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

Grant Cates

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

THE ALGORTIHMS

Euler Method (EM)

- First-point approximation
- Unstable for oscillatory phenomena

$$v_n = v_{n-1} + a(x_{n-1}, t_{n-1})\tau$$
$$x_n = x_{n-1} + v_{n-1}\tau$$

Euler-Aspel Method (EAM)

- Last-point approximation
- Stable for oscillatory phenomena

$$v_n = v_{n-1} + a(x_{n-1}, t_{n-1})\tau$$
$$x_n = x_{n-1} + v_n\tau$$

Beeman Method (BM)

- Uses weighted average of information from previous two timesteps
- Not self-starting

$$x_n = x_{n-1} + v_{n-1}\tau + \frac{\tau^2}{6}\left(4a(x_{n-1}, t_{n-1}) - a(x_{n-2}, t_{n-2})\right)$$
$$v_n = v_{n-1} + \frac{\tau}{6}\left(2a(x_n, t_n) + 5a(x_{n-1}, t_{n-1}) - a(x_{n-2}, t_{n-2})\right)$$

THE FIGURES

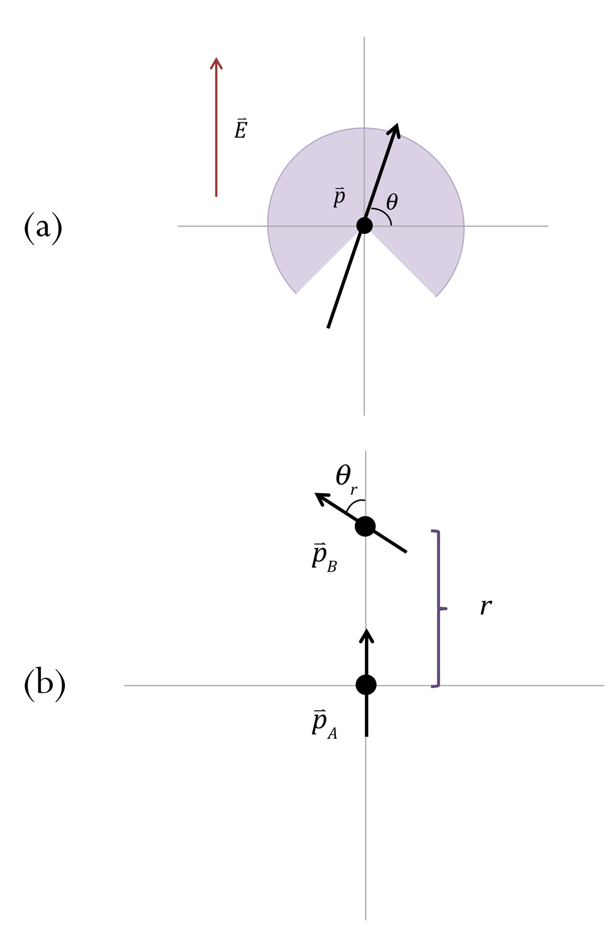

FIG. 1 (a) The setup for The Methods is given. The purple region represents possible initial angles. (b) The setup for The Future Works is given. Two dipoles are separated by a distance r and start with initial relative angle $\boldsymbol{\theta}_r$.

$$y = ax^n$$

$$\rho = \left|1 - \frac{n}{n_o}\right|$$

FIG. 2 (a) The equation to which the data is fitted. (b) The definition for the predictive stability coefficient. (Note: Here, $n_o = ½$)

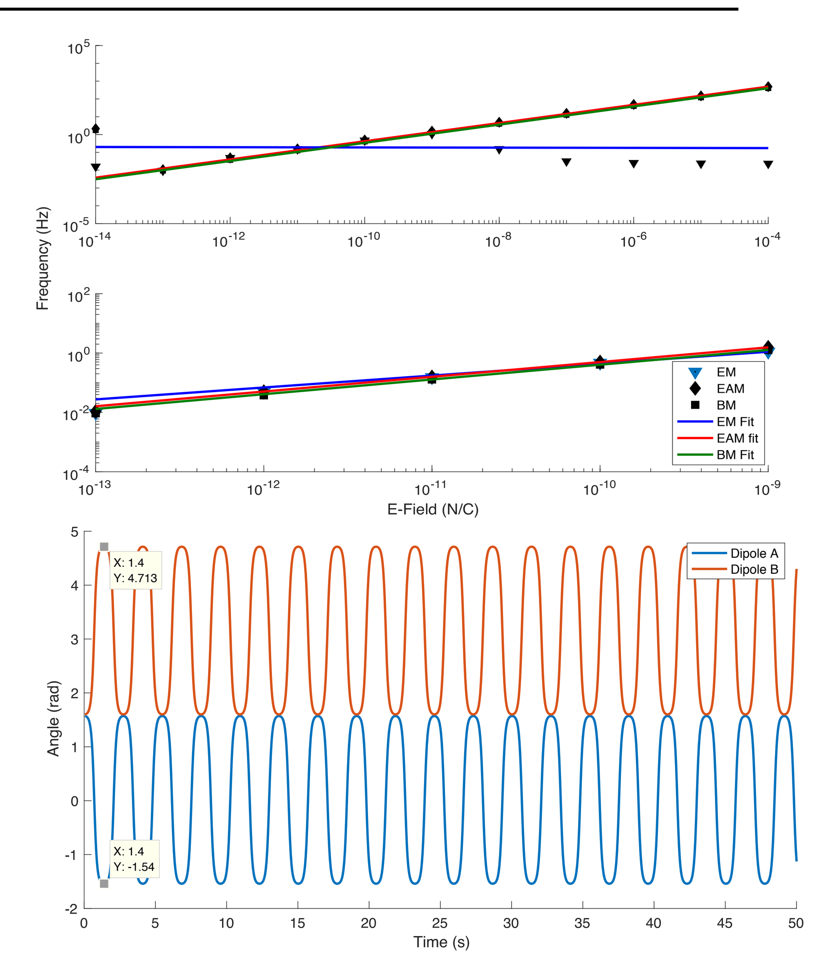

FIG. 3 (a) The results from probing the full range of e-fields (top; $E = 10^{-14}$ to 10^{-4} N/C) and the limited range (bottom; $E = 10^{-13}$ to 10^{-9} N/C) and (b) the preliminary results from The Future Work are shown.

THE ANALYSIS

FIG. 4 The results from fitting the data (to Fig. 2a) and determining the predictive stability coefficient (Fig. 2b) are summarized. The units for a are $\left(\sqrt{C/_{kg\cdot m}}\right)$. Data and best-fits given in Fig. 3a.

Model	a		n		ρ	
	full	*limited*	*full*	*limited*	*full*	*limited*
EM	0.16 ± 0.65	4,500 ± 6,200	-0.01 ± 0.17	0.40 ± 0.07	1.02	0.20
EAM	54,000 ± 390	45,000 ± 7,700	0.51 ± 0.01	0.50 ± 0.01	0.02	0.01
BM	44,000 ± 320	38,000 ± 7,500	0.51 ± 0.01	0.50 ± 0.01	0.02	0.01

- 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

[1]M. Dressel, B. Gorshunov *Broad-band optical spectroscopy of low-energy excitations of water molecules confined in nano-cages of beryl crystal lattice* (2016).