



GREGORY A. BABBITT

Associate Professor

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PROFILE

I am a computational biologist with a focused interest in the development of modern statistical tools for comparative molecular dynamic simulation applied to the function and evolution of proteins and their interactions with other molecules. I am interested in the co-evolution of gene regulatory systems and their biophysical implications for the optimization of the genetic code. I am also broadly interested in the evolution of complex and stochastic processes, across all scales, from the molecular to the ecological.

COMPUTER SKILLS

Python, R, Perl, C, Ruby, HTML/CSS/JS/PHP, Amber MD, UCSF ChimeraX, MEGAX, MATLAB,

EXPERIENCE

ACADEMIA

- **Associate Professor**, 2016-present, *T.H Gosnell School of Life Sciences, Rochester Institute of Technology, Rochester NY*
- **Assistant Professor**, 2011-2016, *T.H Gosnell School of Life Sciences, Rochester Institute of Technology, Rochester NY*
- **Visiting Assistant Professor**, 2010-2011, *Department of Biological and Medical Sciences, Rochester Institute of Technology, Rochester NY*
- **Postdoctoral Research Associate**, 2006 - 2009, *under Dr. Yuseob Kim, Center for Evolutionary Functional Genomics, The Biodesign Institute, Arizona State University, Tempe, AZ*
- **Course Instructor** *University of Florida Biological Sciences Program, 2005-2006*
- **Teaching Assistantship**, *University of Florida Biological Sciences Program, 2000-2006*
- **Research Assistantship**, 1998-2000, *under Dr. Peter Frederick, University of Florida, Department of Wildlife Ecology and Conservation, Gainesville, FL*

PERFORMANCE STATISTICS

- **Thompson Reuters** (Web of Science) - h-index = 9, 262 citations/30 pubs, academic age = 14yr
- **ResearchGate** - RG score = 27 (98% percentile), 5K reads/downloads, 400 citations
- **Google Scholar** - h-index = 13, i10 index = 14, 427 citations

INDUSTRY BACKGROUND

- **Animal keeper and aviculturist**, Columbus Zoological Gardens, Columbus, OH, 1983-1997- care of pachyderms, large cats, giraffe and antelope, and birds.
- **Sub-chair, Ciconiiformes Taxon Advisory Group**, American Zoo and Aquarium Association 1996-2000 - Advised member institutions on husbandry and breeding of tropical storks

