Nathan Andrew Baker

Curriculum Vitae

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Nathan A. Baker, Ph.D. is Director of the Advanced Computing, Mathematics, and Data Division at Pacific Northwest National Laboratory (PNNL) and a Visiting Faculty member in the Division of Applied Mathematics at Brown University. His research focuses on the development of new algorithms and mathematical methods in biophysics, nanotechnology, and informatics. Current projects include new computational methods for modeling solvation in biomolecular systems (`http://www.poissonboltzmann.org/`), mathematical methods for mesoscale materials modeling (`http://www.pnnl.gov/computing/cm4/`), and development of new methods for signature discovery (`http://signatures.pnnl.gov`).

Experience

2016–present **Director**, *Advanced Computing, Mathematics, and Data Division, Pacific Northwest National Laboratory*, Richland, WA.

2015–present **Visiting Professor**, *Division of Applied Mathematics, Brown University*, Providence, RI.

2012–2016 **Laboratory Fellow**, *Computational and Statistical Analytics Division, Pacific Northwest National Laboratory*, Richland, WA.

2013–2015 **Technical Group Manager**, *Applied Statistics and Computational Modeling Group, Pacific Northwest National Laboratory*, Richland, WA.

2010–2012 **Chief Scientist**, *Computational and Statistical Analytics Division, Pacific Northwest National Laboratory*, Richland, WA.

2006–2010 **Associate Professor (tenured)**, *Department of Biochemistry and Molecular Biophysics, Washington University in St Louis*, St Louis, MO.

2002–2006 **Assistant Professor**, *Department of Biochemistry and Molecular Biophysics, Washington University in St Louis*, St Louis, MO.

Education

2001–2002 **Postdoctoral Researcher**, *Department of Chemistry and Biochemistry, University of California San Diego*, La Jolla, CA.

1997–2001 **PhD, Physical Chemistry**, *University of California San Diego*, La Jolla, CA.

1993–1997 **BS, Chemistry**, *University of Iowa*, Iowa City, IA, Honors and highest distinction.

Selected honors and awards

2012 **Fellow**, *American Association for the Advancement of Science*.

2010 **Cancer Biomedical Informatics Grid (caBIG) Connecting Collaborators Award**, *National Cancer Institute*.

2007 **Hewlett-Packard Junior Faculty Excellence Award**, *American Chemical Society*.

2004 **Research Fellowship**, *Alfred P Sloan Foundation*.

Service

Selected extramural service

2014–2017 **Associate Editor**, *Biophysical Journal*, Biophysical Society.

2015–2016 **External Advisory Board Member**, *Visual Analytics for sense-making in Criminal Intelligence analysis (VALCRI) Project*, European Commission.

2014–present **Editorial Board member**, *Scientific Data*, Nature Publishing Group.

2012–2016 **Member**, *Macromolecular Structure and Function D Study Section*, National Institutes of Health.

2015 **Advisory board member**, *Data Management and Analysis Advisory Board*, Novozymes.

2012–2014 **Co-Chair**, *Nanotechnology Databases and Ontologies, US-EU Communities of Research*, OSTP National Nanotechnology Coordinating Office.

2011–2014 **Editor-in-Chief**, *Computational Science and Discovery*, Institute of Physics.

2009–2014 **Chair**, *E56.01 Nanotechnology Subcommittee on Informatics and Terminology*, ASTM.

2013 **Reviewer**, *Progress in Research on Environmental, Health, and Safety Aspects of Engineered Nanomaterials*, National Academy of Sciences.

2010–2013 **Advisory committee member**, *Nanomaterial Registry*, RTI International & National Institutes of Health.

2009–2013 **Working group lead**, *Nanotechnology Working Group, caBIG Integrated Cancer Research Workspace*, National Cancer Institute.

2012 **Panelist**, *National Academies Board on Environmental Studies and Toxicology Research Progress on Environmental, Health, and Safety Aspects of Nanotechnology Workshop*, National Academies of Science.

2012 **Member**, *Program Committee, caBIG Annual Meeting*, National Cancer Institute.

Selected intramural service

2014–present **Chair**, *PNNL Institutional Computing Steering Committee*, Pacific Northwest National Laboratory.

