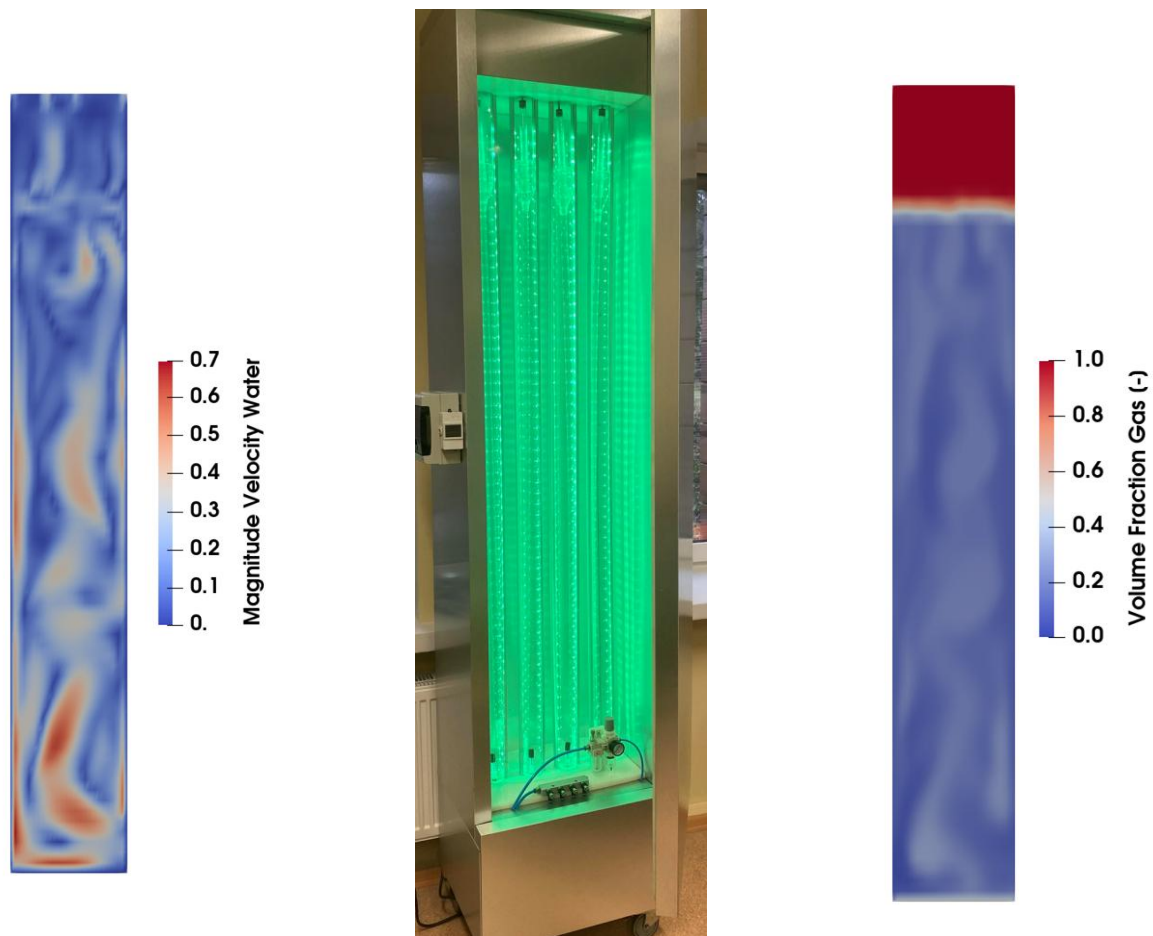


Initial perfectly mixed moving bed and final segregated particles on a forward acting grate.

Contact: Dr Algis Džiugys (algis.dziugys@mail.lei.lt) Prof. Em. Bernhard Peters (bernhard-josef.peters@vilniustech.lt)

Upgrading of Biogas in a Photo-bioreactor

The Multi-Physics Competence Centre at Vilnius Tech is engaged in the development of **biogas upgrading processes using photo-bioreactor systems**. This activity focuses on enhancing the quality of raw biogas by increasing methane concentration while reducing carbon dioxide and other impurities through biologically driven processes. The work supports the integration of **renewable energy production, carbon utilization, and sustainable waste management** within a single technological framework. Photo-bioreactor-based upgrading is being advanced as a pathway toward **low-emission, circular energy systems**, contributing to improved efficiency and environmental performance of biogas facilities. Through this effort, the Centre strengthens its role in advancing innovative bio-energy solutions aligned with European climate and sustainability goals, while supporting industrial applicability and future scale-up of renewable gas technologies.



