

# Nicholas Penha Malaya

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## EDUCATION

**The University of Texas at Austin**, Austin, TX

- Ph.D., Engineering, 2016, Advisor: Professor Robert D. Moser
- M.S., Engineering, 2009

**Georgetown University**, Washington, D.C.

- B.S., Physics & Mathematics, *with honors*, 2007

## RESEARCH INTERESTS

High Performance Computing, Computational Science, Machine Learning, Deep Learning, Exascale Computing, Turbulence, Verification Validation & Uncertainty Quantification, Bayesian Inference

## RESEARCH EXPERIENCE

**AMD**

**Austin, TX**

*Principal Member of Technical Staff*

May 2021 – present

*Senior Member of Technical Staff*

May 2019 – 2021

*Member of Technical Staff*

May 2018 – 2019

*Senior Engineer*

Dec. 2016 – May 2018

**Department of Mechanical Engineering**  
**The University of Texas at Austin**

**Austin, TX**

*Doctoral Candidate*

Jan. 2014 – Dec. 2016

**Institute for Computational Engineering and Sciences**  
**The University of Texas at Austin**

**Austin, TX**

*Research Engineering/Scientist Associate II*

Jan. 2010 – Dec. 2013

**Physics Laboratory, Optical Technology Division**  
**National Institute of Standards and Technology**

**Gaithersburg, MD**

*Assistant Researcher*

May 2005 – August 2005

## AWARDS

- Executive Spotlight Award, June 2020
  - "For the winning LUMI EuroHPC bid"
- Next 5% Award, Q1 2020 & Q3 2022
  - "The Next 5% Award is the highest level of recognition at AMD"
- Datacenter Solution Group's Award of Excellence for work on the Frontier Exascale Proposal, 2019
- "Best Student Paper Finalist" – SC13, Denver, CO
- "Best Paper" – 2012 TACC-Intel Highly Parallel Computing Symposium
- Cockrell School of Engineering Thrust 2000 Ph.D. Fellowship
- 2007 Treado Medal, Georgetown University

## MENTORSHIP

Co-ops Advised:

- Alberto Acevedo, Brett Leroux, Michael Curry (Summer 2020)
- Octavi Obiols Sales (Summer 2019)
- Artem Vysogorets, Tingting Ou, Kuanhao Jiang, Parmida Davarmanesh (Summer 2019)
- Naman Meheshwari (Fall 2018)
- Patrik Gerber, Jiajing Guan, Elvis Nunez, Kaman Phamdo (Summer 2018)
- Zhaoqi Li, Catalina Vajiac, Yu Ma, Yunkai Zhang (Summer 2017)

## TEACHING EXPERIENCE

**The University of Texas at Austin**

*CSE 380 - Tools/Techniques of Computational Science*      **Fall 2015, 2016**

**Los Alamos National Laboratory**

*Computational Physics Student Summer Workshop*      **Summer 2012 - 2017**

## REFEREED JOURNAL PUBLICATIONS

Evaluating GPU Programming Models for the LUMI Supercomputer Markomanolis *et al.* SCFA 2022: Supercomputing Frontiers, Jul 1, 2022

SURFNet: Super-resolution of Turbulent Flows with Transfer Learning using Small Datasets Octavi Obiols-Sales, Abhinav Vishnu, **Nicholas Malaya**, Aparna Chandramowlishwaran Proc. 30th International Conference on Parallel Architectures and Compilation Techniques (PACT), Aug 5, 2021

Vandermonde Wave Function Ansatz for Improved Variational Monte Carlo Alberto Acevedo, Michael Curry, Shantanu H. Joshi, Brett Leroux, **N Malaya** ACM/IEEE Supercomputing Conference 2020, November 11th

CFDNet: a deep learning-based accelerator for fluid simulations O Obiols-Sales, A Vishnu, **N Malaya**, A Chandramowlishwaran, International Conference in Supercomputing (ICS) 2020, June 29th

McMahan JA, Williams BJ, Smith RC, **Malaya N.**, A Linear Regression Framework for the Verification of Bayesian Model Calibration Algorithms. ASME. J. Verif. Valid. Uncert. 2017. doi:10.1115/1.4037705.

