

Particle Based Simulations of Image Quality Defects

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Abstract

We describe a method for investigating and characterizing image-quality defects related to electrographic marking technologies. Using the particle-in-cell method, individual toner particles are tracked in space and time while under the influence of the various forces found in xerographic development subsystems. Using physically realistic models of toner adhesion, cohesion, air drag, and friction; detailed particle trajectories can be calculated and monitored in self-consistent electric fields. We show how this method can be applied to gain a better understanding of phenomena which tend to degrade image quality (*e.g.*, lack of solid-area uniformity, line-edge noise, toner in background areas). Rather than merely measuring and characterizing image-quality defects, we try to induce image artifacts by varying toner and surface properties via computer simulations. In this way, fundamental driving mechanisms for image defects can be identified.

Introduction

In the xerographic process, charged toner particles are accelerated in electric fields and deposited on a photoelectric receiver to form an image. These fields are generated by a combination of surface charge on the receiver (*i.e.*, the latent image), space charge due to the particles, and metallic electrodes with time-varying applied potentials. In order to understand particle transport, detailed simulations of particle trajectories are computed. Using a software system known as *Pic3D*, computer programs can be written which emulate experimental hardware fixtures. Such a program is termed a *digital fixture*. Tens of thousands of particles are tracked over several milliseconds of time using contemporary work-stations. Central to such simulations are models of adhesion and cohesion which capture particle interactions with boundary surfaces and other particles. These models are calibrated by building digital fixtures to emulate existing hardware; parameters which characterize material properties are then adjusted until the models predict the same results as the hardware. When a set of parameters correctly replicates several experiments, the code can then be confidently used to create new digital fixtures for research and product design.

The primary role of *Pic3D* is to automatically compute all forces resulting from space charge and particle collision events while tracking toner particles moving through space. As with most particle-in-cell programs,[1] the code accumulates the net force on each and every particle during a small interval of time, and then twice integrates the equations of motion (*i.e.*, f=ma) during the time step. The force terms consist of both field (*e.g.,* electrostatic, air flow) and collision (*e.g.*, particle-to-surface, particle-to-particle) components. *Particles* are the C++ abstractions (*i.e.*, objects) that represent individual toners. *EventHandlers* are C++ objects that capture the microscopic aspects of adhesion and cohesion. Whenever a particle is “close” to some other particle or surface, the appropriate event handler is invoked to compute the force on that particle.

If all possible particle-to-particle collisions were considered at each time step, the cost of a simulation would grow as $O(N^2)$ for N particles. A way to reduce this cost is to split the forces between particles and boundaries into long-range and short-range components. The short-range compo-nent is calculated explicitly via event handlers while the long-range component (due exclusively to the Coulomb term) is transferred into space-charge and handled as part of the electrostatic field solution. This technique is commonly known as the P^3M (Particle-Particle Particle-Mesh) approach.[1]

Toner-Particle Models

In *Pic3D*, some components of the total force on a particle are empirical relationships that are combined in the manner of pseudopotentials in molecular modeling, we called these components *pseudoforces* by analogy. Each toner particle has a unique pseudoforce that results from its geometry and charge distribution. For our purposes, we wish to find a simple yet representative pseudoforce that can be used by a group of similar particles. Each particle will have a unique size and charge randomly assigned from a measured distribution. For computational simplicity, the force is assumed to be a function of distance only.

Pic3D incorporates a particle-to-particle force model consisting of three regimes: a strongly repulsive hard-core collision force when particles overlap; a short-range attractive cohesion force term; and a long-range Coulomb force term that can be either attractive or repulsive. The particle-to-surface force model is nearly identical except that the “other” particle is assumed to be a mirror image of itself across the interface. In this case, the long-range Coulomb term is always attractive. The model considers four short-range interactions: the inherent cohesion between particles due to atomic and mechanical forces; the force due to irregular charge distributions on the particle; the effective range of the short-term cohesive force; and the permittivities of the particle and the surrounding medium.[2,3] If two particles are physically overlapping, they are experiencing a hard-core collision, so a simple formula based on conservation of energy is used to describe the force between the particles. A coefficient of restitution can be specified to capture the effect of inelastic collisions.

In reality, a toner particle's shape is usually quite irregular and the way a particle lies on a surface will greatly influence is adhesion to that surface. One way to mimic this effect, is to model the particle's adhesion as a random variable governed by the orientation of the particle. This is done by modulating the strength of the short-range force by a stochastic "orientation" parameter which is related to a particle's surface roughness. A particle's orientation is assigned from an appropriate distribution.

