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BRIEF COMMUNICATION

Coefficient of restitution and linear–dashpot model revisited

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Abstract With the assumption of a linear–dashpot interaction force, the coefficient of restitution, $\varepsilon_d^0(k, \gamma)$, can be computed as a function of the elastic and dissipative material constants, k and γ by integrating Newton's equation of motion for an isolated pair of colliding particles. If we require further that the particles interact exclusively repulsive, which is a common assumption in granular systems, we obtain an expression $\varepsilon_d(k, \gamma)$ which differs even qualitatively from the known result $\varepsilon_d^0(k, \gamma)$. The expression $\varepsilon_d(k, \gamma)$ allows to relate Molecular Dynamics simulations to event-driven Molecular Dynamics for a widely used collision model.

Keywords Particle collisions · Coefficient of restitution

1 Introduction

The coefficient of (normal) restitution of colliding spherical particles relates the post-collisional velocities $\mathbf{v}_i'$ and $\mathbf{v}_j'$ and the corresponding pre-collisional velocities $\mathbf{v}_i$ and $\mathbf{v}_j$,

$$\begin{aligned} \mathbf{v}_i' &= \mathbf{v}_i - \frac{1+\varepsilon}{2}\left[\left(\mathbf{v}_i - \mathbf{v}_j\right)\cdot \mathbf{e}_{ij}\right]\mathbf{e}_{ij} \\ \mathbf{v}_j' &= \mathbf{v}_j + \frac{1+\varepsilon}{2}\left[\left(\mathbf{v}_i - \mathbf{v}_j\right)\cdot \mathbf{e}_{ij}\right]\mathbf{e}_{ij} \end{aligned} \tag{1}$$

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where

$$\mathbf{e}_{ij} \equiv \frac{\mathbf{r}_i - \mathbf{r}_j}{\left|\mathbf{r}_i - \mathbf{r}_j\right|} \tag{2}$$

is the unit vector at the instance of the collision. For simplicity, we consider particles of identical mass—the generalization to unequal masses is straightforward.

The coefficient of restitution is the most fundamental quantity in the theory of dilute granular systems. This coefficient together with the assumption of *molecular chaos* is the foundation of the Kinetic Theory of granular gases, based on the Boltzmann or Enskog kinetic equation, see, e.g., [1] and many references therein. On the other hand, the coefficient of restitution is also essential for event-driven Molecular Dynamics simulations which allow for a significant speed-up as compared to traditional force-based simulations, see, e.g., [19] for a detailed discussion. The most important precondition of Eq. (1) is the assumption of exclusively binary collision, that is, the system is assumed to be dilute enough such that multiple-particle contacts can be neglected. The latter condition seems to be rather restrictive, however, it was shown in many examples that event-driven simulations are applicable up to rather high density [16].

The coefficient of restitution is, however, not a fundamental material or particle property. Instead, the particle interaction forces and Newton's equation of motion govern the dynamics of a mechanical many-particle system. Therefore, if we wish to use the concept of the coefficient of restitution and the simple equation (1) to compute the dynamics of a granular system, we have to assure that Eq. (1) yields the same post-collisional velocities as Newton's equation of motion would do.

2 Coefficient of restitution and Newton's equation of motion for frictionless spherical particles

Let us consider the relation between the coefficient of restitution and the solution of Newton's equation of motion. Assume that two approaching particles at velocities $\mathbf{v}_1$ and $\mathbf{v}_2$ come into contact at time $t = 0$. From this instant on they deform one another until the contact is lost at time $t = t_c$. We shall consider the end of the collision at time t_c separately below. For sufficiently short collisions we can treat the unit vector $\mathbf{e}$ as a constant. Then we can describe the collision by the mutual deformation

$$\xi(t) \equiv \max\left(0,\ 2R - |\mathbf{r}_1 - \mathbf{r}_2|\right) \tag{3}$$

where $\mathbf{r}_1(t)$ and $\mathbf{r}_2(t)$ are the time-dependent positions of the particles and R is their radius. The interaction force between the particles is model specific, e.g. [9,19,22], and, in general, a function of the material parameters, the particle masses and radii, the deformation ξ and the deformation rate $\dot{\xi}$. Its time dependence is expressed via $F = F\left(\xi(t), \dot{\xi}(t)\right)$. Newton's equation of motion for the colliding particles reads

$$\frac{m}{2}\ddot{\xi} + F\left(\dot{\xi}, \xi\right) = 0; \quad \xi(0) = 0; \quad \dot{\xi}(0) = v \tag{4}$$

where v is the normal component of the initial relative velocity,

$$v \equiv \frac{1}{2R}\left[\mathbf{v}_1(0) - \mathbf{v}_2(0)\right] \cdot \left[\mathbf{r}_1(0) - \mathbf{r}_2(0)\right] . \tag{5}$$

