SoftComp Roadmap 2025-2030:
From Molecular Topology to Macroscopic Function

The SoftComp Consortium

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Contents

1 Foreword

Soft matter plays a crucial role in nearly every aspect of daily life, such as, for example, food and consumer products, cosmetics and pharmaceuticals, biological systems, and many materials essential to modern technologies. Research in this field is a major driver of innovation across a wide range of sectors, involving numerous large and medium-sized European companies. Despite its clear importance, soft matter research was historically fragmented. Its many subfields - such as surfactants, polymers, colloids, and biomatter - were often pursued separately, and related disciplines including physics, computational science, chemistry, and biophysics tended to work in parallel rather than in close collaboration.

The SoftComp Consortium was first established in 2004 as a Network of Excellence financed by the EU, and then turned into a Consortium, to proactively address this fragmentation, with the aim of strengthening scientific and technological excellence in soft matter research. SoftComp's success story lies in the fact that it was a Network of Excellence from 2004 to 2010 with the ambitious goal of building a durable collaborative and well integrated structure, and more than 15 years after the EU funding ended it remains alive, vibrant, and impactful—demonstrating its lasting value and strength as a research community, bringing together a critical mass of resources and expertise, providing leadership and elevating the strategic integration of soft matter research in Europe to a new level.

A shared research infrastructure has been created, significantly extending the capabilities of individual partner laboratories. This infrastructure offers access to advanced colloidal and polymer synthesis facilities, state-of-the-art experimental techniques for spectroscopy, imaging, and scattering, as well as a joint high-performance computing cluster for simulation and theoretical work. In parallel, a strong emphasis on education and dissemination has led to the organization of numerous schools, workshops, and conferences. A major milestone was the first International Soft Matter Conference in Aachen, Germany, which attracted more than 600 participants from around the world. Its success prompted a follow-up conference series in Europe as well in other continents.

Building on these achievements, SoftComp has demonstrated the substantial added value created through integration—not only for its members, but for the soft matter community at large and, ultimately, for society. The establishment of new university chairs in soft matter science and the growing industrial relevance of the field highlight SoftComp's strong strategic position.

Stephan Förster
SoftComp Coordinator

2 The SoftComp Mission

The Mission of SoftComp is to provide a sustainable environment for the integration of leading European Research Groups in the Field of Soft Matter composites as detailed in the Research Road Map with the clear vision for research, dissemination, education and industrial outreach for the medium-long term. The main objectives of SoftComp are:

- Better science through interdisciplinary communication and joint projects
- Better science through access to joint infrastructure
- Interdisciplinary education of the next generation of soft matter scientists
- Establishing scientific foundations for soft matter–related industrial technologies

To achieve these objectives, SoftComp employs the following instruments:

- Access to research platforms, including:
  - Exchange of samples
  - Mutual use of scientific instrumentation
  - Use of computational facilities and theoretical expertise
- Exchange of scientists
- Web-based communication tools
- Joint dissemination programs
- Joint education programs
- Industrial outreach activities
- Public outreach initiatives

3 Consortium Partners

The SoftComp Consortium brings together leading academic and industrial research groups from across Europe. The consortium comprises 37 partners from 11 countries, uniting expertise in synthesis, characterization, theory, and simulation.

ID	Institution / Laboratory	Short Name	Country
1a	Forschungszentrum Jülich - Neutron Scattering and Biological Matter (IBI-8/JCNS-1)	FZJ	Germany
1b	Forschungszentrum Jülich - Biomolecular Systems and Processes (IBI-4)	FZJ	Germany
1c	Forschungszentrum Jülich - Institute of Biological Information Processing - Theoretical Physics of Living Matter (IBI-5/IAS-2)	FZJ	Germany
2	University of Mainz	Mainz	Germany
7	Universität zu Köln	Köln	Germany
8	Utrecht University	Utrecht	Netherlands
11	University of Leeds	Leeds	United Kingdom
12	University of Edinburgh	Edinburgh	United Kingdom
14	Katholieke Universiteit Leuven	KUL	Belgium
18b	Centre National de la Recherche Scientifique - Montpellier	CNRS	France
18d	Centre National de la Recherche Scientifique - IMMM Le Mans	CNRS	France
19	Universidad de Vigo	Vigo	Spain
20	Universidad del Pais Vasco	San Sebastian	Spain
23	Foundation for Research and Technology	FORTH	Greece
24	A. Mickiewicz University Poznan	Poznan	Poland
33	Imperial College London	Imperial College	United Kingdom
34a	Ecole Supérieure de Physique et de Chimie Industrielles - Laboratoire Matière Molle et Chimie	ESPCI	France
34b	Ecole Supérieure de Physique et de Chimie Industrielles - Physico-chimie des Polymères et des Milieux Dispersés	ESPCI	France
35	University of Fribourg	Fribourg	Switzerland
37	Université Catholique de Louvain	UCL	Belgium
39	Martin Luther University Halle-Wittenberg	Halle	Germany
41	Wageningen University	Wageningen	Netherlands
42	Lund University	Lund	Sweden
43	University of Luxembourg	Luxembourg	Luxembourg
44	Technical University Eindhoven	TUE	Netherlands
45	Institut Laue-Langevin	ILL	France
46	University of Durham	Durham	United Kingdom
48	Universität Tübingen	Tübingen	Germany
50	University of Naples Federico II	Naples	Italy
52	Technical University Darmstadt	TUDa	Germany
53	INSA Lyon	INSA	France
54	Ca' Foscari University of Venice	Ca' Foscari	Italy
55	University of Lyon - Saint Etienne - IMP	Lyon	France
56	Universitat Rovira i Virgili	URV	Spain
57	National Research Council (CNR) - Naples	CNR	Italy

4 The SoftComp Research Road Map

The medium-term perspectives and the long-term vision of the SoftComp Consortium are outlined in this Research Road Map (RRM). The RRM illustrates the coherent framework for scientific, educational, organizational, and infrastructural development and includes the following components:

- **Scientific activity**, describing the main ongoing research directions
- **Joint infrastructure**, describing the research platforms and their use
- **Strategic vision**, describing potential research directions
- **Dissemination**, ensuring effective communication of scientific results
- **Educational**, supporting knowledge transfer to the next generation of soft matter scientists
- **Management**, describing the SoftComp Consortium and its main activities

5 Scientific Activity

The scientific trajectory of the SoftComp Consortium over the past reporting period demonstrates a profound paradigmatic shift. Historically rooted in the equilibrium statistical mechanics of complex fluids—colloids, polymers, and surfactants—the network's research focus has decisively expanded toward non-equilibrium active matter, topologically constrained systems, and biological mechanotransduction. This evolution is driven by the integration of advanced neutron/X-ray scattering techniques with mesoscopic simulations and novel high-throughput imaging modalities. The scientific activity can be mapped onto a landscape defined by the interplay between *activity* (energy consumption), *topology* (connectivity/shape), and *responsiveness* (adaptation).

From Passive Brownians to Chiral Active Fluids

A central theme of the network's recent activity is the transition from describing passive Brownian motion to understanding "living" fluids. The network has moved beyond the single-particle "run-and-tumble" models of bacteria [1] to addressing the hydrodynamic complexity of collective motion.

- **Active Turbulence and Scale-Free Dynamics:** Recent experimental and theoretical work has challenged the universality of active turbulence. Investigating *E. coli* suspensions under confinement, network researchers have demonstrated that bacterial turbulence does not possess an intrinsic vortex length scale but is instead "scale-free," governed largely by the confinement height [2]. This has profound implications for the validity of continuum theories like the Toner-Tu equations in confined geometries.
- **Chirality and Odd Viscosity:** A major theoretical breakthrough, substantiated by simulation, is the characterization of **Chiral Active Matter**. Systems composed of spinning rotors or skyrmions break parity symmetry, leading to the emergence of "Odd Viscosity"—a transverse stress response forbidden in equilibrium fluids. Network groups have simulated how this odd viscosity leads to non-reciprocal interactions [3] and unique flow states where particles are dragged toward vortex centers [4], creating a new class of "meta-fluids" with tunable transport properties.
- **Motility-Induced Phase Separation (MIPS):** The concept of MIPS has been refined to include the effects of surface curvature. Network studies show that on curved surfaces, the interplay between rotational diffusion and the local radius of curvature introduces a new timescale that can suppress phase separation, a finding critical for understanding bacterial colonization in porous media [5, 6].

Topological Polymers and Dynamic Networks

The network has revitalized polymer physics by focusing on topology and dynamic covalency, moving beyond standard reptation models for linear chains.

- **Ring Polymers and "Self-Similar" Dynamics:** Utilizing Neutron Spin Echo (NSE) spectroscopy, the network has provided definitive evidence that ring polymers (which lack chain ends) do not follow the reptation tube model. Instead, they exhibit self-similar dynamics driven by topological constraints that are distinct from entanglements [7, 8]. This work fundamentally challenges existing theories of polymer melts and highlights the role of "threading" in ring-linear blends [9].

- **Vitrimers and Compleximers:** The synthesis of materials combining the robustness of thermosets with the flow of liquids has been a key achievement. The network has characterized *Vitrimers*, where flow is mediated by associative bond exchange reactions (e.g., dioxaborolane metathesis) [10]. Advanced calorimetry (FSC) and rheology have been used to decouple the bond-exchange transition (T_v) from the glass transition (T_g) [11]. Furthermore, "Compleximers"—polyelectrolyte complexes moderated by steric hindrance—have been introduced as water-free, recyclable alternatives to standard plastics [12].

- **Flow-Induced Crystallization (FIC):** Bridging processing and physics, the network has developed the polySTRAND model, which quantitatively links the molecular weight distribution of a melt to the superexponential nucleation rates observing during shear flow [13, 14].

Structural Dynamics of Biomolecular Assemblies

In the biological domain, the network has shifted focus from static structural determination to the dynamics of disordered systems and membrane interfaces.

