Yousef Saad

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Address   Department of Computer Science and Engineering
University of Minnesota
Minneapolis, MN 55455

Education

Doctorat d'Etat	University of Grenoble, France	1983
Doctorat de troisieme cycle	University of Grenoble, France	1974
B. S. in Mathematics	University of Algiers, Algeria	1970

Professional Experience

- I. T. Distinguished Professor, University of Minnesota, Department of Computer Science, May 2005 – present.
- Professor, University of Minnesota, Department of Computer Science, Nov. 1990–present.
- Head of the department of Computer Science and Engineering, University of Minnesota. Jan 1997 – June 2000.
- Senior Scientist, Research Institute for Advanced Computer Science (RIACS), Jul. 1988–Nov. 1990.
- Senior Computer Scientist, Center for Supercomputing Research and Development (CSRD) and Associate Professor, Mathematics Department, University of Illinois at Urbana-Champaign. Aug. 1986–June 1988.
- Research Scientist, then Senior Research Scientist, Computer Science Department, Yale University. July 1984–Aug. 1986.
- Associate professor, University of Tizi-Ouzou, Algeria. Sept. 1983–June 1984.
- Research Scientist, Computer Science Department, Yale University. Aug. 1981–Aug. 1983.
- Visiting Lecturer, Mathematics and Computer Science departments, University of California at Berkeley, Berkeley, CA. January 1981–July 1981.
- Visiting Assistant Professor, Department of Computer Science, University of Illinois at Urbana-Champaign, Urbana, Illinois. January 1980–December 1980.

Research Interests

Iterative methods for solving large sparse linear systems and eigenvalue problems; Tools for sparse matrix computations; Parallel algorithms in numerical linear algebra. Numerical algorithms for materials science. Matrix methods for information sciences

Awards and Honors

- I. T. Distinguished professor (as of May 2005)
- William Norris chair, Jan. 2006 to date

PhD Students (graduated)

- Na Li, PhD, Univ. of Minnesota, Jun. 2006.
- Bernard Sheehan, PhD, Univ. of Minnesota, Nov. 2005.
- Irene Moulitsas, PhD, Univ. of Minnesota, Nov. 2005. [Co-adviser. Main advisor: G. Karypis]
- Abdelkader Baggag, PhD, Univ. of Minnesota, Feb. 2003. [Co-adviser. Main advisor: A. Sameh]
- Edmond Chow, PhD, Univ. of Minnesota, Dec. 1997.
- Kesheng Wu, PhD, Univ. of Minnesota, Mar. 1997.
- Sangback Ma, PhD, Univ. of Minnesota, Aug. 1993.

PhD Students (current)

- J. Chen (Expected graduation: 2010) Passed prelim oral
- S. Sakellaridi (2nd year)
- D. Osei-Kuffuor (2nd year) Grad. Student in Scientific computation
- R. Li (1st year)
- D. Li (1st year) Grad. Student in Scientific computation

Research Grants (Past 5 years)

- "Numerical Linear Algebra and Approximation Theory Methods for Efficient Data Exploration. (sole) PI. $ 275,000 July 2008, 3 years. NSF/DMS.
- "Robust iterative methods for linear systems and least-squares problems", DOE, PI. (Co-PI: M. Sosonkina, Univ. of Iowa and Ames lab.) Start date: 06/15/2008 end Date: 06/14/2011. 405K.
- Scalable methods for electronic excitations and optical responses of nanostructures ... Start date: 05/15/2007 End Date: 05/14/2009 Funding: US Department of Energy. Amount $200,000. (PI: J. Meza, Lawrence Berkeley Lab).
- "MSPA-MCS: Computer Graphics and Visualization Using Conformal Geometry", PI: B. Chen, co-PIs: Xianfeng Gu (SUNY Stony Brook), Yousef Saad. NSF/DMS. Amount $ 312K. Oct. 2005, 3 years.
- "Searching for it: Exploring data with numerical linear algebra and approximation theory", $ 260,000 Sept. 2005, 3 years. NSF/DMS.
- "Virtual Laboratory for Earth and Planetary materials, VLAB", PI: R. Wentkowitz (5 co-PIs). Duration 10/01/04–09/30/08. Total: 1.8M.
- "ITR: Institute for the Theory of Advanced Materials in Information Technology." Period covered: 10/01/2003 – 09/30/08. PI: J. Chelikowsky (4 Co-PIs). Funding: NSF, Total amount of funding: $ 2.5M
- *Parallel Large Scale Sparse Linear System Solvers: New methods and Paradigms* PI: Yousef Saad, Co-PI: Masha Sosonkina, U o Mn, Duluth. Period covered: 06/01/03 – 05/31/2006. Funding: NSF, Total amount of funding: $ 469,839.

