

LOS ALAMOS NATIONAL LABORATORY
Freely Distributable Software
Acknowledgement Form

Primary Author's / Software Steward's Name William Matthew Challacombe
Software Name (include acronym if applicable): Mondo SCF, Version 1.0

It has been decided that it is in the best interest of Los Alamos National Laboratory that this piece of code be distributed freely and with unrestricted use to the public including foreign entities and governments.

I understand that there are no export control restrictions for this software once it has been distributed. Please include your LA-CC number; 01-2

This software is being distributed in the following manner: Freely distributed to the public domain for the following reasons:

1. the quantum chemistry software market is a crowded market with stiff competition with a main vendor who is highly competitive,
2. we would like to attract collaborators to add value to the code,
3. we would like to establish scientific credibility by allowing public scrutiny and comment, and
4. we would like to place the burden of bug fixes and feature enhancements on a pool of collaborators

I certify that this code has been reviewed for its intellectual property issues based on the completed Software Questionnaire:

Hene D'Vazal
Author's signature

Date 2/7/01

I certify that I agree to freely distribute this software and by doing so release all privileges, including any expectations of royalties, associated with commercializing this technology.

Matt Challacombe
Author's signature

Date 2/7/01

Eric Whaley
Author's signature

Date 2/7/2001

C.S. Bishop
Author's signature

Date 2/7/2001

Mike Shultz
Author's signature

Date 2/7/2001

I certify that on behalf of the division management that it is in the best interest of this Laboratory to freely distribute this software:

Alan R. Bishop
Division Leader Signature

Date 2/8/01

Los Alamos

NATIONAL LABORATORY

Copyright Disclosure

C Number
(IBD use only)

Instructions: When completed, submit to Industrial Business Development IPM Copyright Team, MS C334, Phone 5-9091, Fax 5-0154.

1. Copyright Name [If software, list name (acronym, if applicable), version no. Ex: Electronic Chemical Database (ECD), Vers. 1.0]

MondoSCF 1.0

Is this a beta test version? Yes No

Version date 02/01/01

2. External Contributions

(a) Incorporated copyrights: Code obtained from the Internet, canned copyright systems, etc. Attach a copy of the copyright notice(s) for each.

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(b) Non-UC authors (contractors, industrial partners, certain students). Attach individual's employment agreement.

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3. Documentation Is there a user guide or installation instructions with "help" file?

Yes No Under development If under development, estimated date of completion _____

4. Specifics Software Firmware Artwork Schematics

If software, provide:

Computer Platform UNIX Programming Language FORTRAN 90/95 Operating System(s) Mathematica UNIX

5. Funding

Copyright Development Program and B&R Codes	Fiscal year	<u>1999</u>	<u>2000</u>	<u>2001</u>
	Program Code(s)	<u>JAA5</u>	<u>JAA5</u>	<u>JAMP</u>
	Corresponding B&R Code(s)	<u>DP0811030</u>	<u>DP0811030</u>	<u>DP0811030</u>

Major funding source (DOE, DoD, etc.) DoE, NSF

Did this copyright result from some type of collaborative arrangement (CRADA, FIA, etc.)?

Yes No If yes, please list: Agreement number _____ Company Name _____

6. Classification Review Yes No If yes, date 1/28/01
Los Alamos Computer Code (LA-CC) Number 01-2 (Attach copy of review)

7. Export Control Review Yes No If yes, date _____
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8. UC Authors: (Staff Member, Post Doc, GRA, etc.) Note that the employee Z number and country of citizenship are required. If needed, attach list of additional authors listing the same information.

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9. Abstract: Attach a brief description of the software and its functionality, such that someone who is not familiar with the code can understand.

10. Commercial Potential

Does the software (or document) have commercial potential? Yes No If yes, attach explanation.

