The discussion meeting “Simulation of systems under thermodynamic gradients” aimed at addressing the computational challenges and the fundamental aspects of transport and dynamics in systems subject to thermodynamic gradients. The discussion meeting was organized so as to emphasize the unifying phenomenology and principles of a gamut of non-equilibrium systems subject to a variety of gradients with a thermodynamic origin. To that end, we invited researchers with a diverse background and sessions grouped different aspects and approaches to the non-equilibrium behavior and modeling of such systems.

The environment of the discussion meeting was very informal, thus ensuring fluent discussions. Although the meeting only scheduled a specific discussion session at the end of the first day, the chairmen were flexible with the presentations. Hence, the discussions naturally developed along the sessions and there was ample time to address the issues raised by the different contributions.

Specifically, the meeting has raised discussions both on fundamental aspects of the different types of phoretic motion, its computational implementations, and a number of challenging applications. For example, the different types of phoresis relevant in porous media addressed a number of discussions during the whole workshop. The challenges of the different scales which characterize these materials and the corresponding relevant transport mechanisms were discussed critically. The understanding of new porous materials (such as the soft porous crystals) and their potential to tune and transport matter inside them was also addressed. For example, the relevance of cross transport modes and their molecular basis raised concern due to the lack of an identified systematic trend to determine when they may be relevant. The discussions showed that even the understanding of fundamental heat transfer mechanisms at solid-solid and solid-liquid interfaces are still open and deserve more careful attention.

The role of temperature gradients, either imposed externally or emerging from the inhomogeneous composition of colloidal particles, was amply analyzed. The nature of the induced flows and the implications when coupled mechanisms (such as temperature gradients and electric fields, or the applications of thermal gradients in the presence of gravity to promote transport and mixing) led to a number of discussions related to their crossed implications in order to achieve a more general perspective that allows to assess the inter-relationships between them. The impact of thermal inhomogeneities on electrokinetics and vice versa, or the interplay of these mechanisms in cross transport processes was addressed several times along the meeting.

From a computational perspective, the combination of new mesoscopic methods and standard molecualr dynamics techniques served to better understand the complementarity of the approaches. Critical discussions on the methods clarified the potentiality of coarse-grained methods to capture the collective behavior of phoretic motion induced by local temperature gradients, and to address electrokinetics in porous media. The issue of osmotic gradients and how to capture them in mesoscale simulations was also debated. But the need of molecular simulations was clear to analyze, for example, the origin of the dipolar response in the presence of temperature gradients and the nature of a number of transport cross coefficients.

The possibilty to exploit thermal and electric gradients at the nanoscale to promote more efficient transport also led to lively discussions. The issue of the separation of scales and how to scale up new nanodevices was discussed in detail. Also, the extension of themodynamically induced motion in systems intrinsically out of equilibrium happened to be a lively area that showed the potential of this field.

Overall, the discussion meeting has shown that this field is very active and has a strong potential, thanks to recent developments addressing fundamental questions and exploiting new directions. The meeting has provided a wide perspective of the activity in this area and has revealed the growing interest and potential of thermodynamically controlled transport and its computational challenges. Hence, the meeting has helped us to value the interest of organizing a wider event and we will consider the possibility of submitting a proposal to the CECAM flagship call.