Journal Editorships

- Associate editor, SIAM J. on Matrix Analysis (Oct. 2007 – date)
- Associate editor, Computer Physics Communications, Jan 2007 – Jan 2008.
- Associate editor, Electronic Transactions of Numerical Analysis (ETNA), March 2001 to date.

- Associate editor, J. of Numerical Linear Algebra with Applications, 1992 to date.
- Associate editor, IEEE J. Parallel and Distributed Computing. Jan. '96– Jan. '99.
- Associate editor, SIAM J. on Numerical Analysis (June '85 – '94)
- Associate editor, series *Algorithms and Architectures for Advanced Scientific Computing*, Manchester University Press, 1989 – 1992.

Professional Activities

- Organizing committee for IMA Workshop on "Development and Analysis of Multiscale Methods", U of M, Nov. 3-7, 2008.
- Organizing committee for IMA Workshop on "Classical and Quantum Approaches in Molecular Modeling", U of M, July 23-August 3, 2007.
- Committee co-chair for 5th International Workshop on Parallel Matrix Algorithms and Applications (PMAA'08), 20-22 June 2008, Neuchatel Switzerland.
- Committee co-chair for the series of "Precondiontiong xx" meetings, every 2 years since 1999 (Started the first one in June 1999, in Minneapolis). Precondioning 09 will be held on Hong-Kong.
- Consultant for: Scientific Computing Associates (1985–1986), Kuck and Associates Inc. (1986–1988), Dassault Aviation (1988-1989), Object Reservoir (1996), Chevron-Texaco (2002–2004).

University Service

- MSI committee for seed-grants selection 2008-2009
- IMA committee for post-doc selection, 2008.
- Department Head, Jan. 1997 - June 2000.
- Director of Graduate Studies, Program in Scientific Computation, Sept 15, F 1996 - F 1998.
- Chair, Head search committee, academic year 1992-1993.
- Chair, faculty search committee, Academic year 1991-1992.
- Planning Committee, Minnesota Supercomputer Institute (MSI), 1992-1999. Various other committees with MSI since 1991.

Recent Invited Presentations (2006 to 2008)

- Sep 1 – Sep 5, 2008. 'NumAn-08' Conference in Numerical Analysis, Kalamata, Greece. ""Efficient linear algebra methods in data mining", Invited plenary speaker
- June 1 – June 6th, 2008. Householder Symposium XVII, Zeuthen (Germany). June 6th, 2008 "A brief tour of the spectral problems of data mining". Invited plenary speaker.
- April 30th-May 2nd, 2008. Fifth Montreal Scientific Computing Days, University of Montreal. Montreal, Canada, "A tutorial on: Iterative Methods for Sparse Matrix Problems". Invited tutorial speaker.
- Ninth IMACS Inter. Symp. on Iterative Methods, Lille (France). March. 18th, 2008, "Preconditioning techniques for highly indefinite linear systems". Invited plenary speaker.
- Institut Camille Jordan, Lyon (France) March 25th 2008, Invited colloquium speaker (same talk as above).
- Dec 12 – Dec 14, 2007, Workshop on "Solution Methodologies for Scattering Problems", Pau, France. Invited plenary speaker

