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Pacific Northwest
NATIONAL LABORATORY
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Battelle Memorial Institute, Pacific Northwest Division
Acting Under Contract DE-AC05-76RL01830
With the U.S. Department of Energy
Operating the Pacific Northwest National Laboratory (PNNL) (www.pnnl.gov)

Schedule
Contract Number: 392089

Issued by:	**Name and Address of Contractor:**
Battelle Battelle Boulevard, K9-15 P.O. Box 999 Richland, WA 99352-0999 USA Contracts Specialist: [redacted] Telephone Number: [redacted] Fax Number: [redacted] Email: Bryan.Colley@pnnl.gov	J. Heyrovsky Institute of Physical Chemistry of the Czech Academy of Science, v. v. i. Dolejškova 2155/3 Prague 8, 182 23 CZE Contractor Contact: [redacted] Telephone Number: [redacted] Fax Number: Email: [redacted]
Payment Terms: Net 30	**Contract Type:** Fixed Price
Submit Invoices to ap.invoices@pnnl.gov. **Note:** Invoices must list location(s) of service (US: City, State; Foreign: Country).	**Total Contract Amount:** $25,000.00
Contract Period of Performance: January 22, 2018 through September 30, 2021	
Award Battelle hereby agrees to award this Contract to the Contractor subject to acceptance. The rights and obligations of the parties to this Contract are subject to and governed by this document and any documents attached or incorporated by reference.	**Contractor Agreement** Contractor accepts and agrees to furnish and deliver the items or perform services to the extent stated in this document for the consideration stated in this contract. The rights and obligations of the parties to this contract are subject to and governed by this document and any documents attached or incorporated by reference.

Battelle Memorial Institute **Pacific Northwest Division**	**Contractor shall sign and return a copy of this document**
Signature of person authorized to sign [redacted]	**Signature of person authorized to sign** [redacted]
Name [redacted]	**Name** [redacted]
Title Contracts Specialist	Title Director
Date	Date 22-01-2018

Agreements

Statement of Work

Contractor agrees to perform the scope outlined in the attached Statement of Work dated January 10, 2018.

Firm Fixed Price

The firm fixed price for Year 1 is $25,000.00 and includes $6250 for quarterly deliverables.

Options

Battelle anticipates extending the contract on an annual basis by exercising option years 2-4 as funding becomes available for the dollar values listed below.

Year 2 Option	$25,000.00
Year 3 Option	$25,000.00
Year 4 Option	$25,000.00

Invoice Submittal

Invoices may not be submitted more frequently than quarterly. A fixed billable amount of $6250 per quarter is billable upon PNNL's receipt of the quarterly deliverable detailed in the Statement of Work. Submit invoices electronically to ap.invoices@pnnl.gov and payments will be made electronically by wire (foreign payments). Failure to comply with electronic processing may result in a delay in payment.

Language

In the event of any conflict in the interpretation of this contract, the English language version shall prevail.

Currency

The currency of this contract is U. S. Dollars with the amount fixed for the term of the contract.

Technical Oversight Representative

All technical questions should be directed to the Technical Oversight Representative, [redacted]. The Technical Oversight Representative cannot modify this agreement.

Contracts Representative

All contractual questions should be directed to the Contracts Representative, [redacted].

Approval of Subcontracts

Subcontracts require the prior written approval of the Battelle Contracts Representative.

Contract Contents

In addition to this Schedule, the Contract consists of:

- The General Provisions for Fixed Price Foreign -- Supplies/Services - Form A-110-Foreign-FP-R15, dated, September 2017, are hereby incorporated and can be read in full at http://www.pnnl.gov/contracts/contractdocuments.aspx.
- Statement of Work dated January 10, 2018

Integration

The Contract contains the entire understanding between the parties, and there are no understandings or representations not set forth or incorporated by reference herein. No subsequent modifications of this contract shall be of any force or effect unless in writing signed by the party claimed to be bound thereby. No communications, written or oral, by other than a Battelle Contracts Representative shall be effective to modify or otherwise affect the provisions of the contract.

01/10/18

Statement of Work

[redacted]

J. Heyrovsky Institute of Physical Chemistry, Czech Academy of Sciences

RESEARCH

The research shall focus on the development of self-consistent multi-configurational approaches applicable to strongly correlated systems. The research will utilize elements of the Density Matrix Renormalization Group (DMRG) design to provide diagonalization tools for very large active spaces required in multi-reference coupled-cluster (MRCC) calculations (including universal state selective methods).

TECHNICAL APPROACH

Specifically, [redacted] shall be responsible for the development of parallel self-consistent multi-reference approaches based on the Density Matrix Renormalization Group (DMRG). [redacted] shall design and implement parallel implementation of the DMRG approach and integrate it with MRCC formalisms to guide the design of model space. The parallel implementation of self-consistent DMRG approach shall be applicable to systems involving 50 active orbitals.

The key part of the work is to develop an efficient parallel scheme for multiplication of the superblock Hamiltonian with a vector, which is the most expensive part of the DMRG algorithm. The parallel scheme shall take an advantage of a special structure of the superblock Hamiltonian, which leads to a large number of smaller tasks. These tasks shall be distributed across nodes by a scheduler and the results synchronously gathered as needed. The code shall be written in C++, the pilot implementation shall use of Global Array library combined with a data locality approach. Further, the possibility of reduction of communication by shifting from synchronous to asynchronous mode (for example, using GASPI library) shall be explored. The efficient parallel implementation of DMRG shall be interfaced with the Scalable Predictive methods for Excitations and Correlated phenomena (SPEC) library and used for externally corrected of existing coupled-cluster (CC) and MRCC implementations via the Tensor Algebra for Many-body Methods (TAMM) module.

The following software quality assurance (QA) activities shall be conducted for software development of the SPEC DMRG methods:

1. Identify and document software requirements (features). Involve PNNL SPEC PIs in the review process of these requirements.
   The software will be developed with the advanced C++ standard (C++11 or later), and will include MPI library for parallel execution, Global Arrays library to handle large data, and Libint for integral acquisitions. The code will be interfaced with the SPEC library and used for externally correlated CC methods in NWChem program. The work will be performed closely with SPEC PIs, [redacted] and [redacted], to interface the DMRG code with SPEC.
2. Document the design of the software to the specific software requirements.
   For the DMRG algorithm overview, see G.K.-L. Chan and M. Head-Gordon, J. Chem. Phys., 116, 4462 (2002). Global Arrays is developed and maintained by PNNL.

3. Follow the established coding standards and conventions.
   The parallel DMRG code will be written in C++11 with standard I/O utilities, MPI standard v. 2 and above. The interface with NWChem/NWChemEX will use coding standards of those programs.
4. The Contractor will conduct software activities in accordance with PNNL software quality assurance requirements.

REPORTING

1. The results shall be reported to Pacific Northwest National Laboratory (PNNL) on a quarterly basis.
2. It is anticipated that the results of this activity shall form the basis of joint publications and conference presentations by [redacted] and PNNL.
3. [redacted] shall attend project meetings via Skype or telecom as required by the PNNL Project Director, [redacted].

PERSONNEL AND RESEARCH OPERATION

Overall project management and deliverable shall be the responsibility of [redacted] who shall also conduct the research.

PNNL intends to exercise annual year options upon deliverables met and continuation of funding from sponsor. Deliverables each year are outlined below.

Period 1 DELIVERABLES –Ending 11/30/2018

- Q1: Design of the parallel scheme for DMRG, code for a construction of elements of superblock Hamiltonian (Hsb)
- Q2: Implementation of the parallel scheme for contraction of Hsb with a vector
- Q3: Parallel code performing DMRG sweeps
- Q4: Efficient and fully working parallel DMRG code capable to handle 50 active orbitals

Period 2 DELIVERABLES –Ending 11/30/2019

- DMRG code interfaced with TAMM module of SPEC
- Implementation of the Tailored coupled cluster (TCC) method corrected by DMRG

Period 3 DELIVERABLES -Ending 11/30/2020

- Implementation of (N,M) CCSD externally corrected by DMRG
- Combine Universal State-Selective approach with CC methods externally corrected by DMRG

Period 4 DELIVERABLES – Ending 9/30/2021

- Applications on organometallic systems like iron complexes occurring in many enzymes
- Exploring the possibility of implementation of the tensor network approach

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Battelle Memorial Institute, Pacific Northwest Division
Acting Under Contract DE-AC05-76RL01830
With the U.S. Department of Energy
Operating the Pacific Northwest National Laboratory (PNNL) (www.pnnl.gov)

Schedule **Contract Number: 392089 Modification 1**	
Issued by: Battelle Battelle Boulevard, K9-15 P.O. Box 999 Richland, WA 99352-0999 USA Contracts Specialist: [redacted] Telephone Number: [redacted] Fax Number: [redacted] Email: [redacted]	**Name and Address of Contractor:** J. Heyrovsky Institute of Physical Chemistry of the Czech Academy of Science, v. v. i. Dolejškova 2155/3 Prague 8, 182 23 CZE Contractor Contact: [redacted] Telephone Number: [redacted] Fax Number: Email: [redacted]
Payment Terms: Net 30	**Contract Type:** Fixed Price
Submit Invoices to ap.invoices@pnnl.gov. **Note:** Invoices must list location(s) of service (US: City, State; Foreign: Country).	**Total Contract Amount**: $60,000.00
Contract Period of Performance: January 22, 2018 through September 30, 2021	
Award Battelle hereby agrees to award this Contract to the Contractor subject to acceptance. The rights and obligations of the parties to this Contract are subject to and governed by this document and any documents attached or incorporated by reference.	**Contractor Agreement** Contractor accepts and agrees to furnish and deliver the items or perform services to the extent stated in this document for the consideration stated in this contract. The rights and obligations of the parties to this contract are subject to and governed by this document and any documents attached or incorporated by reference.

