Marc T. Henry de Frahan

US citizen, Applied Mathematics/Mechanical engineer

marchdf@gmail.com
github.com/marchdf

Work Experience

Computational Scientist, National Renewable Energy Laboratory 2019-present
Reacting flows, wind turbine physics, performance portability on GPUs, numerical methods, continuum methods, kinetic Monte-Carlo
Principal investigator for several projects (*Adaptive Mesh and Algorithm Refinement*, 500k; *Scalable Parallel Discrete Events Simulations*, 550k)
Principal developer of several Exascale Computing Project software (Pele, ExaWind)

Post-doctoral Researcher, National Renewable Energy Laboratory 2016-2019
Next-generation simulations of wind farms and reacting flow processes

Education

Ph.D. in Mechanical Engineering 2011-2016
University of Michigan, Ann Arbor, MI
Thesis: *Numerical simulations of shock and rarefaction waves interacting with interfaces in compressible multiphase flows*
Advisor: E. Johnsen, Assistant Professor of Mechanical Engineering

M.S. in Applied Mathematics Engineering 2009-2011
Université Catholique de Louvain, Belgium
Thesis: *Implementation of a Discontinuous Galerkin Method for hyperbolic PDEs on GPUs*
Advisors: Prof. J-F Remacle, Prof. P. Chatelain, Prof. V. Legat.

B.S. in Applied Mathematics Engineering 2007-2009
Université Catholique de Louvain, Belgium

Research Interests

Fluid mechanics - turbulence, multiphase flows, hydrodynamic instabilities
Energy - reacting flows, wind turbines and farms
High order numerical methods for computational fluid dynamics
High performance computing with graphics processing units
Machine learning for improved physics models

Journal Articles

M. Hassanaly, N. T. Wimer, A. Felden, L. Esclapez, J. Ream, M. T. Henry de Frahan, J. Rood, M. Day, **Symbolic construction of the chemical Jacobian of quasi-steady state (QSS) chemistries for Exascale computing platforms**, *Comb. and Flame*, vol. 270, 113740, 2024

I. Barrio Sanchez, A. S. Almgren, J. B. Bell, M. T. Henry de Frahan, W. Zhang, **A New Redistribution Scheme for Weighted State Redistribution with Adaptive Mesh Refinement**, *J. Comp. Phys.*, vol. 504, 1, 112879, 2024

M. T. Henry de Frahan, L. Esclapez, J. Rood, N. T. Wimer, P. Mullowney, B. A. Perry, L. Owen, H. Sitaraman, S. Yellapantula, M. Hassanaly, M. J. Rahimi, M. J. Martin, O. A. Doronina, Sreejith N. A., M. Rieth, W. Ge, R. Sankaran, A. S. Almgren, W. Zhang, J. B. Bell, R. Grout, M. S. Day, and J. H. Chen, **The Pele Simulation Suite for Reacting Flows at Exascale**, *Proc. 2024 SIAM Conf. Parallel Proc. Sc. Comput.*, 15-25, 2024

A. Sharma, M. J Brazell, G. Vijayakumar, S. Ananthan, L. Cheung, N. deVelder, M. T. Henry de Frahan, N. Matula, P. Mullowney, J. Rood, P. Sakievich, A. Almgren, P. S Crozier, M. Sprague, **ExaWind: Open-source CFD for hybrid-RANS/LES geometry-resolved wind turbine simulations in atmospheric flows**, *Wind Energy*, vol 27, 3, 225-257, 2024

N. Wimer, L. Esclapez, N. Brunhart-Lupo, M. T. Henry de Frahan, M. Rahimi, M. Hassanaly, J. Rood, S. Yellapantula, H. Sitaraman, B. Perry, M. Martin, O. Doronina, S. Appukuttan, M. Reith, M. Day, **Visualizations of a Methane/Diesel RCCI Engine using PeleC and PeleLMeX**, *Phys. Rev. Fluids*, 8, 110511, 2023

L. Esclapez, M. Day, J. Bell, A. Felden, C. Gilet, R. Grout, M. T. Henry de Frahan, E. Motheau, A. Nonaka, L. Owen, B. Perry, J. Rood, N. Wimer, and W. Zhang, **PeleLMeX: an AMR Low Mach Number Reactive Flow Simulation Code without level sub-cycling**, *J. Open Source Software*, 8, 90, 5450, 2023

N. T Wimer, M. T. Henry de Frahan, S. Yellapantula, **Deep reinforcement learning to discover multi-fuel injection strategies for compression ignition engines**, *Int. J. Eng. Res.*, vol 24, 9, 2023