The collision model parameters are determined by building digital fixtures to emulate existing hardware fixtures. For example, particle-surface adhesion parameter values are based upon a series of experiments conducted by Eklund. His apparatus, known as an electrostatic detachment cell, is essentially a small parallel plate capacitor operated in a vacuum chamber.[4] We emulate the electrostatic detachment cell with the *Pic3D* code, and fit the model coefficients to the experimental data. In practice, we find that models that reproduce this experiment perform well on more complex fixtures. Other experiments are used to determine the coefficient of restitution and surface friction coefficients. Digital fixtures can also be built for cases where analytical solutions exist to further verify the code.

Examples

Our ability to track large numbers of toner particles in realistic fields and geometry's presents us with the opportunity to generate simulated images (particle-by-particle) as they might appear on a photoreceptor. At present, we are able to run simulations containing tens of thousands of particles for a few milliseconds of process time. Up to several cubic millimeters of space can be repre-sented, with corresponding image areas of several square millimeters. Although full-page images cannot be produced, we have found this region to be sufficient to study solid areas, line edges, and halftone dot structures. Note that the resulting images are in fact three dimensional, as toner pile-height information is inherently present in our generated datasets. In this section we present examples of the type of results *Pic3D* can produce as related to image quality. In the following examples, we only consider unfused images as they form on a photoreceptor.

Graininess and Uniformity

Perhaps the simplest example of an image is an area of uniform density. Using a proprietary development mechanism, particles are detached from a donor surface and attracted to a uniformly charged photoreceptor. As the particles arrive at the receiver's surface, they arrange themselves into a more or less uniform sheet of particles. The actual mechanics of this arrangement is rather complex and amounts to minimizing the energy of N interacting bodies, each responding to a large set of complex nonlinear forces. During the arrangement time, the particles may experience forces due to collisions, adhesion to the photoreceptor, cohesion to other particles, and friction due to sliding. By studying various realistic distributions of particle size and charge, we are able to gain an understanding of how solid areas develop and how uniformity and graininess metrics relate to existing and future toner formulations. In figure 1 we show two possible size distributes of toner. Both distributions have approximately the same mean particle diameter, but one distribution is wider than the other. Figure 2 illustrates the difference in how the particles from each distribution pack onto a surface. In general, narrow size distributions tend to pack into films that reflect a more "crystalline" uniform structure and are not as dense or grainy as films generated from toner with wider size distributions.

One clear advantage of simulations over conventional experiments is the ease with which the raw data can be collected and analyzed. Aside from the position and size of each particle, information is directly available regarding charge, adhesion, and other properties (*e.g.*, "Where to high tribo particles end up after they develop on the receiver?").

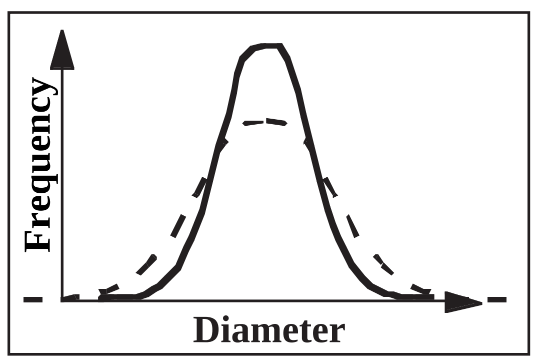

Figure 1. Two toner size distributions; wide and narrow with the same average diameter.

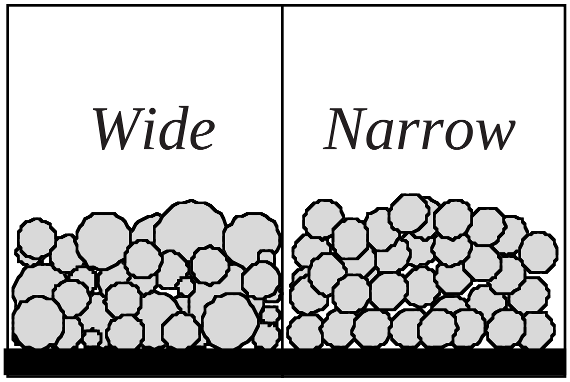

Figure 2. Size distributions affect how toner packs onto a surface.

Line-Edge Noise

If the uniform charge on the receptor surface is replaced by the latent image of a line, negatively charged particles will be attracted towards positive regions of the receptor and repelled away from negative background regions as illustrated in figure 3. In this case, the particles arrange themselves into a line image. Typically, depending upon the exact parameters of the simulation, a developed line will have a different effective width than the latent image written on the photoreceptor. This reflects the well known phenomena of line shrinkage due to fringe fields. Of particular interest is the exact manner in which particles arrange themselves along the edge of the line. Consistent with achieving a state of global minimum energy, particles will rearrange themselves over time to form a remarkably smooth edge as shown along the lower edge in figure 4. The specific particle size distribution and development time (which is related to process speed) can be varied and optimized to achieve high-quality edges consistent with other engineering design goals. Images of arbitrary halftone dots can also be written to the photoreceptor and developed with particles. As development can be easily monitored as a function of time, it is possible to try and optimize toner parameters, such as tribo (Q/M), to improve the growth rate and image quality of line edges and halftone dots (see figure 5).

