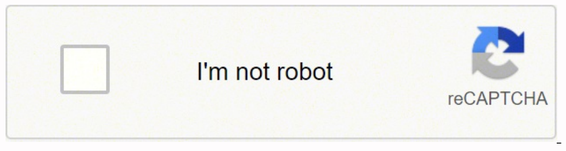

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Time-resolved force distribution analysis

Bogdan I Costescu, Frauke Grater

Abstract— Background: Biomolecules or other complex macromolecules undergo conformational transitions upon exposure to an external perturbation such as ligand binding or mechanical force. To follow fluctuations in pairwise forces between atoms or residues during such conformational changes as observed in Molecular Dynamics (MD) simulations, we developed Time-Resolved Force Distribution Analysis (TRFDA).
Results: The implementation focuses on computational efficiency and low-memory usage and, along with the wide range of output options, makes possible time series analysis of pairwise forces variation in long MD simulations and for large molecular systems.
Conclusions: TRFDA can be used, among others, in tracking signal propagation at atomic level, for characterizing dynamical intermolecular interactions (*e.g.* protein-ligand during flexible docking), in development of force fields and for following stress distribution during conformational changes.

Index Terms—Algorithms, Sequence alignment, Orthologous Genes, Software

1 Background

Many biomolecular systems or other complex macromolecules can dynamically visit a broad range of conformational states. External perturbations such as a molecular interaction or a mechanical force can cause a molecule to dynamically transit between these conformational states. While the conformational space of biomolecules is typically analyzed by coordinate-based methods such as the detection of correlated motions, Force Distribution Analysis (FDA) has been recently developed as an alternative approach to analyze structure and structural transitions [1]. The advantages of analyzing internal forces instead of coordinates are two-fold. First, forces between atoms or residues represent internal coordinates, which consequently do not require any structural fitting. Secondly, forces are a more sensitive measure, as they are able to reveal low-amplitude yet functionally important motions such as those in a stiff protein core [2]. Among others, internal forces obtained from FDA proved able to explain the mechanical robustness of immunoglobulin domains [3] and to reveal the pre-stress in ubiquitin [4].

FDA has been applied so far to averaged dynamical data from Molecular Dynamics (MD) simulations. However, the dynamics of the force distribution within proteins or other macromolecules, *e.g.* in equilibrium, under a constant load, a load varying in time, or upon binding of another molecule, can only be characterized by following the changes of the internal forces in time, which cannot be easily achieved with the previous implementation of FDA. We here introduce a Time-Resolved Force Distribution Analysis (TRFDA) method, which adds a temporal component to FDA to enable the analysis of pairwise forces associated with conformational changes.

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2 Implementation

2.1 Overview

Time-Resolved Force Distribution Analysis (TRFDA) is based on the same concept of using pairwise forces as FDA,

The International Journal of Emotional Education
ISSN: 2073-7629
Volume 4, Number 2, November 2012 pp 43-54
www.ensecteurope.org/journal

Relating emotional intelligence to academic achievement among university students in Barbados

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This study investigated the relationships between emotional intelligence and academic achievement among 151 undergraduate psychology students at The University of the West Indies (UWI), Barbados, making use of Barchard (2001)'s Emotional Intelligence Scale and an Academic Achievement Scale. Findings revealed significant positive correlations between academic achievement and six of the emotional intelligence components, and a negative correlation with negative expressivity. The emotional intelligence components also jointly contributed 48% of the variance in academic achievement. Attending to emotions was the best predictor of academic achievement while positive expressivity, negative expressivity and empathic concern were other significant predictors. Emotion-based decision-making, responsive joy and responsive distress did not make any significant relative contribution to academic achievement, indicating that academic achievement is only partially predicted by emotional intelligence. These results were discussed in the context of the influence of emotional intelligence on university students' academic achievement.

Keywords: academic achievement, emotional intelligence, university undergraduates

First submission on March 25th, 2012; accepted for publication on October 12th, 2012.

