

# Dr. Neil Dalchau

## *Curriculum Vitae*

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## RESEARCH SUMMARY

My research uses computational modelling to both understand and improve the design of biological behaviours. Fundamentally, I believe that in future, modelling will drive design decisions across many biotechnology applications, such as biopharmaceutical manufacturing and therapy development, but is currently limited by a lack of quantitative understanding of cellular components. Therefore, my current efforts are focused on developing techniques that can estimate model parameters that represent biophysically interpretable quantities from observational data, and use the resultant models to suggest new experiments. I am also interested in automating these kinds of workflows, leveraging active learning frameworks such as Bayesian optimization. In recent years, I have worked across several sub-domains of biology, including immunology, DNA computing and pattern formation.

## WORK EXPERIENCE

NOVEMBER 2020 – OCTOBER 2021 (FT)

### Microsoft Research Cambridge *Principal Research Manager*

Led the Station B project at MSR Cambridge, directing a team of 5-10 researchers and software engineers. Initiated a project that used Bayesian optimization to automate biological experiment design.

JANUARY 2012 – OCTOBER 2020 (FT)

### Microsoft Research Cambridge *Scientist (Senior, Principal)*

Transition to permanent scientist following successful postdoctoral work. During these years, I published several high-profile articles in DNA computing, computational immunology and synthetic biology. Also started to co-supervise PhD projects with academic groups. Developed scalable machine learning methodologies for dynamical systems modelling in biology, resulting in two patent filings (one now granted in the US).

OCTOBER 2009 – DECEMBER 2011 (FT)

### Microsoft Research Cambridge *Postdoctoral researcher*

My postdoctoral research focused on computational immunology, in particular antigen presentation on class I molecules of the major histocompatibility complex (MHC). I have continued to develop and published several modelling studies on MHC class I throughout my research career.

DECEMBER 2008 – MAY 2009 (FT)

### Department of Engineering, University of Cambridge *Postdoctoral researcher*

My first postdoctoral position was supervised by Glenn Vinnicombe in the Control group, and was aimed at understanding noise suppression in stochastic models of chemical circuits.

## EDUCATION

- 2005 – 2008 **Doctor of Philosophy (PhD)**  
Department of Plant Sciences  
*University of Cambridge, UK*
- 2001 – 2005 **Master of Mathematics (MMath)**  
Department of Mathematics  
*University of Oxford, UK*

## AWARDS

- 2013 **Honourary Senior Research Associate**  
*University College London, UK*
- 2011 **Tansley Medal**  
*New Phytologist*
- 2007 **Treherne Studentship in the Biological Sciences**  
*Downing College, University of Cambridge*
- 2006 **Frank Smart Studentship**  
*Dept. of Plant Sciences, University of Cambridge*

## SELECTED PUBLICATIONS

For a complete list, please see my [Google Scholar profile](#). I have published over 40 peer-reviewed articles, with an H-index of 22.

Szép G, Dalchau N, Csikász-Nagy A (2021). Parameter inference with bifurcation diagrams. *Neural Information Processing Systems 2021, Accepted*.

Grant PK, Szép G, Patange O, Halatek J, Coppard V, Csikász-Nagy A, Haseloff J, Locke JCW, Dalchau N, Phillips A (2020). Interpretation of morphogen gradients by a synthetic bistable circuit. *Nature Communications*, **11**, 5545.

Spaccasassi C, Yordanov B, Phillips A, Dalchau N (2019). Fast enumeration of non-isomorphic chemical reaction networks. *International Conference on Computational Methods in Systems Biology*, 224-247.

Roeder G, Grant PK, Phillips A, Dalchau N, Meeds E (2019). Efficient Amortised Bayesian Inference for Hierarchical and Nonlinear Dynamical Systems. *International Conference on Machine Learning 2019*, 4445-4455.

Chatterjee G, Dalchau N, Muscat RA, Phillips A, Seelig G (2017). A spatially localized architecture for fast and modular DNA computing. *Nature Nanotechnology*, **12**(9), 920.

Dalchau N\*, Grant PK\*, Brown JR, Federici F, Rudge TJ, Yordanov B, Patange O, Phillips A, Haseloff J (2016). Orthogonal intercellular signaling for programmed spatial behavior. *Molecular Systems Biology*, **12**(1), 849.

