Elements of the Physics 595 Proposal

The Physics 595 Research Initiative
University of Illinois at Urbana-Champaign

Request for Proposals

The Department of Physics at the University of Illinois at Urbana-Champaign (PHYS/UIUC) announces an intensive 1-year program to provide opportunities for talented graduate students to participate in research. Prospective participants are invited to submit proposals for research projects for the 2023 program.

Project Summary "white papers" are due by 5:00 P.M. CST, April 14, 2023. Full proposals are due by 5:00 P.M. CST, April 21, 2023.
Proposals submitted after the deadline will not be considered.

The Initiative
The PHYS/UIUC Phys 595 research program provides resources to enable graduate students to undertake research projects in experimental, theoretical, and computational physics. Of particular interest are projects in condensed matter physics, materials science, theoretical biophysics, theoretical astrophysics, and experimental particle and nuclear physics. Proposed research projects should offer interesting, meaningful research that can be conducted without extensive background knowledge, in a 1-year time frame, and with a broad mix of appropriate techniques and methodologies. An ideal project will offer the student a chance to develop expertise in a particular area while learning techniques applicable to many areas.

Objectives of the Program
- Provide students with a meaningful experience in a first-class research environment.
- Enable students to work closely and directly with practicing researchers.
- Encourage students to develop their own "research literacy," including familiarity with the literature, oral and written communications skills, time management, and teamwork skills.

Terms
Grants are for a 1-year period, beginning August 1, 2023.

Grantees are required to provide a final presentation and a written report that:
- Summarize activities and results as they relate to the proposed objectives.
- Discuss the significance of the results.
- Recommend avenues for future work.

Grantees will participate in programmatic activities and group meetings during the 1-year grant period. Grantees are encouraged to participate in research-group and departmental seminars and colloquia.

Budget and Budget Justification
A maximum of $25,000 may be requested, of which $5,000 must be a student stipend. Other eligible expenses are equipment, materials and supplies, telecommunications, travel, publication/dissemination of results, and institutional overhead.

Institutional overhead is to be calculated at a rate of 52 percent of the modified total direct cost (MTDC) base. Student stipends and equipment costs are to be excluded from the MTDC.
A narrative budget justification of no more than one page must be included in the proposal.

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Criteria

Proposals submitted under this RFP will be peer-reviewed, using the National Science Board merit review criteria. Review panels will present recommendations for awards to the Associate Head for Graduate Programs, Professor S. Lance Cooper. Selection criteria include:

- Overall scientific and technical merit of the project.
- Feasibility.
- Qualifications, capabilities, and experience of the applicant.
- Realism of the proposed project costs.
- The potential of the project to improve the student's knowledge and skills.
- The inclusion of specific evaluation mechanisms for measuring the success of the proposed project.

Proposals

Proposals may be *no longer than 9 pages* and should include the following:

- Cover page—maximum one page.
- Project summary, including explicit statements regarding the "intellectual merit" and "broad impact" of the proposed work—maximum one page.
- Project narrative, including a comprehensive description of the problem to be studied, expected outcomes and how they will be measured, and a discussion of the project's potential contribution to the applicant's graduate education—maximum 5 pages.
- References cited—doesn't count toward total page limit.
- Budget and justification (use the budget categories mentioned above under "Budget")—maximum one page.
- Proposer's *curriculum vitae*—maximum one page.

Submission

Deliver *an electronic copy* of your proposal to S. Lance Cooper (slcooper@illinois.edu), by 5:00 P.M. on Friday, April 21, 2023.

Proposal Time Line

- Project Summary 'white paper' submitted by Friday, April 14, 2023.
- Written proposals submitted by Friday, April 21, 2023.
- Assigned proposals will be sent to students starting on Monday, April 24, 2023.
- Proposal Panel Review on Friday, April 28, 2023.
- Awards announced by Friday, May 5, 2023.
- Project implementation to start August 1, 2023.

For further information about this RFP, contact:

S. Lance Cooper, Department of Physics
227 Loomis Laboratory of Physics
217-333-2589 • *slcooper@illinois.edu.*

The University of Illinois at Urbana-Champaign is an equal employment opportunity employer. Proposals from women and minorities historically underrepresented in science and engineering are particularly welcomed.