The coefficient of restitution follows from the solution of Eq. (4),

$$\varepsilon = -\,\dot{\xi}(t_c) \big/ v\,, \tag{6}$$

where t_c is the duration of the collision.

Thus, the coefficient of restitution due to a specified interaction force law can be determined by solving the equation of motion [20,22,24]. In general, ε is a function of the material parameters, the particle masses and radii and the impact velocity v.

3 Linear–dashpot model

Consider the *linear–dashpot* force,

$$F\left(\xi, \dot{\xi}\right) = -k\xi - \gamma\dot{\xi}\,. \tag{7}$$

This force is problematic as a particle interaction model since particles made of a linear-elastic material do not reveal a linear repulsive force, neither in 3D [7] nor in 2D [4]. The subsequent analysis can be also performed for more realistic force models, such as viscoelastic forces in 3D [2] and 2D [23], however, at much larger mathematical effort. For the important case of viscoelastic 3D spheres the calculation can be found in [25].

The linear–dashpot model is of interest here because this force leads to a *constant* coefficient of restitution, e.g. [22], that is, ε does not depend on the impact velocity but only on the material parameters k and γ. The constant coefficient of restitution in turn is the preferred model in both the Kinetic Theory of granular gases and also in event-driven simulations of granular matter. In contrast, more realistic force models lead to an impact-velocity dependent coefficient of restitution [13,20,24,26,28,30].

The force law Eq. (7) was used in Molecular Dynamics simulations, e.g. [3,10,14,17,18,21,27,29,31] and leads to the coefficient of restitution

$$\varepsilon_d^0 = \exp\left(-\frac{\pi}{\sqrt{2km/\gamma^2 - 1}}\right) \tag{8}$$

which is widely used in the literature.

In most papers on simulation of granular matter it is claimed that the particles interact exclusively repulsive during the entire contact, that is, attracting forces are explicitly excluded. A closer look to Eq. (7) reveals, however, that this force is not strictly positive: For arbitrary (positive) parameters k and γ there is a time when the interaction force becomes attractive. We will discuss this time below in detail. Consequently, the assumption of purely repulsive interaction is in contradiction to the used force, Eq. (7).

Therefore, in many references, e.g. [5,6,8,15,11,19,22,32], only the repulsive part of the force is used,

$$F\left(\xi, \dot{\xi}\right) = \min\left(0,\ -k\xi - \gamma\dot{\xi}\right)\,. \tag{9}$$

that is, the positive (attractive) part of the interaction force is cut off. In the next section we will derive an expression for the coefficient of restitution, ε_d, according to Eq. (9). When using the cut-off force Eq. (9) in a Molecular Dynamics simulation, the expression (8) would systematically underestimate the coefficient of restitution and for some choice of the parameters k and γ yield even qualitatively wrong results.

4 Coefficient of restitution according to the force Eq. (7)

The equation of motion corresponding to Eq. (7)

