Full-scale COmputational design of Porous mesoscale MATerials

Berichterstattung

Projektinformationen

COPMAT

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Projektwebsite

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Periodic Reporting for period 4 - COPMAT (Full-scale COmputational design of Porous mesoscale MATerials)

Berichtszeitraum: 2021-04-01 bis 2023-03-31

Zusammenfassung vom Kontext und den Gesamtzielen des Projekts

What is the problem/issue being addressed?
The problem taken by COPMAT is the full-scale COmputational design of Porous mesoscale MATerials. This entails the computational modeling of microfluidic experiments involving multiphase flows, typically oil and water, in which one of the two species forms droplets (dispersed phase) in a continuum phase. Upon shining UV light into the flow, the continuum species solidifies while the dispersed one evaporates, generating a solid scaffold with holes. The hole distributions depend on microfluidic operational parameters, typically the microfluidic geometry and the mass flow ratio of continuous and dispersed phases. The major appeal of this microfluidic is that the pores' geometry is highly controllable.
This process is governed by the competition of many different mechanisms, pressure, capillarity, near-contact interactions, acting on a broad spectrum of scale of space and time and subject to strong geometric confinement.
Such multiscale nature raises a formidable challenge to both theoretical and experimental science, whence the unique role of leading-edge computational modelling and computer simulations: the hard-core of COPMAT.

Why is it important for society?
The societal impact of new porous mesoscale materials cannot be overestimated: they are potentially useful across a broad range of applications, from manufacturing to food processing (foams, emulsions), to energy production (catalytic materials) to biology (gels) and medicine (tissue and bone repair).

What are the overall objectives?
The overall objective of COPMAT is to leverage the power of the Lattice Boltzmann method, to which the PI has made seminal and internationally acknowledged contributions, to develop a new generation of mesoscale methods and computer codes to handle the aforementioned multiscale problems in a way which would be very unwieldy, if possible at all, to any other numerical method.
This allows not only to interpret existing microfluidic experiments but also to inspire and suggest new ones, leading to new and hitherto unexplored mesoscale porous materials. Besides these practical goals, the development of a new generation of Lattice Boltzmann codes spawns benefits for the general problem of studying complex states of soft flowing matter far from equilibrium, which is a fundamental goal of modern non equilibrium science across many disciplines (see above).

Arbeit, die ab Beginn des Projekts bis zum Ende des durch den Bericht erfassten Berichtszeitraums geleistet wurde, und die wichtigsten bis dahin erzielten Ergebnisse

During the 5 and half years of COPMAT we have performed work along several fronts: theoretical, computational and experimental. For the sake of concreteness we shall refer to the specific workpackages.

WP1: We have explored the effects of near-contact interactions (NCI) on the global rheology of the soft-flowing material at the scale of the experiment, under a broad variety of conditions and regimes of motion. Invariably, the result was that the relative strength of the NCI versus capillary forces is the key control parameter dictating the large-scale rheology of the material. However, NCI need not been modeled down to the supramolecular scale (10 nm) but can be coarsed grained up to micrometric scale without appreciably affecting the material rheology. This finding is the cornerstone of COPMAT and largely responsible for its major success in describing a variety of soft-flowing regimes. In particular, it has relieved us from the extremely demanding task of performing local grid refinement, which would have been a major and very time-consuming ordeal.

WP2: We have developed leading-edge HPC codes (LBsoft and LBCUDA) which represent the state of the art in the field of colloidal bijels. LBCUDA can reach up to 100 GLUPS (hundred billion lattice updates per second) on moderately large GPU clusters, and even on smaller size computers it could allow the computational/experimental design of bijels materials under confinement.

WP3: We have performed very large scale simulations of a very peculiar trabecular-like media, the deep-sea sponge Euplectella-Aspergillum and highlighted the unsuspected role of hydrodynamics not only to relieve mechanical loads but also to facilitate selective feeding and sexual reproduction. This study has been published in Nature (July 2021), a very rare event for simulation-only work, and also made the object of several press-releases, including CORDIS, NSF as well as an article on Scientific American.