2005–2010 **Director**, *Siteman Center for Cancer Nanotechnology Excellence Biocomputing Core*, Washington University in St Louis.

2007–2010 **Director**, *Computational and Molecular Biophysics graduate program*, Washington University in St Louis.

Selected funding

2012–2017 **PNNL lead**, *Collaboratory on Mathematics for Mesoscopic Modeling of Materials (FWP 63024)*, DOE ASCR.

2004–2017 **PI**, *APBS: Nanoscale biomolecular electrostatics software (R01 GM069702)*, NIH NIGMS.

2012–2016 **co-PI**, *DNA-DNA interactions with atomic detail (R01 GM099450)*, NIH NIGMS.

2011–2014 **co-I**, *Mechanism of oxysterol activation of membrane cholesterol (R01 HL067773)*, NIH NHLBI.

2012–2013 **PI**, *ISA-TAB curation of electrostatic data*, OpenEye Software.

2010–2013 **co-I**, *Characterization/bioinformatics-modeling of nanoparticle-complement interactions (U01 NS073457)*, NIH NINDS.

2009–2013 **co-PI**, *Collaborative research: Geometric flow approach to implicit solvation modeling (R01 GM090208-01)*, NIH NIGMS.

2004–2013 **co-I**, *National Biomedical Computation Resource (P41 RR0860516)*, NIH NCRR.

2008–2011 **DBP PI**, *Cancer Nanotechnology Knowledgebase for Nanoparticle Analysis and Design (U54 HG004028)*, NIH NHGRI.

2008–2011 **PI**, *caBIG Integrative Cancer Research Workspace (GS-35F-0306J)*, NIH NCI subcontract.

2007–2010 **PI**, *caNanoLab Data Submission Support (N01-CN-12400)*, NIH NCI subcontract.

2005–2010 **Core PI**, *The Siteman Cancer Center Nanotechnology Excellence at Washington University Biocomputing Core (U54 CA11934205)*.

2008–2010 **co-I**, *New Inhibitors of Acetylcholinesterase that Block Inactivation by Organophosphates (HDTRA1-08-C-0015)*, DoD DTRA.

Selected publications

Purvine, Emilie, Kyle Monson, Elizabeth Jurrus, Keith Star, and Nathan A Baker (in press). "Energy Minimization of Discrete Protein Titration State Models Using Graph Theory". In: *J Phys Chem B*. URL: http://arxiv.org/abs/1507.07021.

Tolokh, Igor S., Aleksander Drozdetski, Lois Pollack, Nathan A. Baker, and Alexey V. Onufriev (in press). "Multi-shell model of ion-induced nucleic acid condensation". In: *Journal of Chemical Physics*.

Gunner, Marilyn R. and Nathan A. Baker (2016). "Continuum electrostatics approaches to calculating pK_as and E_ms in Proteins". In: *arXiv*. URL: http://arxiv.org/abs/1602.07957.

Yang, Xiu, Huan Lei, Nathan A. Baker, and Guang Lin (2016). "Enhancing sparsity of Hermite polynomial expansions by iterative rotations". In: *Journal of Computational Physics* 307, pp. 94–109. DOI: 10.1016/j.jcp.2015.11.038. URL: http://dx.doi.org/10.1016/j.jcp.2015.11.038.

Dowling, Chase P., Sylvia Johnson, Elizabeth Jurrus, and Nathan A. Baker (2015). "An ISA-Tab specification for protein titration data exchange". In: *arXiv*. URL: http://arxiv.org/abs/1511.06431.

Harper, Bryan, Dennis Thomas, Satish Chikkagoudar, Nathan Baker, Kaizhi Tang, Alejandro Heredia-Langner, Roberto Lins, and Stacey Harper (2015). "Comparative hazard analysis and toxicological modeling of diverse nanomaterials using the embryonic zebrafish (EZ) metric of toxicity". In:

Journal of Nanoparticle Research 17.6, pp. 1–12. DOI: 10.1007/s11051-015-3051-0. URL: http://www.ncbi.nlm.nih.gov/pmc/articles/PMC4454819/.

