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 Advanced 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

Summer Co-ops Advised:

• Zhaoqi Li, Catalina Vajiac, Yu Ma, Yunkai Zhang (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

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. 2431.
- 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 sim- ulation 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
- 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.

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 Multipoint 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 Vorticies", 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 N. Malaya, R. Stogner, R. Moser, Numerical Investigation of Synthetic Buoyancy-Presentations 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), Languages: C/C++, Fortran, Python(Num/Scipy), Languages: C/C++, 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.
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Center for Predictive Engineering and Computational Science
Institute for Computational Engineering and Sciences
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