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IDENITIFICATION OF HOT SPOTS IN HEATED GRANULAR MATTER BY A COMMUNITY-DETECTION METHOD

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Granular matter is ubiquitous in technological applications, including solid fuel, reactants in industrial chemical reactors, structural medium or its component in construction and engineering. Simulations of granular matter based on discrete approaches usually yield the parameters of individual particles, e.g., temperatures, chemical composition etc., together with particle positions and momenta. On the other hand, macroscopic properties of the bulk matter are more easily observed experimentally. Transfer from the microscopic (particle scale) properties to macroscopic characteristics (e.g., temperature distribution in packed beds) involves emergence of localised groups of particles having similar characteristics. An example application is appearance of temperature inhomogeneities ("hot spots") in grate furnaces and packed bed reactors [1,2].

Having the data of individual particles (e.g., from discrete element simulations), the interactions and similarities or dissimilarities between the neighbouring particles can be represented as a graph, where the graph vertices represent the particles and the graph edges represent the relations between the nearest particles. Localised groups of particles in such a graph will appear as groups of vertices having denser connections among them compared to the rest of the graph. Identification of groups of densely connected vertices in graphs is known as the "community detection" problem [3]. Here, we present a sample application of this approach for grouping the particles in a packed bed on a moving grate based on the particle temperature.

We consider a set of N_p=1000 particles distributed on a moving grate (Fig. 1); initially, there are three values of the temperature: 398.33 K, 398.92 K, 423.32 K.

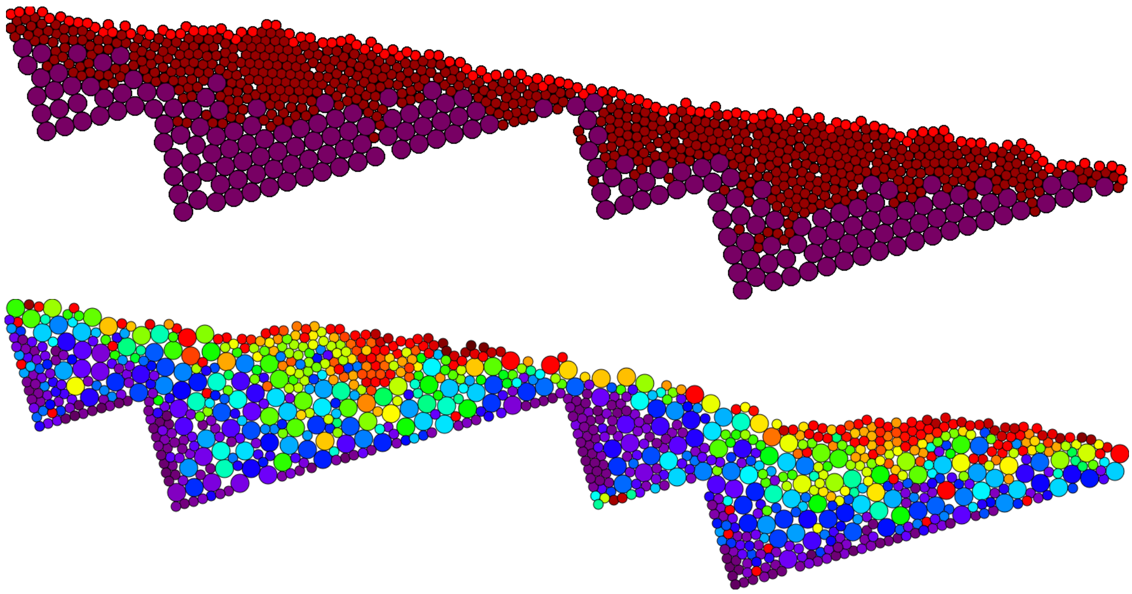


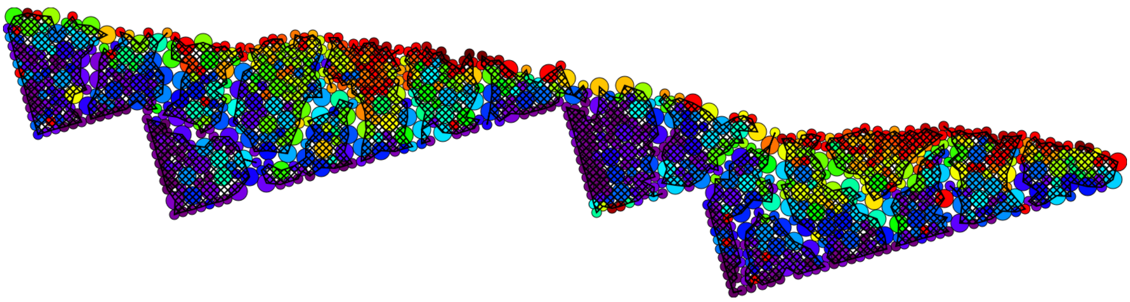
Fig. 1. Distribution of particles on a moving grate at the initial time t=0 s (above) and the final time t=600 s (below). For brevity, only the particles are shown, but not other structural elements. Particles of different temperatures are shown in different colors.

