

EMSL SOFTWARE USER AGREEMENT

This is an agreement between BATTELLE MEMORIAL INSTITUTE, on behalf of the U.S. Department of Energy, through its Contract No. DE-AC06-76RL 01830, located in Richland, Washington, (hereinafter called "BATTELLE"), and

located in _____, (hereinafter called USER).

WHEREAS BATTELLE has rights to the following software systems (1) NWChem, a computational chemistry program (electronic structure and molecular dynamics) for parallel computers, and (2) Extensible Computational Chemistry Environment ("Ecce"), a suite of programs that assists a computational chemist in the building of molecular structures, setup and management of a computational calculation, execution of the calculation on a local or remote system, and visualization of the resultant data properties (both hereinafter, along with associated documentation and all other software furnished by BATTELLE, referred to as "the SOFTWARE"), developed at the Pacific Northwest National Laboratory operated by BATTELLE under Contract Number DE-AC06-76RL 01830 for the U.S. Department of Energy; and

WHEREAS USER desires to use the SOFTWARE for scientific purposes.

NOW THEREFORE, in consideration of mutual covenants contained herein, the parties hereto represent and agree as follows:

1. USE OF THE SOFTWARE

BATTELLE agrees to provide one copy of the SOFTWARE to USER for an unlimited evaluation, testing, and use period subject to termination provisions contained in section 7 below.

2. PROPERTY RIGHTS

- (a) It shall be within BATTELLE's sole discretion whether or not to enter into this Agreement with a prospective USER.
- (b) USER shall take any reasonable action requested by BATTELLE to protect BATTELLE's rights, and to protect the SOFTWARE from unauthorized disclosure.
- (c) USER shall keep the SOFTWARE free and clear of all claims, liens and encumbrances.
- (d) USER shall immediately give notice to BATTELLE of any knowledge it has concerning any infringement of BATTELLE's rights, whether by USER's own employees or any other third party.
- (e) USER has the right to utilize the SOFTWARE in the development of its application programs for its own internal use only.
- (f) USER shall have the right to modify the SOFTWARE.
- (g) BATTELLE shall have a paid-up, irrevocable, nonexclusive license to (i) copy USER's modifications to the SOFTWARE ("USER Modifications"), (ii) use USER Modifications, (iii) modify USER Modifications, (iv) distribute USER Modifications, and (v) grant sublicenses to use, modify and copy USER modifications.

3. RESTRICTIONS ON USE

- (a) USER understands that the SOFTWARE is valuable to BATTELLE and its licensors. USER shall use the SOFTWARE for its own internal operations on computers identified in Attachment A, and shall provide access to its customers who agree to be bound hereunder. All additional entities given access to the SOFTWARE shall be provided a copy of the Software User Agreement and shall agree to comply with all obligations therein. USER shall not directly or indirectly sell, give, offer, or transfer the SOFTWARE or any part thereof to any party outside this Agreement.
- (b) USER shall not permit anyone else to copy the SOFTWARE without the prior written consent of BATTELLE and/or its licensors. USER shall not reverse compile, or reverse assemble the SOFTWARE in whole or in part. Source code is available only on approved special request, and if provided to USER, USER agrees that it will not provide such source code or its associated object code in any form to any third party without BATTELLE's express written consent.

(c) USER's right to possess and use the SOFTWARE shall not be assigned, licensed, or transferred to a successor, affiliate, or any other person, firm, corporation, or organization without the prior written consent of BATTELLE. Any such assignment, license, or transfer without such consent shall be void.

(d) In publicizing results obtained either in part or in full from use of the unmodified SOFTWARE, USER shall place in a conspicuous location on all copies of the document containing the results, the following citations;

For NWChem

Straatsma, T.P.; Aprà, E.; Windus, T.L.; Dupuis, M.; Bylaska, E.J.; de Jong, W.; Hirata, S.; Smith, D.M.A; Hackler, M.; Pollack, L.; Harrison, R.; Nieplocha, J.; Tipparaju V.; Krishnan, M.; Brown, E.; Cisneros, G.; Fann, G.; Fruchtl, H.; Garza, J.; Hirao, K.; Kendall, R.; Nichols, J.; Tsemekhman, K.; Valiev, M.; Wolinski, K.; Anchell, J.; Bernholdt, D.; Borowski, P.; Clark, T.; Clerc, D.; Dachsels, H.; Deegan, M.; Dyall, K.; Elwood, D.; Glendening, E.; Gutowski, M.; Hess, A.; Jaffe, J.; Johnson, B.; Ju, J.; Kobayashi, R.; Kutteh, R.; Lin, Z.; Littlefield, R.; Long, X.; Meng, B.; Nakajima, T.; Niu, S.; Rosing, M.; Sandrone, G.; Stave, M.; Taylor, H.; Thomas, G.; van Lenthe, J.; Wong, A.; Zhang, Z.; "NWChem, A Computational Chemistry Package for Parallel Computers, Version 4.5" (2003), Pacific Northwest National Laboratory, Richland, Washington 99352-0999, USA.

