

Chao Yang

Computational Research Division
Lawrence Berkeley National Laboratory.
One Cyclotron Road, MS-50F,
Berkeley, CA 94720

phone: (510)486-6424
fax: (510)486-5812
email: cyang@lbl.gov

EDUCATION

1994-1998 Rice University

Ph.D in Computational Science and Engineering

1992-1994 The University of Kansas

M.A. in Mathematics

1990-1992 Central Missouri State University

B.S. in Computer Science and Mathematics.

EMPLOYMENT

2000-present Staff Scientist

Computational Research Division
Lawrence Berkeley National Laboratory
Berkeley, CA

2002-2003 On leave from LBNL, Senior Scientist

ILOG, Inc., Mountain View, CA

1999-2000 Householder Fellow in Scientific Computing

Computer Science & Mathematics Division
Oak Ridge National Laboratory, Oak Ridge, TN

1998-1999 Applications Consultant

Advanced Technical Computing Center
NEC Systems Laboratory, Inc., The Woodlands, TX

HONORS

- 2012 Spot Award for contribution to SciDAC projects, CRD, LBNL
- 1999 Householder Fellow in Scientific Computing, Oak Ridge National Laboratory.
- 1998 Ralph Budd Award for best engineering thesis, Rice University.
- 1996 Jack C. Pollard Fellowship, Rice University.

PROFESSIONAL EXPERIENCE

- Associate editor, SIAM Journal on Scientific Computing.

RECENT PUBLICATIONS

- M. Ulbrich, D. Klockner, Z. Wen, C. Yang and Z. Lu, *A Proximal Gradient Method for Ensemble Density Functional Theory*, submitted to SIAM J. Sci. Comp, 2014.
- W. Hu, L. Lin, C. Yang and J. Yang, *Electronic structure of large-scale graphene nanoflakes*, submitted to Journal of Chemical Physics, 2014.
- D. Zuev, E. Vencharynski, C. Yang, A. Krylov, *New algorithms for iterative matrix-free eigensolvers in quantum chemistry*, submitted to Journal of Computational Chemistry, 2014.
- M. Jacquelin, L. Lin and C. Yang, *PSelInv A distributed memory parallel algorithm for selected inversion : the symmetric case*, submitted to ACM Trans. on Math. Software, 2014.
- F. Liu, L. Lin, A. F. Kemper, D. Vigil-Fowler, J. Lischner, F. Jornada, S. Sharifzadeh, J. Deslippe, C. Yang, J. B. Neaton, S. G. Louie, *Numerical integration for ab initio many-electron self energy calculations within the GW approximation*, submitted to Journal of Computational Physics, 2014.
- J. Kaye, L. Lin and C. Yang, *A posteriori error estimator for adaptive local basis functions to solve Kohn-Sham density functional theory*, accepted Communications in Mathematical Sciences, 2014.
- L. Lin, G. Huhs, A. Garcia and C. Yang, *SIESTA-PEXSI: Massively parallel method for efficient and accurate ab initio materials simulation without matrix diagonalization*, J. Phys. Condens. Matter 26, 305503, 2014
- L. Lin, Y. Saad, C. Yang, *Approximating spectral densities of large matrices*, submitted to SIAM Review, 2013.
- Z. Wen, C. Yang, X. Liu and Y. Zhang, *A Penalty-based Trace Minimization Method for Large-scale Eigenspace Computation*, submitted to J. Sci. Comp., 2013.
- H. M. Aktulga, L. Lin, C. Haine, E. G. Ng, and C. Yang, *Parallel Eigenvalue Calculation based on Multiple Shift-invert Lanczos and Contour Integral based Spectral Projection Method*, Parallel Comput. 40, 195, 2014
- S. Marchesini, A. Schirotzek, C. Yang, H. Wu and F. Maia, "Augmented projections for ptychographic imaging", Inverse Problems, vol 29, 2013.
- M. Jung, E. Wilson, W. Choi, J. Shaft, H. M. Aktulga, C. Yang, E. Saule, U. Catalyurek, M. Kandemir, *Exploring the Future of Out-Of-Core Computing with Compute-Local Non-Volatile Memory*, accepted, Supercomputing 2013.