11. Certification I certify that the information contained in this disclosure is accurate to the best of my knowledge. I understand that I will probably be requested to submit source code and documentation to IBD in order for IBD to fulfill the DOE order to submit all copyright asserted software to ESTSC.

Copyright Steward (UC/LANL employee responsible for managing the code)

Printed Name MATT CHALLACOMBE Z Number 121768 Signature M. Challcombe Date 02/01/01

Approval/Signature (Steward's Line Manager or Group Leader)

Printed Name and Title ANTONIO REDONDO, Group Leader Signature A. Redondo Date 02/02/01

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To: mchalla@lanl.gov,
tymczak@lanl.gov,
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From: Mark M Jones <mmj@lanl.gov>
Subject: MondoSCF Review
Cc: joyj@lanl.gov,
johnson@lanl.gov,
irenev@lanl.gov,
sbrockway@lanl.gov,
gallegosjan@lanl.gov
Mime-Version: 1.0
Content-Type: text/html; charset="us-ascii"
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Distribution should be in accordance with LANL's Technology Transfer
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<div>Mark M Jones</div>
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<div>Mail Stop F674, ph. 7-5011, fax 5-4251</div>
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MondoSCF is a suite of programs for performing ab initio electronic structure calculations using Gaussian orbital basis functions. Its primary feature is that it encumbers only an $O(N \lg N)$ computational complexity, where N is proportional to problem size. The code is able to perform self-consistent-field calculations on molecules and systems with periodic boundary conditions using the Hartree-Fock and Density Functional Theories.

Relevant publications:

"Linear scaling computation of the Fock matrix. V.
Hierarchical cubature for numerical integration of
the exchange-correlation matrix"

M. Challacombe
JOURNAL OF CHEMICAL PHYSICS, v. 113(#22) pp. 10037-10043 DEC 8, 2000

"Linear scaling computation of the Fock matrix. IV.
Multipole accelerated formation of the exchange matrix"
E. Schwegler and M. Challacombe, JOURNAL OF CHEMICAL PHYSICS,
v. 111(#14) pp. 6223-6229 OCT 8, 1999

"A simplified density matrix minimization for linear scaling
self-consistent field theory"
M. Challacombe, JOURNAL OF CHEMICAL PHYSICS,
v. 110(#5) pp. 2332-2342 FEB 1, 1999

"Periodic boundary conditions and the fast multipole method"
M. Challacombe, C. White and M Head-Gordon
JOURNAL OF CHEMICAL PHYSICS, v. 107(#23) pp. 10131-10140 DEC 15, 1997

"Linear scaling computation of the fock matrix. II
Rigorous bounds on exchange integrals and incremental Fock build"
E. Schwegler, M. Challacombe and M. Head-Gordon
JOURNAL OF CHEMICAL PHYSICS, v. 106(#23) pp. 9708-9717 JUN 15, 1997

"Linear scaling computation of the Fock matrix."
M. Challacombe and E. Schwegler
JOURNAL OF CHEMICAL PHYSICS, v. 106(#13) pp. 5526-5536 APR 1, 1997

MondoSCF Copyright Disclosure. Attachment 9. Abstract.

MondoSCF is an experimental code for Quantum Chemistry. Quantum Chemistry involves approximate solutions to the Schrodinger equation for the prediction of chemical properties and their theoretical interpretation. The main thrust of MondoSCF is the development of leading edge, reduced complexity algorithms that scale linearly with system size.

Work on MondoSCF began in 1994 with Eric Schwegler when I was a postdoc in Jan Almlöf's group at the Minnesota Supercomputer Institute (NSF funded), and in continued work with Martin Head-Gordon at UC Berkeley in 1997 (DOE funded). I have continued the development of this code since coming to LANL in late 1997. Substantial (~1–2 FTE years) effort has also been put towards its development by myself and Eric Schwegler in our free time.

