

# 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, Computer Modeling, Exascale Computing, Turbulence, Verification Validation & Uncertainty Quantification, Bayesian Inference, Spectral Methods, Machine Learning

## RESEARCH EXPERIENCE

### **HPC Applications Software Technology AMD Research**

**Austin, TX**

*Computational Scientist*

Dec. 2016 – Present

### **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

- “Best Paper” - 2012 TACC-Intel Highly Parallel Computing Symposium, April 10-11, Austin, TX
- Cockrell School of Engineering Thrust 2000 Ph.D. Fellowship
- 2007 Treado Medal, Georgetown University

MENTORSHIP	<p>Summer Co-ops Advised:</p> <ul style="list-style-type: none"> <li>• Zhaoqi Li, Catalina Vajiac, Yu Ma, Yunkai Zhang (2017)</li> </ul>
TEACHING EXPERIENCE	<p><b>The University of Texas at Austin</b></p> <p><i>CSE 380 - Tools/Techniques of Computational Science</i>      <b>Fall 2015, 2016</b></p> <p><b>Los Alamos National Laboratory</b></p> <p><i>Computational Physics Student Summer Workshop</i>    <b>Summer 2012 - 2017</b></p>
REFEREED JOURNAL PUBLICATIONS	<p>McMahan JA, Williams BJ, Smith RC, <b>Malaya N.</b>, A Linear Regression Framework for the Verification of Bayesian Model Calibration Algorithms. ASME. J. Verif. Valid. Uncert. 2017. doi:10.1115/1.4037705.</p> <p>Graham, J., Kanov, K., Yang X.I.A., Lee M.K., <b>Malaya, N.</b>, Lalescu, C.C., Burns, R., Eyink, G., Szalay, A., Moser, R.D. &amp; 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)</p> <p>M. Lee, <b>N. Malaya</b>, Rhys Ulerich, Robert D. Moser, Experiences from Leadership Computing in Simulations of Turbulent Fluid Flows, Computing in Science &amp; Eng., vol. 16, no. 5, 2014, pp. 2431.</p> <p>T. A. Oliver, <b>N. Malaya</b>, R. Ulerich, and R. D. Moser, Estimating uncertainties in statistics computed from direct numerical simulation, Phys. Fluids 26, 035101 (2014). <a href="http://dx.doi.org/10.1063/1.4866813">http://dx.doi.org/10.1063/1.4866813</a></p> <p>M. Lee, <b>N. Malaya</b>, 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</p> <p><b>N. Malaya</b>, 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</p> <p><b>N. Malaya</b>, 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.</p> <p><b>Nicholas Malaya</b>, Karl W. Schulz, Robert D. Moser “Petascale I/O using HDF-5”, Teragrid’10 Technical Paper, Association for Computing Machinery, August 2, 2010.</p>

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

BOOK

CHAPTERS

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. 183190.

PAPERS IN

PREPARATION

**Nicholas Malaya**, Robert D. Moser, “Numerical Simulation of Synthetic Columnar Vortices”, Physics of Fluids

**Nicholas Malaya**, Roy H. Stogner, Robert D. Moser, “A Penalty Method Model for Immersed Boundaries and Control Surfaces”, International Journal for Numerical Methods in Fluids

REFEREED

CONFERENCE

PUBLICATIONS

**Nicholas Malaya**, Shuai Che, Joseph L. Greathouse, Ren 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 NavierStokes equations with a power law viscosity. In 10th World Congress on Computational Mechanics, So 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**, “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 PRESENTATIONS **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, SciPy20164

**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

Extensive experience developing numerical methods for simulation of physical phenomena on workstation and parallel computing environments

**Programming Experience:**

- Languages: C/C++, Fortran, Python(Num/Scipy), L<sup>A</sup>T<sub>E</sub>X, Bash, Mathematica, Octave/Matlab
- Development Env: Linux, Emacs, Git, SVN, Buildbot, TravisCI
- Stanford Certificate in Machine Learning (Online) from Andrew Ng
- Libraries: MPI, OpenMP, HDF-5, FFTW, BLAS, Lapack, Hadoop, Dakota

SERVICE

**Mentorship:**

- Industry Mentor, Research in Industrial Projects for Students (RIPS), IPAM, 2017

**Committees:**

- Program Committee Member, SciPy 2017
- Program Committee Member, PEARC17
- Program Committee, Great Lakes Consortium for Petascale Computation (2012–2015)
- Reviewer, Blue Waters Graduate Fellowship Program (2014–present)

**Journal Referee:**

- Journal of Fluid Mechanics
- Engineering with Computers
- Journal of Computational Physics

MEMBERSHIPS    APS, SIAM, ACM, AIAA

INTERESTS        Marathons, Mountain Climbing, Wine, Go

CITIZENSHIP      United States of America

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## REFERENCES

Jonathan Gallmeier  
Sr. Manager Design Engineering  
AMD Research  
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Todd Oliver, Ph.D.  
Research Scientist  
Center for Predictive Engineering and Computational Science  
Institute for Computational Engineering and Sciences  
University of Texas at Austin  
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Institute for Computational Engineering and Sciences  
and Department of Mechanical Engineering  
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