Battelle Memorial Institute **Pacific Northwest Division**	**Contractor shall sign and return a copy of this document**
Signature of person authorized to sign [redacted]	**Signature of person authorized to sign** [redacted]
Name [redacted] Date: 2018.12.03 13:56:24 -08'00'	**Name** prof. Martin Hof, Dr. rer. nat. DSc., Directo
Title Contracts Specialist	Title J. [redacted]
Date	Date 05 -12- 2018

Modification 1 increases funding by $25,000.00, exercising the year 2 option. The modification also adds a revised statement of work and $10,000.00 of additional funding for a new Total Contract Amount of $60,000.00.

The Schedule of Articles, Article: **Statement of Work, Firm Fixed Price and Contract Contents** should be deleted and the following substituted therefore:

Statement of Work

Contractor agrees to perform the scope outlined in the attached Statement of Work **revised November 06, 2018.**

Firm Fixed Price

The firm fixed price for **Year 1-2 is $60,000.00 and includes $8,750 for Year 2 quarterly deliverables.**

Options

Battelle anticipates extending the contract on an annual basis by exercising option years 3-4 as funding becomes available for the dollar values listed below.

Year 3 Option	$25,000.00
Year 4 Option	$25,000.00

Contract Contents

In addition to this Schedule, the Contract consists of:

- The General Provisions for Fixed Price Foreign -- Supplies/Services - Form A-110-Foreign-FP-R15, dated, September 2017, are hereby incorporated and can be read in full at http://www.pnnl.gov/contracts/contractdocuments.aspx.
- **Statement of Work revised November 06, 2018.**

It is understood and agreed that all other terms and conditions of Contract No. 392089 shall remain unchanged.

2018/231

Contract No. 392089
Revised 11/06/18

Statement of Work

[redacted]

J. Heyrovsky Institute of Physical Chemistry, Czech Academy of Sciences

PROPOSED RESEARCH

The proposed research shall focus on the development of self-consistent multi-configurational approaches applicable to strongly correlated systems. The proposed research will utilize elements of the Density Matrix Renormalization Group (DMRG) design to provide diagonalization tools for very large active spaces required in multi-reference coupled-cluster (MRCC) calculations (including universal state selective methods).

TECHNICAL APPROACH

Specifically, [redacted] shall be responsible for the development of parallel self-consistent multi-reference approaches based on the Density Matrix Renormalization Group (DMRG). [redacted] shall design and implement parallel implementation of the DMRG approach and integrate it with MRCC formalisms to guide the design of model space. The parallel implementation of self-consistent DMRG approach shall be applicable to systems involving 50 active orbitals.

The key part of the work is to develop an efficient parallel scheme for multiplication of the superblock Hamiltonian with a vector, which is the most expensive part of the DMRG algorithm. The parallel scheme shall take an advantage of a special structure of the superblock Hamiltonian, which leads to a large number of smaller tasks. These tasks shall be distributed across nodes by a scheduler and the results synchronously gathered as needed. The code shall be written in C++, the pilot implementation shall use of Global Array library combined with a data locality approach. Further, the possibility of reduction of communication by shifting from synchronous to asynchronous mode (for example, using GASPI library) shall be explored. The efficient parallel implementation of DMRG shall be interfaced with the Scalable Predictive methods for Excitations and Correlated phenomena (SPEC) library and used for externally corrected of existing coupled-cluster (CC) and MRCC implementations via the Tensor Algebra for Many-body Methods (TAMM) module.

The following software quality assurance (QA) activities shall be conducted for software development of the SPEC DMRG methods:

1. Identify and document software requirements (features). Involve PNNL SPEC PIs in the review process of these requirements.
   The software will be developed with the advanced C++ standard (C++11 or later), and will include MPI library for parallel execution, Global Arrays library to handle large data, and Libint for integral acquisitions. The code will be interfaced with the SPEC library and used for externally correlated CC methods in NWChem program. The work will be performed closely with SPEC PIs, [redacted] and [redacted], to interface the DMRG code with SPEC.
2. Document the design of the software to the specific software requirements.

For the DMRG algorithm overview, see G.K.-L. Chan and M. Head-Gordon, J. Chem. Phys., 116, 4462 (2002). Global Arrays is developed and maintained by PNNL.

3. Follow the established coding standards and conventions.
   The parallel DMRG code will be written in C++11 with standard I/O utilities, MPI standard v. 2 and above. The interface with NWChem/NWChemEX will use coding standards of those programs.
4. The Contractor will conduct software activities in accordance with PNNL software quality assurance requirements.

REPORTING

1. The results shall be reported to Pacific Northwest National Laboratory (PNNL) on a quarterly basis.
2. It is anticipated that the results of this activity shall form the basis of joint publications and conference presentations by [redacted] and PNNL.
3. [redacted] shall attend project meetings via Skype or telecom as required by the PNNL Project Director, [redacted].

PERSONNEL AND RESEARCH OPERATION

Overall project management and deliverable shall be the responsibility of [redacted] who shall also conduct the research.

PNNL intends to incrementally fund this Contract each year upon deliverables met and continuation of funding from sponsor. Deliverables each year are outlined below.

Period 1 DELIVERABLES (12/01/2017 – 11/30/2018)

- Q1: Design of the parallel scheme for DMRG, code for a construction of elements of superblock Hamiltonian (Hsb)
- Q2: Implementation of the parallel scheme for contraction of Hsb with a vector
- Q3: Parallel code performing DMRG sweeps
- Q4: Efficient and fully working parallel DMRG code capable to handle 50 active orbitals

Period 2 DELIVERABLES (12/01/2018 – 11/30/2019)

- **Q1: Implementation of the interface between DMRG parallel code and TAMM module of SPEC**
- Q2: Implementation of the efficient parallel C++ module to DMRG program for generation of active amplitudes from the MPS wave function (needed for tailored CCSD)
- **Q3: Implementation of the tailored CCSD method corrected by DMRG**
- **Q4: Implementation of the multireference tailored methods corrected by DMRG, extension of the parallel C++ module for generating amplitudes within the multireference framework.**

Period 3 DELIVERABLES (12/01/2019 – 11/30/2020)

- Implementation of (N,M) CCSD externally corrected by DMRG
- Combine Universal State-Selective approach with CC methods externally corrected by DMRG

Period 4 DELIVERABLES (12/01/2020 – 9/30/2021)

- Applications on organometallic systems like iron complexes occurring in many enzymes
- Exploring the possibility of implementation of the tensor network approach

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With the U.S. Department of Energy
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Schedule
Contract Number: 392089 Modification 2

Issued by:	**Name and Address of Contractor:**
Battelle Battelle Boulevard, K9-15 P.O. Box 999 Richland, WA 99352-0999 USA Contracts Specialist: [redacted] Telephone Number: [redacted] Fax Number: [redacted] Email: [redacted]	J. Heyrovsky Institute of Physical Chemistry of the Czech Academy of Science, v. v. i. Dolejškova 2155/3 Prague 8, 182 23 CZE Contractor Contact: [redacted] Telephone Number: [redacted] Fax Number: Email: [redacted]
Payment Terms: Net 30	**Contract Type:** Fixed Price
Submit Invoices to ap.invoices@pnnl.gov. **Note:** Invoices must list location(s) of service (US: City, State; Foreign: Country).	**Total Contract Amount: $85,000.00**
Contract Period of Performance: January 22, 2018 through September 30, 2021	
Award Battelle hereby agrees to award this Contract to the Contractor subject to acceptance. The rights and obligations of the parties to this Contract are subject to and governed by this document and any documents attached or incorporated by reference.	**Contractor Agreement** Contractor accepts and agrees to furnish and deliver the items or perform services to the extent stated in this document for the consideration stated in this contract. The rights and obligations of the parties to this contract are subject to and governed by this document and any documents attached or incorporated by reference.

Battelle Memorial Institute **Pacific Northwest Division**	**Contractor shall sign and return a copy of this document**
Signature of person authorized to sign [redacted] Date: 2019.12.15 15:15:23 -08'00'	**Signature of person authorized to sign** [redacted]
Name [redacted]	**Name** prof. Martin Hof, Dr. rer. nat. DSc., Director
Title Contracts Specialist	Title
Date	Date 19 -12- 2019

Modification 2 increases funding by $25,000.00, exercising the year 3 option, to a new contract amount of $85,000.00.