- H. M. Aktulga, C. Yang, E. G. Ng, P. Maris, J. P. Vary, *Improving the Scalability of a Symmetric Iterative Eigensolver for Multi-core Platforms*, in press, *Concurrency and Computation: Practice and Experience*, 2013.
- L. Lin and C. Yang, *Elliptic preconditioner for accelerating the self-consistent field iteration in Kohn-Sham Density Functional Theory*, in press, *SIAM J. Sci. Comp.*, 2013.
- L. Lin, M. Chen, C. Yang and L. He, *Accelerating Atomic Orbital-based Electronic Structure Calculation via Pole Expansion and Selected Inversion*, *J. Phys. Cond. Matter*, vol 25, 295501, 2013.
- J. Qian, C. Yang, A. Schirotzek, F. Maia, and S. Marchesini, *Efficient Algorithms for Ptychographic Phase Retrieval*, to appear in *Contemporary Mathematics*, 2013.
- H. Hu, C. Yang and K. Zhao, *Absorption correction A^* for cylindrical and spherical crystals with extended range and high accuracy calculated by Thorkildsen & Larsen analytical method*, accepted, *Acta Crystallographica*, A 2012.
- Z. Wen, C. Yang, X. Lin and S. Marchesini, *Alternating Direction Methods for Classical and Ptychographic Phase Retrieval*, vol 28, *Inverse Problems*, 2012.
- D. Y. Parkinson, C. Yang, C. Knoechel, C. A. Larabell and M. Le Gros, *Automatic alignment and reconstruction of images for soft X-ray tomography*. *Journal of Structure Biology*, vol 177, no. 2, pp. 259-266, 2012.
- J. C. Meza and C. Yang, *Large-scale Electronic Structure Calculation*, book chapter to appear in *Encyclopedia of Applied Mathematics*, 2012.
- H. M. Aktulga, C. Yang, E. Ng, P. Maris and J. P. Vary, *Topology-aware Mappings for Large-scale Eigenvalue Problems*, *Proceedings of 2012 EuroPar Conference*, 2012.
- Z. Zhou, E. Saule, H. M. Aktulga, C. Yang, E. G. Ng, P. Maris and J. P. Vary, *An out-of-core dataflow middleware to reduce the cost of large scale iterative solvers*. *Proceedings of ICPP conference*, 2012.
- H. M. Aktulga, C. Yang, E. Ng, P. Maris and J. P. Vary, *Large-scale Parallel Null Space Calculation for Nuclear Configuration Interaction*, *Proceedings for High Performance Computational Science Conference*, 2011.
- F. Maia, C. Yang and S. Marchesini, *Compressive auto-indexing in femtosecond nanocrystallography*, *Ultramicroscopy*, vol. 111, pp. 807-811, 2011.
- C. Yang and J. Meza, *Minimizing the Kohn-Sham Total Energy for Periodic Systems*, *Linear Algebra and Its Applications*, vol 436, pp. 2764-2779, 2012.
- L. Lin, C. Yang, J. C. Meza, J. Lu, L. Ying and W. E. SelInv - *An Algorithm for Selected Inversion of a Sparse Symmetric Matrix*, LBNL-2746E, *ACM Trans. on Math. Software*, vol, 37, number 4, 2011.
- C. Yang, Z. Wang and S. Marchesini, *Orientation Determination for 3D Single Molecule Diffraction Imaging*. *Proc. SPIE*, vol, 7800, 2010.

- M. G. Vergniory, C. Yang, A. Garcia-Lekue and L. Wang, *Calculation of complex band structure for plane-wave nonlocal pseudopotential Hamiltonian*. Computational Material Science, vol 48, no. 3, pp 544-550, 2010.
- L. Lin, C. Yang, J. Lu, L. Ying and W. E. *A Fast Parallel Algorithm for Selected Inversion of Structured Sparse Matrix with Application to 2D Electronic Structure Calculations*, LBNL-2677E, 2009, SIAM J. Sci. Comp., vol 33, pp. 1329–1351, 2011.
- J.P. Vary, H. Honkanen, J. Li, P. Maris, S. J. Brodsky, A. Harindranath, G. F. de Teramond, P. Sternberg, C. Yang and E. Ng. *Hamiltonian light-front field theory within an AdS/QCD basis*, Nuclear Physics B, vol. 199, pp 64-73, 2010
- J. P. Vary, H. Honkane, J. Li, S. J. Brodsky, A. Harindranath, G. F. de Teramond, P. Sternberg, E. G. Ng and C. Yang, *Hamiltonian light-front field theory in a basis function approach*, Phys. Rev. C, vol. 81, no. 3. 2010.
- P. Maris, M. Sosonkina, J. P. Vary, E. Ng and C. Yang. *Scaling of ab-initio nuclear physics calculations on multicore computer architectures*. Procedia Computer Science, vol 1, no. 1, pp 97-106, 2010.

