Prof. Raghuveer Parthasarathy
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Physics 351

Computer Programming: A Brief Introduction

SOLUTIONS: Exercises P1-P3

P1. Chang *et al.*, retract the conclusions of several of their recent papers, stating that their results are incorrect. The error is attributed to a software mistake that leads to an incorrect sign in some parameter – i.e. a "human" programming error (3 pts). The letter by Miller stresses the importance of knowing what one's software actually does. The editorial by Matthews argues that the error acknowledged by Chang *et al.* does not in itself lead to the authors' erroneous conclusions, but requires a broader ignorance of crystallography.

P2. Bowen *et al.*'s simulation of the DLVO equations of colloidal interactions reproduce experimentally observed inter-particle attractions (1 pt.). Neu's analytic analysis of the DLVO equations proves mathematically that they *cannot* lead to attraction (1 pt.). Therefore, even without knowing what the error in Simulation 2a is, we can be sure it is wrong (2 pts.) – it is as if a computer program had shown that an integer ending in "0" is not divisible by 10, a conclusion that can be proved analytically to be wrong. Bowen *et al.*'s conclusion is likely be due to errors in the computation, perhaps related to numerical errors, or perhaps due to modeling the system on a finite spatial grid (the "adaptive finite element method"), or perhaps due to other issues.

P3. Brunini simply states that his program was wrong, and retracts the paper. He comments that the program was unreliable, implying that there was some numerical error in it, but this explanation is very vague. This explanation is vague and unsatisfying. (2 pts.)