$$m\ddot{\xi} + 2\gamma\dot{\xi} + 2k\xi = 0 \tag{10}$$

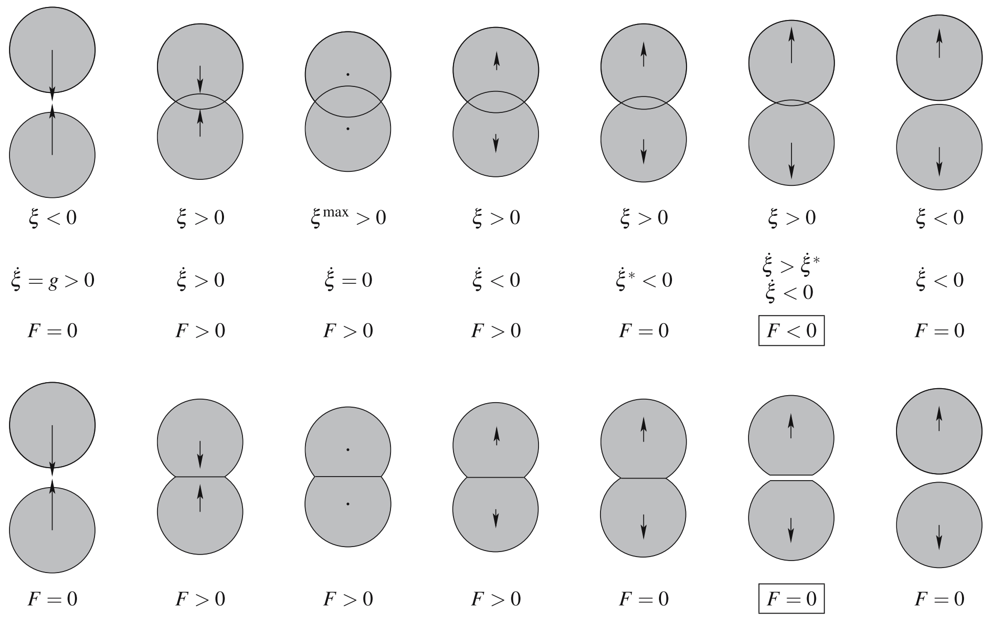

Fig. 1 Sketch of a particle collision. The *upper part* of the figure visualizes the condition (16) for the end of the collision. As an artifact of the model, there appear attracting forces towards the end of the collision (*boxed notation*). *Lower part* the condition (19) for the end of the collision avoids this artifact

with initial conditions

$$\xi(0) = 0\,; \qquad \dot{\xi}(0) = v \tag{11}$$

has two solutions. With the abbreviations

$$\omega_0^2 \equiv \frac{2k}{m}\,; \qquad \beta \equiv \frac{\gamma}{m}\,; \qquad \omega \equiv \sqrt{\omega_0^2 - \beta^2} \tag{12}$$

we can write the solution for the case of low damping ($\beta < \omega_0$) as

$$\xi(t) = \frac{v}{\omega} e^{-\beta t} \sin \omega t\,, \tag{13}$$

while for the case of high damping ($\beta > \omega_0$) we have

$$\xi(t) = \frac{v}{\Omega} e^{-\beta t} \sin \Omega t\,, \tag{14}$$

with

$$\Omega = \sqrt{\beta^2 - \omega_0^2}\,. \tag{15}$$

To determine the coefficient of restitution by means of Eq. (6) we need the duration of the collision t_c. The uncut force, Eq. (7) terminates at time t_c^0 with

$$\xi\left(t_c^0\right) = 0\,; \qquad t_c^0 > 0\,, \tag{16}$$

that is, the collision is finished when $\left|\mathbf{r}_i - \mathbf{r}_j\right| = 2R$. With this condition we obtain $t_c^0 = \pi/\omega$ and the coefficient of restitution

$$\varepsilon_{\mathrm{d}}^0 \equiv \frac{\dot{\xi}\left(t_c^0\right)}{\dot{\xi}(0)} = e^{-\beta\pi/\omega}\,, \tag{17}$$

for the case of low damping, which agrees with Eq. (8). Inserting the time at the end of the collision, $t_c^0 = \pi/\omega$, into the second derivative of Eq. (13) we obtain

$$m\ddot{\xi}\left(\frac{\pi}{\omega}\right) = -\frac{2mv\beta}{\omega} e^{-\beta\pi/\omega} < 0\,, \tag{18}$$

that is, the particles feel an attractive force, see Fig. 1. Consequently, using the force Eq. (7) is not in agreement with the assumption of exclusively repulsive interaction between granular particles. Moreover, for the case of high damping Eq. (16) has no real solution, that is, the particles stick together after a head-on collision (see Fig. 2). One can call this situation *dissipative capture*.

5 Coefficient of restitution according to the force Eq. (9)

When using the interaction force Eq. (9), we require that granular particles interact always repulsive. In this case, obviously, Eq. (16) is not the appropriate condition for the end of a collision as it leads to an artificial attractive force. This fact was already mentioned earlier, e.g. [11,12]; here we want to elaborate a *quantitative* expression for the coefficient of restitution as obtained from integrating Newton's equation of motion using a more suitable boundary condition.