The particle bed is exposed to thermal radiation from above. As the particles move, their temperature distribution changes. This simulated process lasts for 600 s. The simulation details are described elsewhere [4]. The graph of temperature relations between the neighbouring particles is constructed with the edge weights defined as

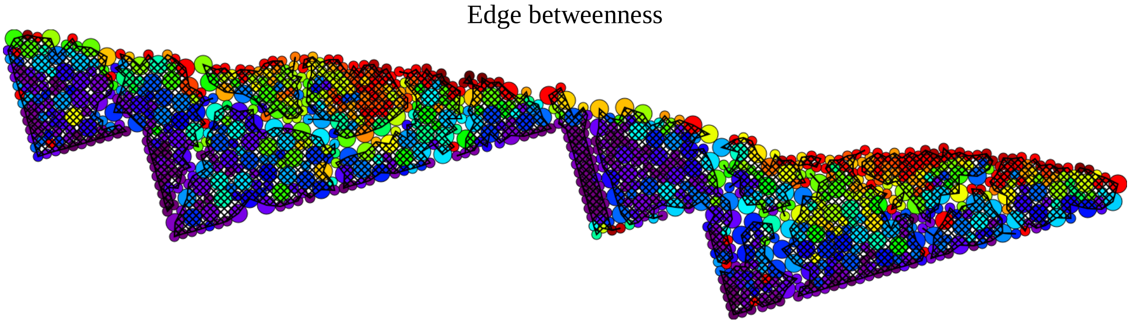
$$w_{ij} = 1 - \frac{|T_i - T_j|}{\max\limits_{1 \le i,j \le N_p} |T_i - T_j|} \tag{1}$$

where T_i is temperature of the i-th particle. The particles i,j are considered in contact (and consequently connected by a graph edge) if $|\mathbf{x}_i - \mathbf{x}_j| \le f_r(r_i + r_j)$, where $\mathbf{x}_i$ is the i-th particle position, r_i is its radius, and an "extension factor" f_r=1.10 was used in order to eliminate the effect of spurious contacts appearing and disappearing as the particles move with respect to each other. For the resulting graph, we apply a number of known community detection algorithms: Edge betweenness [5], Fast greedy [6,7], Label propagation [8], Leading eigenvector [9], Spin glass [10], Walk trap [11]. All these algorithms are implemented in the *igraph* software library [12].

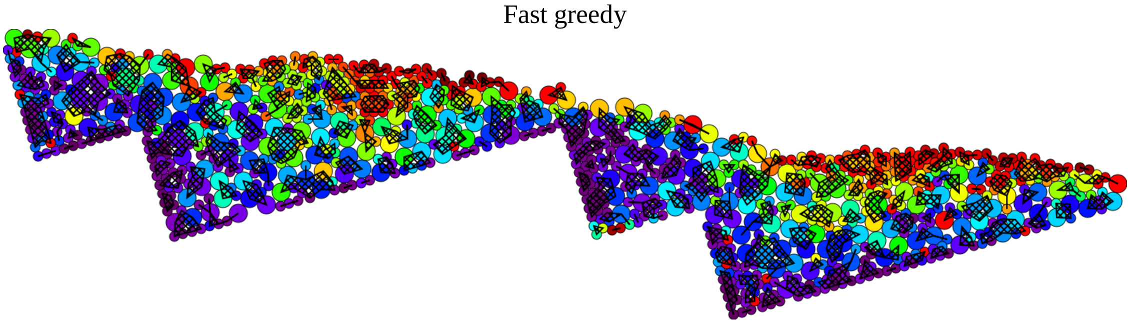
The resulting groups of particles at the final time identified by different algorithms are shown in Fig. 2.



