Available online at www.sciencedirect.com
ScienceDirect
Comput. Methods Appl. Mech. Engrg. 282 (2014) 218–238
Computer methods in applied mechanics and engineering
www.elsevier.com/locate/cma

Bayesian uncertainty quantification and propagation for discrete element simulations of granular materials

P.E. Hadjidoukas[a], P. Angelikopoulos[a], D. Rossinelli[a], D. Alexeev[a], C. Papadimitriou[b], P. Koumoutsakos[a,*]

[a] Computational Science and Engineering Laboratory, ETH Zürich, CH-8092, Switzerland
[b] Department of Mechanical Engineering, University of Thessaly, Pedion Areos, GR-38334 Volos, Greece

Received 31 January 2014; received in revised form 30 June 2014; accepted 18 July 2014
Available online 11 August 2014

Abstract

Predictions in the behavior of granular materials using Discrete Element Methods (DEM) hinge on the employed interaction potentials. Here we introduce a data driven, Bayesian framework to quantify DEM predictions. Our approach relies on experimentally measured coefficients of restitution for single steel particle–wall collisions. The calibration data entail both tangential and normal coefficients of restitution, for varying impact angles and speeds of the bouncing particle. The parametric uncertainty in multiple Force–Displacement models is estimated using an enhanced Transitional Markov Chain Monte Carlo implemented efficiently on parallel computer architectures. In turn, the parametric model uncertainties are propagated to predict Quantities of Interest (QoI) for two testbed applications: silo discharge and vibration induced mass-segregation. This work demonstrates that the classical way of calibrating DEM potentials, through parameter optimization, is insufficient and it fails to provide robust predictions. The present Bayesian framework provides robust predictions for the behavior of granular materials using DEM simulations. Most importantly the results demonstrate the importance of including parametric and modeling uncertainties in the potentials employed in Discrete Element Methods.

Keywords: Uncertainty quantification; Bayesian model selection; Discrete Element Method; Contact force models; Granular flow

1. Introduction

The Discrete Element Method (DEM) [1] is a powerful technique for simulating particle models of engineering systems. It is the main tool of computational investigation in engineering applications [2] including Silo discharge [3–6], wave propagation through granular media [7], particle mixing on grates and in drums [8–10], fluidized beds [11,12] and plug flows [13].

* Correspondence to: Computational Science and Engineering Laboratory, ETH Zürich, Clausiusstrasse 33, CH-8092, Switzerland. Tel.: +41 44 632 52 58; fax: +41 44 632 17 03.
E-mail address: petros@ethz.ch (P. Koumoutsakos).

http://dx.doi.org/10.1016/j.cma.2014.07.017

The core of DEM is the selected Force–Displacement (F–D) model that updates the rotational and translational movement for each particle following pairwise collisions with other particles and obstacles. The F–D model reflects the nature of the material and is a low order model of the detailed viscoelastic interactions of each particle with its environment. However F–D models are semi-empirical and often contain several parameters to be identified. The sensitivity of various Quantities of Interest (QoIs) in DEM simulations to the F–D model parameters has been the subject of several investigations [5,14–17]. The common practice is that DEM parameters are calibrated using experimental measurements, without taking into account the experimental and model uncertainty. The search for an optimal DEM model has led to extensive comparative studies [18,19] of different models and parameters. The studies reported in [19] demonstrated the difficulty in defining and asserting the superiority of one model over the others.

Here we investigate the parameters and structure of F–D models in DEM using a Bayesian framework [20–26]. A probabilistic Bayesian Uncertainty Quantification and Propagation (UQ+P) framework is used to quantify and calibrate parameter uncertainties in DEM simulations based on available experimental measurements from system components. Furthermore we propagate these uncertainties in DEM simulations to make robust predictions for relevant QoI.

We focus on evaluating the quantitative predictions of three different F–D models using experimental data for normal and tangential restitution coefficients. The uncertainty in the parameters of these models is estimated, and the most probable model is identified. In turn we propagate uncertainties to QoI in simulations of applications such as Silo Discharge blocking and the "Brazil Nut" effect [27]. We employ an enhanced parallel variant of the Transitional Markov Chain Monte Carlo (TMCMC) algorithm [28,29] along with a parallel framework to distribute the large number of system runs in clusters with heterogeneous computer architectures [30]. Our results help demonstrate the value of the Bayesian framework for DEM simulations and provide credible intervals for their predictions.

The paper is organized as follows: In Section 2 we outline the elements of DEM simulations and in particular the parametric F–D models. Section 3 presents the Bayesian framework and in Section 4 we give the results for the Bayesian Calibration of the F–D model parameters. Section 5 showcases two UQ+P studies on relevant industrial applications using the calibrated uncertainty models from Section 4. Our summary and conclusions are presented in Section 6.

2. The DEM and its implementation

The DEM is a widely used method to simulate granular material with a broad range of industrial applications ranging from oil and gas to pharmaceutical and metallurgy. The granular material is modeled as a set of particles of various shapes with translational and rotational degrees of freedom accompanied by models of interparticle collisions. Each particle has its own mass, velocity and contact properties. The contact forces between particles consist of elastic, viscous and frictional resistance forces.

In this work we consider two-dimensional systems. Two disks with radii R_i, R_j are assumed to be in mechanical contact if $\xi_{ij} \equiv R_i + R_j - \left|\mathbf{r}_i - \mathbf{r}_j\right| > 0$. Here $\mathbf{r}_i - \mathbf{r}_j = \mathbf{r}_{ij}$ is the vector connecting the center of particle i to the center of particle j and ξ_{ij} is the mutual compression between the particles (see Fig. 1). The force exerted on particle i due to contact with particle j is given as $\mathbf{F}_{ij} = \mathbf{F}^n_{ij} + \mathbf{F}^t_{ij}$ where $\left(F^t\right)$ and (F^n) are its tangential and normal contributions (see 1). Following the notation of [31] the normal and the tangential contact force components can be written as

$$\mathbf{F}^n_{ij} = F^n_{ij}\mathbf{e}^n_{ij}, \quad \mathbf{F}^t_{ij} = F^t_{ij}\mathbf{e}^t_{ij} \tag{1}$$

with the unit vectors

$$\mathbf{e}^n_{ij} = \frac{r_j - r_i}{\left|r_j - r_i\right|}, \qquad \mathbf{e}^t_{ij} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \cdot \mathbf{e}^n_{ij}.$$

Particles evolve according to the two-dimensional Newton's equations of motion (2):

$$m_i\ddot{\mathbf{r}}_i = m_i\mathbf{g} + \sum_{j,j\neq i}^{N} \mathbf{F}_{ij}, \qquad I_i\ddot{\phi}_i = \sum_{j,j\neq i}^{N} \left(\mathbf{l}_{ij} \times \mathbf{F}_{ij}\right) \cdot \mathbf{e}^z_{ij}$$
$$\mathbf{r}_i = \mathbf{r}_{i0}, \quad \dot{\mathbf{r}}_i = 0, \qquad \phi_i = 0, \quad \dot{\phi}_i = 0 \tag{2}$$