A. Giuliani, A.S. Almgren, J.B. Bell, M.J. Berger, M.T. Henry de Frahan, D. Rangarajan, **A weighted state redistribution algorithm for embedded boundary grids**, *J. Comp. Phys.*, 111305, 2022

M. T. Henry de Frahan, J. S. Rood, M. S. Day, H. Sitaraman, S. Yellapantula, B. A. Perry, R. W. Grout, A. Almgren, W. Zhang, J. B. Bell, J. H. Chen, **PeleC: An adaptive mesh refinement solver for compressible reacting flows**, *Int. J. High. Perf. Comp. App.*, vol. 37, 2, 2022

B. Perry, M. T. Henry de Frahan, S. Yellapantula, **Co-optimized machine-learned manifold models for large eddy simulation of turbulent combustion**, *Comb. and Flame*, 244, 112286, 2022

H. Sitaraman, N. Brunhart-Lupo, M. T. Henry de Frahan, S. Yellapantula, B. Perry, J. Rood, R. Grout, M. S. Day, R. Binyahib, K. Gruchalla, **Visualizations of direct fuel injection effects in a supersonic cavity flameholder**, *Phys. Rev. Fluids*, 6, 110504, 2021

J Quick, R. King, M. T. Henry de Frahan, S. Ananthan, M. Sprague, P. Hamlington, **Field Sensitivity Analysis of Turbulence Model Parameters for Flow Over a Wing**, *Int. J. Uncert. Quant.*, vol. 12, 1, 85–106, 2022

H. Sitaraman, S. Yellapantula, M. T. Henry de Frahan, B. Perry, J. Rood, R. W. Grout, M. S. Day, **Adaptive mesh based combustion simulations of direct fuel injection effects in a supersonic cavity flame-holder**, *Comb. and Flame*, 232, 111531, 2021

M. T. Henry de Frahan, N. T Wimer, S. Yellapantula, R. W. Grout, **Deep reinforcement learning for dynamic control of fuel injection timing in multi-pulse compression ignition engines**, *Int. J. Eng. Res.*, vol 23, 9, 2021

S. Yellapantula, M. T. Henry de Frahan, R. King, M. S. Day, R. W. Grout, **Machine learning of combustion LES models from reacting direct numerical simulation**, *Data Analysis for Direct Num. Sim. of Turb. Comb.*, Pages 273-292, 2020

M. T. Henry de Frahana, S. Yellapantula, R. King, M. S. Day, and R. W. Grout, **Deep learning for presumed probability density function models**, *Comb. and Flame*, 208:436–450, Pages 436-450, 2019

P. Mohan, M. T. Henry de Frahan, R. King, and R. Grout, **A block-random algorithm for learning on distributed, heterogeneous data**, *arXiv:1903.00091*, 2019

M. T. Henry de Frahan, and R. Grout, **Data recovery in computational fluid dynamics through deep image priors**, *arXiv:1901.11113*, 2019

M. T. Henry de Frahan, J. L. Belof, R. M. Cavallo, V. A. Raevsky, O. N. Ignatova, A. Lebedev, D. S. Ancheta, B. S. El-dasher, J. N. Florando, G. F. Gallegos, E. Johnsen, and M. M. LeBlanc, **Experimental and Numerical Investigations of Beryllium Strength Models Using the Rayleigh-Taylor Instability**, *featured article in J. Appl. Phys.*, 117(22):225901, 2015

M. T. Henry de Frahan, S. Varadan, and E. Johnsen, **A new limiting procedure for discontinuous Galerkin methods applied to compressible multiphase flows with shocks and interfaces**, *J. Comput. Phys.*, 280(0):489 – 509, 2015

M. T. Henry de Frahan, P. Movahed, and E. Johnsen, **Numerical simulations of a shock interacting with successive interfaces using the Discontinuous Galerkin method: the multilayered Richtmyer-Meshkov and Rayleigh-Taylor instabilities**, *Shock Waves*, 25(4):329–345, 2015

C. A. Di Stefano, G. Malamud, M. T. Henry de Frahan, C. C. Kuranz, A. Shimony, S. R. Klein, R. P. Drake, E. Johnsen, D. Shvarts, V. A. Smalyuk, and D. Martinez, **Observation and modeling of mixing-layer development in high-energy-density, blast-wave-driven shear flow**, *Phys. Plasmas*, 21(5):056306, 2014

