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Novel mesoscopic approach for modeling Carbon Nanotube System IGOR OSTANIN[1], ROBERTO BALLARINI[2], TRAIAN DUMITRICA[3], University of Minnesota, DAVID POTYONDY[4], Itasca Consulting Group Inc, UNIVERSITY OF MINNESOTA/ITASCA CG COLLABORATION — We present a distinct spherical element concept for simulating morphologies and mechanical properties of carbon nanotube systems. The important interactions present at the microscopic level are encapsulated into two types of contact models that act simultaneously. Each individual nanotube is coarse-grained into a chain of spherical elements interacting by parallel contact bonds, representing the microscopic covalent bonding. An anisotropic model with aligning moments acts at the contact between elements located in different tubes to represent the van der Waals long-ranged interactions. The accuracy, computational efficiency, and capabilities of the created mesoscopic model are discussed along with illustrative examples, including self-folding of individual nanotubes, mechanical testing of nanotube ropes, self-assembly of a high-porosity nanotube paper, and mechanical testing of a low-porosity nanotube paper.

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