SOFTWARE

- **ARPACK** (developer), a widely used package for large-scale eigenvalue calculations
- **arec3d** (main developer), a code for image alignment and 3D tomographic reconstruction of cell structures
- **SPARX** (contributor), a suite of software tools for single-particle cryo-electron microscopy image analysis
- **SelInv** (main developer), a code for computing selected entries of the inverse of a symmetric sparse matrix
- **PEXSI** (main developer), a code for performing pole expansion and selected inversion for electronic structure calculations.
- **KSSOLV** (main developer), a MATLAB toolbox for solving the Kohn-Sham equation with planewave discretization
- **Eigpen** (main developer), a code for computing many smallest eigenvalues of a large, sparse symmetric matrix

RECENT TALKS

1. Green's function Method for electron excitation, invited talk at the workshop on multiscale and nanooptics, Michigan State Univeristy, Aug 2014
2. Green's function Method for electron excitation, Invited talk at the workshop on PDE eigenvalue problems, Chinese Academy of Sciences, Beijing, July 2014

3. Eigenvalue problems in electron excitation, SIAM Annual meeting, July 2014
4. Recent progress on Large-scale eigenvalue problem in nuclear CI calculations, SciDAC NUCLEI annual meeting, Santa Fe, 2014.
5. Greens function theory for electron excitation and computational issues, Workshop on Mathematical and Numerical Analysis of Electronic Structure Theory. Berlin, Germany, Apr, 2014
6. Computational Issues in GW calculations, Invited talk at the Institute of Computational Mathematics, Chinese Academy of Science, September, 2013.
7. Numerical integration of the self energy in GW calculations, Workshop on Green's function methods, University of California, Davis, November, 2013.
8. Preconditioners for Accelerating a Fixed Point Iteration in Electronic Structure Calculations, International Conference on Continuous Optimization, Lisbon, Portugal, July, 2013.
9. Computational Techniques for Accelerating Nuclear Configuration Interaction Calculations in MFDn, International Conference on Nuclear Theory in Supercomputing Era, Ames, Iowa, 2013.
10. Techniques for accelerating electronic structure calculation, SIAM Computational Science and Engineering Conference, Portland, 2013.
11. Large-scale eigensolvers for multicore systems, SIAM Computational Science and Engineering Conference, Portland, 2013.
12. Solving Nonlinear Eigenvalue Problems in Electronic Structure Calculations, joint Math/Chemistry Colloquium, UC-Merced, Oct 5, 2012
13. Phase Retrieval for X-ray Diffractive Imaging, SIAM Annual Meeting, July, 2012
14. Solving Nonlinear Eigenvalue Problems in Electronic Structure Calculation, invited talk at the International Workshop on Mathematical and Numerical Analysis of Electronic Structure Models, Beijing, June, 2012
15. Selected Inversion, Sparse Day Workshop, Toulouse, France, June, 2012
16. Solving Nonlinear Eigenvalue Problems in Electronic Structure Calculations, plenary talk at SIAM Applied Linear Algebra Conference, Valencia, Spain, June, 2012
17. Algorithms for Single Molecule Diffractive Imaging, SIAM Conference on Imaging Science, Philadelphia, PA, May 2012
18. Computational building blocks for large-scale electronic structure calculations, invited talk at the Workshop on Nano-optics, Michigan State University, March 2012
19. Numerical Optimization for Materials Design, Chinese Academy of Sciences, Beijing, Nov. 2011
20. Large-scale X-ray Data Analysis, Shanghai Jiao Tong University, Shanghai, Nov. 2011