The **Agreements**, Subarticle: **Firm Fixed Price,** shall be deleted and the following substituted therefore:

Firm Fixed Price
The firm fixed price for **Year 1-3 is $85,000.00** and includes $6,250.00 per quarter for deliverables.

Options
Battelle anticipates extending the contract on an annual basis by exercising option years 4 as funding becomes available for the dollar values listed below.

Year 4 Option	$25,000.00

It is understood and agreed that all other terms and conditions of Contract No. 392089 shall remain unchanged.

2020/079

Pacific Northwest
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Battelle Memorial Institute, Pacific Northwest Division
Acting Under Contract DE-AC05-76RL01830
With the U.S. Department of Energy
Operating the Pacific Northwest National Laboratory (PNNL) (www.pnnl.gov)

Schedule - Contract No. 524799

Issued by:	**Name and Address of Contractor:**
Battelle Battelle Boulevard, K9-15 P.O. Box 999 Richland, WA 99352-0999 USA Contracts Specialist: [redacted] Telephone Number: [redacted] Email: [redacted]	J. Heyrovsky Institute of Physical Chemistry Department of Theoretical Chemistry Dolejškova 2155/3 Prague 8, 18223 CZE Contractor Contact: [redacted] Telephone Number [redacted] Email: [redacted]
Payment Terms: Net 30	**Contract Type:** Fixed Price
Submit Invoices and Invoice/Payment Inquiries to ap.invoices@pnnl.gov. **Note:** Invoices must list location(s) of service (US: City, State; Foreign: Country).	**Total Contract Amount:** $40,000.00
Contract Period of Performance: July 1, 2020 through May 31, 2022	
Award Battelle hereby agrees to award this Contract to the Contractor subject to acceptance. The rights and obligations of the parties to this Contract are subject to and governed by this document and any documents attached or incorporated by reference.	**Contractor Agreement** Contractor accepts and agrees to furnish and deliver the items or perform services to the extent stated in this document for the consideration stated in this contract. The rights and obligations of the parties to this contract are subject to and governed by this document and any documents attached or incorporated by reference.

Battelle Memorial Institute **Pacific Northwest Division**	**Contractor shall sign and return a copy of this document**
Signature of person authorized to sign: [redacted] Digitally signed by [redacted] Date: 2020.07.01 17:08:35 -07'00'	**Signature of person authorized to sign** [redacted] Datum: 2020.07.27 15:18:14 +02'00'
Name [redacted]	**Name** prof. Martin Hof, Dr. rer. nat. DSc., Director
Title Contracts Specialist	Title
Date	Date

IMPORTANT NOTE: Any domestic and foreign travel associated with this contract (including contractor travel within a country of presence) shall be approved in writing by the Battelle Contracts Representative in advance of travel arrangements being finalized. Without the advance approval of the Battelle Contracts Representative for any such travel, any invoiced costs related to such travel will not be paid.

Statement of Work

Contractor agrees to perform the scope outlined in the attached Statement of Work dated May 19, 2020.

Performance Schedule

If at any time the Contractor has reason to believe that a production milestone or delivery date may not be met, Contractor shall immediately notify the Battelle Contracts Representative in writing, outlining the milestone or delivery date in jeopardy, the reasons, and steps the Contractor will take to recover the schedule in order to meet delivery requirements.

Milestone Payment Schedule

Payments will be made upon completion and acceptance of the tasks described in the Statement of Work according to the following milestone payment schedule:

	Deliverable	Payment Amount USD
4.1	Implementation of the construction of PAO orbitals, DOI integrals and sparse maps, performing prescreening based on dipole approximation	$5,000.00
4.2	Implementation of RI integrals and prescreening of occupied pairs at MP2 level	$5,000.00
4.3	Implementation of pair density matrices and obtaining PNO orbitals, and estimation of the ΔE (MP2) correction	$5,000.00
4.4	Working closed-shell DLPNO-CCSD implementation for RHF reference	$5,000.00
4.5	Derivation of the open-shell DLPNO-CCSD equations	$5,000.00
4.6	Modification of the PNO construction and prescreening algorithm for open-shell calculations	$5,000.00
4.7	Implementation of the open-shell DLPNO-CCSD algorithm	$5,000.00
4.8	Applications of the DLPNO implementations to large- size molecular systems	$5,000.00
	Total USD	**$40,000.00**

Technical Oversight Representative

All technical questions should be directed to the Technical Oversight Representative, [redacted] at [redacted]. The Technical Oversight Representative cannot modify this agreement.

Battelle Contracts Representative

All contractual questions should be directed to the Battelle Contracts Representative, [redacted] at [redacted]

Contract Contents

In addition to this Schedule, the Contract consists of:

- Representations and Certifications dated June 11, 2020
- The General Provisions for Fixed Price Foreign - Supplies/Services - Form A-110-Foreign-FP-R18, dated, March 2020, are hereby incorporated and can be read in full at http://www.pnnl.gov/contracts/contractdocuments.aspx
- Statement of Work dated May 19, 2020

Integration

This Contract contains the entire understanding between the parties, and there are no understandings or representations not set forth or incorporated by reference herein. No subsequent modifications of this Contract shall be of any force or effect unless in writing signed by the party claimed to be bound thereby.

No communications, written or oral, by other than a Battelle Contracts Representative shall be effective to modify or otherwise affect the provisions of this Contract.

Statement of Work
NWChemEx
J. Heyrovsky Institute of Physical Chemistry, Czech Academy of Sciences
Principal Investigator: [redacted]
May 19, 2020

I. Background

The overall objective of the NWChemEx project is to provide a community infrastructure for computational chemistry that takes full advantage of exascale computing technologies with a high performing, flexible, and portable structure to support a broad range of chemistry research on a broad range of computing systems, from terascale workstations and petascale servers to exascale computers.

The research focuses on the development of parallel implementation of the domain-based local pair natural orbital coupled cluster method with singles and doubles (DLPNO-CCSD) into the NWChemEx code. In contrast to existing CCSD implementations, DLPNO formulation scales nearly linearly with the system size allowing for very fast evaluation of energies at the CCSD level for large-size molecular systems.

II. Scope and Technical Approach

Dr. [redacted] will be responsible for the implementation of the following steps required in the DLPNO-CCSD algorithm:

1. Determination the projected atomic orbital (PAO) basis and transformation of intermediates into this basis.
2. Calculation of differential overlap integrals (DOI), construction of sparse maps.
3. Pair pre-screening procedures based on dipole approximation
4. Construction of RI integrals at O(N) cost (by modifying existing 3-index integral framework already existing in NWChemEx library).
5. Pair prescreening at the MP2 level.
6. Construction of pair density matrices and obtain PNO orbitals.
7. Derivation of DLPNO-CCSD equations.
8. Carrying out DLPNO-CCSD iterations and obtain DLPNO-CCSD energies.

The following software quality assurance (QA) activities shall be conducted for software development of the DLPNO-CC methods:

1. *Identify and document software requirements (features). Involve PNNL NWChemEx PIs in the review process of these requirements.*
   The software will be developed with the advanced C++ standard (C++11 or later) and will include Global Arrays library to handle large data with the option of involving MPI library (version 2.0 or later) for specific parallel operations. The code will be a part of the NWChemEx code. The work will be performed in close collaboration with NWChemEx team including teams led by [redacted] and [redacted] [redacted]hy.

2. *Document the design of the software to the specific software requirements.*
   For the DLPNO CC algorithm overview, see P. Pinski et al., J. Chem. Phys. 143, 034108 (2015) and Riplinger et al., J. Chem. Phys. 144, 024109 (2016).

3. *Follow the established coding standards and conventions.*
   The parallel DLPNO-CCSD code will be written in C++11 with standard I/O utilities, including Global Arrays using Tensor Algebra for Many-body Methods (TAMM). The parallel implementation of DLPNO-CCSD will utilize the Global Arrays library.

4. The Contractor will conduct software activities in accordance with PNNL software quality assurance requirements.

III. Reporting

1. The results shall be reported to Pacific Northwest National Laboratory (PNNL) on a quarterly basis.
2. It is anticipated that the results of this activity shall form the basis of joint publications and conference presentations by [redacted] and PNNL.
3. Dr. [redacted] shall attend project meetings via Skype or telecom as required by the PNNL with [redacted] and [redacted].

