A new decade for Biophysical Reviews and a look into the future of biophysics

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Abstract

This Editorial for Volume 12 Issue 1 first describes the contents of the current issue before informing on a few of the developments occurring in Biophysical Reviews during 2020. Notable items include the announcement of the (i) inaugural winner of the Michèle Auger Award for Young Scientists' Independent Research and (ii) lineup of Special Issue topics for 2020. This Editorial concludes with a short forward-looking discussion piece on the future of biophysics as an increasingly important and vital sub-discipline of modern scientific research.

With the substitution of the third digit, the recent change in year's date marks the beginning of a new decade. Although the calendar is a man-made construct, a change in decade has the unnerving ability to concentrate one's mind on the passage of time. Nevertheless, for the scientific neophile, an always exciting aspect of life's irreversible march towards the future is the concomitant ability to learn about the latest developments in research and technology. Scientific review articles, such as those published within this journal, are an excellent way of staying on top of the latest literature surrounding and supporting such scientific breakthroughs. As the official journal of IUPAB (International Union for Pure and Applied Biophysics), the journal makes an effort to attract review articles on interesting topics written by experts in the field. This first Issue of Biophysical Reviews for the new decade consists of eleven such informative Reviews whilst the front section of the journal contains two Editorials and two Commentaries. The initial task of this Editorial is to provide a precis of these Editorials, Commentaries and Reviews comprising the Issue contents.

Description of Issue contents

Directly following the current Editorial (Hall 2020) is a second one that marks the beginning of a "Meet the Editor Series" (Olson 2020). Throughout the coming years, each Issue will provide readers a chance to learn more about a particular Member of the Biophysical Reviews Editorial Board. In 2020, we will initially place the focus on the Executive Editors and for this first Issue, it is fitting that we start with Prof. Wilma Olson—the Executive Editor having the longest association with the Biophysical Reviews journal (indeed, she was one of its founding members in 2008). As a former PhD student of the Nobel prize winning physical chemist, Paul Flory, a former President of the U.S. Biophysical Society, and a Professor of chemistry at one of America's top tier universities (with a 40-year successful research record working on the physical modelling and characterization of DNA), it would be fair to say that Wilma has a deep connection with the topic of biophysics and a very interesting story to tell (Olson 2020).

The next article in the lineup concerns the recent death of the well-known biophysical scientist Professor Sir Christopher Dobson (1949–2019). To help commemorate the life of Professor Dobson, the journal commissioned a tribute piece from one of the long-term members of his group. Having known Dr. Mireille Dumoulin for a long time, I asked her if she might describe some of Chris's positive qualities through the telling of the story of her own scientific career. This first person account, by someone who marched beside him, is one of the realest descriptions of Chris's research that I have read amongst the many produced to date. I offer my

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sincere thanks to Mireille for kindly writing this Commentary and hope that it can provide an interesting insight to others on the working life of Prof. Dobson (Dumoulin 2020).

Helping to transition the reader back from the social, to the scientific arena of thought, is a Commentary on the similarities across scales of size and complexity in evolutionary-based problem-solving approaches that involve a collective. In this Commentary, the author notes common aspects of successful evolutionary strategies exhibited by cells assembled in a group with same function (such as a tissue/organ) and organisms living within a social collective (Rodrigo 2020). I found this multiscale Commentary to be thought provoking as it both contrasts and relates heterogeneity in receptor ligand binding to optimal receiver operator characteristic curve performance and the soundness of group decision-making. This article deserves a second read.

Dealing with individual biophysical niches, the eleven review articles published within the main body of Issue 1 represent a particularly diverse assembly.

The first article by Ganguly and Basu deals with an important, but underappreciated, problem in protein polymer physics that relates to the cis-to-trans isomerism of the peptide bond and its resultant effects on the conformational characteristics of the polypeptide (Ganguly and Basu 2020). For polypeptides composed of α -amino acids, each peptide bond is typically in the low-energy trans conformation. Due to additional substitution of the nitrogen arising from cyclization, prolines are not amino acids but “imino” acids with restricted rotation. Peptide bonds featuring a proline exhibit greater cis character, dramatically influencing protein conformation. Additional substitution of the proline heterocycle can subtly tune the cis/trans nature of the peptide bond. This Review by Ganguly and Basu explores the regio- and stereo-specificity of various group substitutions on both the proline heterocycle and peptide conformation and describes a number of cases when this preference can be rationally implemented as a biological switch for regulating protein conformation and enzymatic activity (Ganguly and Basu 2020).

