

# On granular gases and projective integration

Thomas Rey

February 1, 2019

## Granular gases equation.

A granular gas is a set of particles which interact by energy dissipating collisions also known as **inelastic collisions**. This inelasticity is characterized by a collision mechanics where mass and momentum are conserved and kinetic energy is dissipated. Thus, the collision phenomenon is a non-*microreversible* process. The velocities of the colliding pairs  $(v, v_*)$  and  $(v', v'_*)$  are related by

$$v' = v - \frac{1+e}{2} ((v - v_*) \cdot \sigma) \sigma, \quad v'_* = v_* + \frac{1+e}{2} ((v - v_*) \cdot \sigma) \sigma,$$

where  $\sigma \in \mathbb{S}^{d-1}$  and the constant  $e \in [0, 1]$  is the dissipation parameter, known as *restitution coefficient*. One has

$$\begin{cases} v' + v'_* = v + v_*, \\ |v'|^2 + |v'_*|^2 - |v|^2 - |v_*|^2 = -\frac{1-e^2}{2} |u \cdot \sigma|^2 \leq 0. \end{cases} \quad (1)$$

This type of system can be described by a Boltzmann-like **collisional kinetic equations**. More precisely, for a given nonnegative initial condition  $f_0$ , the gas is described by a particle distribution function  $f^\varepsilon = f^\varepsilon(t, x, v)$ , for  $t \geq 0$ ,  $x \in \Omega \subset \mathbb{R}^d$  for  $d \leq 3$  and  $v \in \mathbb{R}^3$ , solution to the scaled, initial-boundary value problem

$$\begin{cases} \varepsilon^\alpha \frac{\partial f^\varepsilon}{\partial t} + v \cdot \nabla_x f^\varepsilon = \frac{1}{\varepsilon^\beta} \mathcal{Q}_\mathcal{I}(f^\varepsilon) \\ f^\varepsilon(0, x, v) = f_0(x, v), \end{cases} \quad (2)$$

where the collision operator  $\mathcal{Q}$  will be given later, and  $\varepsilon$  is a small parameter describing the *rarefaction* of the gas. The open set  $\Omega$  is a bounded Lipschitz-continuous domain of  $\mathbb{R}$ , which means that the model (2) will also have to be supplemented with boundary conditions.

The microscopic mechanism (1) allows us to describe the granular collision operator  $\mathcal{Q}_\mathcal{I}$ . If the nonnegative particles distribution function  $f$  depends only on  $v \in \mathbb{R}^{d_v}$  for  $d_v \leq 3$ , the collision operator  $\mathcal{Q}_\mathcal{I}(f, g)$  can be expressed in the following weak form: given a smooth test function  $\psi$ ,

$$\int_{\mathbb{R}^{d_v}} \mathcal{Q}_\mathcal{I}(f, f) \psi dv := \frac{1}{2} \int_{\mathbb{R}^{d_v} \times \mathbb{R}^{d_v} \times \mathbb{S}^{d_v-1}} |v - v_*| f_* f (\psi' + \psi'_* - \psi - \psi_*) d\sigma dv dv_*, \quad (3)$$

where the classical shorthand notation  $\psi' = \psi(v')$  is used.

Taking  $\psi(v) = 1, v$  and  $|v|^2$  in (3), the relations (1) yield conservation of mass and momentum at the kinetic level and dissipation of kinetic energy  $\int_{\mathbb{R}^{d_v}} \mathcal{Q}_\mathcal{I}(f, f) |v|^2 dv \leq 0$ . The decrease of the energy, together with conservation of mass and momentum, imply that the equilibria of the collision operator are Dirac distributions  $\rho \delta_u(v)$ , where the density  $\rho$  and momentum  $\rho u$  are prescribed by the initial condition (see [BCG00] for the earliest results on the topic). A major difficulty with this equation is the **lack of decaying entropy** functional: a discussion on this question can be found in [GdSMM<sup>+</sup>15].