Conference Proceedings

N. T. Wimer, L. Esclapez, M. T. Henry de Frahan, M. Rahimi, M. Hassanaly, B. Perry, J. Rood, S. Yellapantula, H. Sitaraman, M. Martin, O. Doronina, S. Nadakkal Appukuttan, M. Rieth, M. Day, **Examination of a Methane/Diesel RCCI Engine Using Pele**, 13^{th} *U.S. National Combustion Meeting*, 2023

P. T. Bauman et al, **Experiences Readying Applications for Exascale**, *Supercomputing*, 2023

M. T. Henry de Frahan, M. Rahimi, O. Doronina, B. Perry, S. Yellapantula, I. Cormier, M. Day, M. Martin, **Simulation of Methane Oxycombustion in Supercritical Carbon Dioxide**, *Turbomachinery Technical Conference and Exposition, ASME*, doi: 10.1115/GT2023-101568, 2023

S. A Beig, G. R. Whitehouse, A. H. Boschitsch, A. Sharma, M. J. Brazell, M. T Henry de Frahan, M. A. Sprague, **Developing a Vorticity-Velocity-Based Off-Body Solver to Perform Multifidelity Simulations of Wind Farms**, *2022 AIAA SCITECH Forum. American Institute of Aeronautics and Astronautics*, doi: 10.2514/6.2023-1542, 2022

C. Adcock, M. T. Henry de Frahan, J. Melvin, G. Vijayakumar, S. Ananthan, G. Iaccarino, R. D. Moser,

and M. Sprague, **Hybrid RANS-LES of the Atmospheric Boundary Layer for Wind Farm Simulations**, *2022 AIAA SCITECH Forum. American Institute of Aeronautics and Astronautics*, doi: 10.2514/6.2022-1922, 2021

J. Melvin, M. T. Henry de Frahan, S. Ananthan, G. Vijayakumar, M. Sprague, R. Moser, **Using the Active Model Split Hybrid Turbulence Model for the Simulation of Blade-Resolved Wind Turbines**, *Wind Energy Science Conference*, 2021

S. Yellapantula, B. A. Perry, M. T. Henry de Frahan, M. E. Mueller, and R. W. Grout, **Machine Learning based models for joint PDF shapes for multi-scalar mixing in turbulent flows**, 11^{th} *U.S. National Combustion Meeting*, 2019

M. T. Henry de Frahan, L. Khieu, and E. Johnsen, **High-order Discontinuous Galerkin Methods Applied to Multiphase Flows**, 22^{d} *AIAA Computational Fluid Dynamics Conference. American Institute of Aeronautics and Astronautics*, doi: 10.2514/6.2015-3045, 2015, AIAA CFD Best Student Paper Award (3^{d} place)

M. T. Henry de Frahan and E. Johnsen, **Discontinuous Galerkin method for multifluid Euler equations**, *In 21st AIAA Computational Fluid Dynamics Conference. American Institute of Aeronautics and Astronautics*, doi: 10.2514/6.2013-2595, 2013

M. T. Henry de Frahan, P. Movahed, and E. Johnsen, **Investigating the multilayered Richtmyer-Meshkov instability with high-order accurate numerical methods**, *In 29th International Symposium on Shock Waves 2, Springer International Publishing*, 2015

Awards and Fellowships

President's Team Award 2024
National Renewable Energy Laboratory

Best Visualization Award 2023
Supercomputing 2023

Chairperson's Team Award 2023
National Renewable Energy Laboratory

Milton van Dyke Award 2022
American Physical Society - Division of Fluid Dynamics

President's Award for Exceptional Performance 2022
National Renewable Energy Laboratory

Gallery of Fluid Motion Award Winners 2020
American Physical Society - Division of Fluid Dynamics

President's Team Award 2019
National Renewable Energy Laboratory

Better Scientific Software Fellowship (honorable mention) 2018
Better Scientific Software (Department of Energy organization)

AIAA CFD Best Student Paper Award (3^{d} place) 2015
American Institute of Aeronautics and Astronautics

Rackham Predoctoral Fellowship 2015
University of Michigan

Rackham Centennial Fellowship 2013
University of Michigan

High Distinction 2011
M.S. in Applied Mathematics Engineering at the Université Catholique de Louvain

Leadership Experience

Acting Group Manager for the High Performance Algorithms and Complex Fluids group, NREL 2020-2021
Group lead for a team of 15+ scientists