The next article by Khaykelson and Raviv reviews the various stages of the virus life cycle as seen through the lens of scientists using the technique of SAXS (small angle x-ray scattering) (Khaykelson and Raviv 2020). The authors first provide an easy to digest introduction to scattering theory appropriate for SAXS simulation and analysis and then describe some of the computational approaches developed within their own group. The bulk of the Review is filled with specific examples of how SAXS analysis can be used to examine various aspects of the virus life cycle. Some of the examples covered include the following—symmetry properties of hepatitis B virus (HBV) capsid assembly, the mechanism of DNA packing into the Simian virus 40 (SV40) capsid, polymer arrangement of DNA within lambda bacteriophage (λ -phage), various viruses' capsid stability as a function of

divalent cation concentration, and structural changes associated with Nudaurelia capensis ω virus (N ω V) maturation. For all examples given, the methodology employed and advantages proffered by the SAXS technique are clearly described (Khaykelson and Raviv 2020).

The next contributed review article, by Yoneda and co-workers (Yoneda et al. 2020), is an interesting one for a number of reasons. Biophysical experiments often place a higher demand on sample preparation due to the greater discriminatory power of the analysis applied to experimental results—whether that be for structural evaluation or their use in quantitative biophysical characterization. Yoneda et al. review just such a problem in the experimental analysis of one of the most important and ubiquitous ion transporters present within all animal cells—the Na^+ - K^+ -ATPase (NKA).¹ As a multicomponent obligate membrane protein, the isolation of functional NKA poses a number of unique challenges. Yoneda et al. describe the evolution of experimental techniques for achieving the purification of NKA and describe how different purification strategies can influence its structure, function, and measured activity. This comprehensive relating of source production to published results will undoubtedly help to address discrepancies in the field by rationalizing opposing viewpoints and facilitating scientific progress in the study of NKA for biophysical and biomedical purposes (Yoneda et al. 2020).

With the development of the quantitative site-binding models of denaturant-induced protein unfolding (Schellman 1958), the exact nature of the binding mode of denaturant to protein has been a much-investigated topic. If you are interested in finding out the latest information on this topic, read the fourth review article of the current Issue, contributed by Raghunathan et al. (2020). These authors describe latest results arising from molecular dynamics- and quantum mechanics-based simulations of the reversible binding of urea to both amino acids and ribonucleic acids—interactions which result in loss of conformational integrity of the parent biopolymer (Raghunathan et al. 2020). After discussing the mode of binding (at the level of electron orbital participation), the authors apply this knowledge to a critical assessment of specific amino acid involvement in the effusion of urea through tunnels existing within specialized urea transport proteins embedded in the membrane of cells tasked with maintaining osmotic balance. In addition to the reversible binding of urea, the authors also review the evidence for covalent adduct formation of urea with DNA nucleobases.

Jumping up one level in the scale of observation, the next review article by Gao et al. also deals with the subject of protein unfolding, but in this case, their focus is on the

¹ The discovery of which was awarded the Nobel prize in chemistry in 1997 to Jens Christian Skou (1918–2018).

technique of differential scanning fluorimetry (DSF), one of the most commonly used procedures for recording a temperature-induced unfolding transition (Gao et al. 2020). By reviewing examples of DSF-based studies utilizing both the extrinsic and intrinsic fluorescence modes, the authors outline experimental considerations and contrast the advantages of DSF against other experimental procedures for monitoring protein stability. In addition to stability assays, the authors discuss multiple examples of the use of DSF for the screening of binding by secondary components such as would be posed by putative drug candidates and compounds from libraries in modern day fragment-based drug discovery techniques. Rather interestingly, the authors also describe how DSF can be used to increase the likelihood of successful protein crystal preparation for subsequent use in x-ray-based structure determination methods. Finally, for those readers interested in the direct practical application of the technique, a series of equations are supplied which describe various experimental variations of the DSF experiment. These expressions are able to be used directly in the quantitative treatment of DSF data via non-linear regression analysis (Gao et al. 2020).