To avoid the mentioned artifacts, instead of Eq. (16), we now explicitly take into account the condition of no attraction. That is, the collision is finished when the force becomes zero,

$$\ddot{\xi}(t_c) = 0; \quad t_c > 0; \quad \dot{\xi}(t_c) < 0 . \tag{19}$$

At time t_c when the repulsive force between the particles vanishes, the surfaces of the particles separate from one another. This condition takes, thus, into account that Eq. (7) applies to *particles in contact*—also close to the end of a collision when the distance of the centers of the particles, ξ, increases more rapidly than the particles recover to their spherical shape. Consequently, the particles lose contact even befor they completely recovered their spherical shape (see Fig. 1, lower row) [19,32].

For the case of low damping Eqs. (13) and (19) yield an equation for t_c:

$$\tan \omega t_c = -\frac{2\beta\omega}{\omega^2 - \beta^2} . \tag{20}$$

One has to take care to select the correct branch of the arc tangent for $\beta < \omega_0/\sqrt{2}$ (or $\beta < \omega$) and for $\beta > \omega_0/\sqrt{2}$. The solution reads

$$t_c = \begin{cases} \dfrac{1}{\omega}\left(\pi - \arctan\dfrac{2\beta\omega}{\omega^2 - \beta^2}\right) & \text{for} \quad \beta < \dfrac{\omega_0}{\sqrt{2}} \\ \dfrac{1}{\omega}\arctan\dfrac{2\beta\omega}{\omega^2 - \beta^2} & \text{for} \quad \beta > \dfrac{\omega_0}{\sqrt{2}} \end{cases} \tag{21}$$

For the coefficient of restitution we find

$$\varepsilon_d = e^{-\beta t_c} \tag{22}$$

regardless of the branch of the solution of Eq. (20). Together with the solution for the case of high damping which can be obtained by straight-forward computations we obtain the coefficient of restitution,

$$\varepsilon_d = \begin{cases} \exp\left[-\dfrac{\beta}{\omega}\left(\pi - \arctan\dfrac{2\beta\omega}{\omega^2 - \beta^2}\right)\right] & \text{for} \quad \beta < \dfrac{\omega_0}{\sqrt{2}} \\ \exp\left[-\dfrac{\beta}{\omega}\arctan\dfrac{2\beta\omega}{\omega^2 - \beta^2}\right] & \text{for} \quad \beta \in \left[\dfrac{\omega_0}{\sqrt{2}}, \omega_0\right] \\ \exp\left[-\dfrac{\beta}{\Omega}\ln\dfrac{\beta + \Omega}{\beta - \Omega}\right] & \text{for} \quad \beta > \omega_0 \end{cases} \tag{23}$$

In agreement with physical intuition we have $\varepsilon_d > \varepsilon_d^0$ since the result given in Eq. (23) does not suffer from the artifact of attractive forces implied in Eq. (17). The unphysical dissipative capture does not occur—even for large damping constant the particles separate eventually. For very high damping the coefficient of restitution can be approximated as

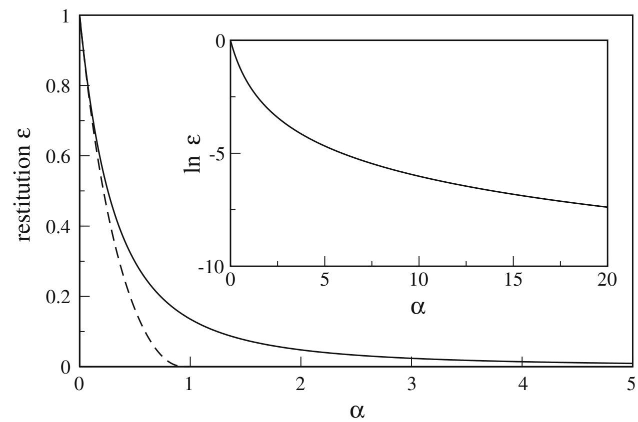

Fig. 2 Coefficient of restitution as a function of $\alpha \equiv \beta/\omega_0$. The *dashed curve* is the result for the termination condition $\xi(t_c^0) = 0$. Obviously, for high damping $\alpha > 1$ we have dissipative capture. The *full line* and the *inlay* show ε as a function of α for the termination condition $F(t_c) = 0$. There is no dissipative capture even for very high damping

$$\varepsilon_d \approx \frac{\omega_0^2}{4\beta^2} \quad \text{for} \quad \beta \gg \omega_0 \tag{24}$$