- **Intrinsically Disordered Proteins (IDPs) and Phase Separation:** The network has pioneered the study of IDPs (e.g., Tau, TDP-43, FUS) using a combination of Small-Angle Scattering (SAS) and "Hierarchical Chain Growth" simulations [15]. Research has elucidated how local stiffness and transient secondary structures dictate the global dimensions of IDPs and drive Liquid-Liquid Phase Separation (LLPS) into biomolecular condensates [16]. Crucially, modifications like phosphorylation have been shown to act as switches for this condensation [17].

- **Membrane Mechanics and Asymmetry:** The mechanical coupling between lipid leaflets ("transleaflet coupling") has been resolved using neutron reflectometry on asymmetric vesicles. The network has demonstrated that lipid asymmetry leads to anomalous membrane stiffening [18]. Additionally, the interaction of antimicrobial peptides with membranes has been re-evaluated, revealing that peptides can induce transient water channels for permeabilization without forming stable pores [19].

- **Mechanobiology of Infection:** Innovative work on the malaria parasite has led to the "Passive Compliance" hypothesis, where simulations proved that the parasite's alignment is driven by the mechanics of the red blood cell membrane and stochastic adhesion, rather than active motor forces [20].

Soft Interfacial Engineering

The engineering of interfaces remains a stronghold, with a move toward adaptive and sustainable systems.

- **Pickering Stabilization with Bio-Colloids:** The network has advanced the understanding of Pickering emulsions stabilized by sustainable particles, such as plant protein microgels [21] and cellulose nanocrystals. Microfluidic studies have revealed that stability can be maintained even at low surface coverage through particle bridging [22].

- **Responsive and Active Surfaces:** Research on "adsorption-active" polymer brushes has demonstrated tunable gating properties [23]. Furthermore, the development of "mechano-bactericidal" nanostructures (e.g., black silicon, gold nanostars) provides a physical route to antimicrobial surfaces, killing bacteria via membrane stretching [24].

Methodological innovation: The Digital Turn
Underpinning these advances is a transformation in methodology. The network is pioneering the integration of *Physics-Informed Machine Learning* with experimental techniques. This includes the use of neural networks to solve the inverse scattering problem for GISAXS/SANS data [25, 26] and the application of Deep Learning to *Tomographic Flow Cytometry*, enabling label-free, 3D identification of circulating tumor cells with unprecedented accuracy [27].

5.1 Network Area 1: Colloidal Composites, Gels and Glasses

Rationale: This pillar leverages the network's dominance in scattering (ILL, FZJ) and rheology to link particle architecture (shape, softness) to macroscopic flow and interfacial stability.

5.1.1 Complex Colloids: Microgels and Soft Glasses

Leading scientists: J. van der Gucht / M. Cloitre

State-of-the-art: From Jamming to Microstructural Control The SoftComp Consortium has firmly established itself at the forefront of "Soft Particle Glasses" (SPGs), a class of materials where the constituent particles—unlike hard spheres—are compressible and deformable. This softness introduces a new degree of freedom to the jamming phase diagram, allowing packing fractions (ϕ) to far exceed the random close packing limit ($\phi_{rcp} \approx 0.64$). The network's research has moved beyond phenomenological rheology to providing a microscopic, particle-level understanding of how these dense suspensions yield and flow.

A pivotal achievement has been the detailed mapping of the **yielding transition**. Using large-scale 3D particle dynamics simulations corroborated by experiments, network researchers have deciphered the link between the transient microstructure and the macroscopic stress overshoot observed during startup shear [28]. It was revealed that yielding is not an instantaneous event but involves the buildup of structural anisotropy—specifically, the accumulation of particles along the compression axis and depletion along the extension axis—coupled with the elastic deformation of the particles themselves. This work provided a universal scaling for the static yield strain and stress, unifying behaviors across diverse soft colloid systems (e.g., star polymers, microgels, core-shell particles).

Furthermore, the network has pioneered the investigation of **transport anomalies** in these crowded environments. The observation of "Fickian yet Non-Gaussian Diffusion" (FnGD) has challenged standard hydrodynamic theories. In this regime, the mean squared displacement (MSD) scales linearly with time (implying normal diffusion), yet the displacement probability distribution exhibits exponential tails (implying heterogeneity). Network studies have shown that this phenomenon is a generic feature of glass-forming liquids and have proposed a "universal" evolution of these non-Gaussian tails, linking them to cage-jump dynamics and the onset of cooperativity [29, 30].

Crucially, the internal architecture of the microgels themselves has been shown to dictate bulk properties. Through contrast-variation SANS and **zero-average contrast** experiments, the network has resolved the different bulk moduli within individual nanogels (core vs. shell) [31]. This has allowed for the precise tuning of softness and deswelling behavior by varying monomer chain length and cross-linker density, directly influencing the colloidal phase behavior from fluid to crystal to glass [32].

The **18b-Montpellier** group has advanced the understanding of jamming and plasticity in soft composites, focusing on the spontaneous dynamics of concentrated emulsions and their failure modes under mechanical forcing. Meanwhile, researchers at **42-Lund** are applying these concepts to food science, using scattering and coarse-grained modeling to decipher the structure and assembly of sustainable plant proteins, effectively treating food as a complex soft matter system.

The **35-Fribourg** group contributes expertise in light and X-ray scattering to probe the dynamics of soft colloids and arrest transitions in dense suspensions, providing critical data for mode-coupling theory validations.

Future Challenges: Programming Disorder and Flow The next frontier lies in actively manipulating this disorder and designing interactions to avoid it when desired.

- **Dynamic Heterogeneity and Memory Erasure under Load:** Current understanding focuses largely on the quiescent glass transition or steady shear. A major open challenge is understanding the *transient* response to complex mechanical histories. Glassy materials solidify in out-of-equilibrium configurations, trapping residual stresses that encode "memories" of their processing. Recent breakthrough work in the network suggests that these memories (and the associated directional anisotropy) can be erased or "tuned" via oscillatory shear training [33]. The challenge is now to link this macroscopic "memory erasure" to specific microscopic rearrangements—identifying the "soft spots" or localized plastic events that mediate rejuvenation. This requires combining time-resolved rheology with real-time structural probes (e.g., Rheo-XPCS or Rheo-SANS).

- **Inverse Design of Packings and Crystals:** While glasses are useful, the ability to avoid the glass transition and self-assemble into specific, open crystalline lattices (e.g., diamond, pyrochlore) is the "holy grail" of photonics. The network has demonstrated the theoretical feasibility of this via "Inverse Design" algorithms [34], which determine the precise patchy interactions required to stabilize a target structure against competing polymorphs and kinetic traps. The challenge is to translate these *in silico* designs into experimental reality using DNA-origami colloids or programmable microgels [35], bridging the gap between Boolean satisfiability algorithms and wet-lab synthesis.

- **Active Microrheology of Soft Glasses:** Moving beyond passive observation, future work should exploit *active* probes (e.g., magnetic particles, laser-driven colloids) embedded within the soft glass. This allows for the measurement of local yielding and non-affine displacements at the scale of the cage itself, testing theories of "Odd Viscosity" and non-reciprocal interactions in dense passive media driven by active dopants.

List of Groups & Capabilities

- **34a-ESPCI (M. Cloitre):** Rheology of soft pastes and jamming.
- **41-Wageningen (J. van der Gucht):** Polymer-colloid mixtures and microrheology.
- **18b-Montpellier (L. Cipelletti):** Jamming, plasticity, and material failure.
- **42-Lund (P. Schurtenberger/A. Stradner):** Scattering of food colloids and protein mixtures.
- **45-ILL (L. Porcar):** SANS/NSE for internal microgel dynamics.

5.1.2 Interfacial Soft Matter: Reactive Foams, Emulsions, and 3D Printing

Leading scientists: C. Monteux / D. Harbottle

State-of-the-art: From Passive Stabilization to Functional Interfaces The network has fundamentally advanced the field of interfacial soft matter by moving beyond simple surfactant stabilization to complex, particle-stabilized (Pickering) systems with tunable functionality. A key strength lies in the diverse library of stabilizing agents developed and characterized by member groups, ranging from sustainable **plant protein microgels** (e.g., pea protein, zein) [36, 37] to high-performance **graphene oxide (GO) laminates** [38] and **stimuli-responsive microgels** [32].

Significantly, the network has elucidated the microscopic mechanisms that confer ultra-stability to these systems. In Pickering emulsions, researchers have demonstrated that stability is not solely dependent on high surface coverage. Microfluidic studies have revealed that even "poorly covered" droplets can remain stable against coalescence through the formation of **particle bridges** and heterogeneous "crown" structures at the droplet contact points [21]. This insight challenges the conventional view that a dense monolayer is required for stability and opens pathways for resource-efficient formulations.

Methodologically, the network has pioneered the coupling of macroscopic interfacial rheology with microscopic structural probes. The development of Rheo-SANS and Rheo-NMR setups for interfaces allows for the simultaneous measurement of surface shear moduli and the in-situ determination of polymer/particle conformation under stress. This has been pivotal in understanding how "transleaflet coupling" in lipid bilayers [18] and "interfacial polymer gradients" in nanocomposites [39] dictate macroscopic material properties.

Future Challenges: Reactivity and Additive Manufacturing The next phase of research will focus on dynamic, non-equilibrium interfaces that are chemically active or processed under extreme conditions.

- **Reactive Interfaces for Urban Mining and Catalysis:** A major emerging theme is the use of liquid foams not just as materials, but as chemical reactors ("Process Intensification"). The network has provided proof-of-concept for *Leaching Foams* capable of recovering critical metals (Copper, Silver) from electronic waste [40, 41]. The challenge now lies in coupling the *chemical kinetics* of oxidation/dissolution with the *physical transport* of reactants through the foam's liquid channels (Plateau borders) and thin films. Understanding how surfactants and particles influence the transfer of gas (e.g., O_2, O_3) across the interface while simultaneously stabilizing the foam against drainage and coalescence is critical for scaling up these green recycling technologies.