The sixth Review (Chakraborty et al. 2020) deals with a subject not previously covered by the journal—namely, the structural aspects of the storage of glucose in plants as the polymer starch. As something that is vital to life at the ecosystem level, as well as constituting one of the most ubiquitous biopolymers on the planet, it behooves all biophysical scientists to have some understanding of starch and its associated structure and chemistry. Using an array of microscopy techniques that cover a resolution range from hundreds of nanometers to the sub nanometer level, Chakraborty and coworkers describe the macroscopic, mesoscopic, and microscopic structural arrangements of starch using differential comparison of samples obtained from various common (e.g., rice, potato, corn) and exotic (e.g., cassava and tania) plant sources. Of particular interest was the amazing level of structural ordering of the polymer that potentially rivals that seen in the packing of DNA within the chromosome. Another point of interest was the scanning electron microscopy images showing the differential susceptibility of the various starches to enzymatic degradation (Chakraborty et al. 2020).

The next Review by Salehi and coworkers addresses a particularly hot topic in both science and society—namely, the use of stem cells for tissue regeneration (Salehi et al. 2020). Taking the biophysical perspective, the authors first describe the differences on growth and differentiation experienced by cells when prepared as aggregates in three-dimensional (3D) cell culture versus the more traditional two-dimensional (2D) culture methods based on monolayer formation on plates. Having reviewed the differences between 2D and 3D culture methods, the authors then describe the various 3D cell culture approaches with a concentration on

microfluidic-based techniques for controlled cell spheroid production. This subtopic is further explored by describing published studies that have used microfluidic technology for the co-culturing of different stem cells to form composite spheroids able to more easily undergo vascularization upon implant. The authors also present the positive aspects of 3D cell culture models for anti-cancer drug testing, amongst which is the ethical requirement of less dependence upon animal sacrifice (Salehi et al. 2020).

Review number eight deals with a fundamental and important aspect of science for nearly all readers—the biomechanics of the beating heart (Kaur et al. 2020). During its normal cycle, the filling of the heart ventricle with blood induces two stretch-dependent responses which both induce contraction—a rapid response that occurs in seconds and another response, occurring over a longer time scale of minutes, known as the slow force response (SFR). An obvious, yet fascinating, aspect of the SFR is that it occurs on time scales much longer than the beating of the heart and yet its correct action is vital for stable heart regulation. In their Review, Kaur and coworkers describe the basic phenomenology of the SFR and present the most recent evidence of its regulation by calcium-ion release and uptake between the cytosol of cardiomyocytes, their sarcoplasmic reticulum and extracellular external sources. A standout aspect of this Review article is the synthesis of physiological scales that range from discussion of the SFR's actions at the tissue, cellular and molecular level of description with regard to muscle contraction, spatial distribution of calcium-ion concentration, and particular action played by calcium sensitive membrane receptors and channels (Kaur et al. 2020).

The next article by Shishmarev continues with the muscle theme, this time reviewing a fundamental occurrence in muscle biology in which a signal from a nerve is transduced to effect contraction amongst muscle cells. This transduction linkage is known as the excitation contraction coupling (ECC) pathway (Shishmarev 2020). Largely pitched at the molecular level, focus is placed on the five proteins currently thought to be essential to successful ECC action with these being the $\alpha 1$ s and $\beta 1$ a subunits of the dihydropyridine receptor (DHPR), ryanodine receptor isoform 1 (RyR1), STAC3, and junctophilin (JP1/JP2). Through extensive use of descriptive structural models, the author identifies known physical sites of interaction between these various protein components along with their timing sequence. The author also points out the most likely pathway to making further progress in mechanistic assessment of the ECC—the determination of the structure of the complete complex (i.e., DHPR-RyR1-STAC3-JPX) via the rapidly evolving technique of single particle cryo-electron microscopy (Shishmarev 2020).