Figure 2 shows both the coefficient of restitution as derived from criterion (16) (dashed line) and the coefficient of restitution derived from the criterion (19) (full line). As the solution Eq. (23) only depends on the ratio $\alpha = \beta/\omega_0$ we draw the coefficient of restitution as a function of this parameter. Figure 2 shows that the unphysical attraction indeed yields a too low coefficient of restitution. The inset shows a logarithmic plot of the same curve showing that there is no capture if the improved criterion, Eq. (19), is applied.

6 Conclusion

Assuming a linear–dashpot interaction force we computed ε as a function of the elastic and dissipative material properties by integrating Newton's equation of motion for a pair of colliding particles.

Using the uncut interaction force law, Eq. (7), implies the assumption that the interaction terminates at time t_c^0 when the centers of the particles have the distance $\left|\mathbf{r}_i - \mathbf{r}_j\right| = 2R$, that is, $\xi(t_c^0) = 0$. As $\ddot{\xi}(t_c^0) < 0$, consequently the use of Eq. (7) is not in agreement with the assumption of exclusively repulsive particle interaction.

For certain choices of the force parameters, k and γ, the equation for the duration of the collision t_c^0 does not have a real solution, that is, it would take infinite time for the particles to separate. In other words, at any finite time one would need to supply energy to separate the particles from one another, that is the particles are in an agglomerated state.

As this agglomeration is solely due to dissipative forces we find this behavior unacceptable. Therefore, to our point of view attractive forces should be excluded by cutting off the interaction force (see Eq. 9) in accordance with standard procedure in the literature. To account for the fact that the interaction force can never become attractive, we characterize the end of the collision by means of the condition $\ddot{\xi}(t_c) = 0$ which avoids the mentioned artifacts. This condition takes into account that the collision may be completed even before $\xi = 0$, that is, the surfaces of the particles lose contact slightly before the distance of their centers exceeds the sum of their radii. Thus, the deformation of the particles may last longer than the time of contact and the particles gradually recover their spherical shape only *after* they lost contact.

The resulting coefficient of restitution is always larger than the value based on $\xi\left(t_c^0\right) = 0$. In agreement with the repulsive character of the interaction force, the coefficient of restitution is always well defined and non-zero (no dissipative capture).

Although the calculation in this paper is limited to a pair of particles which interact by the linear–dashpot force, Eq. (9), being a strong simplification of the interaction of colliding spheres, the effect of premature separation of the particles after a collision applies for a much wider class of interaction laws. The quantitative investigation of the effect for more realistic interaction laws requires the integration of the equation of motion which turns out to be a rather involved mathematical problem. As an example, for the case of viscoelastic 3D spheres the calculation can be found in [25].