- **3D Foam Printing and Bubble Dynamics:** Additive manufacturing of porous materials is a frontier where rheology meets processing. The network is leading the development of *3D Foam Printing*, using physical blowing agents (like supercritical CO_2) to generate hierarchical porosity within printed polymer strands (e.g., PLA, PCL) [42, 43]. The scientific challenge is to predict and control bubble nucleation and growth in a non-Newtonian, cooling polymer melt exiting a nozzle. This requires mastering the interplay between the *solubility/diffusion* of the blowing agent, the *viscoelasticity* of the matrix (which resists bubble expansion), and the *crystallization kinetics* (which freezes the structure). Future work must integrate high-pressure microfluidics and X-ray tomography to visualize these rapid dynamics in-operando, enabling the design of "orientation-graded" foams with spatially tailored mechanical properties [44].

- **Bio-Instructive Interfaces:** Expanding into the biological realm, the network aims to design interfaces that actively direct cellular behavior. This involves "Adsorption-Active" polymer brushes [23] that can gate the transport of specific biomolecules, and "Mechano-Bactericidal" nanostructures [24] that physically rupture bacterial membranes. The challenge is to decipher the thermodynamic determinants of **superselectivity** [45]—how multivalent interactions at an interface can distinguish between cell types or pathogenic states with extreme sensitivity—and to translate these principles into synthetic "glycocalyx-mimetic" coatings.

List of Groups & Capabilities

- **34b-ESPCI (C. Monteux):** Interfacial rheology and microfluidics.
- **11-Leeds (D. Harbottle):** Functional particles for separation processes.
- **50-Naples (P.L. Maffettone):** 3D Foam printing and bubble dynamics simulations.
- **45-ILL (R. Schweins):** Contrast-variation SANS for interfacial layers.

5.1.3 Functional Nanomaterials: From Chiral Assembly to Mechano-Active Surfaces

Leading scientists: V. Baulin / S. Förster

State-of-the-art: Anisotropy and Mechano-Activity The SoftComp Consortium has established a leading position in the synthesis and application of **anisotropic functional nanomaterials**, moving decisively beyond simple spherical colloids. This includes the precise fabrication of complex shapes such as gold nanostars, magnetic nanorods, and hematite-silica core-shell particles. A key achievement has been the development of **"Mechano-Bactericidal" surfaces**—nanostructured landscapes (e.g., black silicon, biomimetic insect wings) that kill bacteria not through chemical antibiotics, but via physical rupture [24]. Theoretical modeling within the network has elucidated the specific mechanism: the stretching of the bacterial cell membrane across sharp nanofeatures until the elastic limit is exceeded [46].

Simultaneously, the network has advanced the field of **magnetic soft matter**. Research has focused on "Skyrmions"—topologically stable, particle-like spin textures in thin films. These quasi-particles exhibit unique "active" behaviors, such as the skyrmion Hall effect, and can form lattices that melt via intermediate hexatic phases [47]. The ability to simulate their dynamics using coarse-grained particle models [48] and visualize them in real-time [49] positions the network at the cutting edge of topological spintronics.

Future Challenges: Chirality and Intelligent Response The future trajectory for this pillar involves harnessing *chirality* for novel optical and rheological properties, and integrating *responsiveness* for smart biomedical applications.

- **Chiral Nanomaterials and Odd Viscosity:** The assembly of chiral structures from achiral building blocks represents a major frontier. Recent work has demonstrated the transformation of achiral semiconductor magic-sized clusters (MSCs) into large-scale **chiral domains** with exceptional circular dichroism through controlled meniscus evaporation [50]. The challenge is now to extend this to the dynamic realm: creating "Chiral Active Fluids" composed of spinning magnetic nanorods. Theoretical predictions suggest these fluids should exhibit **"Odd Viscosity"**—a transverse stress response that breaks parity symmetry [4]. Verifying this experimentally requires the synthesis of monodisperse, magnetic chiral rotors and the development of specialized rheological protocols to measure non-reciprocal stresses in bulk suspensions.
- **Smart Response: Hyperthermia and Drug Delivery:** Coupling physical stimuli with biological action is a key goal. Magnetic nanoparticles offer a route to remote actuation. The network aims to develop **"Smart Vectors"** that combine magnetic hyperthermia (heat generation) with triggered drug release. This requires mastering the "lock-and-key" interactions of functionalized nanoparticles with cell membranes. SANS and Cryo-TEM

studies are essential to resolving the structure of the **"Protein Corona"** that forms around these particles in biological fluids, which can drastically alter their targeting and uptake efficiency [51].

- **Topological Protection in Active Matter:** Investigating how topological defects (like skyrmions or vortices in bacterial swarms) can "protect" material properties against disorder. This involves understanding the "topological protection" mechanisms that allow active flow states to persist in the presence of noise and confinement [52], potentially leading to robust, self-healing active materials for flux control or logic operations.

List of Groups & Capabilities

- **24-Poznan (NanoBioMedical Centre):** Synthesis and HR-TEM (Jeol ARM 200F).
- **2-Mainz (M. Hirtz/F. Schmid):** Lithography and simulation of magnetic colloids.
- **56-URV (V. Baulin):** Modeling of nanoparticle-membrane interactions.

5.2 Network Area 2: Self-assembling and Biomimetic Systems

Rationale: This pillar unifies the study of energy-consuming systems, from synthetic microswimmers to living tissues, supported by high-resolution imaging and mesoscopic simulations.

5.2.1 Active Soft Matter: Swimmers, Topology, and Collective Flow

Leadin scientists: G. Gompper / M. Ripoll

State-of-the-art: Simulating the "Living" Fluid The SoftComp Consortium has defined the state-of-the-art in the theoretical and computational description of active fluids. A cornerstone of this success is the development and application of mesoscopic simulation techniques, specifically **Multiparticle Collision Dynamics (MPC)** and **Dissipative Particle Dynamics (DPD)**. These methods bridge the gap between atomistic detail and continuum hydrodynamics, capturing the essential thermal fluctuations and hydrodynamic interactions that govern microswimmer behavior.

Theoretical work at **42-Lund** further expands this domain by modeling non-equilibrium dynamics in active matter systems controlled by hydrodynamic interactions. Their statistical analysis of the fluid-mediated transition to active turbulence in motile bacteria provides a crucial link between analytical modeling and the large-scale computational studies performed at FZJ and Mainz.

Major recent breakthroughs include:

- **Active Turbulence:** The network has challenged the universality of "bacterial turbulence." By investigating *E. coli* suspensions under varied confinement, researchers demonstrated that the collective chaotic flow does not possess an intrinsic vortex size but is instead "scale-free," bounded only by the confinement height [2]. This finding forces a re-evaluation of continuum theories (like Toner-Tu) for confined active matter.
- **Odd Viscosity in Chiral Fluids:** Network theorists have pioneered the description of **"Odd Viscosity"** (η^O) in fluids composed of spinning rotors (chiral active matter). Simulations have shown that this parity-breaking transport coefficient leads to non-reciprocal interactions [3] and unique flow phenomena, such as the centripetal accumulation of particles in vortices [4].

- **Swimmer Synchronization:** Detailed DPD simulations have elucidated how the viscoelasticity of the suspending medium (e.g., mucus) influences the synchronization of flagella. It was found that synchronization forces are non-monotonically dependent on the Deborah number, with viscoelasticity enhancing in-phase beating at specific relaxation times [53].

Future Challenges: Topology and Complex Environments The next frontier is to harness these active behaviors for function and to understand them in realistic, topologically complex environments.

- **Topological Protection and Defect Dynamics:** Topological defects (vortices, skyrmions) are not just artifacts of active matter; they are fundamental organizing centers. Future work will investigate **"Topological Protection"**—how the topology of the order parameter field can shield active flow states from disorder and dissipation. This involves studying the dynamics of defects in active nematics and hexatics, and exploring how they can be guided by substrate geometry or activity gradients to perform logic operations or directed transport [52].

- **Active Transport in Porous Media:** Most real-world active matter (bacteria in soil, sperm in the reproductive tract) exists in complex, porous environments. The network will focus on **Motility-Induced Phase Separation** (MIPS) in confinement. Simulations have already shown that surface curvature introduces a new timescale that can suppress MIPS [5]. The challenge is to extend this to random porous media, understanding how pore size distribution and connectivity dictate the percolation and colonization of active swarms [6]. This has direct relevance for bioremediation and understanding infection pathways.

- **Chemotaxis and "Smart" Swimmers:** Moving toward "Intelligent Active Matter," the network will integrate sensing and information processing into swimmer models. This includes simulating "Run-and-Tumble" dynamics with memory, where swimmers adapt their tumbling frequency based on the history of chemical concentrations [1]. The goal is to design synthetic microswimmers that can navigate chemical gradients in complex, viscoelastic environments as efficiently as biological organisms.

List of Groups & Capabilities

- **1c-FZJ (G. Gompper/D. Fedosov):** DPD simulations of swimmers and blood flow.
- **2-Mainz (P. Virnau/M. Ripoll):** Simulations of chiral matter and skyrmions.
- **12-Edinburgh (W. Poon/V. Martinez):** Experiments on bacterial motility (DDM).

5.2.2 Living Soft Matter: Holographic Imaging and Mechanobiology

Leading scientists: A. Sengupta / P. Ferraro

State-of-the-art: Label-Free Quantification of Life The SoftComp Consortium has revolutionized the study of living matter by developing and deploying non-invasive, high-throughput imaging technologies. Central to this is Digital Holography (DH) and Tomographic Flow Cytometry. Unlike traditional fluorescence microscopy, which requires staining (perturbing the sample), these techniques measure the intrinsic refractive index distribution of cells in 3D. This has allowed network researchers to identify Circulating Tumor Cells (CTCs) with $> 97\%$ accuracy based solely on their 3D morphology and density, paving the way for "Liquid Biopsy" applications [27].

Simultaneously, the network has advanced the **mechanobiology of tissues and biofilms**. By combining microfluidics with time-lapse imaging, researchers have uncovered how physical forces shape biological architecture. For instance, in growing bacterial colonies, "active biomechanical forces" have been shown to drive a "genealogical demixing," where cell lineages separate into distinct enclaves to minimize mechanical stress, a process governed by the thermodynamics of phase separation [54]. In blood rheology, the network has characterized the "acanthocyte sedimentation rate" as a novel biomarker for neurodegenerative diseases, linking cell shape deformability to macroscopic sedimentation velocity [55].