Requirements of the Physics 595 Proposal

Phys 595 Proposal Cover Sheet (1 page)

Cover Page (1 page)

Today ⇒ Project Summary (1 page) ('white paper' due on April 14)

Project Narrative (5 pages)

Next class ⇒ Budget and Budget Justification (1 page)

References Cited (no limit, but keep ~ 1 page)

Next class ⇒ Curriculum Vitae (1 page)

Full proposal due 5 pm on April 21

Cover Page (maximum one page)

Proposal for implementing the diffusion Monte Carlo method in investigations of few-electron systems

Ko, Wing Ho

Contact Information:

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Project Summary (maximum one page)

Project Summary

The application of *ab initio* methods in calculating electronic structures is an important aspect of theoretical condensed matter physics, and its importance is currently growing as the need for understanding novel materials increases. The goal of this proposed project is to investigate one *ab initio* electronic structure method known as the diffusion Monte Carlo (DMC) method. To achieve this goal, an undergraduate student will write computer programs to apply the DMC method in calculating the ground-state energies of various few-electron systems.

The project is expected to produce results that can be cross-examined with those produced for the same systems using different methods. It is also expected to produce results for comparisons between different implementations of the DMC method.

This proposed project has substantial intellectual merit for the following reasons: it provides a better understanding of the electronic structures of various few-electron systems; it gives insights for improving the DMC algorithm, without using too many computational resources; and it reveals the strengths and weaknesses of the DMC method as compared to other electronic structure methods. This project will benefit from the capabilities of the proposer, who has experience in working on similar projects. It will also be benefit from the institution where the project will be carried out, where experienced faulty members in computational physics (e.g., Prof. Richard Martin and Prof. David Ceperly) can provide an extensive network for help and discussion.

The proposed project will have broader impact on the community for the following reasons: the student will acquire the skill of writing computer programs to solve physical problems and will be introduced to important concepts in theoretical physics; the results of the project will be disseminated in the form of a research proceeding, a senior thesis, a talk given in the annual undergraduate research symposium at the University of Illinois, and a talk given at the American Physical Society March 2006 meeting; attractive visualizations that can be used for educational purposes will also be produced.

Explicit statements of "intellectual merit" and "broad impact"

Project Narrative (maximum five pages)

Project Narrative

INTRODUCTION

Theoretically, all electronic properties of a quantum system can be obtained by solving the time-independent Schrödinger equation (TISE) of the system. Since the TISE cannot be solved analytically in many cases, it is necessary to obtain numerical solutions. Commonly used numerical methods include mean-field methods (e.g., Hartree-Fock), configuration-interaction (CI) methods, and quantum Monte Carlo (QMC) methods. In general, as compared to the QMC methods, mean-field methods are cheap but prone to systematic errors, while configuration-interaction methods are accurate but expensive.

The proposed project will center on one particular QMC method known as the diffusion Monte Carlo (DMC) method, which can be derived from writing the time-dependent Schrödinger equation in imaginary time [2,3,6,7]. In the DMC method, wavefunctions are treated as probabilistic distributions and are represented by an ensemble of random samples. Upon applying random walks on an initial ensemble generated from a trial wavefunction, the ensemble evolves until its distribution is essentially that of the ground-state wavefunction.

In the proposed project, the DMC method will be applied to various few-electron systems. Few-electron systems are investigated since they do not require extensive computational resources, and since data obtained from other approaches are available for comparisons.

METHOD

A schematic of how the DMC algorithm is implemented in computer programs is shown on Fig. 1. The various components are explained below. For further discussion, see refs. [3,5], and the references therein.

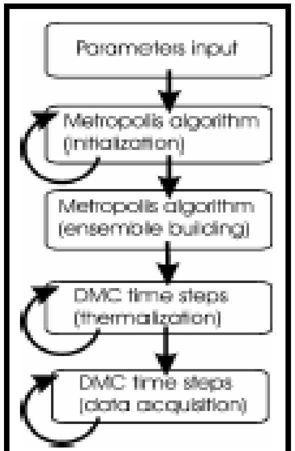

Fig. 1. Schematic for the implementation of the DMC algorithm.

This section summarizes the goals, motivations, methods to be used, and expected results in your project – this should include data and diagrams!

You should be able to generate this quickly from your already-completed introduction, procedure, and results sections!

A Good Project Narrative Should Answer These Questions (also for Research Statement in fellowship and job applications)

1. What research do you propose to do?
2. Why is this research important?
3. Why are you ideally suited to conducting this research (e.g., because of your access to personnel, experiences, and/or unique facilities)?
4. How do you plan to accomplish this research?
5. How will you know if the research is successful?
6. What is the timeline for the research?
7. What will be the benefits to the scientific community if the research is successful?

Budget and Budget Justification (maximum one page)

Budget

The main component for the budget of the proposed project is the student stipend. A student stipend of $4000 is requested.