Distribution of velocity of water and volume fraction of bio gas in a cylindrical Photo-bioreactor

Contact: Assoc Prof Dr Alvydas Zagorskis (alvydas.zagorskis@vilniustech.lt), Prof. em. Bernhard Peters (bernhard-josef.peters@vilniustech.lt)

Bioreactors for Biogas Generation

The Multi-Physics Competence Centre at Vilnius Tech supports the **analysis and development of bioreactors for biogas generation based on fermentation processes**. This activity focuses on understanding and predicting the coupled physical, chemical, and biological phenomena that govern biogas production, including mass and heat transfer, multiphase flow, and microbial activity. By integrating multi-physics modelling and system-level analysis, the Centre enables evaluation of reactor performance, process stability, and operational efficiency under realistic conditions. The work supports optimization of bioreactor design and operating strategies for improved methane yield, reduced energy losses, and enhanced process reliability. These efforts contribute to the advancement of sustainable bioenergy technologies and support industry-driven solutions for renewable gas production, waste valorization, and circular economy applications.

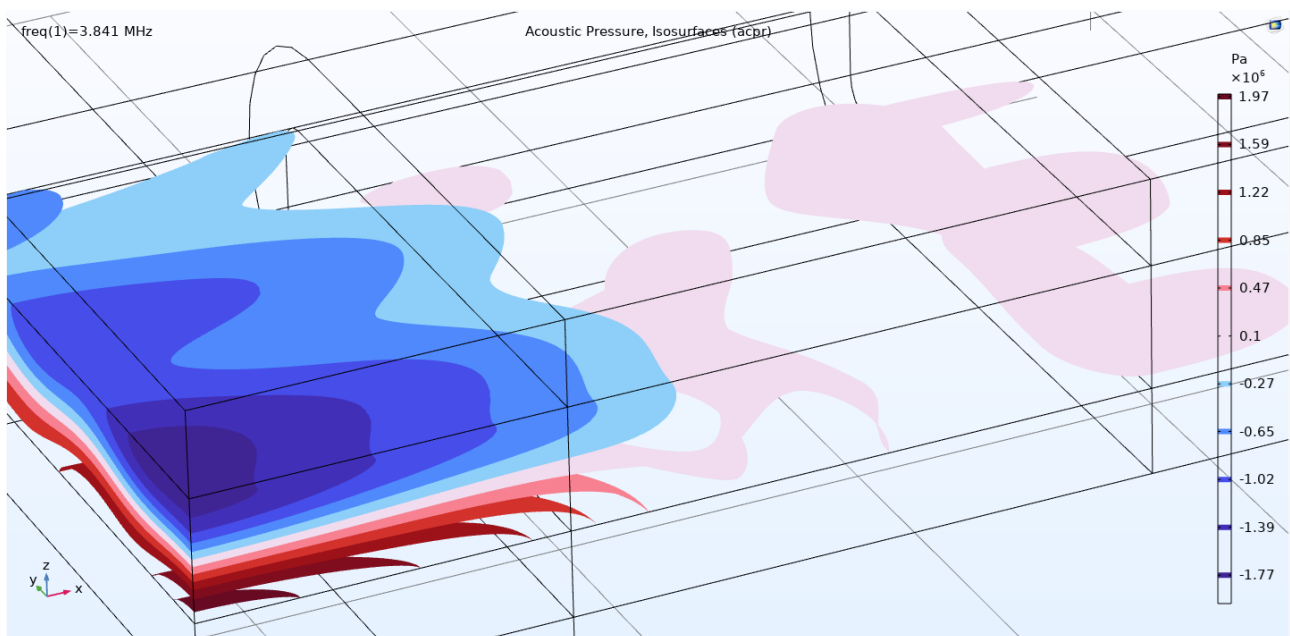


Biogas reactors under different operating conditions

Contact: Assoc Prof Dr Alvydas Zagorskis (alvydas.zagorskis@vilniustech.lt), Prof. em. Bernhard Peters (bernhard-josef.peters@vilniustech.lt)