EDUCATION

Ph.D. / Biology

University of Florida

M.S. / Ecology

University of Florida

B.A. / Zoology

Ohio Wesleyan
University

Post-Doctoral / Genomics

Biodesign Institute
Arizona State University

PUBLICATIONS – student co-authors are italicized

1. *Rajendran M.* Ferran M.C. **Babbitt G.A.** 2022. Identifying vaccine escape sites via statistical comparisons of short-term molecular dynamics (in review, preprint: <https://www.biorxiv.org/content/10.1101/2021.12.06.471374v2>)
2. **Babbitt G.A.** Fokoue E.P. *Srivastava H.R. Callahan B. Rajendran M.* 2022. Statistical machine learning for comparative protein dynamics with the DROIDS/maxDemon software pipeline. In press. STAR Protocols CELL Press.
3. *Rynkiewicz P.* **Babbitt G.A.** Cui F Hudson A.O. Lynch M.L. 2021. Functional binding dynamics relevant to the evolution of zoonotic spillovers in endemic and emergent *Betacoronavirus* strains. JOURNAL OF BIOMOLECULAR STRUCTURE AND DYNAMICS. DOI: [10.1080/07391102.2021.1953604](https://doi.org/10.1080/07391102.2021.1953604)
4. **Babbitt G.A.** 2021. Information theoretics for the machine learning detection of functionally conserved and coordinated protein dynamics. (in preparation, preprint: <https://www.biorxiv.org/content/10.1101/2020.05.29.089003v4>)
5. *Salmon D.* Babbitt C.W. **Babbitt G.A.** Wilmer C.E. 2021. A framework for modeling fraudulent e-waste recycling. RESOURCES CONSERVATION AND RECYCLING. 171: 105613. Elsevier.
6. Babbitt C.W. **Babbitt G.A.** *Oehman J.* 2021. Behavioral impacts on residential food provisioning, use, and waste during the COVID-19 pandemic. SUSTAINABLE PRODUCTION AND CONSUMPTION. 28: 315-325. Elsevier.
7. **Babbitt G.A.** Lynch M. McCoy. M. Fokoue E.P. Hudson A.O. 2020. Function and evolution of B-Raf loop dynamics relevant to cancer recurrence under drug inhibition. JOURNAL OF BIOMOLECULAR STRUCTURE AND DYNAMICS doi: [10.1080/07391102.2020.1815578](https://doi.org/10.1080/07391102.2020.1815578)
8. *Adams L.E. Rynkiewicz P.* **Babbitt G.A.** *Mortensen J. S. North R.A., Dobson R.C.J. Hudson A.O.* 2020. Comparative Molecular Dynamics Simulations Provide Insight Into Antibiotic Interactions: A Case Study Using the Enzyme L,L-Diaminopimelate Aminotransferase (DapL) FRONTIERS IN MOLECULAR BIOSCIENCES doi: [10.3389/fmolb.2020.00046](https://doi.org/10.3389/fmolb.2020.00046)
9. **Babbitt G.A.** Fokoue E. *Evans J.R. Diller K.I. Adams L.E.* 2020. DROIDS 3.0 - Detection of genetic and drug class variant impact on conserved protein binding dynamics. BIOPHYSICAL JOURNAL 118: 541-551 CELL Press.
10. Ryen E.G. Gaustad G. Babbitt C.W. **Babbitt G.A.** 2018. Ecological foraging models as inspiration for optimized recycling systems in the circular economy. RESOURCES CONSERVATION AND RECYCLING 135: 48-57. Elsevier.
11. **Babbitt G.A.** *Coppola E.E. Mortensen J.S. Adams L.E. Liao J. K.* 2018. DROIDS 1.2 – a GUI-based pipeline for GPU-accelerated comparative protein dynamics. BIOPHYSICAL JOURNAL 114: 1009-1017. CELL Press.
12. **Babbitt G.A.** *Coppola E.E. Mortensen J.S. Ekeren P.X. Viola C. Goldblatt D.* Hudson A.O. 2018. Triplet codon organization optimizes the impact of synonymous mutation on nucleic acid molecular dynamics. JOURNAL OF MOLECULAR EVOLUTION 86:91-102. Springer.
13. **Babbitt G.A.** *Coppola E.E. Alawad M.A.* Hudson A.O. 2016. Can all heritable biology really be reduced to a single dimension? GENE 578(2):162-168. *Note: Altmetric ranks this paper as #62 out of a total of 3831 outputs from this journal (i.e. 98th percentile) and #4 out of 130 papers of similar age.*
14. *Fortin C.H. Schulze K.V.* **Babbitt G.A.** 2015. TRX-LOGOS - a graphical tool to demonstrate DNA information content dependent upon backbone dynamics in addition to base sequence. BMC SOURCE