IV. Deliverables

Period 1 deliverables (06/2020 – 05/2021):
Q1: Implementation of the construction of PAO orbitals, DOI integrals and sparse maps, performing prescreening based on dipole approximation.
Q2: Implementation of RI integrals and prescreening of occupied pairs at MP2 level.
Q3: Implementation of pair density matrices and obtaining PNO orbitals, and estimation of the ΔE (MP2) correction.
Q4: Working closed-shell DLPNO-CCSD implementation for RHF reference

Period 2 deliverables (06/2021 – 05/2022):
Q1: Derivation of the open-shell DLPNO-CCSD equations
Q3: Modification of the PNO construction and prescreening algorithm for open-shell calculations
Q3: Implementation of the open-shell DLPNO-CCSD algorithm
Q4: Applications of the DLPNO implementations to large-size molecular systems

2021/001

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Battelle Memorial Institute, Pacific Northwest Division
Acting Under Contract DE-AC05-76RL01830
With the U.S. Department of Energy
Operating the Pacific Northwest National Laboratory (PNNL) (www.pnnl.gov)

Schedule
Contract Number: 392089 Modification 3

Issued by:	**Name and Address of Contractor:**
Battelle Battelle Boulevard, K9-15 P.O. Box 999 Richland, WA 99352-0999 USA Contracts Specialist: [redacted] Telephone Number: 5[redacted] Fax Number: [redacted]8 Email: [redacted]	J. Heyrovsky Institute of Physical Chemistry of the Czech Academy of Science, v. v. i. Dolejškova 2155/3 Prague 8, 182 23 CZE Contractor Contact: [redacted] Telephone Number: [redacted] Fax Number: Email: [redacted]
Payment Terms: Net 30	**Contract Type:** Fixed Price
Submit Invoices to ap.invoices@pnnl.gov. **Note:** Invoices must list location(s) of service (US: City, State; Foreign: Country).	**Total Contract Amount: $120,000.00**
Contract Period of Performance: January 22, 2018 through September 30, 2021	
Award Battelle hereby agrees to award this Contract to the Contractor subject to acceptance. The rights and obligations of the parties to this Contract are subject to and governed by this document and any documents attached or incorporated by reference.	**Contractor Agreement** Contractor accepts and agrees to furnish and deliver the items or perform services to the extent stated in this document for the consideration stated in this contract. The rights and obligations of the parties to this contract are subject to and governed by this document and any documents attached or incorporated by reference.

Battelle Memorial Institute **Pacific Northwest Division**	**Contractor shall sign and return a copy of this document**
Signature of person authorized to sign [redacted] Date: 2021.01.03 15:09:10 -08'00'	**Signature of person authorized to sign** [redacted]
Name [redacted]	**Name** prof. Martin Hof, Dr. rer. nat. DSc., Director
Title Contracts Specialist	Title [redacted]
Date	Date 07-01-2021

Modification 3 increases funding by $25,000.00, exercising the year 4 option. The modification also adds a revised statement of work and $10,000.00 of additional funding for year 4 and a new Total Contract Amount of $120,000.00.

The Schedule of Articles, Article: Statement of Work, Firm Fixed Price and Contract Contents should be deleted and the following substituted therefore:

2021/001

Statement of Work

Contractor agrees to perform the scope outlined in the attached Statement of Work revised November 20, 2020.

Firm Fixed Price

The firm fixed price for:

Year 1 is $25,000.00 and includes $6,250.00 per quarterly deliverables.
Year 2 is $35,000.00 and includes $8,750.00 per quarterly deliverables.
Year 3 is $25,000.00 and includes $6,250.00 per quarterly deliverables.
Year 4 is $35,000.00 and includes $8,750.00 per quarterly deliverables.

Contract Contents

In addition to this Schedule, the Contract consists of:

- The General Provisions for Fixed Price Foreign -- Supplies/Services - Form A-110-Foreign-FP-R15, dated, September 2017, are hereby incorporated and can be read in full at http://www.pnnl.gov/contracts/contractdocuments.aspx.
- Statement of Work revised November 20, 2020.

It is understood and agreed that all other terms and conditions of Contract No. 392089 shall remain unchanged.

2022/004

Pacific Northwest
NATIONAL LABORATORY

Battelle Memorial Institute, Pacific Northwest Division
Acting Under Prime Contract DE-AC05-76RL01830
With the U.S. Department of Energy
Operating the Pacific Northwest National Laboratory (PNNL) (www.pnnl.gov)

BATTELLE MEMORIAL INSTITUTE, PACIFIC NORTHWEST DIVISION'S CONTRACT NUMBER 607400
J. Heyrovsky Institute of Physical Chemistry, Czech Academy of Sciences and Principal Investigators [redacted] and [redacted] to support the "Scalable Predictive methods for Excitations and Correlated phenomena (SPEC)" project

Issued By: Battelle Memorial Institute, Pacific Northwest Division 902 Battelle Boulevard Richland, WA 99352	**Contractor:** J. Heyrovsky Institute of Physical Chemistry of the CAS, v.v.i. Dolejskova 2155 3 Prague 8, 18223 CZE,
Contracts Specialist: Name: [redacted] Telephone Number: [redacted] Email: [redacted]	**Contractor's Point of Contact:** Name: [redacted] Telephone Number: [redacted] Email: [redacted]
Payment Terms: Net 30	**Contract Type:** Firm Fixed Price
Completion Date: December 31, 2025	**Total Price:** $140,000.00 (USD) **Incremental Funding Amount:** $35,000.00 (USD)
Submit Invoices and Invoice/Payment Inquiries To ap.invoices@pnnl.gov. Note: Invoices must list location(s) of service (U.S.: City, State; Foreign: Country).	
Award Battelle hereby awards this Contract to the Contractor subject to acceptance. The rights and obligations of the parties to this Contract are subject to and governed by this document and any documents attached or incorporated by reference.	**Contractor Agreement** Contractor accepts and agrees to furnish and deliver the items and/or perform the services to the extent stated in this document for the consideration stated in this Contract. The rights and obligations of the parties to this Contract are subject to and governed by this document and any documents attached or incorporated by reference.

Battelle Memorial Institute, Pacific Northwest Division	**Contractor shall sign and return a copy of this document**
Signature of person authorized to sign [redacted] Digitally signed by [redacted] Date: 2022.01.04 09:47:06 -08'00'	Signature of person authorized to sign [redacted]
Title Contracts Specialist	Name prof. Martin Hof, Dr. rer. nat. DSc., Director Title
Date	Date 05-01-2022

Note: Captions in this document and in Battelle's General Provisions are included for convenience of reference only and in no other way define or delineate any of the provisions hereof or otherwise affect their construction or effect.

1. SCOPE AND PRICING

Scope: Contractor agrees to perform the scope outlined in the attached Statement of Work dated October 26, 2021 for this Contract (hereinafter referred to as "Contract").

Deliverable and Payment Schedule: Payment shall be made upon receipt of acceptable deliverables as outlined in the Statement of Work. The payment for all Deliverables respectively shall be made upon concurrence by the Technical Oversight Representative (see below) or delegate. The following Payment Schedule shall apply throughout completion of all deliverables.

Deliverable	Description	Due Date (No Later Than)	Fixed Amount (USD)
Year 1, Quarter 1	Report on the progress of preliminary C++ implementation of DMRG-AC0 and DMRG-AC methods	31 March 2022	$8,750.00
Year 1, Quarter 2	Report on the progress of design of the parallel scheme for DMRG-AC0	30 June 2022	$8,750.00
Year 1, Quarter 3	Report on the progress of implementation of the parallel DMRG-AC0, Extension of DMRG by ML features	30 September 2022	$8,750.00
Year 1, Quarter 4	Report on the progress of DMRG-AC0 benchmark study	31 December 2022	$8,750.00
Year 2, Quarter 1	Report on the progress of implementation of the parallel DMRG-AC	31 March 2023	$8,750.00
Year 2, Quarter 2	Report on the progress of design of the DMRG-AC/AC0-in-DFT scheme	30 June 2023	$8,750.00
Year 2, Quarter 3	Report on the progress of implementation of the parallel DMRG-AC0-in-DFT method	30 September 2023	$8,750.00
Year 2, Quarter 4	Report on the progress of DMRG-AC0-in-DFT benchmark studies	31 December 2023	$8,750.00
Year 3, Quarter 1	Report on the progress of GPU parallel scheme for DMRG-AC/AC0: design	31 March 2024	$8,750.00
Year 3, Quarter 2	Report on the progress of GPU parallel scheme for DMRG-AC/AC0: implementation	30 June 2024	$8,750.00
Year 3, Quarter 3	Report on the progress of efficient and fully working parallel DMRG-AC/AC0 code capable of handling 60 active orbitals and 2000 basis functions	30 September 2024	$8,750.00
Year 3, Quarter 4	Report on the progress of applications of the developed methods on extended strongly correlated systems, i.e. transition metal complexes with multiple transition metal atoms	31 December 2024	$8,750.00

Year 4, Quarter 1	Report on the progress of application of DMRG-AC/AC0-in-DFT on extended strongly correlated systems	31 March 2025	$8,750.00
Year 4, Quarter 2	Report on the progress of ML studies harnessing the developed parallel computational methods	30 June 2025	$8,750.00
Year 4, Quarter 3	Report on the progress of improvements of the code: adaptation to the new hardware.	30 September 2025	$8,750.00
Year 4, Quarter 4	Report on the progress of Further possible improvements of the code: improvements of the methods (higher order approximations, tensor network extensions beyond DMRG, employment of the local fermionic mode transformation, etc.)	31 December 2025	$8,750.00
		Total Price (USD)	$140,000.00

