Theory and simulations of branched gels

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Let us consider polymer gels based not on cross-linked linear chains but molecular brushes. They can be described by three parameters, namely degree of polymerization (or length for brevity) of the backbone strand *M*, length between side-chains *m*, and length of side-chains *n*. Having two more adjustable parameters over simple gels we can hope for a possibility to adjust gel properties, *e.g.* swelling ratio and osmotic modulus, as needed for applications.

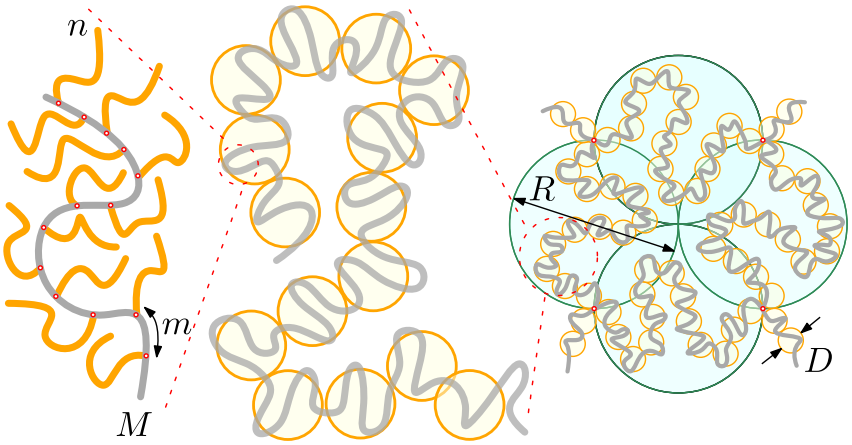

Figure: Geometry parameters of a branched gel.

In this contribution we review predictions of a scaling theory of branched gels in a good solvent and their comparison with Monte Carlo simulations [1–2]. Four interesting regimes according to {*n*,*m*} values are expected, namely either hollow or filled gel mesh and each either with partially or fully stretched spacers of length *m*. The scaling exponents with respect to geometry parameters {*M*,*n*,*m*} are predicted for each regime. The swelling ratio is predicted to pass thru a maximum and osmotic modulus thru a minimum as *n*/*m* ratio increases at fixed *M*. The simulations used Hamiltonian Monte Carlo method with up to 10^5 coarse-grained particles in *NPT* ensemble. The agreement of simulations and scaling theory predictions is fair despite the limited range of accessible {*M*,*n*,*m*} parameters for simulations as theory assumes all of them going to infinity.

References

[1] E. B. Zhulina, F. Uhlik, O. V. Borisov, *Macromolecules* **57**, 6860 (2024).
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[2] F. Uhlik, O. V. Rud, O. V. Borisov, E. B. Zhulina, *Gels* **8**, 793 (2022).
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