- Oct 15 – Oct 19 , 2007, Workshop on "Matrix Analysis and Applications", CIRM, Luminy, France. Invited plenary speaker.
- Sep 23 – Sep 28, 2007. 51st Annual Meeting of the Australian Mathematical Society Melbourne, Australia, invited mini-symposium speaker.
- Sep 14th, and Sep. 21st, 2007, Invited colloquium speaker at University of Queensland and at the Queensland University of Technolology (Brisbane,Australia)
- Jul 23 – Aug 03 , 2007, Classical and Quantum Approaches in Molecular Modeling IMA, University of Minnesota, Twin cities. Tutorial speaker and symposium organizer.
- Apr 16 – Apr 18 , 2007, TAMTAM 3rd colloquium on "Trends in Applications of Mathematics in Tunisia, Algeria, Morrocco". Algiers, Algeria. Invited plenary speaker.
- Mar 22 – Mar 23 , 2007, "Third Berlin-Manchester Workshop on Nonlinear Eigenvalue Problems," University of Manchester, England. Invited Plenary Speaker.
- Nov. 7th–8th, 2006 NASA/IA workshop on Higher order Methods and High-Fidelity Flow Simulations. Norfolk, VA. Invited plenary speaker.
- Jun 22 – Jun 23, 2006. AMI06 Workshop on Numerical Linear Algebra, Lille, France. Invited plenary speaker.
- Jun 13 – Jun 17,2006. 15th International Workshop on Matrices and Statistics (IWMS' 2006), Uppsala, Sweden. Invited plenary speaker.
- Feb 23 – Feb 25, 2006, SIAM conf. on Parallel processing for scientific computing , San Francisco. Invited Mini-Symposium speaker.
- Feb 10 – Feb 14, 2006, Center for research in Mathematics (CRM), and University of Montreal (Applied Mathematics Laboratory), Montreal, Canada. Invited colloquium speaker
- Jan 19 – Jan 21, 2006. 22nd GAMM-Seminar on Large Scale Eigenvalue Computations, Leipzig, Germany.   Invited plenary speaker.

Publications: Books

[1] Y. Saad. *Iterative Methods for Sparse Linear Systems, 2nd edition.* SIAM, Philadelpha, PA, 2003.

[2] Y. Saad. *Numerical Methods for Large Eigenvalue Problems.* Halstead Press, New York, 1992.

[3] A. Ferreira, J. Rolim, Y. Saad, and T. Yang. *Parallel Algorithms for Irregularly Structured Problems, Proceedings of Third International Workshop, IRREGULAR'96 Santa Barbara, CA USA, August 19-21, 1996.* Lecture notes in Computer Science, No 1117. Springer Verlag, Berlin, Heidelberg, New-York, 1996. (Conference proceedings).

[4] D. E. Keyes, Y. Saad, and D. G. Truhlar. *Domain-Based Parallelism and Problem Decomposition Methods in Computational Science and Engineering.* SIAM, Philadelphia, PA, 1995. (Conference proceedings).

[5] D. L. Boley, D. G. Truhlar, Y. Saad, R. E. Wyatt, and L. E. Collins. *Practical Iterative Methods for Large Scale Computations.* North Holland, Amsterdam, 1989. (Conference proceedings).

Publications: Journal Articles

[1] M. Bellalij, Y. Saad, and H. Sadok. Analysis of some Krylov subspace methods for normal matrices via approximation theory and convex optimization. *Electronic Transactions on Numerical Analysis*, 33:17–30, 2008.

[2] Dario Rocca, Ralph Gebauer, Yousef Saad, and Stefano Baroni. Turbo charging time-dependent density-functional theory with Lanczos chains. *The Journal of Chemical Physics*, 128(15):154105, 2008.

[3] Zhengkun Feng, Azzeddine Soulaimani, and Yousef Saad. Nonlinear Krylov acceleration for CFD-based aeroelasticity. *Journal of Fluids and Structure*, pages –, 2008. To appear.

[4] C. Bekas, E. Kokiopoulou, and Y. Saad. Polynomial filtered Lanczos iterations with applications in density functional theory. *SIAM Journal on Matrix Analysis and Applications*, 30:397–418, 2009.

[5] J. Chen and Y. Saad. Lanczos vectors versus singular vectors for effective dimension reduction. *IEEE-TKDE*, –:–, 2008. To appear.

[6] J. Chen and Y. Saad. On the tensor SVD and optimal low rank orthogonal approximations of tensors. *SIAM Journal on Matrix Analysis and Applications*, 30(4):–, 2009.

[7] Yunkai Zhou and Yousef Saad. A Chebyshev-Davidson algorithm for large symmetric eigenproblems. *SIAM Journal on Matrix Analysis and Applications*, 29(3):954–971, 2007.

[8] Haw ren Fang and Yousef Saad. Two classes of multisecant methods for nonlinear acceleration. *Numerical Linear Algebra with Applications*, 16(3):197–221, 2009.

