Physica A 407 (2014) 312–331

Contents lists available at ScienceDirect

Physica A

journal homepage: www.elsevier.com/locate/physa

# A community-detection based approach to identification of inhomogeneities in granular matter

Robertas Navakas [a,*], Algis Džiugys [a], Bernhard Peters [b]

[a] Lithuanian Energy Institute, Laboratory of Combustion Processes, Breslaujos g. 3, 44403 Kaunas, Lithuania

[b] Université du Luxembourg, Campus Kirchberg, 6, rue Coudenhove-Kalergi, L-1359 Luxembourg, Luxembourg

## HIGHLIGHTS

- A granular packed bed is represented as an interaction graph.
- Particle property inhomogeneity is treated as a community structure in the graph.
- A few algorithms are applied for identification of community structure in the graph.
- The community structure is compared to temperature distribution in the packed bed.
- The results are compared to those obtained by two other inhomogeneity identifying algorithms.

## ARTICLE INFO

*Article history:*
Received 23 May 2013
Received in revised form 27 March 2014
Available online 13 April 2014

*Keywords:*
Granular matter
Community detection
Discrete Element Modelling

## ABSTRACT

Interparticle interactions in granular matter are commonly represented by appropriate graphs, therefore, inhomogeneities in granular matter can be possibly reflected by community structure in the respective graphs. Approaches and algorithms for community detection are being actively developed and the achievements in this area can be utilized for analysis of granular systems, where bridging the gap from microscopic configuration to macroscopic phenomena is of great interest.

Here, we analyse applicability of graph community detection algorithms for identification of inhomogeneities of particle parameter distribution in granular matter, in order to explore the relevance of the selected approach in general. As an example application, we analyse identification of temperature distribution inhomogeneities in a simulated packed bed of fuel particles on a moving grate. We build a graph based on particle parameter similarity from the particle temperature data, available from Discrete Element/Particle Modelling, and the problem of identification of particle temperature inhomogeneities is thereby made equivalent to community detection in graphs. We apply a number of well-known community detection algorithms: Edge Betweenness, Walktrap, Infomap, Label Propagation, Spinglass and compare the resulting partitions. We apply this approach to a number of graphs, corresponding to different particle configurations, in order to identify regularities characteristic of partitions produced by different algorithms. We propose a procedure for additional postprocessing of the partitions in order to improve the quality of clusterization. In addition, we apply two alternative algorithms (not related to community detection in graphs) to identify particle distribution inhomogeneities. We also introduce a parameter to evaluate the cluster structure in particle systems.



* Corresponding author. Tel.: +370 37 401872.
*E-mail address:* rnavakas@mail.lei.lt (R. Navakas).

http://dx.doi.org/10.1016/j.physa.2014.04.003
0378-4371/

## 1. Introduction

Granular matter exhibits complex behaviours stemming from underlying simultaneous interactions of the constituent particles. The related phenomena can be observed at different scales, ranging from "microscopic" level of individual particles to "macroscopic" effects involving the bulk of the material; the latter is usually the level most easily accessible to experimental analysis, while the raw output of simulations based on the discrete element method (DEM) [1] or molecular dynamics provides the "microscopic" data. A number of approaches are proposed to bridge the gap between these two extreme scales [2–5].

Moving up from the level of individual particles, localized groups or clusters of particles behaving in a coordinated manner or having similar characteristics emerge in many situations. The related phenomena include particle clustering in cooling granular gas [6,7], particle clusters in circulating fluidized beds [8–10], drag coefficient dependent on the cluster structure in gas–solid flows [11]. Other potential applications include detection of localized groups of particles possessing similar values of certain parameters of interest, e.g., detection of "hot spots" in grate furnaces [12] and packed bed reactors [13–20], inhomogeneous concentrations of absorbed species in fixed bed granular adsorbents [21], nonhomogeneity of particle packings [22], etc., provided the parameters of individual particles are known from, e.g., DEM-based simulations (the exact simulation technique is not important for applicability of the approach presented here, as long as the parameters of interest of the individual particles are known). As the discrete element simulations are becoming more popular with the increasing available computing power, postprocessing of the data available at the scale of individual particles or other discrete objects becomes more important. It is therefore of interest to develop the techniques enabling to recreate larger-scale structures from the particle data.

Since the macroscopic phenomena in granular matter arise due to interactions between multiple particles, a natural approach is to represent such interactions by means of interaction graphs, where the particles are represented by the graph vertices, and the relevant interactions or relations between them are represented by the graph edges. The intensity of interaction can be taken into account by the respective edge weights. Force networks in granular media is commonly represented by graphs [23]. Analysis of graph structure is a subject of ongoing research, in particular, identification of cluster (or community) structures [24]. Earlier, we have suggested a possible relation between the structure of force chains and community structure in loaded granular media, in particular, a case of biaxial compression [25]. Relation between the sound propagation in granular matter and the community structure of the underlying force chains has been analysed as well [26]. In the present contribution, we focus more on the general applicability of the approach based on the community detection algorithms for analysis of granular matter rather than analysis of the selected specific particle system or details of the specific algorithms.

It is generally agreed that the results produced by the community detection (CD) algorithms, as well as their usability, is largely application dependent and the universally applicable rules for selecting the most suitable algorithm(s) are not clearly stated. Analysis of the community detection algorithms is therefore an important area of research [27–30]. Many of the works in this area deal with specifically constructed benchmark graphs [31]. For the purposes of most applications considered so far, a community is usually perceived as a group of graph vertices that have more edges among them than with the vertices outside the community. Granular media is a notable example of a system involving multiple interactions among its constituent parts. Inhomogeneities in such systems, i.e., emergence of localized groups of particles having the parameter values statistically differing from those outside the groups, can be treated as a community structure. The community in this case can be defined as a localized group of particles having more similar values of the parameter of interest than the appropriate values of the particles outside the group. The community structure of the representative graph can be evaluated based on the statistical characteristics of the particle parameter distribution, e.g., mean standard deviation of the parameter value in a particle community is thus expected to be lower than that for the entire system. This approach provides a different perspective to evaluate the community structures and can serve as an additional benchmark for evaluating the community detection algorithms.

Here, we present an approach aimed to identify groups of particles located close to each other and having similar characteristics (similarity of characteristics is defined depending on the particular problem to be considered) in granular matter. As an application example, we use the data from a DEM simulation of packed bed of particles on a moving grate [32], the setup frequently encountered in industrial applications, e.g., in solid fuel combustors [33]. As a specific application in the present study, we demonstrate this approach for a packed bed of bidisperse particles with varying temperatures located on a moving grate [34]. The community detection method is used to evaluate the particle temperature distribution, where nonhomogeneities emerge as the particles move on the moving grate; the appearance of certain temperature zones can be mapped to community structure in the representative graph. Although the data used here is taken from a discrete element simulation of the specific industrial setup, the methods presented here are applicable to any multiparticle configurations for which the appropriate inter-particle relation graphs can be constructed, therefore, the specific details of the underlying system are not important.

In order to reveal the cluster structure in the multi-particle system, we apply a number of known algorithms: Edge betweenness (EB) [35], Infomap (IM) [36,37], Label propagation (LP) [38], Spin glass (SG) [39], Walk trap (WT) [40]. We use here the implementation of these algorithms in the `igraph` library [41]. We compare the identified community structures to the actual distribution of the particle parameters. Since the straightforward application of the readily available algorithms produce noticeably varying results for the same particle configurations, we propose two simple algorithms that result in