Limitation of Funds (Fixed-Price Contract):

(a) Of the Total Price of items through 31 December 2025, the sum of $35,000.00 (USD) is presently available for payment and allotted to this contract. It is anticipated that from time-to-time additional funds will be allocated to the contract in accordance with the following schedule, until the total price of said items is allotted:

SCHEDULE FOR ALLOTMENT OF FUNDS	
Funded – Deliverable Year 1, Quarter 1 Due 31 March 2022	$8,750.00
Funded – Deliverable Year 1, Quarter 2 Due 30 June 2022	$8,750.00
Funded – Deliverable Year 1, Quarter 3 Due 30 September 2022	$8,750.00
Funded – Deliverable Year 1, Quarter 4 Due 31 December 2022	$8,750.00
To Be Funded by 1 January 2023 – Deliverable Year 2, Quarter 1 Due 31 March 2023	$8,750.00
To Be Funded by 1 January 2023 – Deliverable Year 2, Quarter 2 Due 30 June 2023	$8,750.00
To Be Funded by 1 January 2023 – Deliverable Year 2, Quarter 3 Due 30 September 2023	$8,750.00
To Be Funded by 1 January 2023 – Deliverable Year 2, Quarter 4 Due 31 December 2023	$8,750.00
To Be Funded by 1 January 2024 – Deliverable Year 3, Quarter 1 Due 31 March 2024	$8,750.00
To Be Funded by 1 January 2024 – Deliverable Year 3, Quarter 2 Due 30 June 2024	$8,750.00
To Be Funded by 1 January 2024 – Deliverable Year 3, Quarter 3 Due 30 September 2024	$8,750.00
To Be Funded by 1 January 2024 – Deliverable Year 3, Quarter 4 Due 31 December 2024	$8,750.00
To Be Funded by 1 January 2025 – Deliverable Year 4, Quarter 1 Due 31 March 2025	$8,750.00

To Be Funded by 1 January 2025 – Deliverable Year 4, Quarter 2 Due 30 June 2025	$8,750.00
To Be Funded by 1 January 2025 – Deliverable Year 4, Quarter 3 Due 30 September 2025	$8,750.00
To Be Funded by 1 January 2025 – Deliverable Year 4, Quarter 4 Due 31 December 2025	$8,750.00
Total Price (USD)	**$140,000.00**

(b) Contractor agrees to perform work on the items specified in Section 1 of this Contract up to the point at which, if this contract is terminated pursuant to the Termination for Convenience clause of this contract, the total amount payable by Battelle (including amounts payable for subcontracts and settlement costs) would, in the exercise of reasonable judgment by the Contractor, approximate the total amount at the time allotted to the contract. The Contractor is not obligated to continue performance of the work beyond that point. Battelle is not obligated in any event to pay or reimburse the Contractor more than the amount from time to time allotted to the contract, anything to the contrary in the Termination for Convenience clause notwithstanding.

(c) It is contemplated that funds presently allotted to this contract will cover the work to be performed until 31 December 2022.

(d) The provisions of this clause with respect to termination shall in no way be deemed to limit the rights of Battelle under the default clause of this contract. The provisions of this Limitation of Funds clause are limited to the work on and allotment of funds for the items set forth in paragraph (a) of this clause. Battelle may by unilateral modification provide additional funding up to the Total Price specified above. This clause shall become inoperative upon the allotment of funds for the Total Price of said work except for rights and obligations then existing under this clause.

(e) Nothing in this clause shall affect the right of Battelle to terminate this Contract pursuant to the Termination for Convenience clause of this contract.

Currency: The currency of this Contract is U.S. Dollars with the amount fixed for the term of the Contract.

2. PERIOD OF PERFORMANCE/DELIVERY

Period of Performance: The Completion Date is on Page 1. The Deliverable and Payment Schedule is in Section 1.

3. CONTRACTUAL REQUIREMENTS/INFORMATION

Travel Notice: Request for any domestic and foreign travel associated with this Contract (including Contractor travel within a country of presence) shall be approved in writing by the Battelle Contracts Specialist in advance of travel arrangements being finalized. Without the advance approval of the Battelle Contracts Specialist for any such travel, any invoiced costs related to such travel may not be paid.

4. CONTRACT ADMINISTRATION

Battelle Contracts Specialist: The Battelle Contracts Specialist, [redacted], is the sole point of contact for any contractual/administrative communications or questions regarding this acquisition. Contact information is on Page 1.

Technical Oversight Representative: All technical questions should be directed to the Technical Oversight Representative (TOR), [redacted] The TOR cannot modify this Contract.

5. TERMS AND CONDITIONS

The General Provisions for Fixed Price Foreign - Supplies/Services - Form A-110.21-FP-Foreign, dated, July 2021, are hereby incorporated and can be read in full at https://www.pnnl.gov/contracts/contractdocuments.aspx.

6. CONTRACT ATTACHMENTS

In addition to the above, the Contract consists of:

- Statement of Work dated October 26, 2021
- Representations and Certifications dated November 15, 2021

7. ENTIRE AGREEMENT

This Contract contains the entire agreement and understanding between the parties, and there are no agreements, understandings or representations not set forth or incorporated by reference herein. This Contract supersedes all prior proposals, understandings and agreements, whether oral or written, between the parties with respect to the subject matter hereof. No subsequent Modifications of this Contract shall be of any force or effect unless in writing by authorized representatives of each party to this Contract. No communications, written or oral, by other than a Battelle Contracts Specialist shall be effective to modify or otherwise affect the provisions of this Contract.

2022/079

Pacific Northwest
NATIONAL LABORATORY

Battelle Memorial Institute, Pacific Northwest Division
Acting Under Contract DE-AC05-76RL01830
With the U.S. Department of Energy
Operating the Pacific Northwest National Laboratory (PNNL) (www.pnnl.gov)

Schedule - Contract No. 524799, Modification No. 1	
Issued by: Battelle Battelle Boulevard, K9-15 P.O. Box 999 Richland, WA 99352-0999 USA Contracts Specialist: [redacted] Telephone Number: [redacted] Email: [redacted]	**Name and Address of Contractor:** J. Heyrovsky Institute of Physical Chemistry Department of Theoretical Chemistry Dolejškova 2155/3 Prague 8, 18223 CZE Contractor Contact: [redacted] Telephone Number: [redacted] Email: [redacted]
Payment Terms: Net 30	**Contract Type:** Fixed Price
Submit Invoices and Invoice/Payment Inquiries to ap.invoices@pnnl.gov. **Note:** Invoices must list location(s) of service (US: City, State; Foreign: Country).	**Total Contract Amount:** $50,000.00
Contract Period of Performance: July 1, 2020 through November 30, 2022	
Award Battelle hereby agrees to award this Contract to the Contractor subject to acceptance. The rights and obligations of the parties to this Contract are subject to and governed by this document and any documents attached or incorporated by reference.	**Contractor Agreement** Contractor accepts and agrees to furnish and deliver the items or perform services to the extent stated in this document for the consideration stated in this contract. The rights and obligations of the parties to this contract are subject to and governed by this document and any documents attached or incorporated by reference.

Battelle Memorial Institute **Pacific Northwest Division**	**Contractor shall sign and return a copy of this document**
Signature of person authorized to sign Digitally signed by [redacted] Date: 2022.06.08 16:20:41 -07'00'	**Signature of person aut[redacted] to sign**
Name [redacted]	**Name** prof. Martin Hof, Dr. [redacted]at. DSc., Director
Title Contracts Specialist	Title
Date	Date 24-06-2022

IMPORTANT NOTE: Any domestic and foreign travel associated with this contract (including contractor travel within a country of presence) shall be approved in writing by the Battelle Contracts Representative in advance of travel arrangements being finalized. Without the advance approval of the Battelle Contracts Representative for any such travel, any invoiced costs related to such travel will not be paid.

Recitals

This Modification No. 1 is issued to add scope, cost, and time. Consequently, a revised Statement of Work is incorporated below. The Contract Period of Performance is extended through November 30, 2022. The Total Contract Amount of $40,000 is increased by $10,000 for a revised Total Contract Amount of $50,000. All other terms and conditions remain unchanged.

Statement of Work

Contractor agrees to perform the scope outlined in the attached Statement of Work dated May 19, 2020, revised May 25, 2022.

Performance Schedule

If at any time the Contractor has reason to believe that a production milestone or delivery date may not be met, Contractor shall immediately notify the Battelle Contracts Representative in writing, outlining the milestone or delivery date in jeopardy, the reasons, and steps the Contractor will take to recover the schedule in order to meet delivery requirements.