Lei, Huan, Xiu Yang, Bin Zheng, Guang Lin, and Nathan A Baker (2015). "Constructing Surrogate Models of Complex Systems with Enhanced Sparsity: Quantifying the Influence of Conformational Uncertainty in Biomolecular Solvation". In: *Multiscale Modeling & Simulation* 13, pp. 1327–1353. DOI: 10.1137/140981587. URL: http://arxiv.org/abs/1408.5629.

Pabit, Suzette A., Andrea M. Katz, Igor S. Tolokh, Aleksander Drozdetski, Nathan Baker, Alexey V. Onufriev, and Lois Pollack (2015). "Understanding Nucleic Acid Structural Changes by Comparing Wide-Angle X-ray Scattering (WAXS) Experiments to Molecular Dynamics Simulations". In: *arXiv preprint arXiv:1512.08074*. URL: http://arxiv.org/abs/1512.08074.

Pan, Wenxiao, Michael Daily, and Nathan A Baker (2015). "Numerical calculation of protein-ligand binding rates through solution of the Smoluchowski equation using smoothed particle hydrodynamics". In: *BMC Biophysics* 8.1, p. 7. DOI: 10.1186/s13628-015-0021-y. URL: http://www.biomedcentral.com/2046-1682/8/7/abstract.

Sushko, Maria L, Dennis G Thomas, Suzette A Pabit, Lois Pollack, Alexey V Onufriev, and Nathan A Baker (2015). "The role of correlation and solvation in ion interactions with B-DNA". In: *arXiv*. URL: http://arxiv.org/abs/1506.07951.

Bielska, Agata A, Brett N Olsen, Sarah E Gale, Laurel Mydock-McGrane, Kathiresan Krishnan, Nathan Andrew Baker, Paul H Schlesinger, Douglas F Covey, and Daniel S Ory (2014). "Side-Chain Oxysterols Modulate Cholesterol Accessibility through Membrane Remodeling". In: *Biochemistry* 53.18, pp. 3042–3051. DOI: 10.1021/bi5000096. URL: http://www.ncbi.nlm.nih.gov/pmc/articles/PMC4020583/.

Daily, Michael D, Brett N Olsen, Paul H Schlesinger, Daniel S Ory, and Nathan A Baker (2014). "Improved coarse-grained modeling of cholesterol-containing lipid bilayers". In: *Journal of Chemical Theory and Computation* 10.5, pp. 2137–2150. DOI: 10.1021/ct401028g. URL: http://www.ncbi.nlm.nih.gov/pmc/articles/PMC4044725/.

Gosink, Luke J, Emilie A Hogan, Trenton C Pulsipher, and Nathan A Baker (2014). "Bayesian model aggregation for ensemble-based estimates of protein pKa values". In: *Proteins: Structure, Function, and Bioinformatics* 82.3, pp. 354–363. DOI: 10.1002/prot.24390. URL: http://www.ncbi.nlm.nih.gov/pmc/articles/PMC3946329/.

Pham, Christine TN et al. (2014). "Application of a hemolysis assay for analysis of complement activation by perfluorocarbon nanoparticles". In: *Nanomedicine: Nanotechnology, Biology and Medicine* 10.3, pp. 651–660. DOI: 10.1016/j.nano.2013.10.012. URL: http://www.ncbi.nlm.nih.gov/pmc/articles/PMC3966962/.

Richardson, C et al. (2014). *Materials Frontiers to Empower Quantum Computing*. Technical report. Los Alamos National Laboratory.

Thomas, Dennis G, Satish Chikkagoudar, Alejandro Heredia-Langner, et al. (2014). "Physicochemical signatures of nanoparticle-dependent complement activation". In: *Computational Science & Discov-*

ery 7.1, p. 015003. DOI: 10.1088/1749-4699/7/1/015003. URL: http://www.ncbi.nlm.nih.gov/pmc/articles/PMC4169987/.