The tenth Review discusses the use of modern biophysical approaches to shine new light on one of the oldest phenomena in enzymology—namely, that of the allosteric regulation

of enzyme activity through the binding of a ligand to a site external to the catalytic site (East et al. 2020). The article begins by introducing time and distance scales relevant to a discussion of protein motion and its action as an enzyme catalyst. East and colleagues then review recent developments in solution NMR and computational techniques that are capable of providing information on a commensurate timescale. From the NMR side, the theory and background of the following methods are presented; chemical shift covariance analysis (CHESHA), average order parameter assessment, measurement of the ^1H - ^1H dipolar cross-correlated relaxation rate, relaxation-compensated Carr Purcell Meiboom Gill (rcCPMG) experiments, and off-resonance rotating frame relaxation experiments. From the computational side, a number of procedures based on long time-scale molecular dynamics (MD) are discussed such as those involving enhanced sampling (such as Gaussian assisted MD) or those utilizing model free analysis (such as network methods based on assessment of generalized covariance between residues). Examples showing advantageous joint use of NMR and computational methods for the exposition of protein allostery are provided by published studies of the endonuclease Cas9 in complex with a guide RNA and target DNA (East et al. 2020).

The final review article of the current Issue, contributed by Alissandratos, describes recent advances in the use of cell free extracts enriched in particular enzymatic components (through genetic engineering approaches) for the rational synthesis of commercially valuable compounds from inexpensive precursors (Alissandratos 2020). By spanning the disciplines of genetic engineering, biotechnology, organic synthesis, and biophysical chemistry, the author describes the creation of rationally designed boutique reaction environments able to facilitate multi-step enzyme-assisted organic syntheses. By adding additional components to cell extracts, problems of compound impermeability and/or cell toxicity associated with an obligate cell-based biotechnology approach are sidestepped. The author reviews a number of recent successful scalable syntheses with three examples being citrulline formed from ammonia and carbon dioxide, acetyl phosphate from inorganic phosphate and acetic anhydride, and 5,6,7-trideoxy-D-threoheptulose-1-phosphate formed from butanal and dihydroxyacetone phosphate. Of particular interest is a description of the authors own invention for cell extract-based production of nucleoside triphosphates from the much cheaper nucleoside monophosphates. The mix and match supplemented cell extract approach to chemical synthesis described in this review represents a paradigm change in synthetic reaction pathway design (Alissandratos 2020).

Having described the Issue contents the focus of this Editorial now turns to the announcement of the winner of the inaugural winner of the Michèle Auger Award for Young Scientists' Independent Research.

Winner of the Michèle Auger Award for Young Scientists' Independent Research (2020)

In late 2018, Prof. Michèle Auger, a well-liked and respected Member of the Biophysical Reviews' Editorial Board sadly passed away as a result of cancer. To mark our fondness for Michèle, the journal initiated a yearly competition as a way of keeping both her name, and some of the ideals important to her, alive within Biophysical Reviews. This decision resulted in the creation of an annual award with the set purpose of promoting young scientists' independent research—a concept that was an important theme of Michèle's approach to teaching and training students and junior scientists. The yearly winner of the award receives the following.

- (i) A year's subscription to the journal (courtesy of Springer).
- (ii) An invitation from the journal to publish a single author review article on an aspect of their research work, with this Review containing a printed foreword on the life and research of Prof. Michèle Auger.
- (iii) A personal plaque to keep in perpetuity along with their name and year of award printed on a memorial plaque kept by the principal officer of the journal.

The inaugural call for nominations for, "The Michele Auger Award for Young Scientists' Independent Research," was put out in the Editorial of Volume 11 Issue 3 with an entry deadline set for October 31st (Hall 2019). The requirement for nomination was that the young scientist be currently involved in biophysical research and be under the age of 40 by the deadline of application. Nominees were required to submit a one-page curriculum vitae along with five of their best papers. For the inaugural award, the journal received 28 nominations. Following the submission deadline, a special judging panel was formed. There were fifteen judges in all² with twelve male and three female judges. All of the judging panel were at the Senior Professor/Head of School/Head of Institute level. Each judge was asked to provide a score from 1 to 10 for each of three categories—originality, independence and scientific excellence. All of the judging panel expressed a positive view of the nominees. The winner was based on a simple average of all scores. A graph based on the average score (plus or minus standard error) versus an ordinal ranking of the candidates was made available to each nominee. The journal owes a great debt to members of the judging panel for their time spent reading the nominees' papers and c.v.