At **54-Ca' Foscari**, the focus extends to intelligent optical imaging and sensing within biological microenvironments. By tailoring the surface chemistry of nanomaterials, they design smart luminescent sensors capable of remotely probing physical and chemical parameters in cells and animal models, bridging the gap between materials science and in-vivo diagnostics.

Future Challenges: From Observation to Prediction The next steps involve integrating these imaging capabilities with predictive modeling to control biological organization.

- **High-Throughput 3D Tomographic Sorting:** While identification is possible, real-time physical sorting based on holographic signatures remains a challenge. Future work will develop "smart" microfluidic chips where Deep Learning algorithms analyze 3D refractive index maps on-the-fly (latency < 1 ms) to trigger downstream sorting actuators. This "Intelligent Cytometer" will enable the isolation of rare metastatic cells or drug-resistant bacteria from complex biofluids without labels.

- **Stress-Responsive Biofilms and Tissues:** Biofilms are not static; they adapt mechanically. The network has identified "stress-hardening" in biofilm streamers, where the extracellular DNA backbone stiffens under flow [56]. Future research will map the full viscoelastic landscape of biofilms and tissues (e.g., tumor spheroids) under dynamic loading. The goal is to predict how mechanical cues—like substrate stiffness or shear stress—trigger phenotypic switches (e.g., planktonic-to-biofilm transition [57]) or collective migration modes.

- **Organ-on-Chip Mechanotyping:** Scaling down, the network aims to build "Organ-on-Chip" platforms that mimic the mechanical microenvironment of specific tissues (e.g., the stiffness of a tumor or the shear of a capillary). By coupling these chips with Brillouin microscopy or holographic tomography, researchers will perform "mechanotyping" of single cells in situ, correlating their mechanical stiffness with their gene expression or drug response [58].

List of Groups & Capabilities

- **43-Luxembourg (A. Sengupta):** Topological microfluidics and microbial ecology.

- **50-Naples (P. Ferraro/L. Miccio):** Digital Holography and Tomographic Flow Cytometry.

- **11-Leeds (L. Dougan):** Single-molecule force spectroscopy (AFM).

5.2.3 Self-Assembled Biological Matter: Disordered Proteins and Membrane Biophysics

Leading scientists: R. Richter / F. Schreiber

State-of-the-art: Unraveling Disorder and Multivalency The network has established a world-leading position in the structural and dynamic characterization of **Intrinsically Disordered Proteins (IDPs)** and their interactions with lipid membranes. By combining Small-Angle Scattering (SAS) with advanced "Hierarchical Chain Growth" (HCG) simulations, researchers have demonstrated that the global dimensions and phase behavior of IDPs (such as Tau and TDP-43) emerge directly from their local stiffness and transient secondary structures [15]. This "local-to-global" understanding has been crucial for deciphering the molecular grammar of **Liquid-Liquid Phase Separation (LLPS)**, identifying specific residues and post-translational modifications (like phosphorylation) that act as switches for condensation [17].

In parallel, the network has redefined our understanding of cell surface interactions through the concept of **"Superselectivity"**. Using model surfaces grafted with glycans and receptors, researchers have shown that multivalent binding (*e.g.*, of viruses or toxins) exhibits a sharp, step-like dependence on receptor density. This non-linear response allows biological systems to distinguish between cells with only slightly different surface compositions, a principle now being translated into the design of superselective nanoprobes [45, 59]. Neutron Reflectometry has further provided Ångström-resolution maps of how these multivalent ligands restructure the membrane interface [60].

Future Challenges: Dynamics within Condensates and Synthetic Glycocalyx The focus now shifts from static structures to the internal dynamics of these assemblies and the engineering of biomimetic interfaces.

- **Dynamics inside Biomolecular Condensates:** While the formation of condensates is well-studied, the physical state of the matter *inside* them remains elusive. Is it a liquid, a glass, or a gel? The network will employ Neutron Spin Echo (NSE) and fluorescence lifetime imaging (FLIM) to probe the "internal friction" and hydration dynamics of proteins within dense condensates [61]. Understanding how confinement alters water mobility and chain relaxation is critical for explaining how condensates regulate biochemical reaction rates (e.g., in transcription factories).
- **Synthetic Glycocalyx Engineering:** The cell's "sugar coat" (glycocalyx) is a complex regulator of adhesion and immunity. The network aims to construct "Synthetic Glycocalyx" models using precision polymer brushes functionalized with specific glycans (e.g., hyaluronic acid, heparan sulfate). By tuning the grafting density and chain length, researchers will mimic the steric and specific filtering properties of the native glycocalyx. This will serve as a platform to study viral entry mechanisms and to design "stealth" coatings for drug delivery vectors that evade immune recognition [23, 62].
- **Membrane Mechanics and Antimicrobial Action:** Investigating how the mechanical properties of the membrane (bending rigidity, tension) modulate the activity of antimicrobial peptides (AMPs) and nanoparticles. Recent work suggests that AMPs may not need to form stable pores to kill cells but can induce "transient water channels" by perturbing lipid packing [63]. Confirming this "disordered toroidal pore" model requires time-resolved scattering experiments that can capture millisecond-scale permeabilization events.

List of Groups & Capabilities

- **11-Leeds (R. Richter):** QCM-D and surface functionalization.
- **48-Tübingen (F. Schreiber):** Protein phase behavior and scattering.
- **45-ILL (A. Martel):** Membrane diffraction and deuteration lab.

5.3 Network Area 4: Polymer-based Complex Systems

Rationale: Moving beyond standard polymer physics, this pillar focuses on topology (rings), dynamic covalent chemistry (vitrimers), and sustainability.

5.3.1 Polymeric "Arrested" Matter: Vitrimers, Gels, and Processing

Coordinators: *(Suggested: E. Di Maio / T. Thurn-Albrecht)*

State-of-the-art: Dynamic Networks and Topological Control The network has made pioneering contributions to the class of polymers that bridge the gap between thermoplastics and thermosets: **Vitrimers** and **Compleximers**. By exploiting dynamic covalent chemistry (e.g., dioxaborolane metathesis), researchers have synthesized vitrimers that exhibit Arrhenius-like flow at high temperatures while maintaining full network integrity at service temperatures. A key methodological advance has been the use of **Fast Scanning Calorimetry (FSC)** to decouple the bond-exchange transition temperature (T_v) from the glass transition temperature (T_g), proving that these are distinct physical processes [11].

Simultaneously, the network has introduced "Compleximers"—polyelectrolyte complexes where the ionic bonds are "moderated" by bulky hydrophobic groups. This moderation prevents the brittle fracture typical of dried salts, yielding water-free, tough, and recyclable plastics that can be processed like thermoplastics [12].

Researchers at **46-Durham** complement this by focusing on the molecular rheology of complex polymer architectures, utilizing advanced synthesis to create well-defined branched and ring polymers to test tube-model theories.

In the realm of processing, the network has advanced the understanding of **Flow-Induced Crystallization (FIC)**. The development of the polySTRAND model has provided a quantitative link between the molecular weight distribution of a polymer melt and its nucleation rate under shear. This model explains the "superexponential" increase in nucleation density observed in industrial flows by identifying high-molecular-weight chains as the critical precursors that stretch and align to form shish-kebab structures [13].

The mechanical integrity of these advanced polymers is a key focus for **53-INSA Lyon**, where researchers are investigating crack propagation in filled elastomers and the deformation behaviors of semi-crystalline polymers under cyclic loading. Their work on the elastocaloric effect in rubbers opens new avenues for solid-state cooling applications. Simultaneously, the **18d-Le Mans** group is establishing rules for the self-assembly of amphiphilic block copolymers, using light scattering and rheology to understand how block topology controls the structure of aggregates at thermodynamic equilibrium.

Future Challenges: Sustainable Processing and Topological Engineering The future focus is on applying these fundamental insights to sustainable materials and advanced manufacturing processes.

- **Sustainable Foaming with Vitrimers:** Conventional polymer foams are difficult to recycle. The network aims to develop "Vitrimeric Foams" using biodegradable polymers (like PLA or starch) cross-linked with dynamic bonds. The challenge is to tune the bond exchange kinetics to match the timescale of bubble growth during supercritical CO_2 foaming. If the exchange is too fast, the foam collapses; if too slow, it fractures. Mastering this "Deborah number matching" will enable the production of high-strength, recyclable, bio-based foams [42].
- **Topology-Directed Crystallization in Processing:** How do topological constraints (knots, rings, branches) influence crystallization under flow? The network will investigate how ring polymers—which lack chain ends and cannot reptate—crystallize compared to

linear chains. Hypotheses suggest that rings might exhibit suppressed FIC due to the absence of reptation-induced orientation, or conversely, enhanced nucleation due to topological interlocking. Testing this requires combining high-shear rheology with in-situ X-ray scattering (Rheo-SAXS) on pure ring polymer melts synthesized within the network [9].

- **Molecularly-Informed Additive Manufacturing:** Applying the polySTRAND model to 3D printing (Fused Deposition Modeling). The thermal history in 3D printing involves rapid cooling and layer-by-layer reheating, which is distinct from injection molding. The goal is to predict and control the "welding" strength between layers by modeling the interdiffusion and co-crystallization of polymer chains across the interface, optimizing the print parameters for maximum mechanical integrity [43].

List of Groups & Capabilities

- **39-Halle (T. Thurn-Albrecht):** Fast Scanning Calorimetry (FSC) and NMR.
- **53-INSA Lyon (L. Chazeau):** Mechanical characterization and fracture mechanics.
- **18d-Le Mans (C. Chassenieux):** Self-assembly of block copolymers and rheology.
- **50-Naples (E. Di Maio):** High-pressure foaming and 3D printing.