Most computational resources required for the completion of the proposed project are available through the Engineering Work Stations (EWS) maintained by the Campus Information Technologies and Educational Services (CITES) of the University of Illinois. The resources provided include compilers (e.g., GCC for C/C++) for compiling computer codes, high-level computer programs (e.g., Microsoft Excel and Mathematica) for analyzing the data, and computer storage space. However, since a large amount of data is expected to be generated, additional storage space for computer data is required; $150 fund is requested for such storage space. The storage may take the form of computer hard disk, CD-ROMs, and/or storage space in network servers.

To disseminate the results obtained in the proposed project, $600 is requested for one student's travel, to give a talk at the American Physical Society (APS) 2006 March meeting at Baltimore, MD.

The requested fund for the items listed above is summarized in the table below:

Item	**Request fund (institutional overhead excluded)**
Student stipend	$4000
Storage space for computer data	$150
Student's travel to APS March meeting	$600

With a 43 percent institutional overhead applied to the storage space and to student travel, the total budget requested for the proposed project is $5072.50.

This section summarizes (in table form) your requested budget, and provides a brief justification as to why the items requested are needed for your project.

References Cited (no page limit)

References Cited

[1] Michal Bajdich, Lubos Mitas, Gabriel Drobny, and Lucas K. Wagner, "*Approximate and exact nodes of fermionic wavefunctions: coordinate transformation and topologies*," ArXiv Preprint.

[2] Foulkes et. al., "*Quantum Monte Carlo simulations of solids*," Rev. Mod. Phys. **73**, 33 (2001).

[3] B.L. Hammond, W.A. Lester, Jr., and P.J. Reynolds, *Monte Carlo methods in Ab Initio quantum chemistry* (World Scientific, River Edge, NJ, c1994).

[4] W. Kolos and L. Wolniewicz, "Improved Theoretical Ground-State Energy of the Hydrogen Molecule," J. Chem. Phys. **49**, 404 (1968).

[5] Steven E. Koonin, *Computational Physics* (Benjamin, Reading, MA, 1986).

[6] Ioan Kosztin, Byron Faber, and Klaus Schulten, "*Introduction to the Diffusion Monte Carlo Method*," Am. J. Phys. **64**, 633 (1996).

[7] Peter J. Reynolds, David M. Ceperley, Berni J. Alder, and William A. Lester, Jr. "*Fixed-node quantum Monte Carlo for molecules*," J. Chem. Phys. **77**, 5593 (1982).

[8] P.A. Sundqvist, S. Yu. Volkov, Yu. E. Lozovik, and M. Willander, "*Phase transitions of a few-electron system in a spherical quantum dot*," Phys. Rev. B **66**, 075335 (2002).

[9] M. Taut, "*Two electrons in an external oscillator potential: Particular analytic solutions of a Coulomb correlation problem*," Phys. Rev. A. **48**, 3561 (1993).

Curriculum Vitae (maximum one page)

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EDUCATION

2001–Present: University of Illinois at Urbana-Champaign, Urbana, IL USA
Bachelor of Science in Physics with honors expected in May 2005
Bachelor of Science in Mathematics with honors expected in May 2005
Overall GPA: 4.0

2000: Hong Kong Certification of Education Examination
A in English Language (Syllabus B), Biology, Chemistry, Physics, Mathematics, Additional Mathematics, and Economics
B in Chinese Language and Religious Studies

1995–2001: Diocesan Boys' School, 131 Argyle Street, Mongkok, Hong Kong

EMPLOYMENT

2002–Present: *Mentor (Mathematics)*, Netmath Distance Education Program, Department of Mathematics, University of Illinois at Urbana-Champaign, Urbana, IL USA

Summer 2004: REU (Research Experience for Undergraduates) at the University of Illinois under Prof. Richard Martin, investigating the application of quantum Monte Carlo methods on few-electron systems

MEMBERSHIPS AND ACTIVITIES

Vice Chairman, Science Society, Diocesan Boys' School, 2000–2001
Chairman, Astronomy Club, Diocesan Boys' School, 2000–2001
Member, Phi Eta Sigma National Society, University of Illinois Chapter, 2002
Participant, Physics Van, University of Illinois at Urbana-Champaign, 2002–Present
Treasurer, Physics Society, University of Illinois at Urbana-Champaign, 2003–Present

AWARDS AND HONORS

Dean's List, College of Liberal Arts and Sciences, University of Illinois at Urbana-Champaign, Fall 2001–Spring 2004
James Scholar, College of Liberal Arts and Sciences, University of Illinois at Urbana-Champaign, Fall 2001–Spring 2004
Salma Wanna Memorial Award, Department of Mathematics, University of Illinois at Urbana-Champaign, 2004
Undergraduate Outreach Achievement Award, Physics Department, University of Illinois at Urbana-Champaign, 2004
Lorella M. Jones Summer Research Fellowship, Physics Department, University of Illinois at Urbana-Champaign, 2004