MiMM Day 2026:

Can We Design a Stable Gyro-Wire? A Multiphase Modelling Challenge for MiMM Day

Background

Modern adhesive-tape development increasingly relies on virtual methods to reduce experimental effort and identify promising formulation windows earlier in the development process. One emerging challenge is the design of a stable **gyro-wire morphology**, a complex three-dimensional network structure that could enable directed transport of functional additives through the material while maintaining overall mechanical integrity.

Experimental investigations provide only limited insight into the mechanisms governing morphology formation, network connectivity, and long-term stability. A predictive simulation framework is therefore needed to understand whether such structures can emerge in realistic material systems and under which thermodynamic and processing conditions they remain stable.

The Physical System

The target formulation consists of a multiphase material system containing:

- **Matrix A**
- **Additive Y**
- **Triblock Copolymer X**
  - **A-block:** compatible with Matrix A but incompatible with Additive Y
  - **B-block:** compatible with Additive Y but incompatible with Matrix A
  - **C-block:** incompatible with both A and Y

The desired outcome is the spontaneous self-assembly of a continuous **gyro-wire-like network** formed by the B-block domains. This network should remain connected across the material and serve as a transport pathway for Additive Y. Conceptually, the system resembles a morphology-engineering problem in which molecular architecture and thermodynamic interactions must be tuned to create a functional mesoscale structure with targeted transport properties.

The Modelling Challenge

From a thermodynamic perspective, the material system is highly complex and potentially unstable. Competing interactions between the different phases may naturally drive macrophase separation, network breakup, or collapse of connected structures.

The ***key research questions*** are:

- Can a physically realistic model predict the emergence of stable gyro-wire morphologies?
- Which combinations of composition, temperature, interaction parameters, and polymer architecture promote network formation?
- Under which conditions does a percolating B-block network exist?
- Can Additive Y effectively migrate through the connected network?
- Which parameters control the transition between stable and unstable morphologies?

Answering these questions experimentally would require extensive screening campaigns and would provide only limited mechanistic understanding of the governing physics.

Proposed Simulation Approach

The first objective is to identify the most suitable modelling methodology for describing morphology formation in the multiphase system. Candidate approaches include:

- Phase-field modelling

- Coarse-grained molecular simulations
- Hybrid multiscale approaches

A phase-field framework appears particularly promising because it can describe the coupled evolution of multiple interacting phases through nonlinear partial differential equations derived from thermodynamic free-energy functionals.

The model would account for:
- Phase interactions
- Copolymer architecture
- Diffusion processes
- Interfacial energies
- Temperature effects
- Composition-dependent thermodynamics

Simulation results would be coupled with automated parameter screening and optimization methods to identify regions of the design space where stable and connected gyro-wire structures emerge.
In a second step, transport simulations could be performed on the predicted morphologies to evaluate whether Additive Y can efficiently migrate through the generated network.

How is the problem connected to MiMM?
The problem combines several challenges that are highly relevant to the modelling and simulation community:
- Phase separation and self-assembly
- Multiphase thermodynamics
- Nonlinear PDE modelling
- Morphology optimization
- Topology and connectivity analysis
- Transport phenomena in complex microstructures
- Automated exploration of high-dimensional parameter spaces

The challenge therefore provides an attractive benchmark problem at the interface of materials science, applied mathematics, and computational engineering.

Discussion Questions

1. Which simulation approach provides the best balance between physical fidelity and computational efficiency?
2. Can phase-field models reliably predict percolating gyro-wire structures? Or should we follow a different approach?
3. How should connectivity and transport capability be quantified?
4. Which optimization strategies are best suited for identifying stable morphology regimes?
5. What level of molecular detail is required to obtain meaningful predictions?
6. How can such a workflow be transferred into a reusable industrial development service?

Contact at tesa

Kai Ellringmann
Julia Strebe
Nils Hendrik Kröger