One of the consequences of the dissipation of kinetic energy by collisions — and a major feature of the granular gases equation — is the seminal *Haff's Law* [Haf83], which states that the kinetic energy of a granular gas decays polynomially:

$$\int_{\mathbb{R}} \theta^\varepsilon(t, x) dx \lesssim \frac{1}{(1+t)^2}.$$

This asymptotic behavior of the macroscopic temperature is characteristic of granular gases, and has been proved to be optimal in the space homogeneous case for constant restitution coefficient in [MM06]. These results have then been extended to a more general class of collision kernel and restitution coefficients in [AL10, AL13, Rey12]. Nevertheless, in all these works, additional constraints on the smoothness of the initial data (a somehow nonphysical  $L^p$  bound for  $p > 1$ ) are required for the results to hold. Adding friction of stochastic heat bath allows for a richer large time behavior, see [CCG00, MM09]

The existence in the general  $\mathbb{R}_x^3 \times \mathbb{R}_v^3$  setting, for a large class of velocity-dependent restitution coefficient but close to vacuum was obtained in [Alo09]. The stability in  $L^1(\mathbb{R}_x^3 \times \mathbb{R}_v^3)$  under the same assumptions was derived for instance in [Wu09]. Finally the existence and convergence to equilibrium in  $\mathbb{T}_x^3 \times \mathbb{R}_v^3$  for a diffusively heated, weakly inhomogeneous granular gas was proved in [Tri16].

As one can imagine, the theory in the one dimensional case is much simpler. The existence of solutions for the granular gases equation in one dimension of physical space and velocity, with a constant restitution coefficient was proved in [BCP97] for compact initial data. The velocity-dependent restitution coefficient case, for small data, was then proven in [BP02]. The main argument is reminiscent from a work due to Bony in [Bon87] concerning discrete velocity approximation of the Boltzmann equation in dimension 1.

Finally, the problem of the hydrodynamic limit was first tackled formally, and in the quasi-elastic setting  $e \rightarrow 1$ . The first mathematical results for this case can be found in [BCGP99] for the one dimensional case. The review paper [Tos08] summarizes most of the known formal results for the higher dimensional case. Together with P. E. Jabin, we proved rigorously in [JR17] the validity of the hydrodynamic limit of this one dimensional equation, for any value of the restitution coefficient, towards the **pressureless Euler** system

$$\begin{cases} \partial_t \rho + \partial_x(\rho u) = 0, \\ \partial_t(\rho u) + \partial_x(\rho u^2) = 0. \end{cases} \quad (4)$$

This work actually proves this convergence result for a very large class of energy dissipative kinetic equation, by introducing a generalization of the Bony-Cercignani functional appearing in [Cer92], allowing to prove that the solution to (2) becomes monokinetic when  $\varepsilon \rightarrow 0$ .

Finally, in [Rey13], I've performed a spectral analysis of the stochastically heated granular gases operator, linearized closed to a space homogeneous equilibrium. In particular, I proved that one can expand the eigenvalues of the this linear operator as a function of both the radial component  $\rho$  of the spatial Fourier variable  $\mathbf{e}_n$  of the restitution coefficient  $e$ : the eigenvalue  $\lambda_j$  can be written for  $\rho \ll 1$ ,  $e$  close to 1 as

$$\lambda^{(j)}(\rho, e) = i\lambda_1^{(j)}\rho - \lambda_2^{(j)}\rho^2 - \gamma_1^{(j)}(1 - e) + \mathcal{O}(\rho^3 + (1 - e)^2),$$

for explicit constants  $\lambda_1^{(j)} \in \mathbb{R}$ ,  $\lambda_2^{(j)} > 0$ , and  $\gamma_1^{(j)} > 0$ . This result extends the seminal work [EP75].

Any **deterministic numerical method** for the computation of Boltzmann-like collision operator requires to work on a *bounded* velocity space. The approach considered in **MANAKINEQO** for the majority of the considered collision operators consists in adding some non physical binary collisions by periodizing the particle distribution function and the collision operator, and then using Fourier series to compute the truncated operator. This implies the loss of some local invariants, but a careful periodization allows at least the preservation of mass. This periodization is the basis of spectral methods, that we will use in our numerical simulations.

Fourier techniques (also known as **spectral methods**) for the resolution of the Boltzmann equation have been first introduced independently in [PP96] and in [BR97]. They have since been investigated by a lot of authors. One can find numerous results about this type of method in the article [PR00]. It has been shown to be convergent in [FM11] for the elastic case and allows spectral accuracy [CHQZ88]. Spectral methods have then been derived for the granular gases operator (3) in [FPT05]. Together with F. Filbet, we then generalized this method to the spatially inhomogeneous case using a rescaling velocity approach in [FR13], yielding the first evidences of clustering in a kinetic granular gas. Finally, a fast algorithm for granular gases was developed independently in [WZR15, HM19], paving the way for more physically relevant numerical simulation of the model.