15. **Babbitt G.A.** Alawad M.A. Schulze K.V. Hudson A.O. 2014. Synonymous codon bias and functional constraint on GC3-related DNA backbone dynamics in the prokaryotic nucleoid. NUCLEIC ACIDS RESEARCH. 42: 10915-10926.
16. Ryen E. Babbitt C.W. Tyler A.C. **Babbitt G.A.** 2014. Community Ecology Perspectives on the Structural and Functional Evolution of Consumer Electronics. JOURNAL OF INDUSTRIAL ECOLOGY 18(5):708-721.
17. **Babbitt G.A.** Hanzlik C.A. Busse K.N. 2013. Observing fluorescent probes in living cells using a low cost LED flashlight retrofitted to a common vintage light microscope. JOURNAL OF MICROBIOLOGY AND BIOLOGY EDUCATION 14(1): 121-124.
18. **Babbitt G.A.** Schulze K.V. 2012. Codons support the maintenance of intrinsic DNA polymer flexibility over evolutionary timescales. GENOME BIOLOGY AND EVOLUTION 4(9):870-881.
19. Trotta V. Cavicchi S. Guerra D. Andersen D.H. **Babbitt G.A.** Kristensen T.N. Pedersen K.S. Loeschcke V. Pertoldi C. 2011. Allometric and non-allometric consequences of inbreeding on *Drosophila melanogaster* wings. BIOLOGICAL JOURNAL OF THE LINNEAN SOCIETY 102:626-634.
20. **Babbitt G.A.** Cotter C.R. 2011. Functional conservation of nucleosome formation selectively biases presumably neutral molecular variation in yeast genomes. GENOME BIOLOGY AND EVOLUTION 3:15-22
21. **Babbitt G.A.** 2011. Chromatin Evolving. *Despite our long familiarity with the chromosome, much about its function and evolution remains a mystery.* AMERICAN SCIENTIST 99(1): 48-55. **(Cover Feature Article)** reprinted in INVESTIGACIÓN Y CIENCIA (Spanish language edition of SCIENTIFIC AMERICAN)
22. **Babbitt G.A.** 2010. Relaxed selection against accidental binding of transcription factors with conserved chromatin contexts. GENE 466: 43-48.
23. **Babbitt G.A.** Tolstorukov M.Y. and Kim Y. 2010.The molecular evolution of nucleosome positioning through sequence-dependent deformation of the DNA polymer. Special issue - current perspective in nucleosome positioning. JOURNAL OF BIOMOLECULAR STRUCTURE AND DYNAMICS 27(6):765-780.
24. Kim Y., Lee J.H., and **Babbitt G.A.** 2010.The enrichment of TATA box and the scarcity of depleted-proximal-nucleosome in the promoters of duplicated yeast genes. JOURNAL OF MOLECULAR EVOLUTION 70(1):69-73.
25. Babbitt C.W., Kahhat R., Williams E. and **Babbitt G.A.**, 2009. Evolution of product lifespan and its role in the environmental assessment and management of products: a case study of personal computers in higher education. ENVIRONMENTAL SCIENCE AND TECHNOLOGY, 43(13): 5106-5112.
26. **Babbitt G.A.** and Kim Y. 2008.Infering natural selection on fine-scale chromatin organization in yeast. MOLECULAR BIOLOGY AND EVOLUTION 25: 1714-1727.
27. **Babbitt G.A.** 2008. How accurate is the phenotype? An analysis of developmental noise in a cotton aphid clone. BMC DEVELOPMENTAL BIOLOGY 8:19 (1-9 pp).
28. **Babbitt G.A.** and Frederick P.C. 2008.Phenology of body mass changes during reproduction in a nomadic, tropical waterbird, the Scarlet Ibis (*Eudocimus ruber*). ZOO BIOLOGY 27:360-370.
29. **Babbitt G.A.** and Frederick P.C. 2007. Selection for bill dimorphism in ibises: an evaluation of hypotheses. WATERBIRDS. 30: 199-206.
30. **Babbitt G.A.** 2006. Inbreeding reduces power law scaling in the distribution of fluctuating asymmetry: an explanation of the basis of developmental instability. HEREDITY 97: 258-268.

31. **Babbitt G.A.**, Kiltie R., and Bolker B. 2006. Are fluctuating asymmetry studies adequately sampled? Implications of a new model for size distribution. *AMERICAN NATURALIST* 167: 230-245.
32. **Babbitt G.A.** 1996. The effect of collection size on reproduction in captive Caribbean flamingos: direct stimulation, social facilitation or random chance? Proceedings of the AZA Western Regional Conference, Denver, CO.
33. **Babbitt G.A.** 1995. Seasonality and captive management of the Marabou Stork. Proceedings of the American Zoo and Aquarium Association Great Lakes Regional Conference, Louisville, KY.
34. Burt E.H., *Chow W.*, **Babbitt G.A.** 1991. The occurrence and demography of mites in Tree Swallow, House Wren and Eastern Bluebird nests. In Bird-Parasite Interactions, J.E. Loye and M. Zuk, Eds. Oxford Ornithology Series, Oxford University Press.

