The maturation of computational work and its place within the scope of *JGP*

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As the summer nears its peak, we welcome a new Associate Editor to *JGP*, José Faraldo-Gómez. As you may read in his biography (http://www.faraldolab .org), José's research aims to rationalize how the mechanisms of membrane proteins emerge from their structure, dynamics, and interplay with substrates and environment. The appointment of José as an Associate Editor will bring expertise to our weekly editorial meetings in the application of computational methods to biological problems. Slowly but surely, such methods have become mainstream in many of the research areas that interest our authors and readers. To a large degree, this trend reflects the increasing ability of computational researchers to contribute unique mechanistic insights. However, we must also acknowledge that it has been challenging for our community to ensure that the best standards of quality and significance are consistently applied, probably because these kinds of methods remain fairly esoteric for the majority of us. With José's appointment, we bolster our embracement of computational work in *JGP*, either as standalone articles or in conjunction with experimental work, while also affirming our commitment to a rigorous review involving the foremost experts.

The historical strength of *JGP* in kinetics makes this evolution a natural step. Indeed, ion channels were the first type of protein for which single-molecule kinetic data could be obtained. Mathematical models based on such kinetic measurements proved enormously useful, not only to begin to dissect complex structural mechanisms, but also as a means to quantitate, synthesize, and compare experimental observations. A similarly strong tradition exists among physiologists working on complex processes at the organelle, cellular, tissue, and organismal level. While we intend to continue to foster that tradition of mathematical and theoretical modeling of systems, we also seek to broaden our scope. Three areas of particular interest are molecular simulation, i.e., computations aimed at characterizing the structural dynamics and energetics of systems of molecules; structural modeling, i.e., computations designed to predict unknown molecular and macromolecular structures as well as modes of recognition; and bioinformatics, i.e., meta-analyses of functional, structural, and/or sequence-level data.
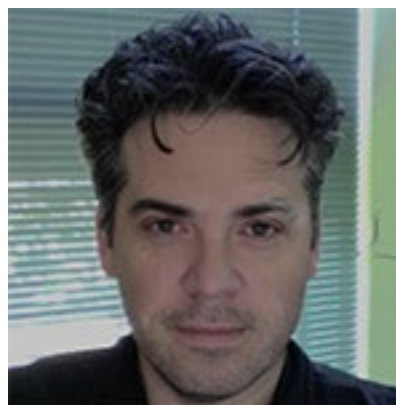

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Needless to say, we will strive to publish only computational work that meets the highest standards of quality, as we do for experimental work. We will value studies that are both systematic and quantitative, as opposed to anecdotal and largely descriptive, and that are based on methodologies whose precision and accuracy are commensurate to the question at hand. Computational articles need not include experimental work, but they ought to integrate or be framed in the context of existing empirical evidence and ideally outline verifiable hypotheses or help design new experiments. And above all, we expect significant mechanistic insights.

The famed statistician George Box once stated, "All models are wrong but some are useful" (Box, 1979). Elaborating on this point, he argued that it is of no interest to ask "Is the model true?" but rather "Is the model illuminating and useful" and is it robust and unbiased? We will be asking ourselves the very same questions.

REFERENCES

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