Characterizing Structure in Particle Systems Using Shape-Matching

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In many computer science applications, a technique known as "shape matching" is used to identify unknown structures. Common applications include retrieving fingerprints from a criminal database or verifying signatures electronically. In the context of materials research, we can use shape matching methods to identify structures formed by particle systems. Our scheme involves associating "shape descriptors" with structural patterns of interest in our particle systems and then characterizing the patterns by comparing shape descriptors with reference structures. We show that shape matching techniques can be applied to a variety of structural characterization problems such as local and global identification and classification, automated phase diagram mapping, and constructing spatial and temporal structure correlation functions. Our techniques are applicable over a wide range of systems, both simulated and experimental, provided particle positions are known or can be detected with high accuracy. To aid in the development and dissemination of these techniques, we have implemented a C++/python library to perform shape matching analysis, which will be made available at matforge.org.