BUILDING AND VALIDATING A MODEL FOR INVESTIGATING THE DYNAMICS OF ISOLATED WATER MOLECULES

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THE INTRODUCTION

• Dressel et. al have found a system in which single water molecules are isolated with only dipole-dipole interactions and expect to find evidence of ferroelectricity.1
• Computational models are desired for proof-of-concept calculations and verifying deduced understanding of this system
• Efficacy of three popular algorithms investigated

THE MOTIVATION

• Models will increase understanding of fundamental interactions in many sciences
• Greatest potential impact is in biology
• Interpreting results of isolation is difficult, because biological systems are too complex and have too much unknown uncertainty

THE METHODS

Consider a dipole at the origin with only rotational degree of freedom in presence of a constant electric field (setup given in Fig. 1a)

for each algorithm
  for each electric field
    for each initial angle
      Model dynamics for total runtime
      Determine frequency of oscillation
    end
  end
end

Examine average frequency vs. e-field
Fit to power function (Fig. 2a)
Determine predictive stability coefficient ρ (Fig. 2b)

THE ALGORITHMS

Euler Method (EM)
- First-point approximation
- Unstable for oscillatory phenomena

Euler-Aspel Method (EAM)
- Last-point approximation
- Stable for oscillatory phenomena

Beeman Method (BM)
- Uses weighted average of information from previous two timesteps
- Not self-starting

THE FIGURES

y = ax^n

THE ANALYSIS

<table>
<thead>
<tr>
<th>Model</th>
<th>n</th>
<th>a</th>
<th>b</th>
<th>p</th>
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<tr>
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• EAM and BM are superior in both ranges
• Limited range in which EM is effective
• EAM determined most effective, because it also better predicts coefficient (a = 56,000)

THE FUTURE WORK

• Determine ρ for more sophisticated algorithms
• Investigate nearest-neighbor interactions (setup given in Fig. 1b)
• Further analyze Prelim. Results for two dipoles (Fig. 3b)
• Look for evidence of ferroelectricity

THE GRATITUDE

• Drs. Michael Crosser, Jennifer Heath, Joelle Murray of Linfield College
• Prof. Dr. Martin Dressel of Stuttgart Universität
• Linfield Physics and Mathematics Departments

Fig. 1 The setup for the Methods is given. The purple region represents possible initial angles. (a) The setup for the Future Work is given. The dipoles are separated by a distance r and start with initial relative angle θ. [1] M. Dressel, J. Grünert, Broad-band optical spectroscopy of low-energy excitations of water molecules confined in aqueous layers of free-standing films (2014).

Fig. 2 (a) The equation to calculate the data is listed. It is the definition for the predictive stability coefficient. (Note: here, a = 0, b = 1).

Fig. 3 (a) The results from simulating the full range of ε-fields (ex. ε = 1.8 ~ 10^12 N/C) and the limited range (electrons ε = 1.8 ~ 10^12 N/C and δ = the preliminary results from the Future Work are shown.

Fig. 4 The results from fitting the data (via Fig. 3) and determining the predictive stability coefficient (Fig. 3b) are summarized. The results for a set of (EAM) data and best fits given in Fig. 1a.