"High Performance Computational Chemistry: an Overview of NWChem a Distributed Parallel Application", Kendall, R.A.; Apra, E.; Bernholdt, D.E.; Bylaska, E.J.; Dupuis, M.; Fann, G.I.; Harrison, R.J.; Ju, J.; Nichols, J.A.; Nieplocha, J.; Straatsma, T.P.; Windus, T.L.; Wong, A.T. *Computer Phys. Comm.*, 2000, 128, 260-283

For Ecce

Black, G.; Didier, B.; Feller, D.; Gracio, D.; Hackler M.; Havre S.; Jones, D.; Jurrus, E.; Keller, T.; Lansing, C.; Matsumoto, S.; Palmer, B.; Peterson M.; Schuchardt, K.; Stephan, E.; Taylor, H.; Thomas, G.; Vorpagel, E.; Windus, T.; Winters C.; "Ecce, A Problem Solving Environment for Computational, Software Version 3.0" (2002), Pacific Northwest National Laboratory, Richland, Washington 99352-0999, USA.

"Ecce – A Problem-Solving Environment's Evolution Toward Grid Services and a Web Architecture," Concurrency and Computation: Practice and Experience 14, 1221-1239, 2002, K.L. Schuchardt, B.T. Didier, G.D. Black

(e) In publicizing results obtained either in part or in full from use of a modified version of NWChem, USER shall place in a conspicuous location on all copies of the document containing the results, the following citations;

Citation:

Straatsma, T.P.; Aprà, E.; Windus, T.L.; Dupuis, M.; Bylaska, E.J.; de Jong, W.; Hirata, S.; Smith, D.M.A; Hackler, M.; Pollack, L.; Harrison, R.; Nieplocha, J.; Tipparaju V.; Krishnan, M.; Brown, E.; Cisneros, G.; Fann, G.; Fruchtl, H.; Garza, J.; Hirao, K.; Kendall, R.; Nichols, J.; Tsemekhman, K.; Valiev, M.; Wolinski, K.; Anchell, J.; Bernholdt, D.; Borowski, P.; Clark, T.; Clerc, D.; Dachsels, H.; Deegan, M.; Dyall, K.; Elwood, D.; Glendening, E.; Gutowski, M.; Hess, A.; Jaffe, J.; Johnson, B.; Ju, J.; Kobayashi, R.; Kutteh, R.; Lin, Z.; Littlefield, R.; Long, X.; Meng, B.; Nakajima, T.; Niu, S.; Rosing, M.; Sandrone, G.; Stave, M.; Taylor, H.; Thomas, G.; van Lenthe, J.; Wong, A.; Zhang, Z.; "NWChem, A Computational Chemistry Package for Parallel Computers, Version 4.5" (2003), Pacific Northwest National Laboratory, Richland, Washington 99352-0999, USA. A modified version.

"High Performance Computational Chemistry: an Overview of NWChem a Distributed Parallel Application", Kendall, R.A.; Apra, E.; Bernholdt, D.E.; Bylaska, E.J.; Dupuis, M.; Fann, G.I.; Harrison, R.J.; Ju, J.; Nichols, J.A.; Nieplocha, J.; Straatsma, T.P.; Windus, T.L.; Wong, A.T. *Computer Phys. Comm.*, 2000, 128, 260-283

(f) The USER is requested to send the citation for any publications using NWChem or a modified version of NWChem to nwchem-support@emsl.pnl.gov or to the address shown in Attachment A. The USER is requested to send the citation for any publications using Ecce to ecce-support@emsl.pnl.gov.

4. CONFIDENTIALITY

USER shall maintain the SOFTWARE in confidence. USER shall not divulge information relating to the SOFTWARE, with the exception of results derived from use of the SOFTWARE, to any third party or use such information for its own benefit without the prior written consent of BATTELLE or make any copies of the SOFTWARE, except that a single copy and a backup copy can be made for installation on the "hard disk" of a single computer system connected, with the appropriate protection, to a network to

ensure that the SOFTWARE cannot be accessed by anyone who is not legally bound to respect the confidentiality herein, provided that such copies reproduce the proprietary rights notices for the SOFTWARE. USER shall treat the SOFTWARE with the same degree of care as it accords to proprietary information in its possession but, in any event, not less than reasonable care. USER agrees not to divulge information concerning the performance (e.g., accuracy of results, computational speed, convergence of calculations, benchmarking) of the SOFTWARE without prior written consent of BATTELLE, except that computer system vendors may report results to customers for a hardware procurement so long as the customer has entered into a non-disclosure agreement with the computer system vendor to protect such information.