Acoustic Agglomeration of Particles

The Multi-Physics Competence Centre at Vilnius Tech investigates the **development and optimization of acoustic agglomeration techniques for particulate systems**. This activity focuses on understanding how sound waves can be used to induce particle collisions and aggregation, enhancing the removal of fine particles from gases and aerosols. By analysing the coupled interactions between acoustic fields, particle dynamics, and fluid flow, the Centre evaluates the effectiveness of acoustic agglomeration under various operating conditions. The insights support the design of systems that improve particulate capture efficiency, reduce emissions, and enhance air quality in industrial and environmental applications. This work advances innovative particle control strategies with potential impact in energy, manufacturing, and environmental engineering.

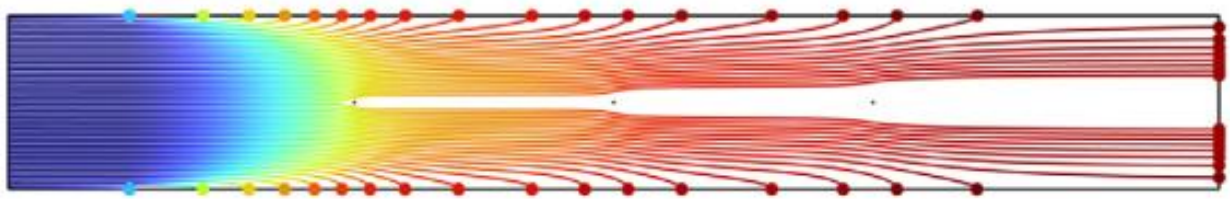


Distribution of acoustic pressure in a particle trap

Contact: Dr Aleksandras Chlebnikovas (aleksandras.chlebnikovas@vilniustech.lt), Prof. em. Bernhard Peters (bernhard-josef.peters@vilniustech.lt)

Precipitation of Particles in an Electric Field

The Multi-Physics Competence Centre at Vilnius Tech conducts advanced analysis of **particle precipitation in electric fields** to support the development of high-efficiency particulate control systems. This activity focuses on understanding the coupled interactions between electric forces, particle dynamics, and fluid flow that govern the capture and removal of fine and ultra-fine particles from gaseous streams. By evaluating the effects of electric field strength, particle properties, and flow conditions, the Centre provides insights for optimizing electrostatic precipitator performance. The work supports the design of systems that maximize particle collection efficiency, reduce emissions, and improve air quality in industrial processes, energy production, and environmental applications. This research contributes to innovative and reliable solutions for sustainable particulate management.



Trajectories of particles ($R = 0.01 \mu\text{m}$) under the influence of an electric field