[9] J. Jones, M. Sosonkina, and Y. Saad. Component-based iterative methods for sparse linear systems. *Concurrency and Computation: Practice and Experience*, 19:625–635, 2007.

[10] E. Kokiopoulou and Y. Saad. Orthogonal neighborhood preserving projections: A projection-based dimensionality reduction technique. *IEEE TPAMI*, 29:2143–2156, 2007.

[11] M. Ilic, I. W. Turner, and Y. Saad. Linear system solution by null-space approximation and projection (snap). *Numerical Linear Algebra with Applications*, 14:61–82, 2007.

[12] B. Philippe and Y. Saad. On correction equations and domain decomposition for computing invariant subspaces. *Computer Methods in Applied Mechanics and Engineering (special issue devoted to Domain Decomposition)*, 196:1471–1483, 2007.

[13] S. MacLachlan and Y. Saad. A greedy strategy for coarse-grid selection. *SIAM Journal on Scientific Computing*, 29(5):1825–1853, 2007.

[14] S. MacLachlan and Y. Saad. Greedy coarsening strategies for non-symmetric problems. *SIAM Journal on Scientific Computing*, 29(5):2115–2143, 2007.

[15] Yunkai Zhou, Yousef Saad, Murilo L. Tiago, and James R. Chelikowsky. Parallel self-consistent-field calculations via Chebyshev-filtered subspace acceleration. *Phy. rev. E*, 74:066704, 2006.

[16] M.L. Tiago, Y. Zhou, M. M. G. Alemany, Y. Saad, and J.R. Chelikowsky. The evolution of magnetism in iron from the atom to the bulk. *Physical Review Letters*, 97:147201–4, 2006.

[17] Z. Li and Y. Saad. SchurRAS: A restricted version of the overlapping Schur complement preconditioner. *SIAM Journal on Scientific Computing*, 27:1787–1801, 2006.

[18] Yousef Saad, Yunkai Zhou, Constantine Bekas, Murilo L. Tiago, and James R. Chelikowsky. Diagonalization methods in PARSEC. *Physica Status Solidi (b)*, 243(9):2188–2197, 2006.

[19] Y. Zhou, Y. Saad, M. L. Tiago, and J. R. Chelikowsky. Self-consistent-field calculation using Chebyshev-filtered subspace iteration. *J. Comp. Phys.*, 219(1):172–184, 2006.

[20] Y. Saad, J. Chelikowsky, and S. Shontz. Numerical methods for electronic structure calculations of materials. *SIAM review*, 2009. To appear.

[21] Leeor Kronik, Adi Makmal, Murilo L. Tiago, M. M. G. Alemany, Manish Jain, Xiangyang Huang, Yousef Saad, and James R. Chelikowsky. PARSEC the pseudopotential algorithm for real-space electronic structure calculations: recent advances and novel applications to nano-structure. *Phys. Stat. Sol. (B)*, 243(5):1063 1079, 2006.

[22] Na Li and Yousef Saad. MIQR: A multilevel incomplete QR preconditioner for large sparse least-squares problems. *SIAM Journal on Matrix Analysis and Applications*, 28(2):524–550, 2006.

[23] C. Bekas, E. Kokiopoulou, and Y. Saad. An estimator for the diagonal of a matrix. *Applied Numerical Mathematics*, 57(11-12):1214 – 1229, 2007. Numerical Algorithms, Parallelism and Applications (2).

[24] Y. Saad. Filtered conjugate residual-type algorithms with applications. *SIAM Journal on Matrix Analysis and Applications*, 28:845–870, 2006.

[25] M. Bollhöfer and Y. Saad. Multilevel preconditioners constructed from inverse–based ILUs. *SIAM Journal on Scientific Computing*, 27:1627–1650, 2006.

[26] Pascal Henon and Yousef Saad. A parallel multistage ILU factorization based on a hierarchical graph decomposition. *SIAM Journal on Scientific Computing*, 28(6):2266–2293, 2006.

[27] N. Li and Y. Saad. Crout versions of the ILU factorization with pivoting for sparse symmetric matrices. *Electronic Transactions on Numerical Analysis*, 20:75–85, 2006.

[28] C. Bekas, Y. Saad, M. L. Tiago, and J. R. Chelikowsky. Computing charge densities with partially reorthogonalized Lanczos. *Computer Physics Communications*, 171(3):175–186, 2005.

