Ray W. S. Grout, Ph.D.
National Renewable Energy Laboratory

Education and Training

University of British Columbia, Mechanical Engineering, B.A.Sc., 2002
University of British Columbia, Mechanical Engineering, M.A.Sc. 2004
University of Cambridge, Engineering, Ph.D. 2007

Professional Experience

2011-Present	Scientist IV – HPC Applications Researcher
2010-2011	Scientist II – HPC Applications Researcher Computational Science Center National Renewable Energy Laboratory, Golden, CO
2007-2010	Postdoctoral Appointee Combustion Research Facility Sandia National Laboratories, Livermore, California
2002	Research Assistant University of British Columbia
2000, 2001	Co-op Student (Injector Design) Westport Innovations, Vancouver, Canada
2005-2007	Undergraduate Supervisor University of Cambridge, Cambridge, England

NATIONAL RENEWABLE ENERGY LABORATORY: Computational Sciences Center
Scientist IV – HPC Applications Researcher Dec 2011-present

- Perform calculations for continuum analysis of biomass intraparticle process, point defect chemistry in photovoltaic devices, CFD analysis of biomass reactors.
- NREL lead and project Co-PI: "ExaCT" combustion exascale co-design center (ASCR/DOE LAB 10-07)
- NREL lead on OLCF-CAAR/S3D effort to prepare DNS code for heterogeneous *Titan* architecture

Scientist II – HPC Applications Researcher June 2010-Dec 2011

- Conduct high fidelity (DNS) simulations of canonical configurations to aid understanding of hydrogen based gas turbine combustion
- Analyze high order finite-difference reacting flows solver to identify porting strategy for heterogenous architectures and implement hybrid parallelization strategy

SANDIA NATIONAL LABORATORY: Combustion Research Facility
Postdoctoral Appointee February 2007 to May 2010

- Perform high fidelity (DNS) simulations and probe fundamental combustion processes
- Develop GPGPU analysis routines for particle dataset interrogation and display on visualization clusters
- Develop models for subgrid chemistry effects in turbulent combustion

Selected Publications

1. R.W. Grout, A. Gruber, H. Kolla, P.T. Bremer, J.C. Bennett, A. Gyulassy, and J.H. Chen. "A direct numerical simulation study of turbulence and flame structure in transverse jets analysed in jet-trajectory based coordinates," Journal of Fluid Mechanics, vol 706, pp 351-383, 2012.
2. R.W. Grout, A. Gruber, C.S. Yoo, and J.H. Chen, "Direct numerical simulation of flame stabilization downstream of a transverse fuel jet in cross-flow," Proceedings of the Combustion Institute, vol. 33, pp. 1629-1637, 2011.
3. J.C. Bennett, V. Krishnamoorthy, S. Liu, R.W. Grout, E.R. Hawkes, J.H Chen, J.Shepherd, V. Pascucci, and P-T Bremer. "Feature-based statistical analysis of combustion simulation data," IEEE Transactions on Visualization and Computer Graphics, vol. 17:12, pp. 1822-1831, 2011.
4. R.W. Grout, N. Swaminathan, and R. S. Cant. "Effects of compositional fluctuations on premixed flames" Combustion Theory and Modelling, 13(5), 823–852, 2009
5. Janine Bennett, Ray Grout, Philippe Pèbay, Diana Roe, and David Thompson. "Numerically stable, single-pass, parallel statistics algorithms." In 2009 IEEE International Conference on Cluster Computing (Cluster 2009), New Orleans, Louisiana, August 31-September 4 2009
6. Kyle Spafford, Jeremy Meredith, Jeffrey Vetter, Jacqueline Chen, Ray Grout, and Ramanan Sankaran. "Accelerating s3d: A GPGPU case study". In HeteroPar'2009: Seventh International Workshop on Algorithms, Models and Tools for Parallel Computing on Heterogeneous Platforms, Delft, The Netherlands, August 25, 2009 2009
7. Ajith Mascarenhas, Ray Grout, Peer-Timo Bremer, Valerio Pascucci, Evatt Hawkes, and Jacqueline Chen. "Topological feature extraction for comparison of length scales in terascale combustion simulation data." Presented at TopoInVis: Topological Methods in Data Analysis and Visualization: Theory, Algorithms, and Applications, February 23–24 2009. Snowbird, Utah
8. R. W. Grout. "An age extended progress variable for conditioning reaction rates." Physics of Fluids, 19:105107–105107–11, 2007.
9. R.W. Grout, W. Kendal Bushe, and Colin Blair. "Predicting the ignition delay of turbulent methane jets using conditional source-term estimation." Combustion Theory and Modelling, 2007.
10. N. Swaminathan and R.W. Grout. "Interaction of turbulence and scalar fields in premixed flames". Physics of Fluids, 18(4), 2006.

Synergistic Activities

The co-investigator has expertise in development of turbulent combustion submodels and has a wealth of experience developing several combustion codes at different institutions. Development of databases for jets in cross flow from large-scale direct numerical simulation in collaboration with the gas turbine industry has resulted in valuable data indicating the importance of low velocity recirculation zones and stratified combustion in the stabilization of flames above a jet in cross flow. Earlier work using DNS to probe fundamental understanding of stratified combustion, investigate appropriate flame markers (progress variables, tracers), and propose new models for the combined effects of flame propagation and mixing integrated provisioning of DNS data with end use. Implementation and validation of theoretically proposed combustion models in commercial CFD codes completes the link between academia and engineer; the co-investigator successfully deployed a model for gaseous auto-ignition using *Fluent,* a commercial CFD code, early in his research career. With an academic background in using direct numerical simulation data for assessment and validation of modeling approaches, and technical experience developing DNS data, the co-investigator represents the client in this endeavor as both the provider and user of DNS data.