5.3.2 Topological Polymers: Rings, Knots, and Active Filaments

Leading scientists: M. Kruteva / P. Virnau

State-of-the-art: Beyond Reptation The network has fundamentally challenged the "Standard Model" of polymer physics—the tube model of reptation—by investigating polymers with non-trivial topology. A landmark achievement has been the definitive characterization of the dynamics of **Ring Polymers**. Unlike linear chains, rings have no ends and cannot reptate. Using Neutron Spin Echo (NSE) spectroscopy, network researchers have shown that ring melts exhibit "self-similar" dynamics over a wide range of time scales, consistent with a "lattice animal" or "fractal loopy globule" conformation, rather than the tube confinement observed for linear chains [7].

This work has been extended to **Ring-Linear Blends**, where a dramatic "threading" effect occurs: linear chains penetrate the open loops of the rings, creating transient topological crosslinks that drastically increase viscosity. The network has quantified this effect, showing that even a small fraction of rings can act as potent rheological modifiers [9].

In the realm of **Knots**, simulations have revealed that the probability of knotting in DNA and synthetic polymers is non-monotonically dependent on chain stiffness and confinement. Recent studies have shown that knots are not static; they can be "tightened" or "delocalized" by external fields, influencing the polymer's ejection from nanopores [64].

Future Challenges: Activity and Non-Equilibrium Topology The next frontier is to introduce *activity* and *flow* into these topological systems.

- **Non-Equilibrium Topology under Shear:** How does a strong shear flow affect a knotted polymer? Does it tighten the knot until the chain breaks, or does it facilitate unknotting? Network simulations suggest that shear flow can "blow up" knots or cause them to slide along the chain contour [65]. Experimental validation is now needed, using microfluidic extension of single DNA molecules combined with fluorescence microscopy to visualize knot dynamics in real-time. This has implications for the stability of long genomic DNA during pipetting or injection.

- **Active Topological Polymers:** Synthesizing "Active Polymers" where the monomers themselves are active agents (e.g., Janus colloids linked by springs) or where the chain is driven by molecular motors. Theory predicts that such "active filaments" should exhibit spontaneous coiling and autonomous motion, but the role of topology (ring vs. linear) in active matter is unexplored. Can an active ring polymer act as a "vesicle-like" container? Can an active knot perform work? The network will leverage its DPD simulation capabilities to explore this "Active Topology" phase space.
- **Topological Glass Transition:** Theoretical predictions suggest that ring polymers might exhibit a unique "Topological Glass Transition" driven by the jamming of threading constraints rather than density. The network aims to test this hypothesis using NSE on high-molecular-weight ring melts, looking for signatures of arrested dynamics that are distinct from the conventional cage effect [8].

List of Groups & Capabilities

- **1a-FZJ (J. Stellbrink/M. Kruteva):** Neutron Spin Echo (NSE) and synthesis.
- **2-Mainz (P. Virnau):** Simulations of knots and polymer topology.
- **11-Leeds (D. Read):** Theoretical modeling of entangled dynamics (Tube theory).

6 Research Platforms: Joint Infrastructure Inventory

To support the ambitious scientific pillars, the SoftComp Consortium leverages a distributed but highly complementary infrastructure. This inventory aggregates the specific equipment, synthesis capabilities, and computational resources available across the member nodes, organizing them into functional platforms.

6.1 Network Capability and Scientific Synergy Analysis

To ensure the strategic alignment of the SoftComp consortium, we performed a quantitative network analysis extracting relationships from bibliographic data and self-reported laboratory capabilities. This data-driven approach visualizes not only the physical infrastructure but the specific scientific intersections connecting the network.

6.2 Platform 1: Advanced Synthesis & Sample Environment

Mission: To provide unique, isotopically labeled, and functionalized soft matter systems that are unavailable commercially.

- **Deuteration & Isotopic Labeling:**
  - **D-Lab (45-ILL):** Large-scale production of deuterated lipids (for membrane asymmetry studies), proteins (for SANS contrast variation), and surfactants.
  - **Polymer Synthesis (1a-FZJ/20-San Sebastian/39-Halle):** Anionic polymerization lines for model polymers (Ring PEO, Star polymers, H-polymers) with specific deuteration patterns.
- **Functional Nanomaterials:**
  - **Chemical Labs (24-Poznan/54-Ca' Foscari):** Synthesis of magnetic nanoparticles (core-shell), quantum dots, functionalized carbon nanotubes, and hybrid organic-inorganic nanomaterials (gloveboxes, autoclaves up to 1100°C).

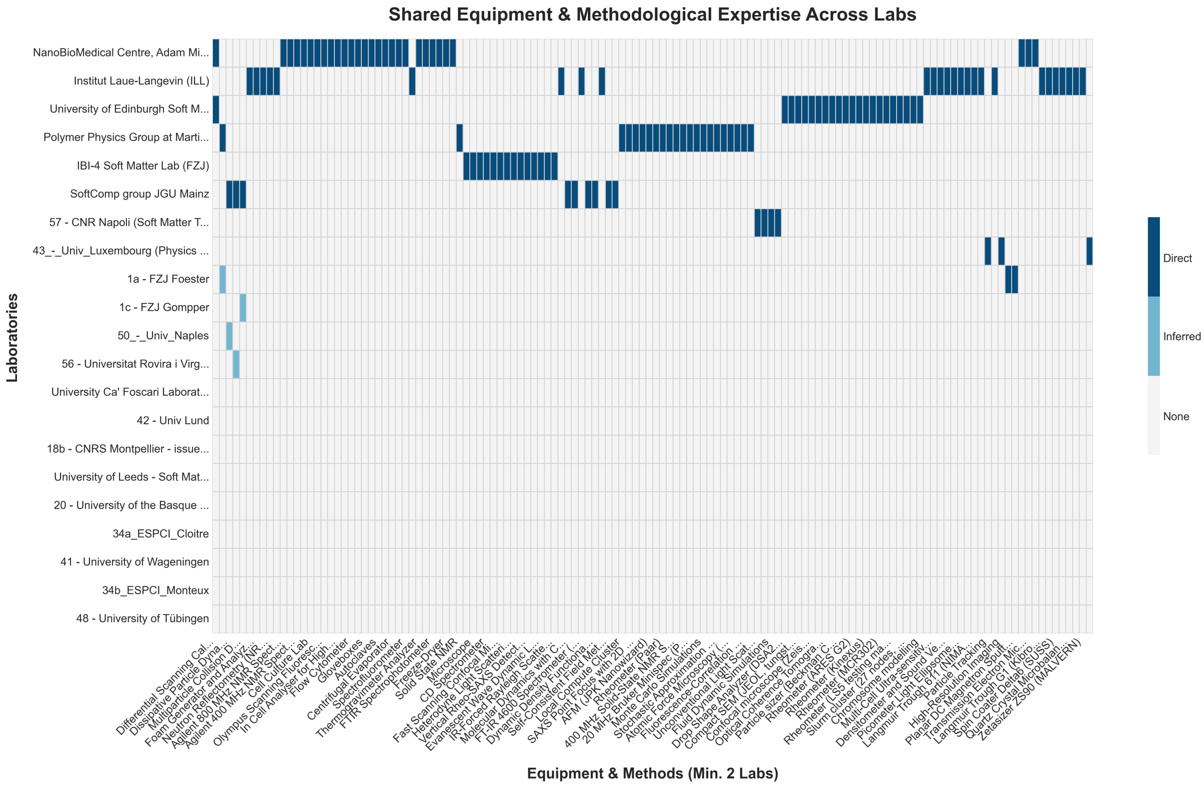

Figure 1: **SoftComp Laboratory Capability Matrix:** A filtered, high-resolution heat map visualizing the distribution of shared experimental methodologies and equipment across member laboratories. By removing isolated nodes and clustering highly connected infrastructure, this matrix serves as a strategic map for the Network Coordination Committee to identify complementary skill sets (e.g., linking computational groups with synthesis labs) and guide the formation of cross-node "Expertise Clusters."

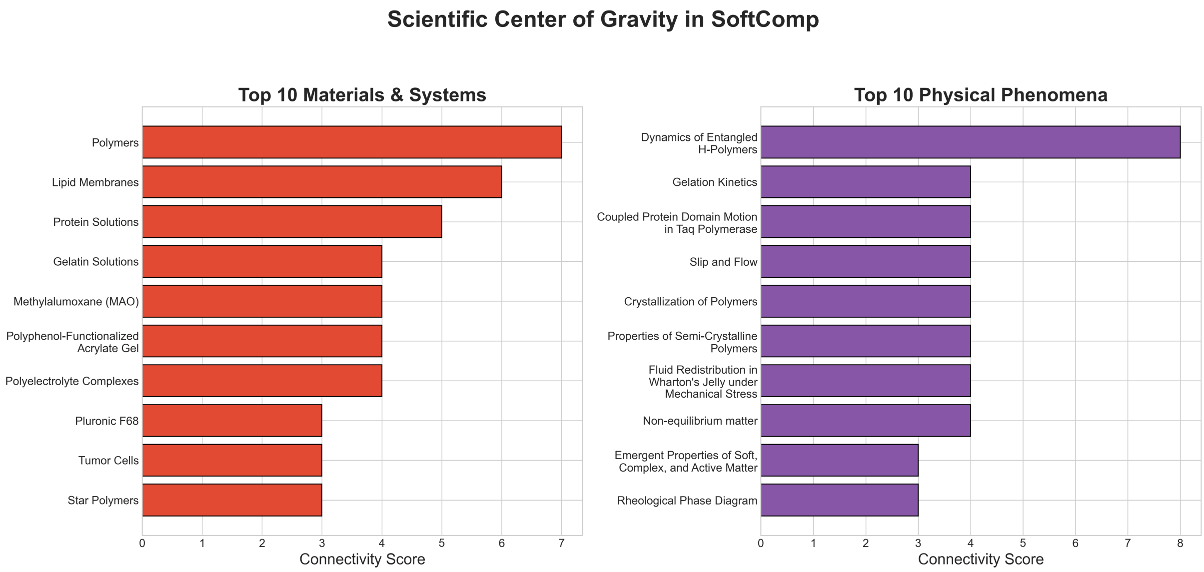

Figure 2: **Core Scientific Focus:** A quantitative ranking of the top specific entities investigated within the network, categorized by Materials (red), and Phenomena (purple). Unlike broad categorizations, this graph highlights the network's deep specific expertise in advanced scattering techniques (Neutron Scattering, SAXS) applied to polymers and their direct application to highly complex systems like entangled polymers, lipid membranes, and phase transitions.

