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Modelling adsorption of charged macromolecules

Jeremy Rosen, Department of Mathematics and Statistics, University of Melbourne

Last summer I worked as a Vacation Scholar on a project with Prof. Derek Chan, exploring the structure of polyelectrolytes adsorbed onto colloidal particles. Since the 1990's these polyelectrolyte-coated particles have aroused a great deal of interest due to their interesting and adaptable surface properties. A clear picture of their internal structure remains to be discovered.

The aim of the project was to use electrophoresis experiments to find possible configurations for the polyelectrolyte layers. We began with experimental electrophoretic data detailing the behaviour of charged particles in an electric field. Working with a physical and chemical model of the charges distributed in and around the particle, we generalised the model to incorporate charged particles coated with successive polyelectrolyte layers. This led to the second-order non-linear differential equation:

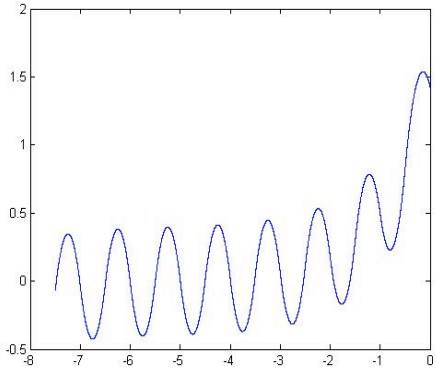
$$\psi''(x) = -\frac{\rho_{el}}{\varepsilon\varepsilon_0} - \frac{\rho_{fix}}{\varepsilon\varepsilon_0}.$$

This relates the potential at a point to the charge distribution around the particle.

No solution of the differential equation for the potential function exists for a general polyelectrolyte charge distribution. To test out different distributions we had to solve the DE numerically using a shooting algorithm we wrote in MATLAB. We had to learn how to program first, and much time was spent making the program more accurate and general. After solving for the potential we could input the distribution found into the model for the electrophoretic mobility and find the theoretical mobilities. Comparisons of the theoretical mobilities of two likely charge distributions showed that they were identical and closely correlated to experimental results, meaning electrophoresis is not a good discriminator.

The Vacation Scholarship was a very rewarding experience. I greatly appreciated working with my two partners, Steve McAteer and Juwen Ho. It was an opportunity to experience mathematics research, including the inevitable lows when nothing seems to work, and the exhilarating highs after a long-sought discovery. I explored areas of maths I didn't know much about before and met some extremely interesting and likeable people.

I highly recommend the Vacation Scholarship program to anyone interested in further studies in Mathematics.



Potential profile of alternating charged layers

Jeremy received an ICE-EM Vacation Scholarship in December 2005. See www.ice-em.org.au/students.html#scholarships05