Tolokh, Igor S, Suzette A Pabit, Andrea M Katz, Yujie Chen, Aleksander Drozdetski, Nathan Baker, Lois Pollack, and Alexey V Onufriev (2014). "Why double-stranded RNA resists condensation". In: *Nucleic Acids Research* 42.16, pp. 10823–31. DOI: 10.1093/nar/gku756. URL: http://www.ncbi.nlm.nih.gov/pmc/articles/PMC4176364/.

Wei, Guo Wei and Nathan A Baker (2014). "Differential geometry-based solvation and electrolyte transport models for biomolecular modeling: a review". In: *arXiv*. URL: http://arxiv.org/abs/1412.0176.

Baker, Nathan A, Juli D Klemm, Stacey L Harper, Sharon Gaheen, Mervi Heiskanen, Philippe Rocca-Serra, and Susanna-Assunta Sansone (2013). "Standardizing data". In: *Nature Nanotechnology* 8.2, pp. 73–74. DOI: 10.1038/nnano.2013.12. URL: http://www.ncbi.nlm.nih.gov/pmc/articles/PMC4054689/.

Baker, Nathan et al. (2013). "Research towards a systematic signature discovery process". In: *Intelligence and Security Informatics (ISI), 2013 IEEE International Conference on*. IEEE, pp. 301–308. DOI: 10.1109/isi.2013.6578848. URL: http://ieeexplore.ieee.org/lpdocs/epic03/wrapper.htm?arnumber=6578848.

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Daily, Michael D, Jaehun Chun, Alejandro Heredia-Langner, Guowei Wei, and Nathan A Baker (2013). "Origin of parameter degeneracy and molecular shape relationships in geometric-flow calculations of solvation free energies". In: *The Journal of Chemical Physics* 139.20, p. 204108. DOI: 10.1063/1.4832900. URL: http://www.ncbi.nlm.nih.gov/pmc/articles/PMC3862591/.

Harper, Stacey L et al. (2013). "Nanoinformatics workshop report: current resources, community needs and the proposal of a collaborative framework for data sharing and information integration". In: *Computational Science & Discovery* 6.1, p. 014008. DOI: 10.1088/1749-4699/6/1/014008. URL: http://www.ncbi.nlm.nih.gov/pmc/articles/PMC3895330/.

Olsen, Brett N, Agata A Bielska, Tiffany Lee, Michael D Daily, Douglas F Covey, Paul H Schlesinger, Nathan A Baker, and Daniel S Ory (2013). "The structural basis of cholesterol accessibility in membranes". In: *Biophysical Journal* 105.8, pp. 1838–1847. DOI: 10.1016/j.bpj.2013.08.042. URL: http://www.ncbi.nlm.nih.gov/pmc/articles/PMC3797575/.

Thomas, Dennis G, Jaehun Chun, Zhan Chen, Guowei Wei, and Nathan A Baker (2013). "Parameterization of a geometric flow implicit solvation model". In: *Journal of Computational Chemistry* 34.8, pp. 687–695. DOI: 10.1002/jcc.23181. URL: http://www.ncbi.nlm.nih.gov/pmc/articles/PMC3578971/.

Thomas, Dennis G, Sharon Gaheen, et al. (2013). "ISA-TAB-Nano: a specification for sharing nanomaterial research data in spreadsheet-based format". In: *BMC Biotechnology* 13.1, p. 2. DOI: 10.1186/1472-6750-13-2. URL: http://www.ncbi.nlm.nih.gov/pmc/articles/PMC3598649/.

Chen, Zhan, Shan Zhao, Jaehun Chun, Dennis G Thomas, Nathan A Baker, Peter W Bates, and GW Wei (2012). "Variational approach for nonpolar solvation analysis". In: *The Journal of Chemical Physics* 137.8, p. 084101. DOI: 10.1002/jcc.23181. URL: http://www.ncbi.nlm.nih.gov/pmc/articles/PMC3578971/.

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Lee, Sun-Joo, Paul H Schlesinger, Samuel A Wickline, Gregory M Lanza, and Nathan A Baker (2012). "Simulation of fusion-mediated nanoemulsion interactions with model lipid bilayers". In: *Soft Matter* 8.26, pp. 7024–7035. DOI: 10.1039/C2SM25847A. URL: http://www.ncbi.nlm.nih.gov/pmc/articles/PMC3375911/.