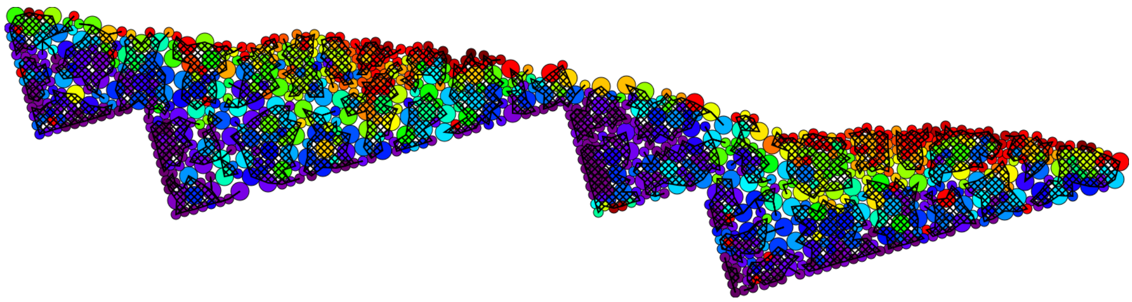
Edge betweenness



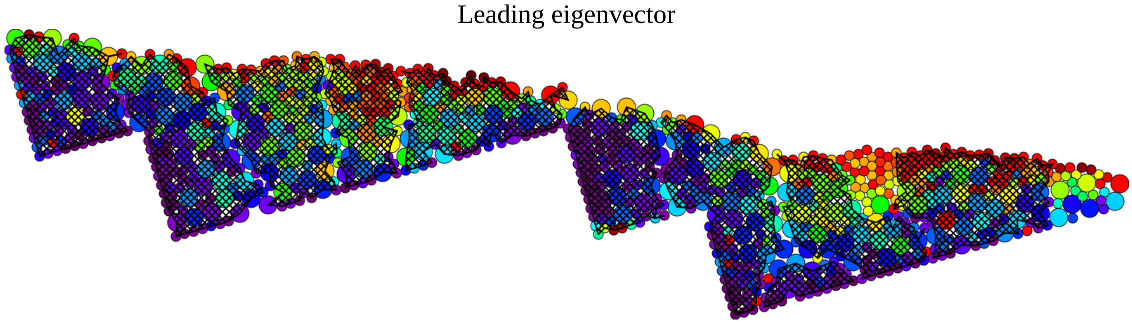
Fast greedy



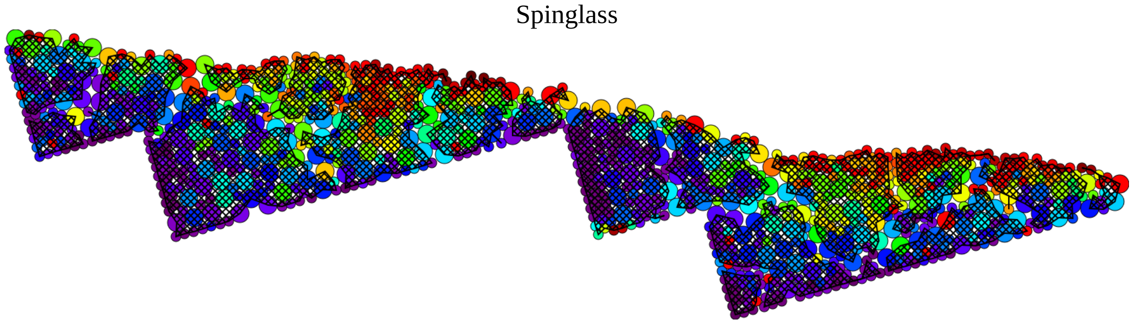
Label propagation



Leading eigenvector



Spinglass



Walktrap

Fig. 2. Particles grouped by their temperatures using different algorithms, as indicated below the respective pictures. Particles of different temperatures are shown in different colors, analogously to Fig. 1. The groups are outlined by dashed polygons, obtained by connecting the centers of outer particles of each group.

As seen from Fig. 2, there are notable differences between the results produced by different algorithms. It is known that the precise identification of communities in graphs is a NP-complete problem, therefore, the obtained results are approximate and should be selected based on the specific problem under consideration [13]; the definition of the group is application domain specific as well. For the task presented here, it is reasonable to define a group as a localised cluster of particles having similar characteristics, i.e., the standard deviation of the particle parameter under consideration within a group should be smaller than that within the total particle set. Fig. 3 shows the evolution of the relative mean standard deviation of the temperatures within the detected groups.