5. WARRANTIES

(a) Nothing in this Agreement shall be deemed to be a representation or warranty by BATTELLE, its licensors, or the U.S. Government of the accuracy or usefulness for any purpose of the SOFTWARE, it being agreed that the SOFTWARE is provided on an "AS IS" basis without warranty. **BATTELLE GRANTS NO WARRANTIES, EITHER EXPRESS OR IMPLIED, ON THE SOFTWARE OR ANY SERVICES PROVIDED OR PERFORMED, INCLUDING THOSE CONCERNING MERCHANTABILITY OR FITNESS FOR A PARTICULAR PURPOSE.**

(b) Neither BATTELLE, nor its licensors nor the U.S. Government shall be liable to USER or any other person for any loss of profits, loss of use, interruption of business, or for any indirect, special, general, incidental, or consequential damages, of any kind in connection with or arising out of the furnishing, performance, or use of the SOFTWARE or services. No obligation or liability shall arise or flow out of BATTELLE's rendering technical or other advice in connection with the SOFTWARE or services.

6. REMEDIES

In the event that any unauthorized use of the SOFTWARE is made or threatened, BATTELLE and/or its licensors may take appropriate action, in law or equity, to seek compensation or prevent such use. BATTELLE's licensors are third party beneficiaries to this Agreement.

7. TERMINATION

This Agreement may be terminated at any time upon thirty (30) days' written notice by either party. Upon such termination, USER shall remove from the computers specified in Attachment A, and return, the original and all reproductions, including partial reproductions of the SOFTWARE and documentation, and so certify in writing to BATTELLE. All copies of the User's Guide and any other documentation shall promptly be returned to BATTELLE.

8. INVALIDITY

If any provision or provisions of this Agreement shall be held to be invalid, illegal, or unenforceable, the validity, legality, and enforceability of the remaining provisions shall not in any way be affected or impaired thereby.

9. EXPORTATION OF THE SOFTWARE

USER shall adhere to the export Laws and Regulations of USER's country. USER agrees to comply with all requirements of the Export Administration Regulations, including the requirement for obtaining any export license, if applicable. USER agrees to indemnify, defend and hold harmless BATTELLE, its officers, agents and employees from all liability involving the violation of any export regulations, either directly or indirectly, by USER.

10. GOVERNING LAW

This Agreement will be construed in accordance with the Laws of the State of Washington of The United States of America and in the English language, and USER agrees that any action brought to enforce any provision or obligation hereunder shall be brought in a court of competent jurisdiction in the State of Washington.

11. ENTIRE AGREEMENT

The parties agree that the terms and conditions herein constitute the entire agreement between the parties and supersede all previous communications, proposals, representations, and agreement, whether oral or written, relating to the subject matter of this Agreement. The provisions of this Agreement are severable.

12. SIGNATURE

USER indicates acceptance of the terms of this Agreement by his or her signature below.

USER_____

SIGNED BY_____

PRINTED NAME_____

TITLE_____

DATE_____

BATTELLE MEMORIAL INSTITUTE

SIGNED BY_____

DATE_____

Attachment A
User Information Request Form

Please TYPE the following information and return with the signed agreement by:

Fax (illegible faxes will be returned)

**Jessica Foreman
PNNL
509/376-0420**

Surface mail

**Jessica Foreman
PNNL
P.O. Box 999 MS K8-91
Richland WA 99352
USA**

1. Name and mailing address of Facility:

2. Facility Point of Contact/USER:

(This is the person responsible for ensuring that the EMSL Software User Agreement is upheld and **must be a faculty member or permanent staff of facility.**)

Job Title:

Phone:

Fax:

email:

3. Facility SOFTWARE support:

(This person is responsible for being the first line of support for SOFTWARE at your site. All issues regarding SOFTWARE will be forwarded to the SOFTWARE development team via this contact.)

Job Title:

Phone:

Fax:

email:

4. Primary system hardware/software configuration:

Vendor:

Model identification:

Number of processors:

Aggregate Memory size:

Aggregate Disk size:

Operating System:

Fortran Compiler version number:

C Compiler version number:

Batch/Queue software used:

5. Do you require NWChem source code? (yes/no)

If yes, please justify your request below.

6. Please describe the User community below (e.g., academic researchers, DOE Weapons, Commercial, etc.) and estimate the number of users on this computer system.

7. Please list all known EMSL collaborative projects which are being conducted on this computer system.