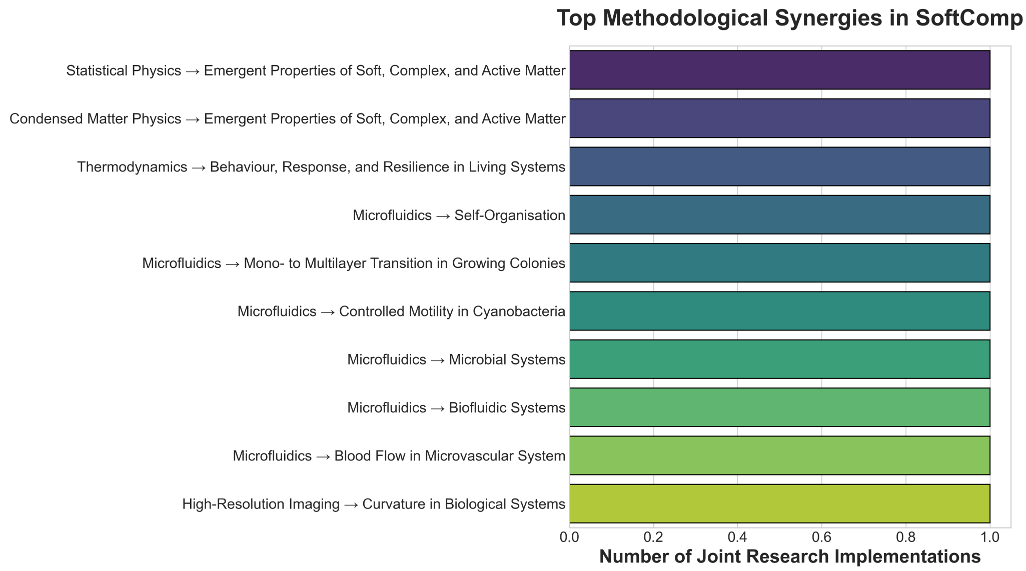

Figure 3: **Methodological Synergy Map:** This interaction matrix illustrates the exact cross-disciplinary linkages between the most prominent investigative methods and target materials/phenomena. The heatmap reveals a strong integration of Molecular Dynamics and Scattering techniques applied toward understanding complex phase behaviours (e.g., crystallization, microphase separation) and biological systems, proving the consortium's unique capability to bridge theory and experiment.

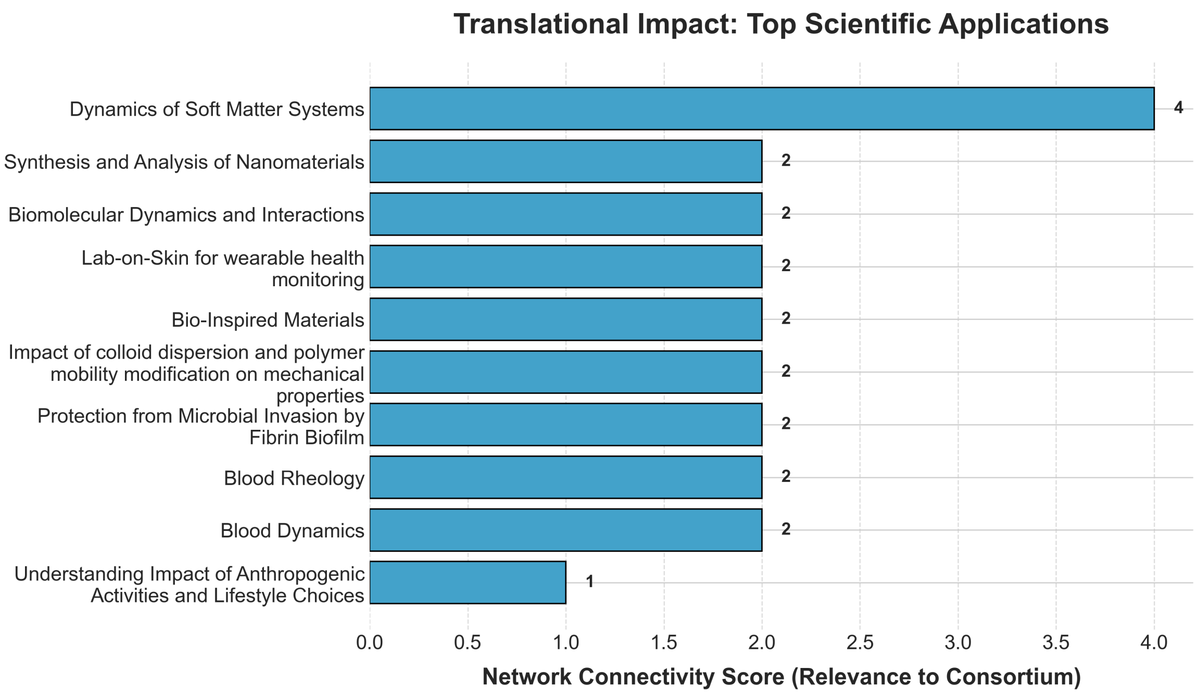

Figure 4: **Scientific Portfolio Distribution:** The proportional distribution of research entities identified across the network's output.

  - **Microfluidic Synthesis (2-Mainz/11-Leeds):** On-chip generation of monodisperse microgels, giant unilamellar vesicles (GUVs), and hierarchically structured particles.

- **Sample Environments:**
  - **Rheo-SANS/SAXS Cells (45-ILL/1b-FZJ):** Couette and cone-plate shear cells transparent to neutrons/X-rays; Vertical Rheo-SAXS detection lines.
  - **High-Pressure/Electric Field Cells (1b-FZJ/45-ILL):** Cells for SANS under electric fields (FZJ) and high pressure (ILL) to study phase transitions.
  - **Langmuir Troughs (45-ILL/11-Leeds/34b-ESPCI):** Advanced troughs (NIMA, Kibron) for interfacial films, adaptable for neutron reflectometry and interfacial rheology.

Strategic Action: Establish a **"Soft Matter Library"**—a centralized database and physical repository of standard deuterated polymers, lipids, and characterized nanoparticles available to all network partners for benchmarking and calibration.

6.3 Platform 2: Scattering, Imaging & Rheology

Mission: To enable multi-scale characterization from the Angstrom to the millimeter, and from femtoseconds to hours.

- **Neutron and X-ray Scattering (including Large Scale Facilities):**
  - **SANS (45-ILL/1a-FZJ):** D11, D22, D33 (ILL); KWS-1, KWS-2 (FZJ). Upgraded with SEC-SANS for biological samples.
  - **Neutron Spin Echo (NSE) (45-ILL/1a-FZJ):** IN11, IN15 (ILL); J-NSE (FZJ) for probing polymer dynamics and membrane undulations.
  - **Reflectometry (45-ILL):** D17, FIGARO for solid-liquid and air-liquid interfaces.
  - **SAXS/WAXS (39-Halle/1a-FZJ/53-INSA/11-Leeds/42-Lund):** High-brilliance lab-scale SAXS/WAXS setups (e.g., Xenocs Xeuss 3.0 at INSA, Anton Paar SAXSpoint at Leeds) with tensile and humidity stages.

- **Advanced Microscopy and Imaging:**
  - **Electron Microscopy (24-Poznan/12-Edinburgh/53-INSA/11-Leeds):** HR-TEM (Jeol ARM 200F), Cryo-TEM (Jeol 1400), Cryo-FIB-SEM (Zeiss Crossbeam 550), and Environmental TEM for in-situ studies.
  - **Optical Microscopy (24-Poznan/42-Lund):** Fast Scanning Confocal (Leica SP8, Zeiss LSM980) with STED and FLIM capabilities.
  - **Label-Free Imaging (50-Naples):** Digital Holographic Microscopes and Tomographic Flow Cytometers for 3D refractive index mapping.
  - **Surface Probes (11-Leeds/39-Halle/12-Edinburgh):** High-speed Atomic Force Microscopes (Bruker NanoRacer, JPK Nanowizard) for single-molecule force spectroscopy and rapid topographical imaging.

- **Rheology and Nanomechanics:**
  - **Macroscopic Rheology:** A comprehensive suite of high-end rheometers (Anton Paar MCR series, TA ARES G2) located at **50-Naples**, **18d-Le Mans**, **34b-ESPCI**, **11-Leeds**, and **12-Edinburgh**.

- **Mechanical Testing (53-INSA/11-Leeds):** Dynamic Mechanical Analysis (DMA) and tensile testing coupled with in-situ X-ray scattering or stereo-correlation.
- **Specialized Rheology:** Counter-rotating shear cells (45-ILL), Microcapillary Rheometers (50-Naples), and Interfacial Shear Rheometers (34b-ESPCI/11-Leeds).

Strategic Action: Develop a **"Correlative In-Operando Service"** that physically couples instruments (e.g., a portable Digital Holography unit mounted on a SANS beamline) to allow simultaneous structural and morphological characterization under flow.

6.4 Platform 3: Theory, Simulation & Data Science

Mission: To provide the theoretical framework for experimental design and the computational tools for data inversion and predictive modeling.

- **High-Performance Computing (HPC):**
  - **Clusters (12-Edinburgh/2-Mainz/39-Halle):** Dedicated Slurm clusters (e.g., Edinburgh: 27 nodes, 64 CPUs/node) and GPU-accelerated nodes for massive parallel simulations.
  - **Software Codes (1c-FZJ/2-Mainz/42-Lund):** Proprietary and open-source codes for DPD, MPC, Lattice Boltzmann, and DFT developed within the network to model active matter and polymer dynamics.
- **Machine Learning and Data Analysis:**
  - **AI for Scattering (56-URV/2-Mainz):** Neural networks (CNNs, Normalizing Flows) for real-time inversion of GISAXS/SANS data.
  - **Inverse Design (57-CNR-Naples/54-Ca' Foscari):** Network theory and computational pipelines for designing self-assembling systems and analyzing complex datasets.
  - **AI for Imaging (50-Naples):** Deep Learning models for cell classification in holographic cytometry.