[29] E. Lorin de la Grandmaison, S. B. Gowda, Y. Saad, M. L. Tiago, and J. R. Chelikowsky. Efficient computation of the coupling matrix in time-dependent density functional theory. *Computer Physics Communications*, 167:7–22, 2005.

[30] Y. Saad. Multilevel ILU with reorderings for diagonal dominance. *SIAM Journal on Scientific Computing*, 27(3):1032–1057, 2005.

[31] K. Bekas and Y. Saad. Computation of smallest eigenvalues using spectral Schur complements. *SIAM Journal on Scientific Computing*, 27(2):458–481, 2005.

[32] Riyad Kechroud, Azzeddine Soulaimani, Yousef Saad, and Shivaraju Gowda. Preconditioning techniques for the solution of the Helmholtz equation by the finite element method. *Math. Comput. Simul.*, 65(4-5):303–321, 2004.

[33] M. Sosonkina, Y. Saad, and X. Cai. Using the parallel algebraic recursive multilevel solver in modern physical applications. *Future Generation Computer Systems*, 20:489–500, 2004.

[34] Y. Saad, A. Soulaimani, and R. Touihri. Variations on algebraic recursive multilevel solvers (ARMS) for the solution of CFD problems. *Applied Numerical Mathematics*, 51:305–327, 2004.

[35] W. R. Burdick, Y. Saad, L. Kronik, Manish Jain, and James Chelikowsky. Parallel implementations of time-dependent density functional theory. *Computer Physics Communications*, 156:22–42, 2003.

[36] Z. Li, Y. Saad, and M. Sosonkina. pARMS: a parallel version of the algebraic recursive multilevel solver. *Numerical Linear Algebra with Applications*, 10:485–509, 2003.

[37] S. Ogüt, R. Burdick, Y. Saad, and J. R. Chelikowsky. Ab initio calculations for large dieletric matrices of confined systems. *Phys. Rev. Lett.*, 90(127401), 2003.

[38] N. Li, Y. Saad, and E. Chow. Crout versions of ILU for general sparse matrices. *SIAM Journal on Scientific Computing*, 25(2):716–728, 2003.

[39] Y. Saad. Finding exact and approximate block structures for ILU preconditionning. *SIAM Journal on Scientific Computing*, 24:1107–1123, 2003.

[40] P. Guillaume, Y. Saad, and M. Sosonkina. Rational approximation preconditioners for general sparse linear systems. *Journal of Computational and Applied Mathematics*, 158:419–442, 2003.

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[42] L. Little, Y. Saad, and L. Smoch. Block LU preconditioners for saddle point problems. *Numerical Algorithms*, 2003. Expanded version appeared in SISC, vol. 25 (2003), pp. 729-748.

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[44] M. Bollhöfer and Y. Saad. On the relations between ILUs and factored approximate inverses. *SIAM Journal on Matrix Analysis and Applications*, 24:219–237, 2002.

[45] M. Bollhöfer and Y. Saad. A factored approximate inverse preconditioner with pivoting. *SIAM Journal on Matrix Analysis and Applications*, 23:692–702, 2002.

[46] L. Little, Z. Li, H. G. Choi, and Y. Saad. Particle partitioning strategies for the parallel computation of solid-liquid flows. *Computers in Math. with Applications*, 43:1591–1616, 2002.

[47] A. Soulaimani, N. B. Salah, and Y. Saad. Enhanced GMRES acceleration techniques for some CFD problems. *Int. J. of CFD*, 16(1):1–20, 2002.

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[49] Y. Saad and J. Zhang. Enhanced multi-level block ILU preconditioning strategies for general sparse linear systems. *Journal of Computational and Applied Mathematics*, 130:99–118, 2001.

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[51] Y. Saad. Further analysis of minimal residual iterations. *Numerical Linear Algebra with Applications*, 7:67–93, 2000.

[52] A. Chapman, Y. Saad, and L. Wigton. High-order ILU preconditioners for CFD problems. *Int. J. Numer. Meth. Fluids*, 33:767–788, 2000.

[53] Y. Saad and H. A. van der Vorst. Iterative solution of linear systems in the 20th century. *Journal of Computational and Applied Mathematics*, 123:1–33, 2000.