Graham, J., Kanov, K., Yang X.I.A., Lee M.K., **Malaya, N.**, Lalescu, C.C., Burns, R., Eyink, G., Szalay, A., Moser, R.D. & Meneveau, C. “A Web Services-accessible database of turbulent channel flow and its use for testing a new integral wall model for LES.” Journal of Turbulence (2015)

M. Lee, **N. Malaya**, Rhys Ulerich, Robert D. Moser, “Experiences from Leadership Computing in Simulations of Turbulent Fluid Flows,” Computing in Science & Eng., vol. 16, no. 5, 2014, pp. 24–31.

T. A. Oliver, **N. Malaya**, R. Ulerich, and R. D. Moser, “Estimating uncertainties in statistics computed from direct numerical simulation,” Phys. Fluids 26, 035101 (2014). <http://dx.doi.org/10.1063/1.4866813>

M. Lee, **N. Malaya**, and R. D. Moser, “Petascale direct numerical simulation of turbulent channel flow on up to 786k cores,” in Proceedings of the 2013 ACM/IEEE International Conference for High Performance Computing, Networking, Storage and Analysis (SC). ACM Press, 2013 (**Best Student Paper Finalist**)

**N. Malaya**, K. C. Estacio-Hiroms, R. H. Stogner, K. W. Schulz, P. T. Bauman, G. F. Carey, “MASA: A Library for Verification Using Manufactured and Analytical Solutions”, Engineering with Computers, 29(4), 487–496, 2013

**N. Malaya**, T. Oliver, K. C. Estacio-Hiroms, “Manufactured Solutions for the Favre-Averaged Navier-Stokes Equations with Eddy-Viscosity Turbulence Models”, Technical Paper, 50th AIAA ASM, 2012.

**Nicholas Malaya**, Karl W. Schulz, Robert D. Moser “Petascale I/O using HDF-5”, Teragrid’10 Technical Paper, Association for Computing Machinery, August 2, 2010.

Robert D. Moser, **Nicholas P. Malaya**, Henry Chang, et. al., “Theoretically based optimal large-eddy simulations”, Physics of Fluids, October 23, 2009.

Damon McDougall, **Nicholas Malaya**, Robert D. Moser, “The Parallel C++ Statistical Library for Bayesian Inference: QUESO”, Handbook of Uncertainty Quantification, edited by Roger Ghanem, David Higdon, Houman Owhadi, (Springer International Publishing, 2017)

**Nicholas Malaya**, Robert D. Moser, Amitabh Bhattacharya. “Modeling Multi-point Correlations in Wall-Bounded Turbulence”, Progress in Wall Turbulence: Understanding and Modeling, edited by M. Stanislas, J. Jimenez, and I. Marusic (Springer, Netherlands, 2011), Vol. 14, pp. 183–190.

#### PATENTS

Deliberate conditional poison training for generative models, N Malaya, US Patent App. 16/208,384

Optimized and scalable sparse triangular linear systems on networks of accelerators, K Hamidouche, MW LeBeane, NP Malaya, JL Greathouse, US Patent App. 16/044,145

Method and system for opportunistic load balancing in neural networks using metadata, N Malaya, Y Eckert, US Patent App. 16/019,374

Configuring Computational Elements for Performing a Training Operation for a Generative Adversarial Network, NP Malaya, US Patent App. 16/009,089

Dynamic hardware selection for experts in mixture-of-experts model, N Malaya, N Jayasena, US Patent App. 15/849,633

Concurrent training of functional subnetworks of a neural network, D Yudanov, NP Malaya, US Patent App. 15/841,030

Dynamic, variable bit-width numerical precision on fpgas for machine learning tasks, NP Malaya, EH Mednick, US Patent App. 15/833,287

Artificial neural network reduction to reduce inference computation time, N Malaya, US Patent App. 15/638,993

#### PAPERS IN PREPARATION

SURFNet: Super-resolution of Turbulent Flows with Transfer Learning using Small Datasets Octavi Obiols-Sales, Abhinav Vishnu, Nicholas Malaya, Aparna Chandramowlishwaran <https://arxiv.org/abs/2108.07667>

#### REFEREED CONFERENCE PUBLICATIONS

**Nicholas Malaya**, Shuai Che, Joseph L. Greathouse, René van Oostrum, Michael J. Schulte, Accelerating Matrix Processing with GPUs Published in the Proceedings of the 24th IEEE Symposium on Computer Arithmetic (ARITH 24), July, 2017

**N Malaya**, D McDougall, C Michoski, M Lee, CS Simmons, Experiences Porting Scientific Applications to the Intel (KNL) Xeon Phi Platform Proceedings of the

Practice and Experience in Advanced Research Computing 2017 on Sustainability, Success and Impact

K. W. Schulz, R. Ulerich, **N. Malaya**, P. T. Bauman, R. Stogner, and Chris Simmons, “Early Experiences Porting Scientific Applications to the Many Integrated Core (MIC) Platform”, TACC-Intel Highly Parallel Computing Symposium, Austin, TX, April 10–11, 2012. Winner - Best Paper.

