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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
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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
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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.

## Collaborators

R.S. Cant (Cambridge Univ.); R. Sankaran (Oak Ridge National Lab.); C. S. Yoo (Sandia National Lab.); E.R. Hawkes (Univ. New South Wales); E. S. Richardson (Sandia National Lab.); A. Gruber (Univ. Trondheim); V. Pascucci (Univ. Utah); K.-L. Ma (University of California, Davis); H. Yu (University of Nebraska.); C. Wang (University of California, Davis); J. Bennett (Sandia National Lab.); P.-T. Bremer (Lawrence Livermore National Lab.); W. K. Bushe (University of British Columbia, Vancouver); C. Blair (Westport Innovations); J. Bei (University of British Columbia, Vancouver); A. Mascarenhas (Google); S. Klasky (ORNL); M. Sprague (NREL); P. Graf (NREL); R. Larsen (NREL); M. Nimlos (NREL); B. Donohoe (NREL); P. Pepiot (Cornell); K. Malhotra (Cornell/NREL); N. Swaminathan (Cambridge Univ.); J. Levesque (Cray); H. Kolla (SNL); J.H. Chen (SNL); K. Gruchalla (NREL); S. Lyra (SNL); A. Gyulassy (UC Davis); W. Jones (NREL).

**Graduate Advisors:** Dr. W.K. Bushe (Masters); Drs. N. Swaminathan and R.S.Cant (Doctoral)

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**Education and Training**

B.S., Symbolic Systems, Stanford University, 1989  
Graduate Research Associate, Lawrence Berkeley National Laboratory, 1998-2002  
Ph.D., Mathematics, University of California at Berkeley, 2003  
Postdoctoral Research Associate, NREL, Scientific Computing Center, 2003-2006

**Research and Professional Experience**

2006– Senior Scientist, NREL, Computational Science Center. High performance computing. Applied mathematics. Modeling, simulation, optimization, data mining in support of a variety of renewable energy research. Mathematical research in simulation optimization and multi-scale simulation.

2003–2006 Postdoctoral Research Associate, NREL, Scientific Computing Center. Simulation optimization for alloys and nanostructures.

1998–2002 Graduate Research Associate, Lawrence Berkeley National Laboratory. Mathematical research in optimal prediction and other model reduction techniques for differential equations.

1992–1997 C/C++ Programmer, Access Softek, Inc. Berkeley, Ca. Windows and Macintosh commercial programmer. Highlights from a wide variety of projects include genetic programming based optimization for physical simulation of articulated figures.

**Selected Publications**

1. S. C. Billups, J. Larson, and P. Graf (2013), Derivative-Free Optimization of Expensive Functions with Computational Error Using Weighted Regression, *SIAM J. Optim.*, Vol. 23 (1), 2753.
2. A. M. Nardes, A. J. Ferguson, J. B. Whitaker, B. W. Larson, R. E. Larsen, K. Maturová, P. A. Graf, O. V. Boltalina, S. H. Strauss, N. Kopidakis, (2012), Beyond PCBM: Understanding the photovoltaic performance of blends of indene-C60 multiadducts with poly(3-hexylthiophene), *Advanced Functional Materials* Vol. 22, (19), pp. 4115-4127.
3. M. Lunacek, A. Nag, D. A. Alber, K. Gruchalla, C. Chang, and P. A. Graf, (2011), Simulation, Characterization, and Optimization of Metabolic Models with the High Performance Systems Biology Toolkit, *SIAM J. Sci. Comput.* Vol. 33, pp. 3402-3424.
4. M. E. Köse, P. A. Graf, N. Kopidakis, S. Shaheen, K. Kim, and G. Rumbles, (2009), Exciton Migration in Conjugated Dendrimers: A Joint Experimental and Theoretical Study, *ChemPhysChem*, Vol. 10, (18), pp. 3285-3294.
5. P. Graf, M. E. Köse and K. Kim, Numerical Formulation of the Effective Medium Approximation: Illustrative Examples and Application to Organic Semiconductors, in *Computational Nanoscience How to Exploit Synergy between Predictive Simulations and Experiment*, (Mater. Res. Soc. Symp. Proc. Volume 1177E, Warrendale, PA, 2009), Z7.

6. P. A. Graf, W. B. Jones, and K. Kim, (2009), A note on the virtual crystal approach to alloy optimization, J. Comput. Phys., Vol. 228, pp. 4309.
7. P. Piquini, P. A. Graf, and A. Zunger, (2008), Band-gap Design of Quaternary (In,Ga)(As,Sb) Semiconductors Via the Inverse-band-structure Approach, Phys. Rev. Lett. Vol. 100, 2008; pp. 186403.
8. P. A. Graf and W. B. Jones (2007), A Projection Based Multiscale Optimization Method for Eigenvalue Problems. J. Global Optim. Vol 39, 2007; pp. 235-245.
9. P. A. Graf, K. Kim, W. B. Jones, and L.-W. Wang, (2007), Surface Passivation Optimization Using DIRECT. J. Comput. Phys. Vol. 224(2), 2007; pp. 824-835.
10. K. Kim, P. A. Graf, and W. B. Jones, W.B. (2005), A Genetic Algorithm Based Inverse Band Structure Method for Semiconductor Alloys, J. Comput. Phys. Vol. 208(2), pp. 735-760.

### **Synergistic Activities**

- Moderator, NREL Systems Engineering for Wind Energy Workshop, 2013
- Reviewer, ASCR Early Career Research Program, 2011
- Reviewer, SuperComputing08 Technical Program Committee
- Reviewer, SuperComputing09 Technical Program Committee

### **Collaborators and Co-Editors (past 48 months)**

David Biagioni (CU-Boulder), Stephen Billups (CU-Denver), Katherine Dykes (NREL), Gi-Heon Kim (NREL), Stephan Lany (NREL), Ross Larsen (NREL), Monte Lunacek (CU-Boulder) Andrew Ning (NREL), Michael Sprague (NREL), Sean Shaheen (Denver Univ.), Kandler Smith (NREL), Vladan Stevanovich (NREL), Alex Zunger (CU-Boulder)

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