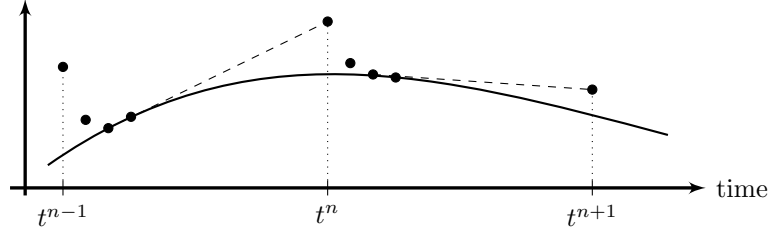


Figure 1: Sketch of PInt: the black dots represent the small  $\delta t$ – time steps, and the dashed line the extrapolation.

## Projective integration in a nutshell

The development of easy-to-implement **AP schemes** for kinetic equations of type (2) is another very important domain that the **MANAKINEQO** project will investigate. Such a scheme needs to provide an **accurate** and **efficient** approximation of the general kinetic equation, while altogether being **stable** in the  $\varepsilon \rightarrow 0$  limit, and providing an accurate approximation of the limiting problem **independently** on the time step or mesh size.

A robust and fully explicit method, which allows for time integration of (two-scale) stiff systems with arbitrary order of accuracy in time, is **projective integration** (PInt, see Fig 1 for a visual summary). PInt was proposed in [GK03a] for stiff systems of ordinary differential equations with a clear gap in their eigenvalue spectrum. In such stiff problems, the fast modes, corresponding to the Jacobian eigenvalues with large negative real parts, decay quickly, whereas the slow modes correspond to eigenvalues of smaller magnitude and are the solution components of practical interest. PInt allows a stable yet explicit integration of such problems by first taking a few small (inner) steps using a step size  $\delta t$  with a simple, explicit method, until the transients corresponding to the fast modes have died out, and subsequently projecting (extrapolating) the solution forward in time over a large (outer) time step of size  $\Delta t > \delta t$ . In [LS12], PInt was analyzed for kinetic equations with a diffusive scaling. An arbitrary order version, based on Runge-Kutta methods, has been proposed recently in [LLS16], where it was also analyzed for kinetic equations with an advection-diffusion limit. In [LMS17], the scheme was used to construct a explicit, flexible, arbitrary order method for general nonlinear hyperbolic conservation laws, based on relaxation to a kinetic equation. Alternative approaches to obtain a higher-order PInt scheme have been proposed in [LG07, RMGK04]. These methods fit within recent research efforts on numerical methods for multiscale simulation [EEL<sup>+</sup>07, KGH<sup>+</sup>03].

For problems exhibiting more than a single fast time scale, telescopic PInt was proposed [GK03b]. In these methods, the PInt idea is applied recursively. Starting from an inner integrator at the fastest time scale, a PInt method is constructed with a time step that corresponds to the second-fastest time scale. This PInt method is then considered as the inner integrator of a PInt method on yet a coarser level. By repeating this idea, telescopic PInt methods construct a hierarchy of projective levels in which each outer integrator step on a certain level serves as an inner integrator step one level higher. The idea was studied and tested for linear kinetic equations in [MS18]. These methods turn out to have a computational cost that is essentially independent of the stiffness of the collision operator.

We do not call PInt methods AP as such, because we cannot explicitly evaluate the scheme for  $\varepsilon = 0$  to obtain a classical numerical scheme for the limiting equation. Nevertheless, PInt and telescopic PInt methods share important features with AP methods. In particular, their computational cost does (in many cases) not depend on the stiffness of the problem. To be specific, it was shown in [MS18], for linear kinetic equations, that the number of inner time steps at each level of the telescopic hierarchy is independent of the small-scale parameter  $\varepsilon$ , as is the step size of the outermost integrator. The only parameter in the method that may depend on  $\varepsilon$  is the *number* of levels in the telescopic hierarchy. For systems in which the spectrum of the collision operator fall apart into a set of clearly separated clusters (each corresponding to a specific time scale), the number of levels equals the number of spectral clusters. In this situation, the computational cost is completely independent from  $\varepsilon$ . When the collision operator represents a continuum of time scales, the number of PInt levels increases logarithmically with  $\varepsilon$ .