References

1. Brilliantov, N.V., Pöschel, T.: Kinetic Theory of Granular Gases. Clarendon, Oxford (2004)
2. Brilliantov, N.V., Spahn, F., Hertzsch, J.M., Pöschel, T.: A model for collisions in granular gases. Phys. Rev. E **53**, 5382 (1996)
3. Campbell, C.S.: Granular shear flows at the elastic limit. J. Fluid Mech. **465**, 261 (2002)
4. Engel, P.A.: Impact Wear of Materials. Elsevier, Amsterdam (1978)
5. Goldenberg, C., Goldhirsch, I.: Small and large scale granular statics. Granul. Matter **6**, 87 (2004)
6. Goldhirsch, I., Goldenberg, C.: Stress in dense granular materials. In: Hinrichsen, H., Wolf, D.E. (eds.) The Physics of Granular Media. Wiley, Weinheim, p. 3 (2004)
7. Hertz, H.: Über die Berührung fester elastischer Körper. J. F Reine U Angewandte Math. **92**, 156 (1882)
8. Kadau, D., Schwesig, D., Theuerkauf, J., Wolf, D.E.: Influence of particle elasticity in shear testers. Granul. Matter **8**, 35 (2006)
9. Kruggel-Emden, H., Simsek, E., Rickelt, S., Wirtz, S., Scherer, V.: Review and extension of normal force models for the Discrete Element Method. Powder Technol. **171**, 157 (2007)
10. Luding, S.: Stress distribution in static two dimensional granular model media in the absence of friction. Phys. Rev. E **55**, 4720 (1997)
11. Luding, S.: Collisions & contacts between two particles. In: Herrmann, H.J., J.-P. Hovi, J.P., Luding, S. (eds) Physics of dry granular Media, Kluwer, Dordrecht, p. 285 (1998a)
12. Luding, S.: Die Physik kohäsionsloser granularer Medien (Habilitation thesis; in german). Logos Verlag, Berlin (1998b)
13. Luding, S., Clément, E., Blumen, A., Rajchenbach, J., Duran, J.: Anomalous energy dissipation in molecular dynamics simulations of grains: The “detachment” effect. Phys. Rev. E **50**, 4113 (1994a)
14. Luding, S., Clément, E., Blumen, A., Rajchenbach, J., Duran, J.: Onset of convection in molecular dynamics simulations of grains. Phys. Rev. E **50**, R1762 (1994b)
15. Matuttis, G., Luding, S., Herrmann, H.J.: Discrete element simulations of dense packings and heaps made of spherical and non-spherical particles. Powder Technol. **109**, 278 (2000)
16. Meerson, B., Pöschel, T., Bromberg, Y.: Close-packed floating clusters: Granular hydrodynamics beyond the freezing point?. Phys. Rev. Lett. **91**, 24,301 (2003)
17. Mouraille, O., Mulder, W.A., Luding, S.: Sound wave acceleration in granular materials. J. Stat. Mech. **2006**, P07,023 (2006)
18. Oger, L., Savage, S.B., Corriveau, D., Sayed, M.: Yield and deformation of an assmebly of disks subjected to a deviatoric stress loading. Mech. Mater. **27**, 189 (1998)
19. Pöschel, T., Schwager, T.: Computational Granular Dynamics. Springer, Berlin (2005)
20. Ramírez, R., Pöschel, T., Brilliantov, N.V., Schwager, T.: Coefficient of restitution of colliding viscoelastic spheres. Phys. Rev. E **60**, 4465 (1999)
21. Schäfer, J., Wolf, D.E.: Bistability in simulated granular flow along corrugated walls. Phys. Rev. E **51**, 6154 (1995)
22. Schäfer, J., Dippel, S., Wolf, D.E.: Force schemes in simulations of granular materials. J. Phys. I **6**, 5 (1996)
23. Schwager, T.: Coefficient of restitution for viscoelastic disks. Phys. Rev. E **75**, 051,305 (2007)
24. Schwager, T., Pöschel, T.: Coefficient of restitution of viscous particles and cooling rate of granular gases. Phys. Rev. E **57**, 650 (1998)
25. Schwager, T., Pöschel, T.: Coefficient of restitution for viscoelastic spheres: the effect of delayed recovery. arXiv:07081434 (2007)
26. Taguchi, Y.: Powder turbulence: Direct onset of turbulent flow. J. Phys. I **2**, 2103 (1992a)
27. Taguchi, Yh.: New origin of a convective motion: elastically induced convection in granular materials. Phys. Rev. Lett. **69**, 1367 (1992b)
28. Tanaka, T., Ishida, T., Tsuji, Y.: Direct numerical simulation of granular plug flow in a horizontal pipe. the case of cohesionless particles (in japanese). Kiron B **57–534**, 456 (1991)
29. Thompson, P.A., Grest, G.A.: Granular flow: friction and the dilatancy transition. Phys. Rev. Lett. **67**, 1751 (1991)
30. Tsuji, Y., Tanaka, T., Ishida, T.: Lagrangian numerical simulation of plug flow of cohesionless particles in a horizontal pipe. Powder Technol. **71**, 239 (1991)
31. Weir, G., Tallon, S.: The coefficient of restitution for normal incident, low velocity particle impacts. Chem. Eng. Sci. **60**, 3637 (2005)
32. Wolf, D.E.: How to simulate granular matter. In: Blügel, S., Gompper, G., Koch, E., Müller-Krumbhaar, H., Spatschek, R., Winkler, R.G. (eds.) Computational Condensed Matter Physics—Lecture Manuscripts of the 37th Spring School of the Institute of Solid State Research, IFF-Ferienkurs, vol 32. Forschungszentrum, Jülich, p. B13 (2006)