## PATENTS

Meeds E (2019), Roeder G, **Dalchau N**. Modelling ordinary differential equations using a variational auto encoder (U.S. Patent No. 11,030,275). U.S. Patent and Trademark Office. <https://bit.ly/3vTkngg>

## SOFTWARE

|            |  |
|------------|--|
| CRN-engine | Collection of simulation and analysis tools for chemical reaction-based systems, and implementation of domain-specific programming languages <i>chemical reaction networks</i> (CRN) and <i>DNA strand displacement</i> (DSD). <ul style="list-style-type: none"><li>• Developed parameter inference techniques using Markov chain Monte Carlo (MCMC) in F#.</li><li>• Developed solvers for analysis of the chemical master equation (F#, C++).</li><li>• Developed solvers for approximate stochastic simulation via moment closure (F#).</li><li>• Developed parameter synthesis methods for stable equilibria using satisfiability modulo theory (F#).</li></ul> |
| VI-HDS     | Variational inference for hierarchical dynamical systems. PyTorch-based implementation of variational autoencoders that map time-series data to parameterized models. <ul style="list-style-type: none"><li>• Co-developed original method (Python, TensorFlow)</li><li>• Translated method to PyTorch (Python)</li></ul>  |
| Station-B  | Set of tools to facilitate applying Bayesian optimization to experiment design. <ul style="list-style-type: none"><li>• Prototyped ABEX (automated biological experimentation) module, which wraps <b>Emukit</b> to recommend a new experiment using batch Bayesian optimization.</li><li>• Co-developed a module that performs <i>static characterization</i>, which extracts a representative quantity for gene expression from time-series fluorescent reporter data.</li></ul>   |
| GenCRN     | Enumeration of non-isomorphic chemical reaction networks.  |

## SKILLS

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|--------|---|
| F#     | <ul style="list-style-type: none"><li>• Core contributor to <b>CRN-engine</b> and associated tools (Visual CRN, DSD and GEC; see above)</li><li>• Developed a variety of numerical solvers for dynamical systems</li><li>• Occasional contributor to community F# libraries</li></ul> |
| Python | <ul style="list-style-type: none"><li>• Co-developed <b>VI-HDS</b> on TensorFlow</li><li>• Translated <b>VI-HDS</b> to PyTorch</li><li>• Led development of tools for Bayesian optimization</li></ul>   |
| Julia  | <ul style="list-style-type: none"><li>• Advised and assisted PhD student in development of <b>BifurcationInference.jl</b>, which provides differentiable optimization of bifurcation diagrams</li></ul>   |
| Matlab | <ul style="list-style-type: none"><li>• Haven't used it for a while, but used to do everything in Matlab!</li></ul>   |

## COMMUNITY ENGAGEMENT

### Conference Organisation

- Dagstuhl Seminar 18082: Formal Methods for the Synthesis of Biomolecular Circuits. February, 2018.

### Advisory Boards

- Compugene Program, TU Darmstadt: 2017–2019

### Program Committees

- Computational Methods in Systems Biology (CMSB): 2020, 2021
- Hybrid Systems & Biology (HSB): 2015, 2019, 2020
- Verification of Engineered Molecular Devices and Programs (VEMDP): 2014, 2015, 2018

### Invited Talks (last 5 years)

- **QuantBio** 2019, EPFL-ETHZ summer school
- NII Shonan Seminar #157, 2019, Japan
- BADS & PNA 2019, Hungary
- CCBI Annual Symposium 2019, University of Cambridge, UK
- Computation in Natural Systems 2018, Chicheley Hall, UK
- **Quantitative System Biology** 2018, King's College London, UK
- Compugene Symposium 2017, TU Darmstadt
- IET/SynbiCITE Engineering Biology Conference 2016

## REFERENCES

### Dr. Aditya Nori

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|----------|---|
| POSITION | Partner Research Manager<br>Health Intelligence |
| EMPLOYER | <i>Microsoft Research Cambridge</i>             |
| PHONE    | +44 (0)1223 479700                              |
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### Dr. Andrew Phillips

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| POSITION | Head of Synthetic Biology           |
| EMPLOYER | <i>Microsoft Research Cambridge</i> |
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