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Thomas, Dennis G, Satish Chikkagoudar, Alan R Chappell, Nathan Baker, et al. (2012). "Annotating the structure and components of a nanoparticle formulation using computable string expressions". In: *Bioinformatics and Biomedicine Workshops (BIBMW), 2012 IEEE International Conference on*. IEEE, pp. 889–894. DOI: 10.1109/BIBMW.2012.6470259. URL: http://www.ncbi.nlm.nih.gov/pmc/articles/PMC3922075/.

Alexov, Emil et al. (2011). "Progress in the prediction of pKa values in proteins". In: *Proteins: structure, function, and bioinformatics* 79.12, pp. 3260–3275. DOI: 10.1002/prot.23189. URL: http://www.ncbi.nlm.nih.gov/pmc/articles/PMC3243943/.

Carstensen, Tommy, Damien Farrell, Yong Huang, Nathan A Baker, and Jens Erik Nielsen (2011). "On the development of protein pKa calculation algorithms". In: *Proteins: Structure, Function, and Bioinformatics* 79.12, pp. 3287–3298. DOI: 10.1002/prot.23091. URL: http://www.ncbi.nlm.nih.gov/pmc/articles/PMC3193850/.

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Lee, Sun-Joo, Paul H Schlesinger, Samuel A Wickline, Gregory M Lanza, and Nathan A Baker (2011). "Interaction of melittin peptides with perfluorocarbon nanoemulsion particles". In: *The Journal of Physical Chemistry B* 115.51, pp. 15271–15279. DOI: 10.1021/jp209543c. URL: http://www.ncbi.nlm.nih.gov/pmc/articles/PMC3245340/.

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Thomas, Dennis G, Fred Klaessig, et al. (2011). "Informatics and standards for nanomedicine technology". In: *Wiley Interdisciplinary Reviews: Nanomedicine and Nanobiotechnology* 3, pp. 511–532. DOI: 10.1002/wnan.152. URL: http://www.ncbi.nlm.nih.gov/pmc/articles/PMC3189420/.

Unni, Samir, Yong Huang, Robert M Hanson, Malcolm Tobias, Sriram Krishnan, Wilfred W Li, Jens E Nielsen, and Nathan A Baker (2011). "Web servers and services for electrostatics calculations with APBS and PDB2PQR". In: *Journal of Computational Chemistry* 32.7, pp. 1488–1491. DOI: 10.1002/jcc.21720. URL: http://www.ncbi.nlm.nih.gov/pmc/articles/PMC3062090/.

Callenberg, Keith M, Om P Choudhary, Gabriel L de Forest, David W Gohara, Nathan A Baker, and Michael Grabe (2010). "APBSmem: a graphical interface for electrostatic calculations at the membrane". In: *PloS ONE* 5.9, e12722. DOI: 10.1371/journal.pone.0012722. URL: http://www.ncbi.nlm.nih.gov/pmc/articles/PMC2947494/.

Chen, Zhan, Nathan A Baker, and Guo-Wei Wei (2010). "Differential geometry based solvation model I: Eulerian formulation". In: *Journal of Computational Physics* 229.22, pp. 8231–8258. DOI: 10.1016/j.jcp.2010.06.036. URL: http://www.ncbi.nlm.nih.gov/pmc/articles/PMC2951687/.

Lee, Sun-Joo, Brett Olsen, Paul H Schlesinger, and Nathan A Baker (2010). "Characterization of perfluorooctylbromide-based nanoemulsion particles using atomistic molecular dynamics simulations". In: *The Journal of Physical Chemistry B* 114.31, pp. 10086–10096. DOI: 10.1021/jp103228c. URL: http://www.ncbi.nlm.nih.gov/pmc/articles/PMC2917838/.

Thomas, Dennis G, Rohit V Pappu, and Nathan A Baker (2010). "NanoParticle Ontology for cancer nanotechnology research". In: *Journal of Biomedical Informatics* 44.1, pp. 59–74. DOI: 10.1016/j.jbi.2010.03.001. URL: http://www.ncbi.nlm.nih.gov/pmc/articles/PMC3042056/.

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