OPEN SOURCE SOFTWARE

DROIDS 2.0 - software suite for comparative protein dynamics GPL3.0 (2018)
 DROIDS 3.0 - software suite for comparative protein dynamics GPL3.0 (2019)
 DROIDS 4.0 - software suite for comparative protein dynamics GPL3.0 (2020)
<http://proteindynamics.net>

PDBmutator – creates structural variants in UCSF Chimera given PDB and alignment file GPL3.0 (2020)
<https://gbabbitt.github.io/PDBmutator>

amberMDgui – a simple GUI interface for Amber Molecular Dynamics simulations GPL3.0 (2020)
<https://gbabbitt.github.io/amberMDgui>

amberENTHALPY – a simple GUI interface for calculating protein-ligand binding enthalpy from Amber Molecular Dynamics simulations GPL3.0 (2020)
<https://gbabbitt.github.io/amberENTHALPY>

AWARDS AND SMALL GRANTS

- Faculty Research Development Grant (FEAD) in 2018 from the College of Science, Rochester Institute of Technology \$5,000
- 2017 Nvidia hardware grant – Nvidia corporation (GTX Titan Xp processor)
- Faculty Research Development Grant (FEAD) in 2015 from the College of Science, Rochester Institute of Technology \$5,000
- Provost's Learning Innovation Grant (FEAD) in 2015 from the Rochester Institute of Technology \$5,000
- Strategic Acceleration of Research for Tenure Track Faculty grant (START) in 2012 from the Office of Sponsored Research Services, Rochester Institute of Technology \$10,000
- Faculty Research Development Grant (FEAD) in 2009 from the College of Science, Rochester Institute of Technology \$3,000
- Best Oral Presentation – Division of Invertebrate Zoology, Society for Integrative and Comparative Biology 2006. Orlando, FL.
- Best Poster – Waterbird Society 1998 meeting in Miami, FL. Runner-up Best Presentation
- Recipient of Student Travel Award to the 1999 meeting of the Waterbird Society in Grado, Italy

COURSES TAUGHT

- Cell and Molecular Biology for Engineers I and II
- Statistics for Bioinformatics
- Computational Statistics and Data Science (graduate)
- Bioinformatics Programming Languages
- Biomimicry for Scientists, Engineers and Artists

- Introduction to Bioinformatics

PROFESSIONAL MEMBERSHIPS AND SERVICE

- Biophysical Society
- Genetics Society of America
- Society of Molecular Biology and Evolution
- Sigma Xi - the Scientific Research Society
- American Society of Naturalists (past)
- The Society for Integrative and Comparative Biology (past)
- American Microscopical Society (past)
- American Zoo and Aquarium Association (past)
- Reviewer for National Science Foundation, National Institutes of Health and many professional journals.

PRESENTATIONS AND INVITED TALKS

Babbitt G.A. 2020. Machine learning-based detection of functionally conserved binding interactions in molecular dynamic simulations. Biophysical Society, San Diego CA USA. (chaired platform session on Molecular Dynamics)

Babbitt G.A. 2019. Machine learning based detection of genetic and drug class variant impact on functionally conserved protein dynamics. Hauptman-Woodward Medical Research Institute, Buffalo, NY USA.

Babbitt G.A. 2019. Machine learning based detection of genetic and drug class variant impact on functionally conserved protein dynamics. Ruder Boskovic Institute, Zagreb, Croatia.

Babbitt G.A. 2020. Machine learning-based detection of functionally conserved binding interactions in molecular dynamic simulations. Biophysical Society, San Diego CA USA.

Babbitt G.A. 2019. Comparative molecular dynamics of the BRAF activation loop reveals a biophysical mechanism of cancer recurrence under drug inhibition. Biophysical Society, Baltimore MD USA.