Milestone Payment Schedule

Payments will be made upon completion and acceptance of the tasks described in the Statement of Work according to the following milestone payment schedule:

	Deliverable	Payment Amount USD
4.1	Implementation of the construction of PAO orbitals, DOI integrals and sparse maps, performing prescreening based on dipole approximation	$5,000.00
4.2	Implementation of RI integrals and prescreening of occupied pairs at MP2 level	$5,000.00
4.3	Implementation of pair density matrices and obtaining PNO orbitals, and estimation of the ΔE (MP2) correction	$5,000.00
4.4	Working closed-shell DLPNO-CCSD implementation for RHF reference	$5,000.00
4.5	Derivation of the open-shell DLPNO-CCSD equations	$5,000.00
4.6	Modification of the PNO construction and prescreening algorithm for open-shell calculations	$5,000.00
4.7	Implementation of the open-shell DLPNO-CCSD algorithm	$5,000.00
4.8	Applications of the DLPNO implementations to large- size molecular systems	$5,000.00
4.9	Integration of GauXC library for computation DOIs	$5,000.00
4.10	Finalize sparse maps for efficient computation and tune thresholds for a set of large molecules	$5,000.00
	Total USD	**$50,000.00**

Technical Oversight Representative

All technical questions should be directed to the Technical Oversight Representative, [redacted] at [redacted] The Technical Oversight Representative cannot modify this agreement.

Battelle Contracts Representative

All contractual questions should be directed to the Battelle Contracts Representative, [redacted].

Contract Contents

In addition to this Schedule, the Contract consists of:

- Representations and Certifications dated June 11, 2020
- The General Provisions for Fixed Price Foreign - Supplies/Services - Form A-110-Foreign-FP-R18, dated, March 2020, are hereby incorporated and can be read in full at http://www.pnnl.gov/contracts/contractdocuments.aspx
- Statement of Work dated May 19, 2020, revised May 25, 2022

Integration

This Contract contains the entire understanding between the parties, and there are no understandings or representations not set forth or incorporated by reference herein. No subsequent modifications of this Contract shall be of any force or effect unless in writing signed by the party claimed to be bound thereby. No communications, written or oral, by other than a Battelle Contracts Representative shall be effective to modify or otherwise affect the provisions of this Contract.

Statement of Work
NWChemEx
J. Heyrovsky Institute of Physical Chemistry, Czech Academy of Sciences
Principal Investigator: [redacted]
May 19, 2020, revised May 25, 2022

I. Background

The overall objective of the NWChemEx project is to provide a community infrastructure for computational chemistry that takes full advantage of exascale computing technologies with a high performing, flexible, and portable structure to support a broad range of chemistry research on a broad range of computing systems, from terascale workstations and petascale servers to exascale computers.

The research focuses on the development of parallel implementation of the domain-based local pair natural orbital coupled cluster method with singles and doubles (DLPNO-CCSD) into the NWChemEx code. In contrast to existing CCSD implementations, DLPNO formulation scales nearly linearly with the system size allowing for very fast evaluation of energies at the CCSD level for large-size molecular systems.

II. Scope and Technical Approach

[redacted] will be responsible for the implementation of the following steps required in the DLPNO-CCSD algorithm:

1. Determination the projected atomic orbital (PAO) basis and transformation of intermediates into this basis.
2. Calculation of differential overlap integrals (DOI), construction of sparse maps.
3. Pair pre-screening procedures based on dipole approximation
4. Construction of RI integrals at O(N) cost (by modifying existing 3-index integral framework already existing in NWChemEx library).
5. Pair prescreening at the MP2 level.
6. Construction of pair density matrices and obtain PNO orbitals.
7. Derivation of DLPNO-CCSD equations.
8. Carrying out DLPNO-CCSD iterations and obtain DLPNO-CCSD energies.
9. Integration of GauXC library for computation DOIs
10. Finalize sparse maps for efficient computation and tune thresholds for a set of large molecules

The following software quality assurance (QA) activities shall be conducted for software development of the DLPNO-CC methods:

1. *Identify and document software requirements (features). Involve PNNL NWChemEx PIs in the review process of these requirements.*
   The software will be developed with the advanced C++ standard (C++11 or later) and will include Global Arrays library to handle large data with the option of involving MPI library (version 2.0 or later) for specific parallel operations. The code will be a part of the NWChemEx code. The work will be performed in close collaboration with NWChemEx team including teams led by [redacted] and [redacted].

2. *Document the design of the software to the specific software requirements.*
   For the DLPNO CC algorithm overview, see P. Pinski et al., J. Chem. Phys. 143, 034108 (2015) and Riplinger et al., J. Chem. Phys. 144, 024109 (2016).

3. *Follow the established coding standards and conventions.*
   The parallel DLPNO-CCSD code will be written in C++11 with standard I/O utilities, including Global Arrays using Tensor Algebra for Many-body Methods (TAMM). The parallel implementation of DLPNO-CCSD will utilize the Global Arrays library.

4. The Contractor will conduct software activities in accordance with PNNL software quality assurance requirements.

III. Reporting

1. The results shall be reported to Pacific Northwest National Laboratory (PNNL) on a quarterly basis.
2. It is anticipated that the results of this activity shall form the basis of joint publications and conference presentations by Dr. [redacted] and PNNL.
3. Dr. [redacted] shall attend project meetings via Skype or telecom as required by the PNNL with [redacted] and [redacted].

IV. Deliverables

Period 1 deliverables (06/2020 – 05/2021):
Q1: Implementation of the construction of PAO orbitals, DOI integrals and sparse maps, performing prescreening based on dipole approximation.
Q2: Implementation of RI integrals and prescreening of occupied pairs at MP2 level.
Q3: Implementation of pair density matrices and obtaining PNO orbitals, and estimation of the ΔE (MP2) correction.
Q4: Working closed-shell DLPNO-CCSD implementation for RHF reference

Period 2 deliverables (06/2021 – 05/2022):
Q1: Derivation of the open-shell DLPNO-CCSD equations
Q3: Modification of the PNO construction and prescreening algorithm for open-shell calculations
Q3: Implementation of the open-shell DLPNO-CCSD algorithm
Q4: Applications of the DLPNO implementations to large-size molecular systems

Period 3 deliverables (06/2022 – 11/2022):
Q1: Integration of GauXC library for computation DOIs
Q2: Finalize sparse maps for efficient computation and tune thresholds for a set of large molecules

2022/134

Pacific Northwest
NATIONAL LABORATORY

Battelle Memorial Institute, Pacific Northwest Division
Acting Under Prime Contract DE-AC05-76RL01830
With the U.S. Department of Energy
Operating the Pacific Northwest National Laboratory (PNNL) (www.pnnl.gov)

BATTELLE MEMORIAL INSTITUTE, PACIFIC NORTHWEST DIVISION'S CONTRACT NO. 607400, MODIFICATION NO. 1
J. Heyrovsky Institute of Physical Chemistry, Czech Academy of Sciences and Principal Investigators [redacted] and [redacted] to support the "Scalable Predictive methods for Excitations and Correlated phenomena (SPEC)" project

Issued By: Battelle Memorial Institute, Pacific Northwest Division 902 Battelle Boulevard Richland, WA 99352	**Contractor:** J. Heyrovsky Institute of Physical Chemistry of the CAS, v.v.i. Dolejskova 2155 3 Prague 8, 18223 CZE,
Contracts Specialist: Name: [redacted] Telephone Number: [redacted] Email: [redacted]	**Contractor's Point of Contact:** Name: [redacted] Telephone Number: [redacted] Email: [redacted]
Payment Terms: Net 30	**Contract Type:** Firm Fixed Price
Completion Date: December 31, 2025	**Total Price:** $144,972.00 (USD) **Incremental Funding Amount:** $39,972.00 (USD)
Submit Invoices and Invoice/Payment Inquiries To ap.invoices@pnnl.gov. Note: Invoices must list location(s) of service (U.S.: City, State; Foreign: Country).	
Award Battelle hereby awards this Contract to the Contractor subject to acceptance. The rights and obligations of the parties to this Contract are subject to and governed by this document and any documents attached or incorporated by reference.	**Contractor Agreement** Contractor accepts and agrees to furnish and deliver the items and/or perform the services to the extent stated in this document for the consideration stated in this Contract. The rights and obligations of the parties to this Contract are subject to and governed by this document and any documents attached or incorporated by reference.

Battelle Memorial Institute, Pacific Northwest Division	**Contractor shall sign and return a copy of this document**
Signature of person authorized to sign Digitally signed [redacted] [redacted] Date: 2022.10.20 11:21:28 -07'00'	Signature of person authorized to sign [redacted]
Title Contracts Specialist	Name prof. Martin Hof, Dr. rer. nat. DSc., Director Title
Date	Date 21-10-2022

Recitals: This Modification No. 1 is issued to add scope and cost to allow the Principal Investigators to attend a project meeting in Seattle, WA. Consequently, the Total Price of $140,000 is increased by $4,972 for a revised Total Price of $144,972. Additionally, the Incremental Funding Amount of $35,000 is increased by $4,972 for a revised Incremental Funding Amount of $39,972.00. A revised Statement of Work is incorporated below. All other terms and conditions remain unchanged.