MondoSCF is highly modular, and has been written in object oriented Fortran90, C and Mathematica. Platform independent IO is supported with HDF5. MondoSCF has incorporated several external contributions. These include PhiPAC for optimized matrix–matrix multiplies, a number of Mathematica packages for producing source code from algebraic equations, and various routines from the SLATEC library. The copyright notices for these contributions are listed in Attachment 2.

Platforms on which MondoSCF is known to run include IRIX/MIPSF90, LINUX/PGF90, LINUX/NAGF95 and AIX/XLF90.

Currently, MondoSCF performs Hartree–Fock, pure Density Functional, and hybrid HF/DFT calculations in a Cartesian–Gaussian basis. All algorithms are linear scaling for non–metallic systems. Work is presently underway to implement periodic boundary conditions, forces and to parallelize the code.

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QUANTUM CHEMISTRY SOFTWARE UPROAR

Gaussian says license policies are needed to protect code, but some chemists say restrictions go too far

Elizabeth K. Wilson

C&EN West Coast News Bureau

Like many of his colleagues in theoretical chemistry, Northwestern University postdoc Vitaly Rassolov occasionally used Gaussian, the popular, all-purpose workhorse software for doing quantum chemistry.

Rassolov's primary adviser was chemistry professor Mark A. Ratner. But Rassolov also worked on projects that included one of Ratner's collaborators, chemistry professor John Pople. Pople was the developer of the original Gaussian programs, for which he shared the 1998 Nobel Prize in Chemistry. He had long since parted ways with Gaussian Inc. --the company that markets the program--and had recently taken up with a competing company called Q-Chem. The license agreement that Northwestern signed with Gaussian Inc. forbade competitors access to the software.



Pople developed original Gaussian programs.

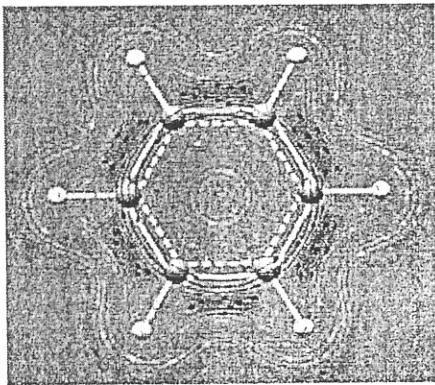
But, the group reasoned, Rassolov himself was not a competitor, and his work was primarily with Ratner, not Pople, and was not related to software development. Besides, Rassolov says he had already notified Gaussian more than a year ago of the collaboration.

So it came as a shock when, on March 19, the university received a letter from Gaussian Inc. saying that the group's failure to notify them of Rassolov's association with Pople violated their

business sense.

Right now, chemists say they're suffering because frequently, nothing does the job as well as Gaussian. It is largely due to Gaussian's ease of use that it has now become commonplace for experimental chemists to augment their results with theory. According to one estimate, Gaussian is used, at least part of the time, by 90% of researchers doing ab initio quantum chemistry.

Ab initio, or "from first principles," refers to the strategy of describing atoms or molecules from the ground up based on their electronic structures. This can be accomplished by solving the Schrödinger equation, which uses wave functions to calculate a molecule's energy, geometry, and other properties. Numerous techniques accomplish this, many based on the method known as Hartree-Fock. The mathematics involved can be prohibitively time consuming and difficult, especially for large molecules. But advances in theory and the increasing power of computers have made many such calculations feasible.



Gaussian predicts properties such as those shown in this current flow diagram for benzene. [Courtesy of Gaussian Inc.]

One revolutionary theoretical shortcut, known as density functional theory (DFT), greatly simplifies things. DFT calculates molecular energies based on a molecule's electron density rather than wave function. As DFT's primary developer, University of California physics professor Walter Kohn shared the 1998 Nobel Prize with Pople.

The Gaussian package contains an enormous number of capabilities based on both Hartree-Fock and DFT. It can run calculations that predict, for example, a molecule's NMR chemical shift, infrared and Raman spectral intensities, or structure.