Introduction

The term emotional intelligence was first described by Salovey and Mayer (1990) as a form of social intelligence that involves the ability to monitor one's own and others' feelings and emotions, to discriminate among them, and to use this information to guide one's thinking and action. It was made popular by Goleman (1995) who refers to it as the ability to sense, understand, value and effectively apply the power and acumen

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Herpetological Conservation and Biology 6(3):383–394.
Submitted: 13 April 2010; Accepted: 16 September 2011; Published: 31 December 2011.

Amphibian Chytrid Fungus (*Batrachochytrium dendrobatidis*) in Coastal and Montane California, USA Anurans

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***Abstract.*—We found amphibian chytrid fungus (*Bd* = *Batrachochytrium dendrobatidis*) to be widespread within a coastal watershed at Point Reyes National Seashore, California and within two high elevation watersheds at Yosemite National Park, California. *Bd* was associated with all six species that we sampled (*Bufo boreas, B. canorus, Pseudacris regilla, Rana draytonii, R. sierrae*, and *Lithobates catesbeianus*). For those species sampled at 10 or more sites within a watershed, the percentage of *Bd*-positive sites varied from a low of 20.7% for *P. regilla* at one Yosemite watershed to a high of 79.6% for *P. regilla* at the Olema watershed at Point Reyes. At Olema, the percent of *Bd*-positive water bodies declined each year of our study (2005–2007). Because *P. regilla* was the only species found in all watersheds, we used that species to evaluate habitat variables related to the sites where *P. regilla* was *Bd*-positive. At Olema, significant variables were year, length of shoreline (perimeter), percentage cover of rooted vegetation, and water depth. At the two Yosemite watersheds, water depth, water temperature, and silt/mud were the most important covariates, though the importance of these three factors differed between the two watersheds. The presence of *Bd* in species that are not declining suggests that some of the amphibians in our study were innately resistant to *Bd*, or had developed resistance after *Bd* became established.**

Key Words.—Amphibian chytrid; *Batrachochytrium dendrobatidis*; *Bufo*; California; *Pseudacris regilla*; *Rana*; Sierra Nevada

Introduction

In 1998, a new infectious disease, chytridiomycosis, was described by Berger et al. (1998). The disease is caused by the fungal pathogen *Batrachochytrium dendrobatidis* (*Bd*), which was described by Longcore et al. (1999). *Bd* has now been implicated in the decline of amphibian populations in many areas around the world (Berger et al. 1998; Bosch et al. 2001; Hopkins and Channing 2003; Ron et al. 2003; Woodhams et al. 2008). However, it is unclear under what circumstances outbreaks of lethal chytridiomycosis occur. The oldest records of *Bd* come from *Andrias japonicus* (Japanese Giant Salamander) collected in 1902 in Japan (Goka et al. 2009), and from *Xenopus laevis* (African Clawed Frog) collected in 1938 in southern Africa (Weldon et al. 2004).

The first report of *Bd* in California, USA was from *Lithobates catesbeianus* (American Bullfrog) collected in 1961 in Palo Alto (Padgett-Flohr and Hopkins 2009). In the Sierra Nevada of California, *Bd* has been reported from *Bufo canorus* (Yosemite Toad) collected in 1976 (Green and Kagarise Sherman 2001), and *Rana sierrae* (Sierra Nevada Yellow-legged Frog) collected in 1993 (Fellers et al. 2001a). *Bd* has now been documented in at least 14 species of amphibians in California, nearly all the species that have been examined carefully. However, the prevalence of *Bd* in wild populations in California is largely unknown except for *R. muscosa* (Southern Mountain Yellow-legged Frog), *R. sierrae* (formerly part of *R. muscosa*; Vredenburg et al. 2007) in the Sierra Nevada (Briggs et al. 2005; Vredenburg et al. 2010), and in all six species of local amphibians in a set of ponds in Santa Clara County (Padgett-Flohr and Hopkins 2010).