## References

- [AL10] R. J. Alonso and B. Lods. Free cooling and high-energy tails of granular gases with variable restitution coefficient. *SIAM J. Math. Anal.*, 42(6):2499–2538, 2010.
- [AL13] R. J. Alonso and B. Lods. Two proofs of Haff’s law for dissipative gases: the use of entropy and the weakly inelastic regime. *J. Math. Anal. Appl.*, 397(1):260–275, 2013.
- [Alo09] R. J. Alonso. Existence of Global Solutions to the Cauchy Problem for the Inelastic Boltzmann Equation with Near-vacuum Data. *Indiana Univ. Math. J.*, 58(3):999–1022, 2009.
- [BCG00] A. V. Bobylev, J. A. Carrillo, and I. Gamba. On some properties of kinetic and hydrodynamic equations for inelastic interactions. *J. Statist. Phys.*, 98(3):743–773, 2000.
- [BCGP99] D. Benedetto, E. Caglioti, F. Golse, and M. Pulvirenti. A hydrodynamic model arising in the context of granular media. *Computers & Mathematics with Applications*, 38(7-8):121–131, oct 1999.
- [BCP97] D. Benedetto, E. Caglioti, and M. Pulvirenti. A One-dimensional Boltzmann Equation with Inelastic Collisions. *Rend. Sem. Mat. Fis. Milano*, LXVII:169–179, 1997.
- [Bon87] J.-M. Bony. Solutions globales bornées pour les modèles discrets de l’équation de Boltzmann, en dimension 1 d’espace. In *Journées “Équations aux dérivées partielles” (Saint Jean de Monts, 1987)*. École Polytechnique, Palaiseau, 1987. Exp. No. XVI, 10 pp.
- [BP02] D. Benedetto and M. Pulvirenti. On the one-dimensional Boltzmann equation for granular flows. *M2AN Math. Model. Numer. Anal.*, 35(5):899–905, April 2002.
- [BR97] A. Bobylev and S. Rjasanow. Difference scheme for the Boltzmann equation based on the fast Fourier transform. *Eur. J. Mech. B Fluids*, 16(2):293–306, 1997.
- [CCG00] J. A. Carrillo, C. Cercignani, and I. M. Gamba. Steady states of a boltzmann equation for driven granular media. *Phys. Rev. E*, 62:7700–7707, Dec 2000.
- [Cer92] C. Cercignani. A remarkable estimate for the solutions of the Boltzmann equation. *Appl. Math. Lett.*, 5(5):59–62, 1992.
- [CHQZ88] C. Canuto, M. Hussaini, A. Quarteroni, and T. Zang. *Spectral Methods in Fluid Dynamics*. Springer Series in Computational Physics. Springer-Verlag, New York, 1988.
- [EEL<sup>+</sup>07] W. E, B. Engquist, X. Li, W. Ren, and E. Vanden-Eijnden. Heterogeneous multiscale methods: a review. *Commun. Comput. Phys.*, 2(3):367–450, 2007.
- [EP75] R. S. Ellis and M. A. Pinsky. The First and Second Fluid Approximations to the Linearized Boltzmann Equation. *J. Math. Pures Appl.*, 54(9):125–156, 1975.
- [FM11] F. Filbet and C. Mouhot. Analysis of Spectral Methods for the Homogeneous Boltzmann Equation. *Trans. Amer. Math. Soc.*, 363:1947–1980, 2011.
- [FPT05] F. Filbet, L. Pareschi, and G. Toscani. Accurate Numerical Methods for the Collisional Motion of (Heated) Granular Flows. *J. Comput. Phys.*, 202(1):216–235, 2005.
- [FR13] F. Filbet and T. Rey. A Rescaling Velocity Method for Dissipative Kinetic Equations - Applications to Granular Media. *J. Comput. Phys.*, 248:177–199, 2013.
- [GdSMM<sup>+</sup>15] M. I. García de Soria, P. Maynar, S. Mischler, C. Mouhot, T. Rey, and E. Trizac. Towards an H-theorem for granular gases. *J. Stat. Mech: Theory Exp.*, 2015(11):P11009, 2015.
- [GK03a] C. W. Gear and I. G. Kevrekidis. Projective methods for stiff differential equations: problems with gaps in their eigenvalue spectrum. *SIAM J. Sci. Comput.*, 24(4):1091–1106, 2003.
- [GK03b] C. W. Gear and I. G. Kevrekidis. Telescopic projective methods for parabolic differential equations. *J. Comput. Phys.*, 187(1):95–109, 2003.
- [Haf83] P. Haff. Grain flow as a fluid-mechanical phenomenon. *J. Fluid Mech.*, 134:401–30, 1983.
- [HM19] J. Hu and Z. Ma. A fast spectral method for the inelastic Boltzmann collision operator and application to heated granular gases. *J. Comput. Phys.*, Accepted 2019. Preprint 2018.
- [JR17] P.-E. Jabin and T. Rey. Hydrodynamic Limit of Granular Gases to Pressureless Euler in Dimension 1. *Q. Appl. Math.*, 75:155–179, 2017.
- [KGH<sup>+</sup>03] I. G. Kevrekidis, C. W. Gear, J. M. Hyman, P. G. Kevrekidid, O. Runborg, C. Theodoropoulos, et al. Equation-free, coarse-grained multiscale computation: Enabling microscopic simulators to perform system-level analysis. *Commun. Math. Sci.*, 1(4):715–762, 2003.
- [LG07] S. L. Lee and C. W. Gear. Second-order accurate projective integrators for multiscale problems.