[54] Y. Saad and J. Zhang. BILUTM: A domain-based multi-level block ILUT preconditioner for general sparse matrices. *SIAM Journal on Matrix Analysis and Applications*, 21:279–299, 2000.

[55] Y. Saad, M. C. Yeung, J. Erhel, and F. Guyomarc. A deflated version of the conjugate gradient algorithm. *SIAM Journal on Scientific Computing*, 21:1909–1926, 2000.

[56] A. Stathopoulos, S. Öğüt, Y. Saad, J.R. Chelikowsky, and H. Kim. Parallel methods and tools for predicting materials properties. *Computing in Science and Engineering*, 2:9–18, 2000.

[57] Andreas Stathopoulos and Yousef Saad. Restarting techniques for (jacobi-) davidson symmetric eigenvalue methods. *Electronic Transactions on Numerical Analysis*, 1999. To appear.

[58] Yousef Saad and Jun Zhang. Diagonal threshold techniques in robust multi-level ILU, preconditioners for general sparse linear systems. *Numerical Linear Algebra with Applications*, 6:257–280, 1999.

[59] C. Le Calvez and Y. Saad. Modified Krylov acceleration for parallel environments. *Applied Numerical Mathematics*, 30:191–212, 1999.

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[61] Y. Saad and M. Sosonkina. Distributed Schur complement techniques for general sparse linear systems. *SIAM Journal on Scientific Computing*, 21(4):1337–1356, 1999.

[62] P. Castillo and Y. Saad. Preconditioning the matrix exponential operator with applications. *J. Scientific Computing*, 13(3):225–302, 1999.

[63] Y. Saad and J. Zhang. BILUM: Block versions of multi-elimination and multi-level ILU preconditioner for general sparse linear systems. *SIAM Journal on Scientific Computing*, 20:2103–2121, 1999.

[64] K. Wu, Y. Saad, and A. Stathopoulos. Inexact Newton preconditioning techniques for eigenvalue problems. *Electronic Transactions on Numerical Analysis*, 7:202–214, 1998. Special issue on eigenvalue methods.

[65] T. F. Chan, E. Chow, Y. Saad, and M. C. Yeung. Preserving symmetry in preconditioned Krylov subspace methods. *SIAM Journal on Scientific Computing*, 20:568–581, 1998.

[66] E. Chow and Y. Saad. Experimental study of ILU preconditioners for indefinite matrices. *Journal of Computational and Applied Mathematics*, 86:387–414, 1997.

[67] E. Chow and Y. Saad. Approximate inverse preconditioners via sparse-sparse iterations. *SIAM Journal on Scientific Computing*, 19:995–1023, 1998.

[68] E. Chow and Y. Saad. ILUS: an incomplete LU factorization for matrices in sparse skyline format. *International Journal for Numerical Methods in Fluids*, 25:739–748, 1997.

[69] Y. Saad. Analysis of augmented Krylov subspace techniques. *SIAM Journal on Matrix Analysis and Applications*, 18:435–449, 1997.

[70] A. Chapman and Y. Saad. Deflated and augmented Krylov subspace techniques. *Numerical Linear Algebra with Applications*, 4:43–66, 1997.

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[73] A. Soulaimani and Y. Saad. An arbitrary Lagrangian-Eulerian finite element method for solving three-dimensional free surface flows. *Comput. Meth. Appl. Mech. Eng.*, 162:79–106, 1998.

[74] E. Chow and Y. Saad. Approximate inverse techniques for block-partitioned matrices. *SIAM Journal on Scientific Computing*, 18:1657–1675, 1997.

[75] Y. Saad and K. Wu. DQGMRES: a direct quasi-minimal residual algorithm based on incomplete orthogonalization. *Numerical Linear Algebra with Applications*, 3:329–343, 1996.

[76] X. C. Cai and Y. Saad. Overlapping domain decomposition algorithms for general sparse matrices. *Numerical Linear Algebra with Applications*, 3:221–237, 1996.

[77] Y. Saad. ILUM: a multi-elimination ILU preconditioner for general sparse matrices. *SIAM Journal on Scientific Computing*, 17(4):830–847, 1996.

[78] Y. Saad, A. Stathopoulos, J. Chelikowsky, K. Wu, , and S. Öğüt. Solution of large eigenvalue problems in electronic structure calculations. *BIT*, 36(3):563–578, 1996.

