MercuryCG - From Discrete Particles to Continuum Fields

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Abstract

Micro–macro transition methods are used to both calibrate and validate continuum models from discrete data, obtained from either experiments or simulations. Such methods generate continuum fields such as density, momentum, stress, etc, from discrete data, i.e. positions, velocity, orientations and forces of individual elements. Performing this micro–macro transition step is especially challenging for heterogeneous and dynamic situations.

Here, we present a mapping technique, called coarse-graining, to perform this transition. This novel method has several advantages: by construction the obtained macroscopic fields are consistent with the continuum equations of mass, momentum and energy balance. Additionally, boundary interaction forces can be taken into account in a self-consistent way and thus allow for the construction of locally accurate stress fields even within one element radius of the boundaries. Similarly, stress and drag forces can be determined for individual constituents, which is critical for several continuum applications, e.g. mixture theory-based segregation models. Moreover, the method does not require ensemble-averaging and thus can be efficiently exploited to investigate static, steady and time-dependent flows. The method presented in this paper is valid for any discrete data, e.g. particle simulations, molecular dynamics, experimental data, etc.; however, for the purpose of illustration we consider data generated from discrete particle simulations of granular mixtures flowing over rough inclined channels. We show how to practically use our coarse-graining extension for both steady and unsteady flows using our open-source coarse-graining tool MercuryCG. The tool is available as a part of an efficient discrete particle solver MercuryDPM (www.MercuryDPM.org).

References

1. DR Tunuguntla and AR Thornton and T Weinhart. From discrete elements to continuum fields: Extension to bidisperse systems. Computational Particle Mechanics 3(3), 349-365 (2016).