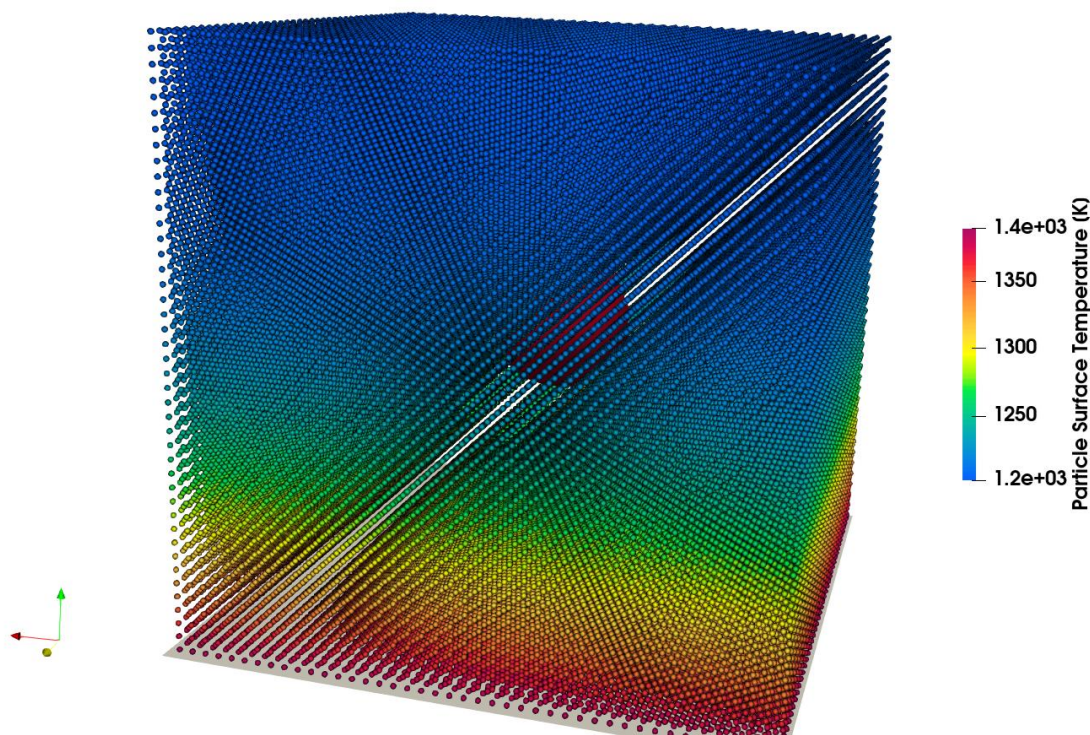
Contact: Dr Aleksandras Chlebnikovas (aleksandras.chlebnikovas@vilniustech.lt), Tautvydas Juknevičius (tautvydas.juknevicius@vilniustech.lt), Prof. em. Bernhard Peters (bernhard-josef.peters@vilniustech.lt)

Insulation properties of refractory materials

This project focuses on the **investigation of heat transport in blocks of granular media** using the **eXtended Discrete Element Method (XDEM)** within a multi-physics modelling framework. Granular materials are widely used in energy, chemical, and thermal engineering applications, where accurate prediction of heat transfer is essential but challenging due to complex particle–particle interactions.

XDEM enables detailed, particle-resolved simulation by coupling discrete element modelling with thermal transport mechanisms, including conduction, convection, and radiation at the grain scale. In this study, XDEM is employed to analyse heat propagation through granular blocks under various boundary conditions, material properties, and packing structures. The numerical approach allows capturing local temperature gradients, contact heat transfer, and transient thermal behaviour that are difficult to access experimentally.

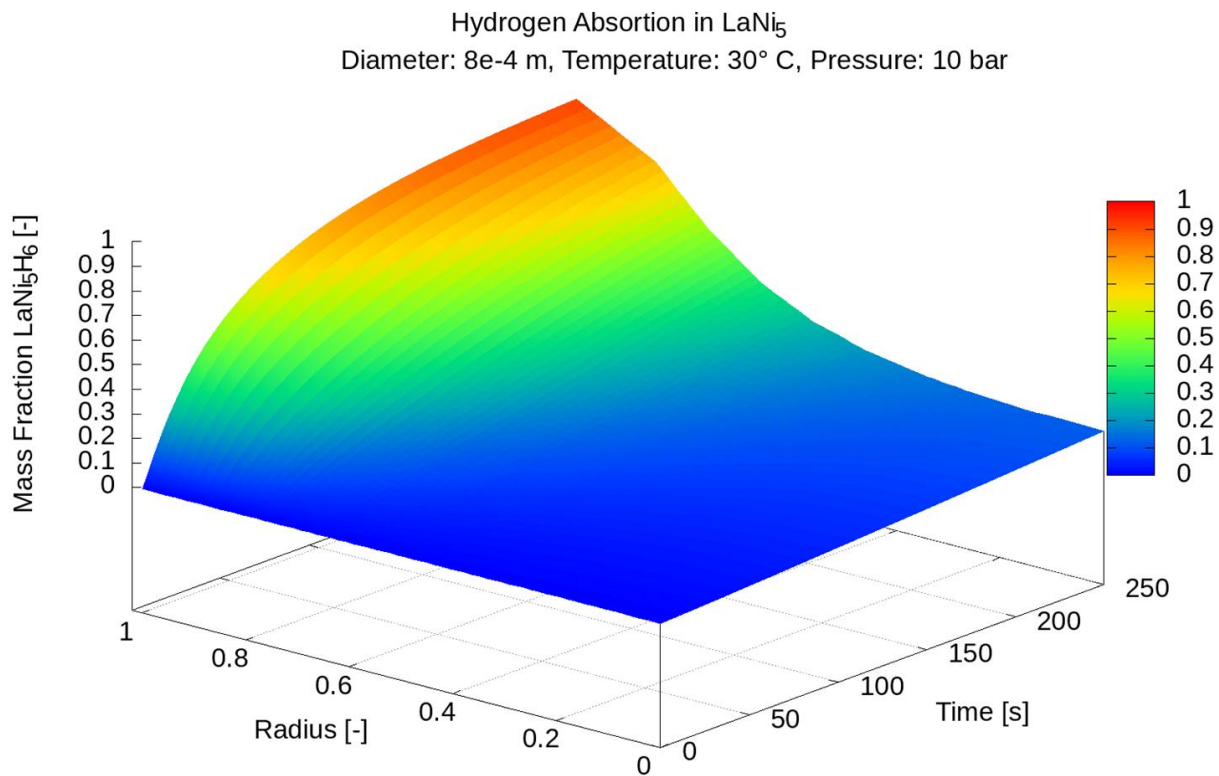
The outcomes of the project contribute to improved understanding and predictive capability of thermal processes in granular systems, supporting the design and optimisation of advanced thermal energy storage, packed-bed reactors, and other multi-physics engineering applications.