[79] J. R. Chelikowsky and Y. Saad. Grids in space: The electronic and structural properties of clusters. *Chemical Design Automation News*, 11:29–38, 1996.

[80] X. Jing, N. Troullier, J. R. Chelikowsky, K. Wu, and Y. Saad. Vibrational modes of Silicon nanostructures. *Solid State Communi.*, 96:231, 1995.

[81] J. R. Chelikowsky, X. Jing, K. Wu, and Y. Saad. Molecular dynamics with quantum forces: Vibrational spectra of localized systems. *Physical Review B*, B 53:12071, 1996.

[82] A. Stathopoulos, Y. Saad, and C.F. Fisher. Robust preconditioning of large, sparse symmetric eigenvalue problems. *Journal of Computational and Applied Mathematics*, pages 197–215, 1995.

[83] N. Troullier, J. R. Chelikowsky, and Y. Saad. Calculating large systems with plane waves: Is it a n^3 or n^2 scaling problem? *Solid State Commun.*, 93:225, 1995.

[84] J. R. Chelikowsky, N. Troullier, X. Jing, D. Dean, N. Binggeli, K. Wu, and Y. Saad. Algorithms for predicting the structural properties of clusters. *Computer Physics Communications*, 85:325, 1995. Feature article.

[85] J. R. Chelikowsky, N. Troullier, and Y. Saad. The finite-difference-pseudopotential method: Electronic structure calculations without a basis. *Physical Review Letters*, 72:1240, 1994.

[86] J. R. Chelikowsky, N. Troullier, K. Wu, and Y. Saad. Higher order finite difference pseudopotential method: An application to diatomic molecules. *Physical Review B*, B 50:11355, 1994.

[87] X. Jing, N. Troullier, D. Dean, N. Binggeli, J. R. Chelikowsky, K. Wu, and Y. Saad. Ab initio molecular dynamics simulations of Si clusters using a high-order finite-difference-pseudopotential method. *Physical Review B*, B 50:12234, 1994.

[88] Y. Saad. ILUT: a dual threshold incomplete ILU factorization. *Numerical Linear Algebra with Applications*, 1:387–402, 1994.

[89] P. N. Brown and Y. Saad. Convergence theory of nonlinear Newton-Krylov algorithms. *SIAM Journal on Optimization*, 4:297–330, 1994.

[90] James R. Chelikowsky, N. Troullier, and Y. Saad. The finite difference pseudo-potential method: electronic structure calculations without a basis. *Phys. Rev. Letters*, 72:1240–1243, 1994.

[91] S. Petiton, Y. Saad, K. Wu, and W. Ferng. Basic sparse matrix computations on the cm-5. *Internat. J. of Modern Physics*, 4:65–83, 1993.

[92] Y. Saad. A flexible inner-outer preconditioned GMRES algorithm. *SIAM Journal on Scientific and Statistical Computing*, 14:461–469, 1993.

[93] Y. Saad. Analysis of some Krylov subspace approximations to the matrix exponential operator. *SIAM Journal on Numerical Analysis*, 29:209–228, 1992.

[94] E. Gallopoulos and Y. Saad. Efficient solution of parabolic equations by polynomial approximation methods. *SIAM Journal on Scientific and Statistical Computing*, 13:1236–1264, 1992.

[95] T. Kerkhoven and Y. Saad. Acceleration techniques for decoupling algorithms in semiconductor simulation. *Num. Mat.*, 60:525–548, 1992.

[96] B. Philippe, Y. Saad, and W. J. Stewart. Numerical methods in Markov chain modeling. *Journal of Operations Research*, 40(6):1156–1179, 1992.

[97] B. Datta and Y. Saad. Arnoldi methods for large Sylvester-like observer problems, and an associated algorithm for partial spectrum assignment. *Linear Algebra and its Applications*, 154-156:225–244, 1991.

[98] P. N. Brown and Y. Saad. Hybrid Krylov methods for nonlinear systems of equations. *SIAM J. Sci. Stat. Comp.*, 11:450–481, 1990.

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[100] T. Kerkhoven, A. Galick, U. Ravaioli, J. Arends, and Y. Saad. Efficient numerical simulation of electron states in quantum wires. *J. Applied Physics*, 68:3461–3469, 1990.

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