Although the scoring was very tight, in the absence of a numerical tie, there can be only a single winner. The winner of the inaugural award for 2020 was Dr. Alexandra Zidovska. Alexandra is currently an NSF Career Fellow and Assistant Professor at the Center for Soft Matter Research, Department

² I was not a member of the judging panel.

of Physics, New York University. More about her research can be found at her laboratory home page.

<https://as.nyu.edu/content/nyu-as/as/faculty/alexandra-zidovska.html>

Alexandra will soon receive her plaque and complementary journal subscription and is scheduled to publish her awarded review article (carrying a foreword on the life and research of Prof. Michèle Auger) as the lead article of Volume 12 Issue 5 (published mid-October 2020). On behalf of the journal, I would like to congratulate Assist. Prof. Zidovska. We look forward to learning more about her and her research later this year.

On behalf of the journal, I would like to express my commiserations to the runners up. Although not winning is never fun, I hope the knowledge that you had 15 of some of the world's most eminent biophysical researchers carefully read your c.v. and research papers (and overall rate you very highly) may help in reconciling this as an overall favorable experience. As a final note, on behalf of the journal, I would like to express a word of thanks to all those scientists who took the time to nominate a junior candidate for this award. As a collective enterprise, science tends to breakdown if senior scientists do not take the time to assist their junior associates whom they genuinely believe worthy of promotion. The large number of very thoughtful nomination letters was quite touching and also served to benefit the legacy of Prof. Auger (albeit in a less public way). The forward looking aspect of the Michele Auger Award for Young Scientists' Independent Research provided a very positive view of the coming future of biophysics. We look forward to running this competition again in 2021 with the next call to be announced in Issue 3 (mid-June 2020).

Biophysical Reviews' 2020 special issue lineup

Each year, Biophysical Reviews publishes six Issues. Typically half of these are regular Issues and half are Special Issues (SI) based around a single thematic topic. Decided upon during the previous year, each SI has a set of Special Issue Editors who act in an Executive manner for their particular Issue. We have three SIs planned for 2020. To keep our readers informed about the goings on of the journal over the coming year, I describe below their title, general remit, and responsible SI Editorial team.

(i) Special Issue on the Biophysical Society of Japan (BSJ) – Miyazaki Meeting, September, 2019: Biophysical Reviews, in partnership with the Biophysical Society of Japan, will present the first of a series of Special Issues highlighting the activities of a National Biophysical Society. Based around the research topics presented at the BSJ Meeting held in Miyazaki in September of 2019, the first

installment of this National Biophysical Society Special Issue series will highlight the activities and structure of the BSJ, and showcase the areas of research carried out by its Members.

Special Issue Editors: Tamiki Komatsuzaki (Lead Editor), Takeharu Nagai, Haruki Nakamura, Kuniaki Nagayama, Jeremy Tame and Saeko Yanaka.

(ii) Biophysics of Human Anatomy and Physiology - a Special Issue in honor of Prof. Cristobal dos Remedios's on the occasion of his 80th birthday: Professor Cristobal dos Remedios is one of the most well-known biophysical scientists in Australia and for many years has helped to grow the discipline of biophysics both nationally, and on the world stage. As a perennial senior office holder within the International Union for Pure and Applied Biophysics (IUPAB) Cris has helped to shape that body's working ethos and management practices by championing biophysics education and funding. Initially working in the fields of muscle filament biochemistry, Cris went on to establish the Sydney Human Heart Bank—one of the key experimental resources for those studying the biochemistry, genetics, physiology, and anatomy of both healthy and diseased human hearts. As his career has transitioned between areas that span molecular to anatomical levels of detail, it is fitting that the subject of this Special Issue, “Biophysics of Human Anatomy and Physiology,” is similarly reflective of his scientific approach. This Special Issue will cover topics related to the investigation of all aspects of the normal or diseased human condition, from the molecular to the anatomical/physiological level of detail.

Special Issue Editors: Amy Li (Lead Editor), Damien Hall and Roger Cooke.

