An inverse problem in the kinetics of fragmentation

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Scientific background

The size reduction of particulate solids, referred to as milling when performed in a mill, is a ubiquitous process throughout the manufacturing chain, used to produce every year billions of tons of low-value-added products (e.g., minerals) and high-value-added products (e.g., pharmaceuticals) alike. Milling is a process of high energy-consumption but low energy-efficiency, expending about 6% (including material waste) of global electricity generated with only a few per cent used for material breakage. Designing a successful mill is a long and expensive process requiring building successive prototypes with trial-and-error. One of the major technical hurdles to improving efficiency of operation and design is the inability to *predict* the evolution of particle size distribution (PSD). Considerable efforts have been spent on experiments and mathematical modelling for PSD prediction in different milling operations. One type of research uses a "bottom-up" approach - starting from understanding single-particle breakage and then deriving breakage functions for population balance modelling (PBM). One difficulty associated with this approach is that complete understanding of the single particle breakage mechanism is a formidable challenge in itself as material fracturing initiates at the atomic/molecular scale. Resolving the full range of relevant scales in a computational model is impossible for the foreseeable future.

In this project we seek to demonstrate proof-of-concept for an alternative approach based on solving the inverse population balance problem. We assume that the population balance equation is a valid model of the evolution of the PSD and then use observational data of the evolution of the PSD to determine the breakage functions most likely to explain the observed data.

Research challenge

We denote the volume fraction of particles with size x at time t, or particle size distribution, by $f(x, t, \mathbf{Y})$. Here $\mathbf{Y}$ denotes a vector of environment and physical variables which can affect the particles such as the local stress or the granular flow conditions. In neglecting to include a spatial dependence, we are implicitly assuming that the mill is homogeneous. The statistical dynamics of the particle size distribution can be modelled with the population balance equation [1]:

$$\partial_t f(x, t, \mathbf{Y}) = -b(x, \mathbf{Y}) \, f(x, t, \mathbf{Y}) \qquad (1)$$
$$+ \int_x^\infty \nu(y, \mathbf{Y}) \, b(y, \mathbf{Y}) \, P(x|y, \mathbf{Y}) \, f(y, t) \, dy$$

where $b(x, \mathbf{Y})$ is the breakage rate for particles of size x, $\nu(y, \mathbf{Y})$ is the average number of fragments produced in the breakage of a particle of size y and $P(x|y, \mathbf{Y})$ is the proportion of particles of size x produced in the breakage of a particle of size y. Typically, these functions are obtained from experimental measurements or numerical simulations and Eq. (1) is integrated forward to predict the evolution of $f(x, t)$. Such experimental measurements are often a pain-staking process and it is sometimes unclear whether the conditions of experiments correspond conditions inside a mill. In this project, we will solve the corresponding *inverse* problem which can be stated as follows: given experimental measurements of $f(x, t)$ at a sequence of stages of the milling process and assuming that the dynamics is described by Eq. (1), find the breakage functions, $b(x, \mathbf{Y})$, $\nu(x, \mathbf{Y})$ and $P(x|y, \mathbf{Y})$, which best describe the measurements. We will begin with the simplest model - binary breakage. In this case (neglecting the environment variables for now) $\nu = 2$ and everything is encoded into a single function, $\beta(x, y)$, which is the rate for the process $(x + y) \rightarrow (x) + (y)$. Eq. (1) becomes

$$\partial_t f(x, t) = -f(x, t) \int_0^x dy \, \beta(x - y, y) \quad (2)$$
$$+ 2 \int_x^\infty dy \beta(x, y) f(y, t)$$
$$\equiv L * \beta,$$

where the right-hand side defines the linear operator, L (which depends on the size-ditribution, $f(x, t)$) acting on the breakage function, $\beta(x, y)$. Solutions (there are typically many) of the inverse problem are minima of the functional, $S[\beta]$, given by

$$S[\beta] = \int_0^\infty \int_0^\infty |\partial_t f(x, t) - L * \beta|^2 \, dx \, dt \quad (3)$$

Such inverse problems are usually ill-posed in the sense that the set of minimising solutions is sensitive to small amounts of noise in the input data, $f(x, t)$. This can be overcome using various "regularisation" techniques. A deterministic regularisation scheme for inverse problems of this type was presented in [2]. In this project, we will adopt a probabilistic regularisation scheme based on the Bayesian formulation of inverse problems put forward in [3] which is implemented using functional Markov Chain Monte Carlo algorithms [4]. This approach is computationally more expensive than the classical approaches but has the advantage of providing good estimates of the uncertainty in the estimate of the breakage function on a scale-by-scale basis.

Pre-requisites

This is a complex project blending ideas from non-equilibrium statistical mechanics and kinetic theory with uncertainty quantification and inverse problems. It will also require a competent programmer since the "observational data" used as input for constructing the functional $S[\beta]$ will have to be obtained by numerically integrating Eq. (1). Nevertheless it might be fun for a student with the right interests and skills.

Additional considerations

This project is offered as a MathSys or an Erasmus Mundus M1 MSc project. It could lead to a follow-on PhD project subject to suitable funding arrangements.

References

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[3] S. L. Cotter, M. Dashti, J. C. Robinson, and A. M. Stuart. Bayesian inverse problems for functions and applications to fluid mechanics. *Inverse Problems*, 25(11):115008, 2009.

[4] Alexandros Beskos and Andrew Stuart. MCMC methods for sampling function space. In Rolf Jeltsch and Gerhard Wanner, editors, *6th International Congress on Industrial and Applied Mathematics Zurich, Switzerland, 16-20 July 2007*, pages 337–364. European Mathematical Society Publishing House, Zurich, Switzerland, 2009.