- J. Comput. Appl. Math.*, 201(1):258–274, 2007.
- [LLS16] P. Lafitte, A. Lejon, and G. Samaey. A high-order asymptotic-preserving scheme for kinetic equations using projective integration. *SIAM J. Numer. Anal.*, 54(1):1–33, 2016.
  - [LMS17] P. Lafitte, W. Melis, and G. Samaey. A high-order relaxation method with projective integration for solving nonlinear systems of hyperbolic conservation laws. *J. Comput. Phys.*, 340:1–25, 2017.
  - [LS12] P. Lafitte and G. Samaey. Asymptotic-preserving projective integration schemes for kinetic equations in the diffusion limit. *SIAM J. Sci. Comput.*, 34(2):A579–A602, 2012.
  - [MM06] S. Mischler and C. Mouhot. Cooling process for inelastic Boltzmann equations for hard spheres, Part II: Self-similar solutions and tail behavior. *J. Statist. Phys.*, 124(2):703–746, 2006.
  - [MM09] S. Mischler and C. Mouhot. Stability, convergence to the steady state and elastic limit for the Boltzmann equation for diffusively excited granular media. *Discrete Contin. Dyn. Syst.*, 24(1):159–185, 2009.
  - [MS18] W. Melis and G. Samaey. Telescopic projective integration for kinetic equations with multiple relaxation times. *J. Sci. Comput.*, 76(2):697–726, 2018.
  - [PP96] L. Pareschi and B. Perthame. A Fourier Spectral Method for Homogeneous Boltzmann Equations. *Transport Theory Statist. Phys.*, 25(3):369–382, 1996.
  - [PR00] L. Pareschi and G. Russo. Numerical Solution of the Boltzmann Equation I : Spectrally Accurate Approximation of the Collision Operator. *SIAM J. Numer. Anal.*, 37(4):1217–1245, 2000.
  - [Rey12] T. Rey. Blow Up Analysis for Anomalous Granular Gases. *SIAM J. Math. Anal.*, 44(3):1544–1561, 2012.
  - [Rey13] T. Rey. A Spectral Study of the Linearized Boltzmann Equation for Diffusively Excited Granular Media. Preprint arXiv 1310.7234, 2013.
  - [RMGK04] R. Rico-Martinez, C. W. Gear, and I. G. Kevrekidis. Coarse projective kmc integration: forward/reverse initial and boundary value problems. *J. Comput. Phys.*, 196(2):474–489, 2004.
  - [Tos08] G. Toscani. *Mathematical Models of Granular Matter*, chapter Hydrodynamics from the Dissipative Boltzmann Equation, pages 59–75. Springer Berlin Heidelberg, Berlin, Heidelberg, 2008.
  - [Tri16] I. Tristani. Boltzmann equation for granular media with thermal force in a weakly inhomogeneous setting. *J. Funct. Anal.*, 270(5):1922–1970, 2016.
  - [Wu09] Z. Wu.  $L^1$  and BV-type stability of the inelastic Boltzmann equation near vacuum. *Continuum Mech. Thermodyn.*, 22(3):239–249, November 2009.
  - [WZR15] L. Wu, Y. Zhang, and J. M. Reese. Fast spectral solution of the generalized Enskog equation for dense gases. *J. Comput. Phys.*, 303:66–79, 2015.