Rhys Ulerich, Kemelli C. Estacio-Hiroms, **Nicholas Malaya**, and Robert D. Moser. A transient manufactured solution for the compressible Navier–Stokes equations with a power law viscosity. In 10th World Congress on Computational Mechanics, São Paulo, Brazil, July 2012. doi: 10.5151/meceng-wccm2012-16661. (pages 108, 223, 227).

Juan Sillero, Javier Jimenez, Robert. D. Moser, **Nicholas Malaya**, “Direct Simulation of a zero-pressure gradient turbulent boundary layer up to  $Re_\theta = 6650$ ”, Technical Paper, 13th European Turbulence Conference, September, 2011.

#### INVITED

PRESENTATIONS **Nicholas Malaya**, “Accelerating CFD with ML/AI at AMD”, ModSim 2021, October 8th, 2021.

**Nicholas Malaya**, “The Frontier System: Computing at Exascale”, Northeastern University, Dec. 1st, 2021.

**Nicholas Malaya**, “Enabling Portable Directive-Based Programming at Exascale”, WACCPD, SC20, November 13th, 2020.

**Nicholas Malaya**, “Hardware and Software Co-design: Preparing and Optimizing Scientific Applications for Exascale Computing”, Institute for Applied Computational Science, Harvard University February, 21st, 2020.

**Nicholas Malaya**, “AMD EPYC CPUs and Radeon Instinct GPUs for HPC”, El Capitan Application Readiness Kick-off Workshop, Lawrence Livermore National Laboratory, January 14th, 2020.

**Nicholas Malaya**, “AMD EPYC CPUs and Radeon Instinct GPUs for HPC”, El Capitan Application Readiness Kick-off Workshop, Sandia National Laboratories, Dec. 3rd, 2019.

**Nicholas Malaya**, “AMD GPU Evolution”, Frontier Application Readiness Kick-off Workshop, Oak Ridge Leadership Computing Facility, Oct. 8th, 2019.

**Nicholas Malaya**, **Max Kiehn**, “Automated Software Testing with Machine Learning”, AMD Software Tech Forum, September 9th, 2019.

**Nicholas Malaya**, “Learning Systems”, Department of Computer Science, University of Chicago, November 28th, 2018.

**Nicholas Malaya**, “Full-Stack Open-Source Supercomputing”, OpenSuCo4 Keynote at SC18 Dallas, TX, November 12th, 2018.

**Nicholas Malaya**, “Technology Directions in AI”, UT McCombs School of Business, Austin, TX, October 9th, 2018.

**Nicholas Malaya**, “Numerical Investigation of Synthetic Dust Devils”, AMD Research, Austin, TX, July 8th, 2016.

**Nicholas Malaya**, “Introduction to Scientific Computation”, Dell HPC Innovation Lab, Austin, TX, September 2nd, 2016.

**Nicholas Malaya**, “Verification, Validation and Uncertainty Quantification in Turbulence Simulations”, Texas Advanced Computing Center, Austin, TX, May 12th, 2016.

**Nicholas Malaya**, “Numerical Investigation of Synthetic, Buoyancy-Induced Columnar Vortices”, Sandia National Laboratories, Albuquerque, NM, March 16th, 2016.

**Nicholas Malaya**, “Verification & Software Quality in Scientific Computing”, Los Alamos Computational Physics Student Summer Workshop, 2014.

**Nicholas Malaya**, “The Method of Manufactured Solutions”, Los Alamos Computational Physics Student Summer Workshop, 2013.

**Nicholas Malaya**, Christopher Simmons, “Scientific Software Engineering Best Practices”, Los Alamos Computational Physics Student Summer Workshop, 2012.