Babbitt G.A. 2018. Taking the measure of mutation in the light of molecular dynamics. Genetics Society of America, Madison, WI USA

Babbitt G.A. Coppola E.E. Mortensen J.M. 2018. DROIDS 1.0 – a GUI-based pipeline for GPU-accelerated comparative protein dynamics. Biophysical Society, San Francisco, CA USA

Babbitt G.A. Coppola E.E. 2017. Triplet codon organization optimizes the impact of synonymous mutation on nucleic acid molecular dynamics. Society for Molecular Biology and Evolution, Austin, TX USA

Babbitt G.A. Coppola E.E. 2016. GC content evolution through the lens of nucleic acid molecular dynamics. Genetics Society of America, Orlando, FL USA

Babbitt G.A. 2015. GC content evolution in light of macromolecular polymer dynamics. Society for Molecular Biology and Evolution Conference, Vienna Austria

Babbitt G.A. 2015. Visualizing Shannon information content on the DNA backbone. Society for Molecular Biology and Evolution Conference, San Juan Puerto Rico

Babbitt G.A. 2014. Chromatin evolving: is DNA the only relevant molecular target of natural selection? Invited talk. Student organized Molecular Biology Symposium UC Denver Medical Center

Babbitt G.A. 2013. Codon bias and the multiplexing of genetic and structural information in DNA. Session Presentation, Society for Molecular Biology and Evolution Conference, Chicago USA.

Babbitt G.A. 2012. Evolving codes –real and imagined manifestations of the genetic code. GSOLS seminar series

Babbitt G.A. 2011. Dynamic DNA-histone interaction as a common currency for quantifying eukaryotic gene regulatory evolution. Presentation, Biophysical Society Meeting: Dynamic DNA packaging across kingdoms; chromatin and beyond. Asilomar, California

Babbitt G.A. and Kim Y. 2008. Evolution at the gateway to transcription: selective forces maintaining chromatin differences at the core promoter. Session Presentation, Society for Molecular Biology and Evolution Conference, Barcelona, Spain.

Babbitt G.A. and Kim Y. 2007. Inferring natural selection on fine-scale chromatin organization in yeast. Session Presentation, Society for Molecular Biology and Evolution Conference, Halifax, Nova Scotia.

Babbitt G.A. 2007. Stress, stability and size: capturing process variation in the development of multicellular organisms. Session Presentation, Annual Meeting of the Society for Integrative and Comparative Biology, Phoenix, AZ. Abstract only to be published in Integrative and Comparative Biology.

Babbitt G.A. Kiltie R., and Bolker B. 2005. Are fluctuating asymmetry studies adequately sampled? Implications of a new model for size distribution. Session Presentation, Annual Meeting of the Society for Integrative and Comparative Biology, Orlando, FL. Abstract only published in Integrative and Comparative Biology 45(6) 959-959. Awarded best student presentation, Invertebrate Zoology Division.

Babbitt G.A. 2004. Population-level power-law distribution of developmental stability is associated with genetic homogeneity. Poster Presentation, Annual Meeting of the Society for Integrative and Comparative Biology, New Orleans, LA. Abstract only published in Integrative and Comparative Biology 43(6) 940-940.

Babbitt G.A. 2003. Population-level power-law distribution of developmental stability is associated with genetic homogeneity. Poster presentation, Fourth Annual Georgia Tech Conference on Bioinformatics, Atlanta, GA.

Babbitt G.A. 1999. When do male ibises have longer bills than females? The evolution of sexual bill dimorphism within colonial ibis species. Session presentation, Proceedings of the 1999 Waterbird Society, Grado, Italy.

Babbitt G.A. 1998. Mathematical description and analysis of reproductive photocues in captive bird populations. Session Presentation, Proceedings of the 1998 North American Ornithological Conference, St. Louis, MO.

Babbitt G.A. and Frederick P.C. 1998. Does body condition limit the reproduction of captive Scarlet Ibis? Session presentation, Proceedings of the 1998 Colonial Waterbird Society, Miami, FL.

Babbitt G.A. and Frederick P.C. 1998. Why do male Scarlet Ibis have longer bills than females? Poster presentation, Proceedings of the 1998 Colonial Waterbird Society, Miami, FL. Awarded best student poster presentation.