7 Strategic Vision: From Characterization to Engineering Life-Like Systems

For the past decade, SoftComp activities have been organized around three traditional domains. While this structure successfully fostered deep expertise, the scientific landscape has shifted. The grand challenges of the next decade—autonomous materials, sustainable plastics, and digital twins for biology—require a transition from **equilibrium to non-equilibrium**, from **passive to active**, and from **observation to prediction**. To maintain global leadership, SoftComp leverages its unique combination of neutrons, photons, and algorithms through specific **Expertise Clusters**. These clusters operationalize the network's distributed infrastructure to address cross-cutting challenges.

7.1 Key Expertise 1: Active Rheology

Goal: To define the constitutive equations of active fluids (bacterial suspensions, chiral colloids) by coupling macroscopic rheology with microscopic dynamics.

- **The Gap:** We understand single swimmers and have advanced rheometers, but lack a systematic link between the two for bulk active fluids.
- **SoftComp Leading Scientists:**
  - **Experimentalists: P.L. Maffettone (50-Naples)**, **W. Poon (12-Edinburgh)**, and **P. Schurtenberger (42-Lund)**.
  - **Theorists: G. Gompper (1c-FZJ)** and **M. Ripoll (1c-FZJ)**.
  - **Key Infrastructure:** Naples' *Microcapillary Rheometer* coupled with FZJ's *Electric Field Light Scattering* and Lund's *Active Matter Modelling.*

7.2 Key Expertise 2: The "Digital Twin" for Soft Matter

Goal: To solve the "inverse problem" in scattering and microscopy using AI, enabling real-time structural determination.

- **The Gap:** Scattering data provides statistical averages, while microscopy provides local snapshots. Neither gives a full 3D dynamic picture alone.
- **SoftComp Leading Scientists:**
  - **Imaging: P. Ferraro (50-Naples)** - Digital Holography.
  - **Scattering: L. Porcar (45-ILL)** - SANS/AI.
  - **AI/Theory: 56-V. Baulin (URV)**, **P. Virnau (2-Mainz)**, and **A. Giacometti (54-Ca' Foscari)**.
- **Key Infrastructure:** ILL's D22/D33 beamlines, Naples' Holographic Flow Cytometer, and Ca' Foscari's network theory algorithms.

7.3 Key Expertise 3: Sustainable "Living" Materials

Goal: To engineer materials that mimic biological adaptation (self-healing, stress-stiffening) using sustainable building blocks.

- **The Gap:** Biological insights and synthetic capabilities need to be translated into "synthetic design."
- **SoftComp Leading Scientists:**

- **Bio-Physics: A. Sengupta (43-Luxembourg)** - Bacterial mechanics.
- **Polymer Physics: T. Thurn-Albrecht (39-Halle)**, **J. Colmenero (20-San Sebastian)**, and **L. Chazeau (53-INSA)**.
- **Processing: E. Di Maio (50-Univ.Naples)** - Bio-foaming.

- **Key Infrastructure:** Halle's *Fast Scanning Calorimetry*, Naples' *3D Foam Printing*, and INSA's *In-situ Tensile Microscopy.*

7.4 Key Expertise 4: The "Synthetic Cell Interface" Initiative

Goal: To engineer and characterize asymmetric, responsive lipid membranes that mimic the complexity of real cell walls.

- **The Gap:** Theoretical models of membrane permeation must be coupled with direct measurements of mechanical forces and transport kinetics.
- **SoftComp Leading Scientists:**
  - **Structural Analysis: U. Perez-Salas (45-ILL)** and **A. Martel (45-ILL)**.
  - **Nanomechanics: S. Connell (11-Leeds)** and **L. Dougan (11-Leeds)**.
  - **Theory: V. Baulin (56-URV)**.
- **Key Infrastructure:** ILL's *FIGARO* and Leeds' *Fast-Scan AFM.*

7.5 Key Expertise 5: "Disorder-to-Function" (IDPs and SCNPs)

Goal: To bridge the gap between biological *Intrinsically Disordered Proteins (IDPs)* and synthetic *Single-Chain Nanoparticles (SCNPs).*

- **The Gap:** Combining the physics of internal friction and conformational entropy across biological and synthetic domains.
- **SoftComp Leading Scientists:**
  - **Synthetic Polymer Physics: J. Pomposo (20-San Sebastian)** and **A. Arbe (20-San Sebastian)**.
  - **Biological Physics: L. Stelzl (2-Mainz)** and **R. Biehl (1a-FZJ)**.
  - **Phase Behavior: F. Schreiber (48-Tübingen)**.
- **Key Infrastructure:** FZJ's *J-NSE* and San Sebastian's *Dielectric Spectroscopy.*

7.6 Key Expertise 6: "Green" Soft Matter for Energy and Recycling

Goal: To utilize Ionic Liquids (ILs) and Deep Eutectic Solvents (DES) for sustainable polymer processing and metal recovery.

- **The Gap:** Integrating synthesis, crystallization physics, and processing for Circular Economy materials.
- **SoftComp Leading Scientists:**
  - **Ionic Liquids: R. Markiewicz (24-Poznan)**.
  - **Crystallization: T. Thurn-Albrecht (39-Halle)**.
  - **Applications: D. Harbottle (11-Leeds)** (Metal extraction) and **S. Förster (1a-FZJ)** (Batteries).
- **Key Infrastructure:** Poznan's *Agilent 800 MHz NMR* and Halle's *SAXS/WAXS* setups.

7.7 Infrastructure Access and Mobility Strategy

To maximize the impact of these Expertise Clusters, the network facilitates seamless access to equipment.

7.7.1 The "Sample-to-Beam" Fast Track

Problem: Synthesizing specialized samples (e.g., deuterated ring polymers) and getting beamtime at large-scale facilities are often disconnected processes. *Solution:* The SoftComp Research Visits programme enables a cohesive workflow: 1. Synthesis and initial characterization at **San Sebastian, Halle, or Poznan**. 2. Advanced scattering experiments at **ILL or FZJ**. 3. Data modelling and simulation via remote access to **Mainz or Edinburgh** clusters.

7.7.2 The "Mobile Instrumentation" Fleet

Problem: Some unique instruments are fixed at specific partner sites. *Solution:* SoftComp supports the transport of portable modules to beamlines. For example, the adaptation of the **Naples Digital Holography** module for mounting directly onto the ILL D22 sample stage enables simultaneous SANS and 3D imaging, a capability unique in the world.

7.8 Implementation Plan

Phase 1 (2025-2026): *Data Integration.* Establish a repository for standardized data formats between Rheology, Imaging, and Scattering groups. Launch pilot collaborative projects within the defined Expertise Clusters.

Phase 2 (2027-2028): *Infrastructure Coupling.* Demonstrate simultaneous Holography-SANS experiments. Expand the "Sample-to-Beam" mobility grants to include new partners (Ca' Foscari, INSA).

Phase 3 (2029-2030): *Translation.* Publish a white paper on the design rules for "Active and Intelligent Soft Matter," derived from the network's integrated experiments and simulations.

The true power of this consortium lies in its potential to function as a **single, distributed meta-facility**. No other network can seamlessly link the **holographic imaging** of Naples with the **neutron scattering** power of the ILL, the **theoretical rigor** of Mainz/Edinburgh, and the **material synthesis** expertise of Halle, San Sebastian, and Poznan. By operationalizing these connections, SoftComp ensures it remains the epicenter of European soft matter research.

The true power of this consortium lies not in its individual labs, but in its potential to function as a **single, distributed meta-facility**. No other network can seamlessly link the **holographic imaging** of Naples with the **neutron scattering** power of the ILL, the **theoretical rigor** of Mainz, and the **material synthesis** expertise of Halle and San Sebastian. By operationalizing the "Collaboration Clusters" and the "Digital Twin" platform proposed herein, SoftComp will do more than just observe the complexity of soft matter, it may transform into strategic, infrastructure-driven alliance. This strategy ensures that SoftComp will not only remain the epicenter of European soft matter research but will also define the paradigm for the next generation of active and functional materials.

8 Dissemination

Effective dissemination of knowledge is a cornerstone of the SoftComp activity. By combining scientific excellence with broad outreach and sustainable practices, SoftComp ensures that scientific results, technological advances, methodologies, and best practices developed within SoftComp are effectively communicated to relevant stakeholders, foster uptake by the research community and industry, and contribute to education, innovation, and societal impact and that its research outputs generate lasting value for science, industry, and society. The SoftComp Consortium's mission statement makes clear that its main goal is to enhance scientific activity in all branches of soft matter research, and the dissemination activities of the SoftComp Consortium are guided by the following objectives:

- Scientific Excellence: Promote high-quality research outcomes in soft matter science through peer-reviewed publications and scientific events.
- Community Building: Strengthen and expand the SoftComp research community across disciplines and regions.
- Knowledge Transfer: Facilitate the transfer of methods, tools, and results to industry and applied research.
- Education and Training: Support capacity building for early-stage researchers and practitioners.

Therefore, the SoftComp dissemination activities are tailored to the needs of

- Academic Researchers: in soft matter science, ranging from established experts to newcomers, and encompassing both experimentalists and theoreticians.
- Industry and SMEs: Companies interested in applying soft computing techniques to real-world problems.
- Early-Stage Researchers and Students: PhD candidates, postdoctoral researchers, and graduate students.

The SoftComp activities include the following means of dissemination:

- Dissemination events, like conferences, workshops and meetings, amongst them:
  - International Soft Matter Conference
  - SoftComp Annual meetings
  - Webinars
- Scientific Publications (or single SoftComp group or joint)
- Newsletters
- SoftComp Forum
- Web portal
- Social Media accounts

Despite, the SoftComp dissemination activities mainly depends on the applications submitted by the members, some events are regularly financed by SoftComp, such as, for example, the International Soft Matter Conference (ISMC) established in 2007 by the SoftComp Network of Excellence that it turned out to be the Softcomp's flagship achievement as it gave birth to a series of conferences that take place every year now in three different continents, i.e. Europe, America and Asia.

