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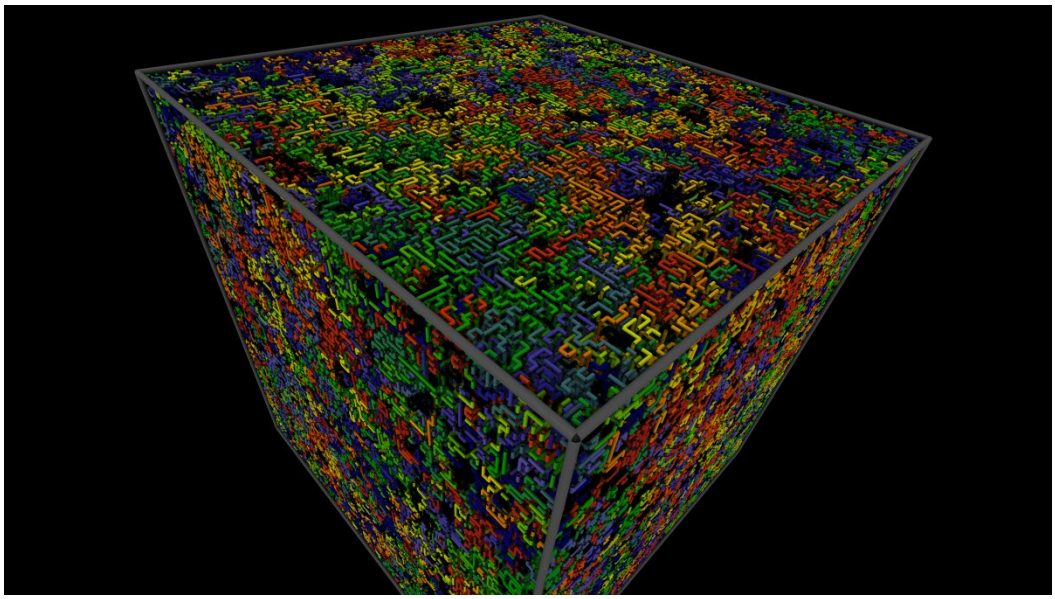
PRESS RELEASE

A new twist in a tangled story

A new self-assembly Monte Carlo method makes it possible to simulate giant dense polymer systems on an unprecedented scale, revealing that their entanglements are not diffuse but rather concentrated in localized knots and links



Trieste, 21 agosto 2026

Long polymer chains are everywhere: in synthetic materials, soft matter, biological systems such as chromosomes, and mathematical models of filaments and knots. When many such chains are densely packed, they form what physicists call a polymer melt. In this crowded environment, each chain is constrained by the others around it. These entanglements are central to the behaviour of polymeric materials, but they also make the systems extremely difficult to simulate: as chain length increases, the time needed to obtain a new independent configuration grows very rapidly. For very large systems, conventional simulations can therefore become computationally prohibitive.

For more than 70 years, scientists have used many “tricks” to speed up this process, including so-called Monte Carlo methods with ingenious moves designed to accelerate the evolution of the system. These methods helped, but the basic

problem remained: in a dense melt, changes still had to propagate through a highly tangled system, slowing down the simulation.

A new SISSA study by Enrico Fornasa, Francesco Slongo and Cristian Micheletti introduces a different way around this bottleneck. Drawing inspiration from ideas in quantum computing, the researchers looked at the problem from a new perspective. Their new method, called Self-Assembly Monte Carlo, or SAMC, stops treating the system as a fixed tangle that must slowly relax; instead, it allows local bonds to break and reform, so that the polymer melt can reorganize more efficiently while still producing physically meaningful equilibrium configurations.
“The key step was to stop asking the tangle to relax by slowly propagating deformations along mutually entangled backbones,” explains Cristian Micheletti, professor of Molecular and Statistical Biophysics at SISSA. “Instead, we let nearby polymers reconnect by swapping bonds, thereby profoundly reorganizing their backbones. This is not meant to reproduce the real microscopic dynamics of a polymer melt, but it is a very efficient way of sampling its equilibrium configurations.”

This extra freedom could have made the method fast but physically meaningless: after many bond swaps, initially long chains might have turned into a dust of much smaller chains, many of them closed on themselves as rings. Instead, giant linear chains emerged spontaneously, taking up almost the entire volume and leaving behind a small background of short rings. The system kept the essential behaviour expected from a dense polymer melt. The result is a major change of scale. SAMC makes it possible to generate configurations with up to 10^9particles, reaching systems far beyond the usual range of conventional approaches. At this size, the bottleneck is no longer producing the configurations: it becomes storing, visualizing and analysing the enormous amount of data produced.

“When producing independent configurations becomes easier than looking at them, you know that the computational problem has changed scale,” says Micheletti. “That is what SAMC gives us: access to a regime where the question is no longer simply whether we can equilibrate the system, but what new physical information we can extract from configurations that were previously too large to handle.”

The simulations also shed new light on how entanglements are distributed in space when long polymers are densely packed. Entanglements within a chain and between pairs of nearby polymers are not spread out in space, but instead manifest as localized knots and links separated by long weakly entangled portions.
The result opens a route to studying dense chain systems beyond idealized polymer physics, including designed materials, polymer networks and biological

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soft matter. Future applications include polymers in spatial confinement, such as channels, slits and cavities, and the use of SAMC-generated configurations as starting points for more detailed molecular dynamics simulations.

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Full Paper
Doi:
https://doi.org/10.1038/s41467-026-74480-4

IMAGE: The image shows a fully packed system of one million particles that self-assembled into ten giant polymers (coloured) and a background of short closed loops (black). Credits: Cristian Micheletti, SISSA.

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