Stefan Endres

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Research interests: global optimisation · computational chemistry · chemical phase equilibria

Education

M.Eng. (*with distinction* (80%)) Chemical Engineering, University of Pretoria, 2018

- Dissertation title: **"A simplicial homology algorithm for Lipschitz optimisation."**
  · Advisers:
  - Prof. Walter Focke (Walter.Focke@up.ac.za)
  - Dr. Carl Sandrock (Carl.Sandrock@up.ac.za)

  · External examiner: Prof. John Hedengren (Brigham Young University) (john_hedengren@byu.edu)
  · Internal examiner: Prof. Daniel Wilke (nico.wilke@up.ac.za)
- Research projects nanomaterial science modelling and simulation. Adviser: Prof. Walter Focke (Walter.Focke@up.ac.za)

B.Eng. (*Honours*) Chemical Engineering, University of Pretoria, 2016

- Specialisation in Materials Science and Optimisation.

B.Eng. Chemical Engineering, University of Pretoria, 2015

- Specialisation in Computational Thermodynamics.

Employment History

University of Pretoria, Department of Chemical Engineering *2018 to present*

- Assistant lecturer (process control) and researcher (Institute of Applied Materials (IAM)).

University of Pretoria, Department of Chemical Engineering *2014 to 2017*

- Teaching assistant duties include running weekly tutorial sessions twice a week that augmented the third-year thermodynamics, process dynamics and fourth year process control courses.
- Supervision of research teams at the IAM.

Sappi Ltd., Sappi Technology Centre, Innovation Hub *November 2014 to February 2015*

- Duties included modelling, simulation and parameter optimisation of novel non-linear reaction-diffusion models for applications in kraft pulping, design and implementation of lab experiments with pilot reactors and analysis of results used in the parameter optimisation. Direct supervisor: Dr. Ron Braunstein (Ron.Braunstein@sappi.com).

ABYX Chemical Manufacturing *November 2011 to January 2012*

- Duties included design work on pneumatic circuitry, manufacturing line optimisation and solar powered heat exchangers which were eventually successfully commissioned in the plant. Supervisor: Wendel Krook (smile@abyx.co.za).

Publications

- Endres, SC, Sandrock, C, Focke, WW (2018) *A simplicial homology algorithm for lipschitz optimisation,* Journal of Global Optimization. http://dx.doi.org/10.1007/s10898-018-0645-y.

Free pre-print download available at https://stefan-endres.github.io/files/shgo_jogo.pdf

Manuscripts

- Endres, SC, Sandrock, C & Focke, WW, *shgo: Simplicial homology global optimisation*, Software X. Pre-print: https://stefan-endres.github.io/shgo/files/shgo_softx.pdf
- Endres, SC, Focke, WW & Sandrock, C, *SHGO invariance and convergence in non-linear, non-continuous spaces for black box simulations*, Optimization Letters. Pre-print: https://stefan-endres.github.io/shgo/files/shgo_letter.pdf
- Endres, SC, Sandrock, C & Focke, WW, *A Memory Efficient Simplicial Complex Structure*. Pre-print: https://stefan-endres.github.io/shgo/files/hyperct.pdf
- Endres, SC, Focke, WW & Sandrock, C, *Multiple Dual Cutting Plane Formulation using SHGO for Multicomponent, Multiphase Phase Equilibria Calculations*.
- Endres, SC, Focke, WW & Sandrock, C, *A Geometric Approach to Bilevel Programming with Applications in Phase Equilibria Parameter Optimization*.

Software

Libraries (core developer and maintainer)

- shgo (https://stefan-endres.github.io/shgo/ · https://pypi.python.org/pypi/shgo)
  - Simplicial homology global optimization is a new global optimization algorithm specialized in solving, efficient local minima mapping and characterization of black and grey box objective functions by utilizing techniques from integral homology theory.
- hyperct (https://github.com/Stefan-Endres/hyperct)
  - Library for low memory mesh grids, hypercube triangulations and sub-triangulations.
- pyddt (https://github.com/Stefan-Endres/pyDDT · https://pypi.python.org/pypi/tgo)
  - Hyperbolic PDE solver using WENO schemes for deflagration-to-detonation transition simulations.
- dwpm (https://github.com/Stefan-Endres/DWPM-Mixture-Model)
  - Phase separation calculation algorithms primarily using the DWPM mixture rule.

Libraries (contributor)

- scipy (https://github.com/scipy/scipy/)
  - SciPy library: Fundamental library for scientific computing. Contributions to scipy.optimize.
- clifford (https://github.com/pygae/clifford)
  - pygae/clifford library: A numerical geometric algebra module for python. Contributions to sparse Clifford algebra initiations.

Skills

Programming, Scientific and Engineering Software and CAD

- Python (including SciPy stack)
- C/C++
- MATLAB/Octave · Simulink
- AspenPlus
- FEM software: ANSYS · FEniCS (FEM using the variational formulation)

Operating Systems, Graphic Design Software and Typesetting

- Linux (Arch) · Inkscape · LaTeX · LibreOffice
- Windows · Adobe Illustrator · MS Office

Practical

- Technical training at Tshwane South College (Pretoria West Campus, 2010).
  Welding · Machining · Soldering · Turning · Panel Wiring · Electrical Motors · Fitting