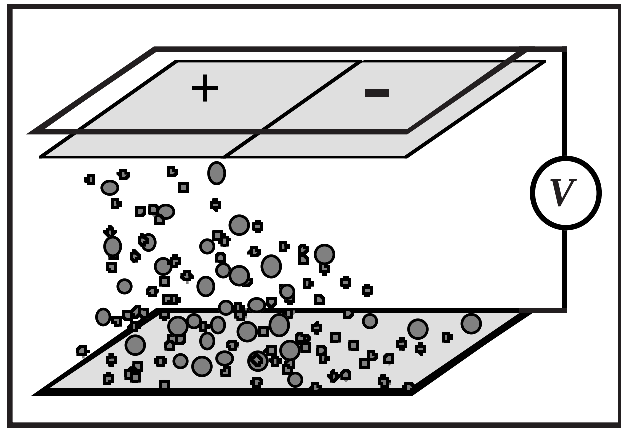

Figure 3. Schematic of a line-edge development apparatus. Toner is ejected from the lower donor surface and either attracted or repelled to areas above.

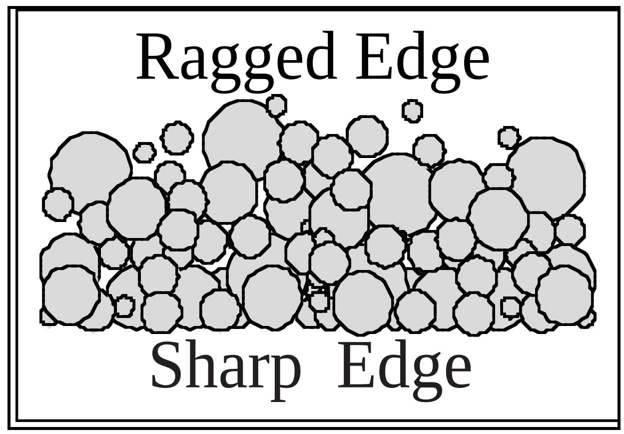

Figure 4. Particle development of a line. The top edge is drawn to illustrate poor edge quality when compared with the lower edge.

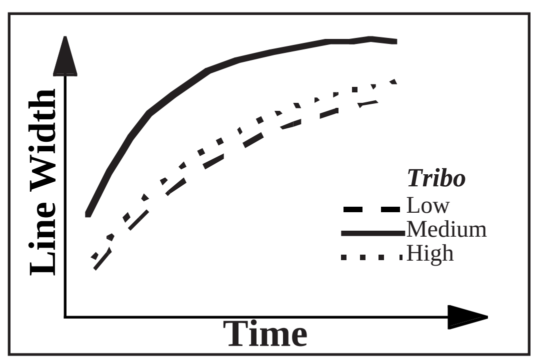

Figure 5. Line width as a function of Q/M (tribo).

Background Development

In a cleaning field, where the particles are normally repelled from the photoreceptor's surface, some toner development is observed. Our digital fixture allows us to determine which portions of the charge and mass distribution tend to contribute to this source of image noise. By varying the distribution and monitoring which particles develop, it might be possible to design toner which minimizes background noise. For example, Figure 6 illustrates regions of Q/M which can be identified by noting the exact charge and mass of each particle that appears in the background region of a simulated image. Such data would be hard to obtain experimentally.

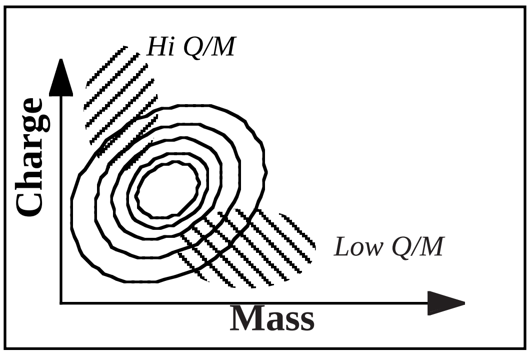

Figure 6. Charge-mass distribution of toner showing regions which may contribute to background noise for a particular development subsystem.

Conclusion

We have used the *Pic3D* system to model and study the microscopic aspects of several types of image-quality defects. The notion of a digital fixture appears useful in the design process, especially as high-performance computers become accessible to engineering development groups. Detailed simulations at the particle level can be used to extract the fundamental driving mechanisms of image artifacts which are related to the inherent particulate nature of xerography. Our software serves as a complementary tool to conventional hardware-based experiments and the use of image-quality metrics in designing high-quality electrographic print engines.

References

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