Note: Captions in this document and in Battelle's General Provisions are included for convenience of reference only and in no other way define or delineate any of the provisions hereof or otherwise affect their construction or effect.

1. SCOPE AND PRICING

Scope: Contractor agrees to perform the scope outlined in the attached Statement of Work dated October 26, 2021, revised September 23, 2022 for this Contract (hereinafter referred to as "Contract").

Deliverable and Payment Schedule: Payment shall be made upon receipt of acceptable deliverables as outlined in the Statement of Work. The payment for all Deliverables respectively shall be made upon concurrence by the Technical Oversight Representative (see below) or delegate. The following Payment Schedule shall apply throughout completion of all deliverables.

Deliverable	Description	Due Date (No Later Than)	Fixed Amount (USD)
Year 1, Quarter 1	Report on the progress of preliminary C++ implementation of DMRG-AC0 and DMRG-AC methods	31 March 2022	$8,750.00
Year 1, Quarter 2	Report on the progress of design of the parallel scheme for DMRG-AC0	30 June 2022	$8,750.00
Year 1, Quarter 3	Report on the progress of implementation of the parallel DMRG-AC0, Extension of DMRG by ML features	30 September 2022	$8,750.00
Year 1, Quarter 4	Report on the progress of DMRG-AC0 benchmark study	31 December 2022	$8,750.00
Project Meeting	[redacted] and [redacted] shall attend the SPEC project meeting	31 December 2022	$4,972.00
Year 2, Quarter 1	Report on the progress of implementation of the parallel DMRG-AC	31 March 2023	$8,750.00
Year 2, Quarter 2	Report on the progress of design of the DMRG-AC/AC0-in-DFT scheme	30 June 2023	$8,750.00
Year 2, Quarter 3	Report on the progress of implementation of the parallel DMRG-AC0-in-DFT method	30 September 2023	$8,750.00
Year 2, Quarter 4	Report on the progress of DMRG-AC0-in-DFT benchmark studies	31 December 2023	$8,750.00
Year 3,	Report on the progress of GPU parallel scheme for DMRG-	31 March	$8,750.00

Quarter 1	AC/AC0: design	2024	
Year 3, Quarter 2	Report on the progress of GPU parallel scheme for DMRG-AC/AC0: implementation	30 June 2024	$8,750.00
Year 3, Quarter 3	Report on the progress of efficient and fully working parallel DMRG-AC/AC0 code capable of handling 60 active orbitals and 2000 basis functions	30 September 2024	$8,750.00
Year 3, Quarter 4	Report on the progress of applications of the developed methods on extended strongly correlated systems, i.e. transition metal complexes with multiple transition metal atoms	31 December 2024	$8,750.00
Year 4, Quarter 1	Report on the progress of application of DMRG-AC/AC0-in-DFT on extended strongly correlated systems	31 March 2025	$8,750.00
Year 4, Quarter 2	Report on the progress of ML studies harnessing the developed parallel computational methods	30 June 2025	$8,750.00
Year 4, Quarter 3	Report on the progress of improvements of the code: adaptation to the new hardware.	30 September 2025	$8,750.00
Year 4, Quarter 4	Report on the progress of Further possible improvements of the code: improvements of the methods (higher order approximations, tensor network extensions beyond DMRG, employment of the local fermionic mode transformation, etc.)	31 December 2025	$8,750.00
		Total Price (USD)	$144,972.00

Limitation of Funds (Fixed-Price Contract):

(a) Of the Total Price of items through 31 December 2025, the sum of $39,972.00 (USD) is presently available for payment and allotted to this contract. It is anticipated that from time-to-time additional funds will be allocated to the contract in accordance with the following schedule, until the total price of said items is allotted:

SCHEDULE FOR ALLOTMENT OF FUNDS	
Funded – Deliverable Year 1, Quarter 1 Due 31 March 2022	$8,750.00
Funded – Deliverable Year 1, Quarter 2 Due 30 June 2022	$8,750.00
Funded – Deliverable Year 1, Quarter 3 Due 30 September 2022	$8,750.00
Funded – Deliverable Year 1, Quarter 4 Due 31 December 2022	$8,750.00
Funded – Attend SPEC Project Meeting	$4,972.00
To Be Funded by 1 January 2023 – Deliverable Year 2, Quarter 1 Due 31 March 2023	$8,750.00
To Be Funded by 1 January 2023 – Deliverable Year 2, Quarter 2 Due 30 June 2023	$8,750.00
To Be Funded by 1 January 2023 – Deliverable Year 2, Quarter 3 Due 30 September 2023	$8,750.00
To Be Funded by 1 January 2023 – Deliverable Year 2, Quarter 4 Due 31 December 2023	$8,750.00

To Be Funded by 1 January 2024 – Deliverable Year 3, Quarter 1 Due 31 March 2024	$8,750.00
To Be Funded by 1 January 2024 – Deliverable Year 3, Quarter 2 Due 30 June 2024	$8,750.00
To Be Funded by 1 January 2024 – Deliverable Year 3, Quarter 3 Due 30 September 2024	$8,750.00
To Be Funded by 1 January 2024 – Deliverable Year 3, Quarter 4 Due 31 December 2024	$8,750.00
To Be Funded by 1 January 2025 – Deliverable Year 4, Quarter 1 Due 31 March 2025	$8,750.00
To Be Funded by 1 January 2025 – Deliverable Year 4, Quarter 2 Due 30 June 2025	$8,750.00
To Be Funded by 1 January 2025 – Deliverable Year 4, Quarter 3 Due 30 September 2025	$8,750.00
To Be Funded by 1 January 2025 – Deliverable Year 4, Quarter 4 Due 31 December 2025	$8,750.00
Total Price (USD)	**$144,972.00**

(b) Contractor agrees to perform work on the items specified in Section 1 of this Contract up to the point at which, if this contract is terminated pursuant to the Termination for Convenience clause of this contract, the total amount payable by Battelle (including amounts payable for subcontracts and settlement costs) would, in the exercise of reasonable judgment by the Contractor, approximate the total amount at the time allotted to the contract. The Contractor is not obligated to continue performance of the work beyond that point. Battelle is not obligated in any event to pay or reimburse the Contractor more than the amount from time to time allotted to the contract, anything to the contrary in the Termination for Convenience clause notwithstanding.

(c) It is contemplated that funds presently allotted to this contract will cover the work to be performed until 31 December 2022.

(d) The provisions of this clause with respect to termination shall in no way be deemed to limit the rights of Battelle under the default clause of this contract. The provisions of this Limitation of Funds clause are limited to the work on and allotment of funds for the items set forth in paragraph (a) of this clause. Battelle may by unilateral modification provide additional funding up to the Total Price specified above. This clause shall become inoperative upon the allotment of funds for the Total Price of said work except for rights and obligations then existing under this clause.

(e) Nothing in this clause shall affect the right of Battelle to terminate this Contract pursuant to the Termination for Convenience clause of this contract.

Currency: The currency of this Contract is U.S. Dollars with the amount fixed for the term of the Contract.

2. PERIOD OF PERFORMANCE/DELIVERY

Period of Performance: The Completion Date is on Page 1. The Deliverable and Payment Schedule is in Section 1.

3. CONTRACTUAL REQUIREMENTS/INFORMATION

Travel Notice: Request for any domestic and foreign travel associated with this Contract (including Contractor travel within a country of presence) shall be approved in writing by the Battelle Contracts Specialist in advance of travel arrangements being finalized. Without the advance approval of the Battelle Contracts Specialist for any such travel, any invoiced costs related to such travel may not be paid. The planned project meeting November 5 and 6 in Seattle, WA is approved.

4. CONTRACT ADMINISTRATION

Battelle Contracts Specialist: The Battelle Contracts Specialist, [redacted], is the sole point of contact for any contractual/administrative communications or questions regarding this acquisition. Contact information is on Page 1.

Technical Oversight Representative: All technical questions should be directed to the Technical Oversight Representative (TOR), [redacted]. The TOR cannot modify this Contract.

5. TERMS AND CONDITIONS

The General Provisions for Fixed Price Foreign - Supplies/Services - Form A-110.21-FP-Foreign, dated, July 2021, are hereby incorporated and can be read in full at https://www.pnnl.gov/contracts/contractdocuments.aspx.

6. CONTRACT ATTACHMENTS

In addition to the above, the Contract consists of:

- Statement of Work dated October 26, 2021, revised September 23, 2022
- Representations and Certifications dated November 15, 2021

7. ENTIRE AGREEMENT

This Contract contains the entire agreement and understanding between the parties, and there are no agreements, understandings or representations not set forth or incorporated by reference herein. This Contract supersedes all prior proposals, understandings and agreements, whether oral or written, between the parties with respect to the subject matter hereof. No subsequent Modifications of this Contract shall be of any force or effect unless in writing by authorized representatives of each party to this Contract. No communications, written or oral, by other than a Battelle Contracts Specialist shall be effective to modify or otherwise affect the provisions of this Contract.