Over the years, other ab initio quantum chemistry software programs, such as Jaguar by Schrödinger, Spartan by Wavefunction, or Q-Chem by Q-Chem, have emerged. But though they can perform many of the functions that Gaussian does--and some of them even better--none of them yet do them all.

Many theorists on the cutting edge use their own specialized programs and so aren't much affected by the loss of Gaussian. But others have found themselves in a real bind.

Lawrence S. Norris, a graduate student at Northwestern, says that without Gaussian, parts of his

theoretical chemistry lecturer. Gill takes up the chair of theoretical and computational chemistry at the University of Nottingham later this year, and "Nottingham has already received their Gaussian letter," he says.

And over the past couple of years, chemistry professor Henry F. Schaefer III, at the University of Georgia, Athens, joined Q-Chem's board, and Thomas R. Furlani, the associate director at SUNY Buffalo's CCR, became a Q-Chem consultant. Both those universities have site licenses for Gaussian 94, but they have been unable to upgrade to Gaussian 98.

At these universities, the individual group licenses have explicit wording designed to make sure competitors stay away from Gaussian: "The licensee will not use or permit any person or third party to use the software in any manner or way that will compete with the business of Gaussian or will provide assistance to any competitor of Gaussian."

But that wording goes beyond what's truly necessary, maintains Walter B. McRae, associate vice president for computing and networking at the University of Georgia, who is also a former theoretical chemist. "I've been in the game a long time. I license millions of dollars of software a year, and I've never seen that," he says.

But Frisch insists such precautions are well within reason and shouldn't interfere with the licensee's research. "Our intention is to allow free access, except to those developing competing products," he says. "Gaussian Inc. bends over backward to publish our scientific developments and to make our software, including source code, available at modest prices."

Some say the current licensing issues are rooted in the history of Gaussian Inc. For example, there were conflicts early on when Pople wished to distribute Gaussian profits among former postdocs and graduate students who helped develop the code, while others at Gaussian wanted to return the money to research.

In 1992, a former Pople graduate student named Benny Johnson, who was helping develop DFT capabilities for Gaussian, squabbled with some members of Gaussian Inc. over the intellectual rights to some of the code. The conflict was serious enough that he, Gill, and former Pople postdoc Carlos Gonzalez formed the competing Q-Chem. Pople left Gaussian Inc., and as part of the agreement, he was forbidden from affiliating with any competitor until Jan. 1, 1999. Shortly after that date rolled around, Pople joined Q-Chem's board of directors.

Soon afterward, the Northwestern situation came to a head, according to several sources. At a seminar to celebrate Pople's winning the Nobel Prize--dubbed the "Pople People Party," held March 6-7, 1999, on Amelia Island, Fla.--Rassolov delivered a talk on density functional theory's ability to describe a chemical bond. The paper included work using Gaussian.

Less than two weeks later, Northwestern's license was revoked.

Rassolov insists, however, that he and Pople deliberately attempted to make their relationship known to Gaussian Inc. by offering them prepublished research results. In an e-mail exchange that began March 10, 1998, Rassolov offered Gaussian a copy of the data, listing Pople, Ratner, and himself as authors. Frisch accepted the offer, and Rassolov sent the data in another e-mail dated March 11, along with a note stating that the data were obtained with Gaussian and again

Frisch argues, however, that "the program is provided to them for their research, not so that they can help to improve competing products." He adds, "None of the users at these sites benchmarks computers as their research activity, so we don't view this limitation as terribly restrictive."

The University of Georgia's Schaefer acknowledges that his affiliation with Q-Chem has created a "rough situation" at his university. He says that despite the difficulties, he still has warm relations with the Gaussian Inc. principals, several of whom were his former postdocs. But when he joined Q-Chem, "it never occurred to me it would cause trouble with the Gaussian license," he says. "It's been something of a gut-wrenching experience."◀

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