Contact: Darius Mačiūnas (darius.maciunas@vilniustech.lt), Prof. em. Bernhard Peters (bernhard-josef.peters@vilniustech.lt), Prof Dr Habil Rimantas Kačianauskas (rimantas.kacianauskas@vilniustech.lt)

Hydrogen Storage

The Multi-Physics Competence Centre at Vilnius Tech advances **hydrogen storage technologies** through high-fidelity multi-physics modelling of metal hydride-based systems. This activity focuses on understanding and predicting hydrogen absorption behavior at the particle and reactor scales, addressing the strong coupling between **heat transfer, mass transport, and thermo-chemical reactions** that governs storage performance. The Centre develops and applies XDEM-based simulation capabilities to represent the complex thermochemical response of metal hydride materials under realistic operating conditions, including transient effects and spatial gradients. These efforts enable accurate and computationally efficient representation of hydrogen storage processes, supporting the analysis of system performance, thermal management, and scalability. The work provides a foundation for the design and optimization of safe, efficient, and robust hydrogen storage solutions, contributing to the broader adoption of hydrogen technologies in energy systems aligned with sustainability and decarbonization goals.

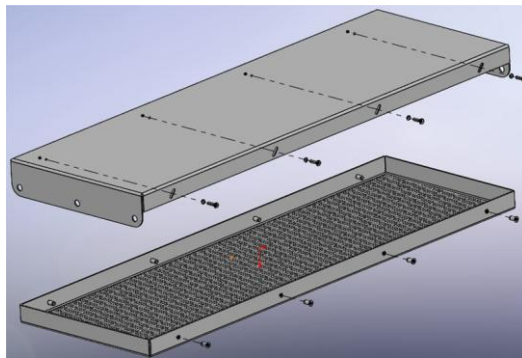


Evolution of the LaNi_5H_6 profile in a particle

Contact: Prof. em. Bernhard Peters (bernhard-josef.peters@vilniustech.lt)

Development of louvred noise barrier

The Multi-Physics Competence Centre at Vilnius Tech conducts advanced analysis supporting the **development of louvred noise barriers** for transportation and urban infrastructure applications. This activity focuses on understanding the interaction between **acoustic performance, airflow, and structural behaviour**, which is critical for noise mitigation solutions that must also meet ventilation, safety, and durability requirements. Through multi-physics analysis, the Centre evaluates sound attenuation, flow-induced effects, and environmental loading under realistic operating conditions. The outcomes support optimized barrier designs that balance noise reduction efficiency with aerodynamic performance and structural integrity. This work contributes to the development of innovative noise control solutions for road, rail, and industrial environments, enhancing environmental quality and supporting sustainable infrastructure development.



Design of a noise reduction barrier

Contact: Darius Mačiūnas (darius.maciunas@vilniustech.lt), Assoc Prof Dr Sergejus Borodinas (sergejus.borodinas@vilniustech.lt)