The SoftComp annual meeting plays a vital role in the dissemination of SoftComp research by bringing together all SoftComp researchers to share progress, align objectives, and foster collaboration. It provides a dedicated forum for presenting scientific results, discussing methodological advances, and highlighting applications developed within the network, ensuring that knowledge generated in SoftComp is effectively communicated across disciplines. Each year, the Annual Meeting welcomes about 130-140 researchers and features a special thematic focus, explored through dedicated sessions, alongside general sessions that cover a broad range of topics, promoting both in-depth discussion and cross-disciplinary exchange. The meeting also strengthens internal dissemination by encouraging cross-project synergies, while supporting external dissemination through the involvement of early-career researchers, invited speakers, and links to related initiatives. Overall, the annual meeting is a key instrument for consolidating SoftComp's scientific identity, amplifying its visibility, and maximizing the impact of its research outputs.

Figure 5: SoftComp Annual Meeting 2025, Venice-Mestre, Italy.

Electronic media, including the SoftComp website, newsletters, user forum and SoftComp accounts on social networks, continuously promote awareness of the network and its partners and enable the exchange of information both within the network and externally.

9 Education

Educating the next generation of scientists in soft matter and soft matter composites is a core responsibility of SoftComp members. Our mission is to provide PhD students with a training environment richer and more diverse than what would be available outside SoftComp. By supporting cross-institution mobility, via the Research Visits funding programme, and organizing many schools and labcourses, SoftComp aims to equip students with both the knowledge and skills needed to excel in academic and industrial research. Many members are actively teaching at all level, Bachelor, Master and PhD, at major European universities, providing the first step in educating future soft matter scientists. The SoftComp opportunities for educational purposes rely on the applications submitted by the members, however a number of labcourses and schools are regularly granted by SoftComp, among which the following ones:

- European School on Rheology, an intensive course on rheological measurements and applications
- Labcourse on Neutron scattering, an impressive tool for investigating soft condensed matter
- NMR Ampere School, for theoretical and experimental aspects of NMR methods
- Summer School on Scattering Methods Applied to Soft Matter, an introduction to instrumentation and experimental methods in scattering, covering both dynamics and structural aspects.

At the SoftComp Annual Meetings, there is strong participation of PhD students, who are trained in improving their communication skills through oral presentations in a friendly as well as expert environment. These meetings provide an important forum for students to present research, receive feedback, and develop confidence in presenting to both peers and senior researchers.

10 Management

10.1 Organization

The SoftComp Consortium is regulated by the SoftComp Consortium Agreement (CA) signed by all the participant groups. The organization of the SoftComp Consortium is described in the following figure.

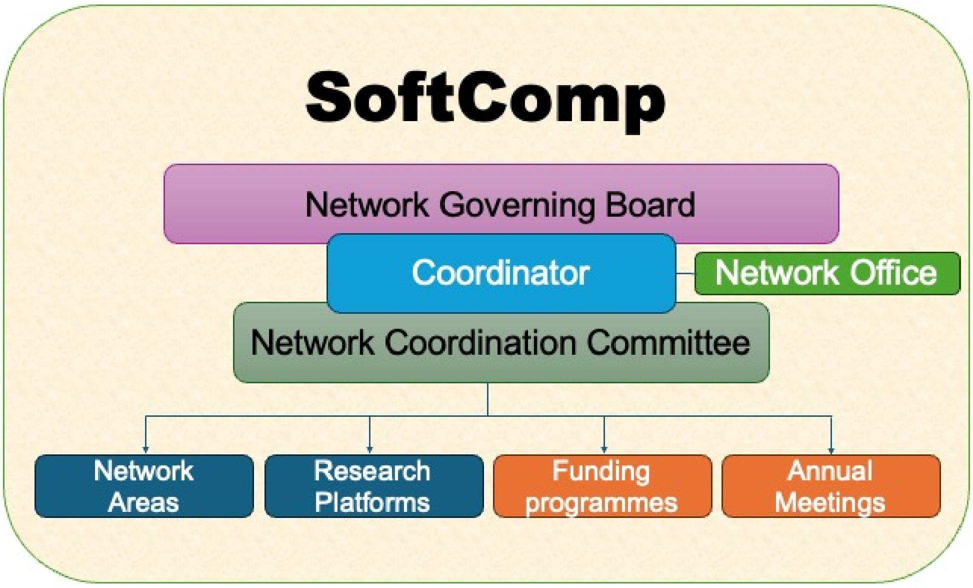

Figure 6: SoftComp organizational structure.

The SoftComp Consortium is governed by the Network Governing Board (NGB), consisting of one delegate per SoftComp group.

Moreover, the Network Coordination Committee (NCC) is in charge to run the SoftComp Consortium, and consists of the following members:

- the SoftComp Coordinator
- the Network Area Chairpersons
- the Research Platform Leaders
- the Dissemination Officer
- the Educational Officer
- the SoftComp Network Manager
- the Industrial Liaison and Exploitation Officer

Additional experts, such as, for example, the Communication and the Social Media Officers, can be invited to the NCC and NGB meetings.

The Coordinator of the SoftComp Consortium has the overall responsibility to run the SoftComp Consortium and the funds are managed according to the internal and national rules of the Coordinator institution. Among others, the Coordinator has following major rights and obligations:

- management of the funds in accordance with the NGB as well as NCC decisions

- obligation not to conclude and/or to fulfil any agreement for which the financing is not assured
- responsibility of the administration
- obtaining audit certificates
- preparation of the NGB and NCC meetings
- updating the SoftComp Research Road Map.

The Coordinator is supported in these tasks by the SoftComp Network Office.

In case of needs, dedicated task forces can be appointed to tackle issues.

The full set of information is available in the SoftComp Consortium Agreement (CA) and it can be downloaded at https://eu-softcomp.net/download/consortium-agreement.

10.2 Fee

Each SoftComp group self-finances the activity with the payment of a yearly fee. There are two level of membership: Academic and Industrial. The SoftComp Network Governing Board at the meeting N. 09 on May 29, 2012, decided to reduce the yarly fee compared to what stated in the original Consortium Agreement. The current yearly fee are then:

- Academic partners 2.500€
- Industrial partners 5.000€

The payment of the yearly fee gives the following rights:

- participation to the SoftComp Annual meeting up to 4 persons of each SoftComp group, free of charge, i.e. accommodation, subsistence, and a financial contribution up to 250 euro per person for the travel costs
- submit unlimited applications to the SoftComp funding programmes

10.3 Funding programmes

After the end of the EU Grant, the SoftComp Consortium decided to self-finance the activities, which include an Annual Meeting and the following funding programmes:

- Dissemination and Educational programme to organize an event (conference, workshop, labcourse, school. . .). If accepted the SoftComp Consortium can contribute up to 50
- Equity programme, for increasing the visibility of underrecognized researchers. If accepted the SoftComp Consortium can contribute up to 100
- Research Visits programme, for facilitating integration through experiments, sample preparation and scientific discussions. If accepted the full travel, accommodation and subsistence costs can be covered by the SoftComp Consortium.
- Topical Workshops and Schools programme, for the organization of workshops and schools on special topics If accepted the SoftComp Consortium can contribute up to 100

All researchers affiliated to SoftComp group can submit applications to any of the SoftComp programme for their scientific activities. The applications will be assessed by internal review panels and the decision is communicated to the applicants usually within 4 weeks after the submission. Detailed information on the SoftComp programmes is available within the Guidelines for Applicants at https://eu-softcomp.net/user-area/proposal. Access to this site is reserved to SoftComp members only.

10.4 Finances

The SoftComp Consortium relies on the yearly fees paid by each SoftComp groups. The following table shows the incomes and the costs of all SoftComp years after the end of the EU grant.

Year	Income	Costs	Balance
2010	205.111,60	93.619,48	111.492,12
2011	299.014,87	106.786,20	192.228,67
2012	240.000,00	108.962,21	131.037,79
2013	102.500,00	44.457,68	58.042,32
2014	110.833,00	111.413,98	-580,98
2015	105.000,00	111.842,34	-6.842,34
2016	105.782,26	107.764,89	-1.982,63
2017	98.750,00	138.706,24	-39.956,24
2018	110.000,00	77.191,45	32.808,55
2019	99.379,93	41.107,55	58.272,38
2020	5.000,00	33.240,67	-28.240,67
2021	2.500,00	9.603,80	-7.103,80
2022	75.000,00	93.811,87	-18.811,87
2023	90.000,00	127.350,63	-37.350,63
2024	87.500,00	128.738,06	-41.238,06
Total	1.736.371,66	1.334.597,05	401.774,61

At the end of 2024, the SoftComp financial picture is described below:

Cash	401.774,61€
Committed costs	61.840,08€
Fee not yet cashed	37.500,00€
Total funds available	377.434,53€

The yearly fees are unable to cover the yearly costs, however with the available funds the SoftComp Consortium has a foreseen lifetime of about 10 more years. As already happened in the past, in case applications for research funding will be accepted by external funding agencies, joint activities with SoftComp can be organized and the costs shared among SoftComp and the project(s), which will reduce the SoftComp yearly costs, extending furtherly the SoftComp lifetime. Audit certificates are requested for each SoftComp year.

10.5 Accession to the SoftComp Consortium

In case you are interested to join the SoftComp Consortium, please find here below detailed information on the accession procedure. The accession procedure to the SoftComp Consortium consists of the following steps:

- letter of interest from someone with legal power at your institution stating that the institution agrees to the Consortium Agreement including the annual fee.
- a short document with the expertise and instrumentation ready to be shared within the SoftComp Consortium

After this step, the SoftComp Network Governing Board will vote for the accession. If the time frame is favourable, the applicant is invited to the Annual Meeting for showing the group and the researches carried out there, together with the expertise and instrumentation to be shared within the Consortium.

When the accession is accepted the proper form available in the Consortium Agreement shall be filled and sent to the SoftComp Project Office.

Only after this step an invoice will be issued for the year or fraction of year, and the members of the group can use the SoftComp resources.

11 Contacts

For any question, please contact the SoftComp Network Manager
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12 Acknowledgment

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