STATEMENT OF WORK
Scalable Predictive methods for Excitations and Correlated phenomena (SPEC)
J. Heyrovsky Institute of Physical Chemistry, Czech Academy of Sciences
[redacted] and [redacted]
October 26, 2021, revised September 23, 2022

I. BACKGROUND AND PROPOSED RESEARCH

The proposed research shall focus on the development of new quantum chemical methods applicable to extended strongly correlated systems, which will involve a treatment of dynamical correlation effects to support the Scalable Predictive methods for Excitations and Correlated phenomena (SPEC) at Pacific Northwest National Laboratory (PNNL). The work will focus on implementation of new tools based on the recently developed massively parallel DMRG program [MOLMPS]. For a proper treatment of the dynamical correlation, methods will be employed based on the adiabatic connection (AC) which are particularly suitable for connection with large complete active space (CAS) wave functions. In addition, the parallel performance currently based on CPU based architectures will be extended for mixed CPU/GPU architectures, which will further improve the performance needed for proposed highly challenging systems. Optimization and scaling on DOE's Leadership Computer Facilities (LCFs) such as Perlmutter (NERSC) and Summit (OLCF) will be targeted. Finally, DMRG calculations will be embedded in a DFT environment by means of the projection-based WF-in-DFT embedding and develop the DMRG-AC-in-DFT methodology. All tools will be extended by machine learning capabilities, for automatic selection of active spaces and very fast estimation of the mutual information for CAS orbital ordering optimization or other applications.

II. REQUIREMENTS

[redacted] and [redacted] shall be responsible for the development of the proposed methods. They shall design and implement the parallel implementation of the DMRG-AC approach, the efficient parallel implementation of DMRG-AC-in-DFT approach, the design and implementation of the GPU parallel scheme, and implement machine learning (ML) features in MOLMPS. For the last task, interactions with the ML/AI group at PNNL will be sought. The parallel implementation of the proposed DMRG-based approaches shall be applicable to systems involving up to about 60-70 active orbitals and more than 2000 basis functions.

The parallel scheme shall maintain an advantage of a special structure of the superblock Hamiltonian, which leads to a large number of smaller tasks. These tasks shall be distributed across nodes by a scheduler and the results synchronously gathered as needed. The code shall be written in C++, the pilot implementation shall use of Global Array library combined with a data locality approach. The efficient parallel implementation of DMRG-based approaches shall be interfaced with the Scalable Predictive methods for Excitations and Correlated phenomena (SPEC) library and used for externally corrected of existing coupled-cluster (CC) and MRCC implementations via the Tensor Algebra for Many-body Methods (TAMM) module.

The adiabatic connection (AC) technique is especially suitable for large CAS wave functions, since it requires only one and two-body reduced density matrices (RDM). The AC formula,

firstly used in the context of DFT, linearly interpolates between the zeroth-order Hamiltonian H(0) and the exact one H. H(0) is chosen to have a form of a sum of group Hamiltonians, which for the case of CASSCF reference wave functions comprises only two terms, one corresponding to the doubly occupied (inactive) part and one corresponding to the active orbitals. The general integral formula of the AC correlation energy can be derived by exploiting the Hellmann-Feynman theorem and the exact relation between the two-body RDMs and one-body reduced functions. An important note is that this energy expression already assumes that one-body density matrix stays constant along the AC path. This approximation is justifiable if the CASSCF reference wave function contains major part of the static correlation and will be valid only if the CAS is large enough. In this respect, AC is especially appealing for connection with DMRG. In other words, AC correction accounts for (mainly) dynamical correlation, which do not alter the one-body RDM. In fact, one can avoid the rather expensive AC integration by linearized-AC-integrand approximation, named AC0, without losing much of accuracy.

Both the full DMRG-AC method as well as the approximated DMRG-AC0 method will be developed. Implementations shall employ RDMs exported from NWChem CASSCF module which has been already interfaced with MOLMPS. The DMRG-AC/AC0-in-DFT approach will make use of the DMRG-SCF-in-DFT methodology, which will be at the end refined by the AC/AC0 energy correction.

[redacted] and Dr. [redacted] shall modify the data handling scheme and task schedulers, to distribute the tasks between CPUs and GPUs efficiently. The large number of tasks sharing the same operators data shall be executed on GPU, while CPU shall execute tasks composed from larger data chunks available only remotely.

The machine learning features to MOLMPS shall be added - ML models for very fast prediction of the lowest state energies, or two-orbital entropies, which will reveal much more detailed information about correlation structure in the system and allow very fast sampling of molecules when searching for perspective candidates with certain properties (singlet-triplet gap, correlation structure, etc.).

The goal for year 1 is the fully working parallel implementation (CPU parallel scheme) of the DMRG-AC0 method, which will be verified by benchmarks, and the implementation of the ML capabilities for DMRG. In the second year, a more general DMRG-AC method and the DMRG-AC0-in-DFT method will be implemented, the code will allow parallel execution and will be benchmarked. In year 3, the work will be focused on optimization of the codes and implementation of the GPU parallel scheme, the result shall be efficient GPU parallel code for DMRG-AC/AC0 methods and the code shall be used for application on extended correlated systems. The goal for year 4 is to apply DMRG-AC0-in-DFT method on extended correlated systems, employ ML capabilities for DMRG-AC0/AC/AC0-in-DFT methods. The code shall be adapted to the newest hardware.

The following software quality assurance (QA) activities shall be conducted for software development of the SPEC DMRG methods:

1. Identify and document software requirements (features). Involve PNNL SPEC PIs in the review process of these requirements.

   The software will be developed with the advanced C++ standard (C++11 or later), and will include MPI library for parallel execution, Global Arrays library to handle large data, and Libint for integral acquisitions. The code will be interfaced with the SPEC library and used for externally corrected CC methods in NWChem program. The work will be performed closely with PNNL SPEC PIs, [redacted] and [redacted], to interface the DMRG code with SPEC.

2. Document the design of the software to the specific software requirements.

   For the DMRG algorithm overview, see G.K.-L. Chan and M. Head-Gordon, J. Chem. Phys., 116, 4462 (2002). Global Arrays is developed and maintained by PNNL. For AC see Pernal, K. Electron Correlation from the Adiabatic Connection for Multireference Wave Functions. Phys. Rev. Lett. 2018, 120, for projection-based DFT embedding see F. R. Manby, M. Stella, J. D. Goodpaster, and T. F. Miller, Journal of Chemical Theory and Computation 8, 2564 (2012).

3. Follow the established coding standards and conventions.

   The parallel DMRG code will be written in C++11 with standard I/O utilities, MPI standard v. 2 and above. The interface with NWChem/NWChemEX will use coding standards of those programs.

4. The Contractor will conduct software activities in accordance with PNNL software quality assurance requirements.

[redacted] and [redacted] shall attend the in person all PI SPEC project meeting for two days currently scheduled for Saturday, 5 November 2022 and Sunday, 6 November 2022 in Seattle, Washington, USA. The airfare shall be refundable in the event the PI SPEC project meeting is delayed.

III. DELIVERABLES

1. The results shall be reported to PNNL on a quarterly basis.

2. It is anticipated that the results of this activity shall form the basis of joint publications and conference presentations by [redacted], [redacted] and PNNL.

3. [redacted] and [redacted] shall attend project meetings via Skype or telecom as required by the PNNL Project Director, [redacted].

Year 1 DELIVERABLES

- Q1: Preliminary C++ implementation of DMRG-AC0 and DMRG-AC methods

- Q2: Design of the parallel scheme for DMRG-AC0
- Q3: Implementation of the parallel DMRG-AC0, Extension of DMRG by ML features
- Q4: DMRG-AC0 benchmark study

- **Project Meeting:** Dr. [redacted] and Dr. [redacted]c shall attend the in person all PI SPEC project meeting estimated to occur 5 November 2022 and 6 November 2022

Year 2 DELIVERABLES

- Implementation of the parallel DMRG-AC
- Design of the DMRG-AC/AC0-in-DFT scheme
- Implementation of the parallel DMRG-AC0-in-DFT method
- DMRG-AC0-in-DFT benchmark studies

Year 3 DELIVERABLES

- GPU parallel scheme for DMRG-AC/AC0, design and implementation
- Efficient and fully working parallel DMRG-AC/AC0 code capable of handling 60 active orbitals and 2000 basis functions
- Applications of the developed methods on extended strongly correlated systems, i.e. transition metal complexes with multiple transition metal atoms

Year 4 DELIVERABLES

- Application of DMRG-AC/AC0-in-DFT on extended strongly correlated systems
- ML studies harnessing the developed parallel computational methods
- Further possible improvements of the code: e.g. adaptation to the new hardware or improvements of the methods (higher order approximations, tensor network extensions beyond DMRG, employment of the local fermionic mode transformation, etc.)