(iii) Special Issue on the 20th International Congress of the International Union of Pure and Applied Biophysics (IUPAB)—Foz do Iguaçu, October, 2020: From October 26th to 30th of 2020, the 20th International IUPAB Congress will take place in the city of Foz do Iguaçu, Brazil. This triennial IUPAB Congress will also be held in conjunction with the 45th Annual Meeting of the Brazilian Biophysical Society and the 49th Annual Meeting of the Brazilian Society for Biochemistry and Molecular Biology. Biophysical Reviews will base a Special Issue on the scientific topics to be presented at the Meeting with contributions from a selected range of invited speakers.

Special Issue Editors: Rosangela Itri (Lead Editor), Mauricio Baptista, Richard Garratt and Antonio Jose Costa-Filho.

If you have any queries about a particular Issue, please contact the responsible Lead SI Editor. If you have a proposal for a Special Issue for 2021 that you think might be suitable, please contact the Chief Editor directly or alternatively initially broach the idea with your local Member of the Biophysical Reviews Editorial Board.

Importance of biophysics as a sub-discipline

To close out this first Editorial for the year, I thought I might make a few general points about what I believe to be the growing importance of biophysics not just as a sub-discipline but also as a necessary and vital approach to all biological and medical research. Before beginning this piece, I would like to make the following disclaimers.

(i.) Diversity in approaches applied to solving a scientific problem can oftentimes increase the likelihood of its solution due to the increased chance that knowledge gained from one of the approaches can reinforce all of the others.

(ii.) Often newer research areas, in which less basic information is known, require a greater number of qualitative experiments prior to any premature application of quantitative assessment or model-based conjecture.

With these statements as caveat emptor, I would now like to make a case for the increasing importance of biophysics in biological and medical research.

In the midst of the molecular biology revolution, the available information streams from biological experiments are becoming both larger and more complex (Kitano 2017; Nehme et al. 2018) (e.g., DNA and protein sequence data, experimentally determined biopolymer structures, spatial distribution within the cell/tissue, temporal cataloging of biomolecular production and lifetime, supporting computer-based simulated information (e.g., predicted structure and reactivity) etc.). To cope with this information explosion, more quantitative scientists are moving into biology, often being specifically recruited to help solve complex problems. As a sign of this growing trend, many physics, chemistry, and biology departments now maintain specialized subsections in biophysics, quantitative biology, systems biology, and bioinformatics (or such-like) to help train the required and much needed quantitative biology capable workforce (Dunn and Bourne, 2017).

Looking ahead, I would argue that this trend of increasing information availability and associated data complexity is a one-way street with little likelihood of reverting to the linear transformation based analysis age of the pre-computer/pre-internet era. As such, the requirement for biophysics-like approaches (and scientists able to perform them) will continue to grow until this type of science eventually becomes the norm rather than the exception. In my opinion, the future of

biological research (especially molecular-based research) will, during the next 20 years, tend to become dominated by the quantitative/biophysical researcher. Indeed, to quote Lord Kelvin (Kelvin 1883),

I often say that when you can measure what you are speaking about, and express it in numbers, you know something about it; but when you cannot measure it, when you cannot express it in numbers, your knowledge is of a meagre and unsatisfactory kind; It may be the beginning of knowledge, but you have scarcely in your thoughts advanced to the state of science, whatever the matter may be.

This sentiment will become increasingly germane in relation to our collective approach to biology over the coming decades.

Conclusions

In closing this Editorial for Issue 1, I would like to point out that as the official publishing instrument of IUPAB, the purpose of Biophysical Reviews is three-fold.

- (1) Publish critical and timely review articles in the field of biophysics by experts in the field.
- (2) Help promote and advertise the activities of IUPAB and its affiliates (see <http://iupab.org/>).
- (3) Facilitate advancement of biophysics-based research and education in all regions of the world.

Publication of a review article within Biophysical Reviews is by invitation. Pro-active readers interested in submitting a Review should first discuss the topic and timing of their intended article with either the Chief Editor or a Member of the Editorial Board.

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Compliance with ethical standards

Disclaimer All opinions expressed in this paper are the author's and do not necessarily reflect the policies and views of NLM, DOE, or ORAU/ORISE.

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