WP4: We have studied the motion of hierarchical emulsions (droplets within droplets) as well as of other new states of soft flowing matter, such as soft granular flows. These numerical studies have unveiled new regimes of motion and new functional regimes which have no counterpart in ordinary fluids. This work has been published in high-profile journals, such as Nature Communications (2021, 2023) and Physical Review Letters (2022). It lays the ground for future studies not only in soft material science but also in computational biology and micro/nanomedicine.

WP5: Our work has been systematically disseminated through the publication of over fifty high level international scientific journals, dozens of seminars and invited talks, over ten press-releases and also a few articles on magazines for the general audience. In addition, COPMAT work has received a dozen of distinctions, namely covers, highlights and Editorial picks. This work has also been exploited to obtain the ERC-PoC DROPTRACK, which was awarded to the PI in October 2022.

WP-Extra: In addition to the planned work, COPMAT has also delivered additional unplanned results in the following areas: 1) COVID-19 research: Computational studies of the COVID-19 spike dynamics (in the framework of a six-month extension due to COVID-19 disruption) ; 2) Active Matter: Dynamics of active droplets under confinement, 3) Machine-learning for microfluidics; development of a machine-learning based software for fast automatic droplet recognition and tracking in microflows. This is making the subject of the ERC-PoC (DROPTRACK).

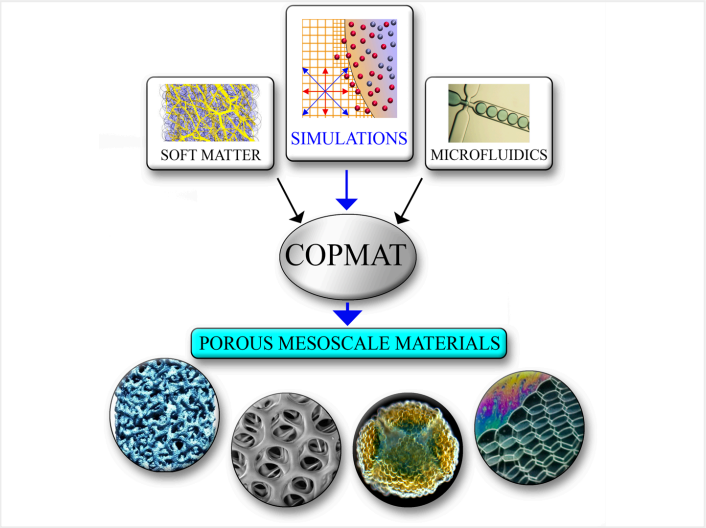
Fortschritte, die über den aktuellen Stand der Technik hinausgehen und voraussichtliche potenzielle Auswirkungen (einschließlich der bis dato erzielten sozioökonomischen Auswirkungen und weiter gefassten gesellschaftlichen Auswirkungen des Projekts)

COPMAT has gone beyond the state of the art in many respects.

Modeling: we have designed a new class of Lattice Boltzmann codes (LBEMU)with near-contact interactions which have proved key to the successful description of soft flowing matter under a rich variety of regimes and materials: soft flowing crystals, hierarchical emulsions, soft dense confined emulsions, granular flows, bijels. No existing LB code prior to COPMAT would have been in a position to describe most the regimes covered by COPMAT, primarily strongly confined dense emulsions.

HPC-LB software: we have developed leading-edge HPC-LB codes for multi-jel materials which goes at least an order of magnitude beyond existing software in the field. Also, HPC versions of LBEMU have been instrumental for the interpretation of a variety of microfluidic experiments (see below).

Experimental: LBEMU has been instrumental in assisting and complementing a series of entirely new microfluidic experiments on hierarchical emulsion (with Weitz's group in Harvard), soft granular flows (with Prof J. Guzowski at the Poland Acad of Sci), flow of dense emulsions in tapered channels (with Prof Tang at Stanford Univ) and new microchip devices (with Prof Pisignano, Uni Pisa, work in progress). It is no exaggeration to state that LBEMU is currently way ahead of any other simulation tool for these kind of experiments (as explicitly recognized by all of the above experimental partners). We regard this is a major sign of success of COPMAT.



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