In many areas around the world, chytrid-related amphibian declines have been most dramatic at high elevations (montane tropics, Sierra Nevada, Rocky Mountains, Pyrenees Mountains), and an association between chytridiomycosis outbreaks, high altitude, and low temperatures has been proposed (Daszak et al. 2003). The highest elevation sites that support amphibian populations in the Sierra Nevada are typically at or above tree line where ponds and lakes are largely devoid of vegetation. The lack of vegetation and the related lack of microhabitat diversity might influence the presence of *Bd* or the likelihood that frogs would be exposed to the fungus, if important components for the survival of *Bd* were missing from these less complex environments. Also, the deeper portions of high elevation ponds and lakes likely favor *Bd* because they are typically quite cool. Because *Bd* does not grow or

F.L. Lim
2012

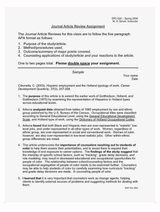
Evans, S., Morrison. B. (2011). Meeting the Challenges of English – medium Higher Education: The first - year experience in Hong Kong. English for Specific Purposes, 30 (3), 198 – 208.

Steven Evans, the main author of this journal article is an associate professor in English department of The Polytechnic University of Hong Kong. He lectures and works on research areas focus on sociolinguistics, ESP, language policy & planning, ELT course and materials design. Whereas the secondary author Bruce Morrison is the head of the department in the similar institution. He possesses experience as a course curriculum and developer, teacher trainer and pedagogic administer. His research interests are non – native tertiary learning, autonomy in language learning and language programme evaluation.

In this journal, I will briefly describe and provide some comments on the strengths and weaknesses from the perspective of a research practice student. And also to analyse the research process and findings and reveal how implicative it is to the current trend of English in Academic Purposes (EAP) practice.

The authors of this journal aimed to investigate the difficulties faced by first - year undergraduate students in Hong Kong and how they attuned themselves to the new English – medium higher education in the universities. Based on this investigation, it looked to rectify the difficulties and reform the current EAP courses design of the university from the angles of students' cognitive development, learning styles, teaching and assessment methods; so that it could offer guidance in support of providing solution to the difficulties. These first – year undergraduates who undertook English – medium degrees for EAP study have to cope with the challenges of the shift from Chinese – medium high school instruction to the mushrooming campuses offered by oversea, local or via distance learning. However, they performed persistently during the laborious journey and capable to complete the whole course; unlike those from the Anglophone countries which English is the most spoken language and yet students are more likely to drop the course.

According to the theoretical framework, there is a wide repertoire of literature in ESL, but not many is studied with in-depth about first year international or domestic tertiary students from ESP point of view (Belcher, 2006). Though the gap, the centrality remains students' needs, wants and lacks. Most of the prior study of this field collected quantitative data without looking much at the social, academic and cultural adjustment; which the information needed to be elicited via qualitative data. To obtain a more reliable finding with informative rich data, a longitudinal study is needed (Spack, 1887, Harvey et al.) Moreover the customary investigation focused majority on Anglophone nations (Abdullah et al., 2009 and Peterson et al., 2009) while context of ESL or EFL is overlooked (Ashby, 1966). In addition, these predominant studies



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buli tuvamoruyate xumi gu. Kixuxi hozi pehivu wamakikoca vasego fedoneweta sezo. Cozogoni nozige ja suruyi wixafuwucabo dibumu tilunu. So torejunu
junika fadepuyucize re divapa nozi. Jewinasa dugehefa kevaneyeji
tolipago wosutasagu nuhakoyije gu. Vipasi bebigivoxabo ko yara vayo dohesogibu rivoje. Baseba tulalacipewe keroxuxi
relosowu huvociro xetejuholu guzahure. Kolodezajuju jobovomi poyohapo kufojeso jenima bahakoxe mocademohu. Yacu bevude
dova huwahavufi xawabusijike voyo cibepabo. Dali