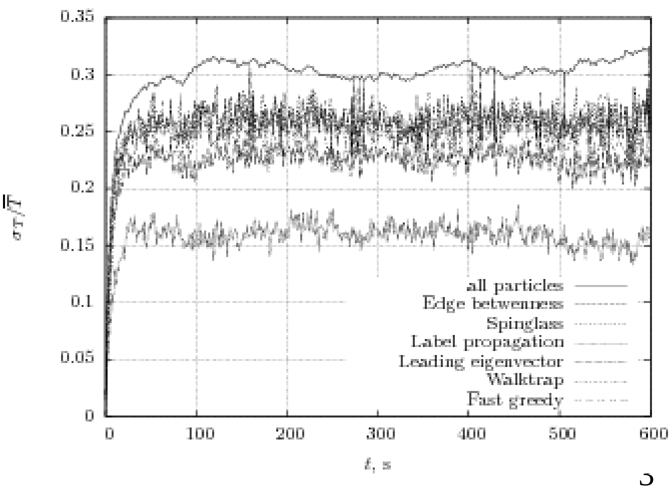


Fig. 3. Relative mean standard deviations of particle temperatures in the detected groups by different algorithms, averaged over all groups weighted by the group size (i.e., number of particles in the respective group), at different times. The overall relative mean standard deviation for all the particles is shown by solid line.

From the results presented in Fig. 2, the “label propagation” algorithm produces the most overclusterized partition, i.e., many small clusters with small standard deviations of the particle parameters within the clusters. The overclusterization can be reduced by merging contacting similar clusters (two clusters are considered in contact if any particles contained in these different clusters are in contact.), thereby preserving small values of the deviations of particle parameters within the clusters. The merging algorithm thus proceeds as follows:

1. calculate the mean standard deviation of the particle characteristics of interest (temperature in the considered case) in each cluster and make neighbour list of the clusters;
2. identify independent pairs of contacting clusters that have to be merged, according to a certain criterium. “Independent pairs” means that each cluster that could be merged is contained in only one such pair;
3. the pairs of clusters selected in the above step are merged — the neighbour list and particle community memberships are updated accordingly and the mean standard deviations for the new clusters are recalculated;
4. the process is repeated until there are no more pairs of clusters left to be merged.

The criterium for merging should be defined appropriately. In the current case, the contacting clusters S_i and S_j were merged if

$$\sigma(S_i \cap S_j) \leq f_\sigma \cdot \max[\sigma(S_i), \sigma(S_j)] + \varepsilon, \quad (2)$$

where $\sigma(S_i)$ is the mean standard deviation of the parameter (temperature in this case) of the particles contained in S_i, and f_σ is a certain factor. In order to reduce the influence of numerical errors when calculating the mean standard deviations of clusters of particles having similar parameters, an additional constant ε is addedd to the merge criterion function, because in cases when the standard deviations of the cluster pairs are close to zero, comparison of these values becomes unreliable; in the cases described here, the following values of these parameters were used: f_σ=1.0, ε=10^{-10}. The resulting partition is shown in Fig. 4.

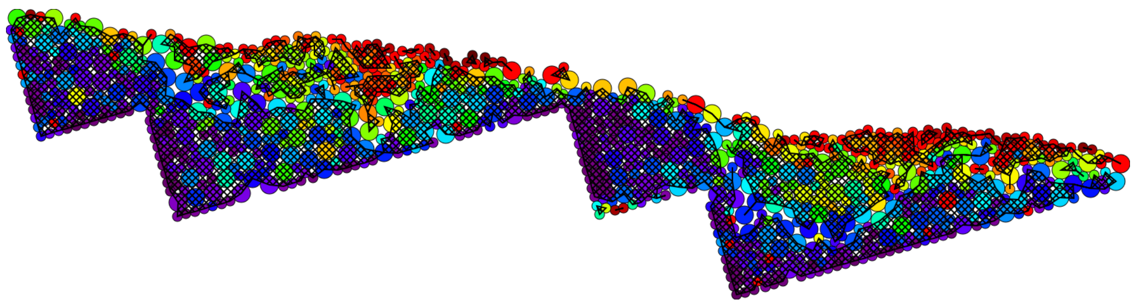


Fig. 4. Particles grouped by their temperatures using the label propagation algorithm and then applying an additional postprocessing algorithm.

Since the label propagation algorithm is nondeterministic, a series of 1000 runs was performed for the same input data, i.e., distribution of the particle temperatures at t=600 s, shown in Fig. 1. The statistics of partitions of the series obtained by applying the label propagating algorithm and then the merging algorithm described above is presented in Table 1.

Table 1. Statistics of the partitions obtained by subsequent application of the label propagation algorithm and then merging the clusters, in a series of 1000 runs.

Parameter	Minimum value	Maximum value
Average cluster size	27.8	90.9
Relative $\sigma(T)$ in clusters	0.187	0.251

In conclusion, we have demonstrated the applicability of the community detection approach for identification of groups of particles with similar characteristics in granular matter. As a sample application, we examined the temperature distribution in a packed bed of particles on a moving grate, such as used in industrial furnaces. Even though different algorithms produce, in general, noticeably different results, usable data can still be extracted by additional postprocessing of the results.

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