Mechanical Engineering Graduate Council, University of Michigan 2013-2016
- STEM Communication Chair
  Communicate graduate student research to lay audiences
- President
  Promote social, academic and professional development for ME graduate students
- Graduate Seminar Chair
  Organize monthly seminars to showcase graduate student research

Graduate Student Advisory Committee, University of Michigan 2014-2015
Representative for Department of Mechanical Engineering
Identify and plan activities to promote community among engineering graduate students

Mentorship and Teaching Experience

Prakash Mohan, National Renewable Energy Laboratory 2022-Present
Postdoctoral research mentor

Arth Sojitra 2023
Mentor for summer internship on the lattice boltzmann method

Grace Wei 2023
CSGF practicum mentor on the kinetic Monte-Carlo methods

Nick Wimer, National Renewable Energy Laboratory 2019-2021
Postdoctoral research mentor

Bruce Perry, National Renewable Energy Laboratory 2019-2021
Postdoctoral research mentor

Likhit Ganedi, Carnegie-Mellon Univeristy 2021
Mentor for summer internship on hybrid particle-continuum solvers

Jani Adcock, Stanford University 2020-2023
CSGF practicum mentor, Ph.D. committee member

Julia Ream, Florida State University 2019-2023
Co-advisor of Ph.D. committee for work on turbulent supercritical CO2 simulations

Prakash Mohan, University of Texas-Austin 2018
Mentored Ph.D. graduate student for a project on deep learning for LES models

Jalil Alidoost, University of Michigan 2015-2016
Mentored senior undergraduate for a project on diffusive and kinetic properties of chair motion in the Shapiro Library

Colby Hanley, University of Michigan 2015-2016
Mentored freshman undergraduate for a project on multi-GPU profiling for high-performance computing

Graduate Student Instructor for ME 523: Computational Fluid Dynamics Fall 2013
University of Michigan, Ann Arbor, MI

Research Experience

DOE I-Corps Cohort 15 Fall 2022
Department of Energy
Immersive two-month training for researchers to define technology value propositions, conduct stakeholder discovery interviews, and develop viable market pathways for their technologies.

Deep Learning Specialization 2017-2018
Coursera
Topics: neural networks (CNN, RNN), deep learning frameworks (Keras, Tensorflow)

Argonne Training Program on Extreme-Scale Computing, Argonne National Laboratory Summer 2017
Invited to an intensive 2-week workshop on high performance computing

NextProf Engineering Future Faculty Workshop, University of Michigan Fall 2015
Invited to participate in a workshop to prepare for faculty positions

International High Performance Computing Summer School, Hungary Summer 2014
Invited to attend NSF workshop to learn new paradigms in scientific computing

Lawrence Livermore National Laboratory, Livermore, CA Summer 2012
Student intern
Comparing Beryllium strength models with experimental data
Supervisors: Dr. B. Remington and Dr. R. Cavallo

Computational Methods in High Energy Density Plasmas, UCLA, CA Spring 2012
Invited to attend a 6 week long workshop by the Institute for Pure and Applied Mathematics at the University of California - Los Angeles

Lawrence Livermore National Laboratory, Livermore, CA Summer 2010
Student intern
Studied hydrodynamic instabilities in inertial confinement fusion targets
Characterized growth factors during capsule compression
Supervisors: Dr. L. J. Suter and Dr. D. S. Clark

Lawrence Livermore National Laboratory, Livermore, CA Summer 2009
Student intern
Studied hot electron signatures and capsule preheat in the context of inertial confinement fusion as developed at the National Ignition Facility
Supervisors: Dr. L. J. Suter and Dr. C. A. Thomas

Lawrence Livermore National Laboratory, Livermore, CA Summer 2008
Student intern
Studied and optimized National Ignition Facility inertial confinement fusion target geometries using view factor calculations
Supervisors: Dr. L. J. Suter and Dr. C. A. Thomas

Volunteer Service and Outreach

NREL Postdoctoral Committee 2016-2018
Organizing networking and professional development activities

DAPCEP Instructor Spring 2015
Organized and taught a 6-week long engineering discovery course for Detroit-area middle school students

Volunteer Instructor, Adams Academy Engineering Club 2014-2016
Instructed fun basic science and engineering projects at a local primary school

Graduate Student Recruiter, University of Michigan 2012-2016
Organized and participated in recruitment events graduate students visiting the Mechanical Engineering department

Skills

Scientific programming
C/C++, Python, GPU (CUDA, SYCL, ROCM, Kokkos, AMReX), MPI, OpenMP, OpenACC, Git

Operating systems
GNU/Linux, OSX

Languages
English, French