**Nicholas Malaya** & Robert D. Moser, “Tools and Techniques for Code Verification using Manufactured Solutions.”, SIAM Conference on Uncertainty Quantification, April 2-4, 2012, Raleigh, North Carolina

**Nicholas Malaya**, Karl W. Schulz, “Verification through the MASA Library”, Los Alamos Computational Physics Student Summer Workshop, 2011.

**Nicholas Malaya**, Rhys Ulerich, Robert Moser, “Petascale Direct Numerical Simulations of Turbulent Channel Flow”, ESP Kick-off Workshop and Project Plan Presentation, Oct. 18th, 2010.

**Nicholas Malaya** “Theoretically Based Optimal LES”, TFS/NRE Seminar, Department of Mechanical Engineering, Oct. 29th, 2009.

CONFERENCE    **N. Malaya** The AMD MI250X Crusher Workshop, OLCF, 2022  
PRESENTATIONS

**N. Malaya** Frontier Center of Excellence Update: AMD hardware and software ECP All-Hands, April. 16th, 2021

**N. Malaya** Accelerated Computing at AMD Research UT Austin ECE Speaker Panel, October 23rd, 2020

**N. Malaya** Preparing Scientific applications for Exascale Computing UCLA IPAM, July 15th, 2020

**N. Malaya** The Frontier Node Architecture Design ECP All-Hands, Feb. 6th, 2020

**N. Malaya** Preparing Scientific Applications for Frontier SC19 Booth Talk, Nov. 20th, 2019

**N. Malaya** Porting Scientific Applications using HIP SC18 Booth Talk, Nov. 13th, 2018

**N. Malaya** AMD Exascale Applications and Software Technologies PathForward Review Meeting, March 21st, 2018

**N. Malaya**, R. Stogner, R. Moser, Numerical Investigation of Synthetic Buoyancy-Induced Columnar Vortices, Bulletin of the American Physical Society 60, 2015

**Nicholas Malaya** MASA: A Tool for the Verification of Scientific Software, SciPy2016

**N. Malaya**, R. Ulerich, T. Oliver, R Moser, Estimating Uncertainties in Statistics Computed from DNS, APS Meeting Abstracts 1, 21004, 2012

**Nicholas Malaya**, Karl Schulz, “Verification through the MASA Library”, DOE PSAAP Annual Review, 2011

**Nicholas Malaya**, Pk Yeung, “Collaborative Research: Enabling Discovery in High Reynolds Number” Turbulence via Advanced Tools for Petascale Simulation and Analysis, 2010

**Nicholas Malaya**, Amitabh Bhattacharya, Robert Moser, “Theoretically Based Optimal LES”, APS DFD, 2008.

## TECHNICAL SKILLS

### Programming Experience:

- Languages: C/C++, Fortran, Python(Num/Scipy), L<sup>A</sup>T<sub>E</sub>X, ROCm/HIP/HCC, CUDA, Bash, Mathematica, Octave/Matlab
- Development Env: Linux, Emacs, Git, SVN, Buildbot, TravisCI
- Stanford Certificate in Machine Learning (Online) from Andrew Ng
- Libraries: MPI, OpenMP, Tensorflow, PyTorch, FFTW, BLAS, Lapack, Dakota, Petsc

## SERVICE

### Mentorship:

- Industry Mentor, RIPS IPAM UCLA, 2017, 2018, 2019, 2020
- Senior Judge, Austin Energy Regional Science Festival 2014-present

#### **Committees:**

- Technical Program Committee Member, Session Chair, Programming Frameworks and System Software area at SC22
- Steering Committee Member, WACCPD SC21 and SC22
- Program Committee for Cluster 2021
- Program Committee HiPar at SC21
- Program Committee Member, SciPy 2017, 2018, 2019
- Program Committee Member, PEARC17
- Program Committee, Great Lakes Consortium for Petascale Computation (2012–2015)
- Reviewer, Blue Waters Graduate Fellowship Program (2014–2018)

#### **Companies Advised:**

- Board Member, kWh Analytics (2012-2016)

#### **Journal Referee:**

- Machine Learning and the Physical Sciences, NeurIPS, 2019-2020
- Parallel Computing
- Journal of Fluid Mechanics
- Engineering with Computers
- Journal of Computational Physics
- Neural Information Processing Systems

MEMBERSHIPS    ACM, SIAM

INTERESTS       Marathons, Motorsport, Mountain Climbing, Wine, Go

CITIZENSHIP     United States of America

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