OAK RIDGE NATIONAL LABORATORY
CENTER FOR NANOPHASE MATERIALS SCIENCES
Research Proposal

Workflow History

Action	Actor	Date/Time
Submitted	tconley22@ensworth.com	2021-5-05 23:53

Award Information

Award Status
Approved with Special Conditions

Review Comments

Start Date
Aug 1, 2021

End Date
Jul 31, 2022

Technical Contact(s)
Ganesh, Panchapakesan
Kumar, Rajeev

General Information

Proposal Number	Proposal Type
CNMS2021-B-00825	General

Title of Proposal
Simulation of Feynman's Ratchet and Pawl

Does any part of the proposed work represent an industrial collaboration and/or partnership?
No

CNMS staff members contacted to discuss feasibility of project
None

Participants

Name	Email Address	Institution	Role	On-Site
Conley, Trent	tconley22@ensworth.com	Ensworth School	Principal Investigator	Y

CNMS Facilities Requested

Facility Group	Facility	Requested Usage
(LEAD) Nanomaterials Theory Institute	NTI staff support, theoretical project	1 days
	NTI Computational Cluster, capacity computing	1 K cpu-hours

Samples and Identification of Hazards

Research samples used in this project will be
Wholly supplied by user, only characterized at CNMS

Indicated hazards
No major safety issues

Categorization

Indicate any subjects that apply to this project
Engineering
Physics (excluding condensed matter physics)

Funding

Source of Support	Funding Source
Other	Personal

Funding Status
Funding has been obtained

Review Suggestions

List a few keywords to help in matching potential reviewers
Thermodynamics, Entropy, Ratchet, Simulation

Suggested reviewers from CNMS Review Committee
Arya, Gaurav
Kuroda, Marcelo

Review Comments

Comments

Special Conditions

Description of Proposed Research

1) What is/are the main scientific or technological question(s) that you plan to address?

Under special conditions, it is possible that a Feynman ratchet and pawl system of specific design could induce asymmetric distributions of molecular gas dynamics which would enable novel applications such as thermal management of nano-machinery and semiconductors and could possibly be a source or energy production in exothermic systems. The Feynman ratchet has been extensively studied in various configurations, but none of the approaches have considered design features that will be possible in just a few years based upon advances in carbon nanotube technology and the interaction of such nano structures in such proximity that non-Boltzmann distributions of gas molecules arise due to the atomic scale of the mechanical structures. As an example, Feynman asserted that the ratchet and pawl system fails due to equilibrium boundary conditions arising from the randomness of Brownian motion. However, if the distance between the pawl and the ratchet teeth is small enough relative to the size of the gas atoms themselves such that non-Boltzmann distributions arise, will the pawl still slip between the ratchet's teeth? Furthermore, if the ratchet's paddle has a large surface area but the ratchet's teeth and pawl are much smaller, will particles with higher kinetic energy on the tail end of the Maxwell-Boltzmann distribution occasionally cause an imbalance, allowing the ratchet to produce work? While current semiconductor manufacturing resolutions are too large for producing a network of these ratchets and pawls, this simulation opens the door to these possibilities as Moore's Law progresses to smaller feature sizes. However, even if the simulation proves the ratchet to not perform as hypothesized, such research will be important for the scientific community by advancing our understanding of the interaction of molecular gas dynamics at nanoscale when interacting with mechanical devices.

2) Outline the overall technical approach that you plan to use to address the above questions. This section should provide the context for research tasks described below in sections (3), home institution activities, and (4), CNMS research.

In proving how the ratchet and pawl system would generate heat, Richard Feynman detailed that the pawl would slip and cause the ratchet to fall back a notch the same rate at which the Brownian motion would cause it to move forward a notch(1). However, Feynman assumed that the forces applied on the pawl and the paddle are statistically uniform, and used this assumption in proving that no net force can be generated by the ratchet. This simulation will include a simple ratchet and pawl system, with a paddle connected via a shaft in the z axis, where a spring acts on the pawl. The ratchet system will be subject to the collisions of surrounding gas particles, but the pawl, spring, ratchet wheel, shaft, and paddle will be attached to a fixed point yet allowed to pivot. I have proposed to run simulations using Simbody(2), an open source physics engine developed in C++ that runs in O(N) time with a high degree of accuracy, to test Feynman's hypothesis. The size of the ratchet, total number of particles in the gas, average kinetic energy of the gas particles, and the spring strength will all be varied to calibrate each of the key design parameters and their impact on the system efficiency.

3) What research tasks will be carried out at the users' home institution or elsewhere outside of the CNMS? Include any preliminary syntheses, measurements, or tests that have been/will be performed in preparation for the proposed research at the CNMS.

I will run simulations of a smaller scale to best leverage the computational resources available.
As a junior at the Ensworth High School in Nashville, our computational resources are very limited. I have built a simulation of the system using a Macbook Pro with the new M1 chip. While this early development has proven the software's ability to simulate the system, the magnitude of the computations needed to accurately model the atomic level interactions is far too great to be simulated on a laptop.

4) Describe very clearly and specifically the research tasks to be carried out at the CNMS and the expected outcomes from the CNMS tasks. Include any technical milestones that must be met and the need for specialized capabilities and/or expertise at the CNMS for the research to be successful.

The objective of this simulation is to determine the optimal parameters for a novel Feynman ratchet and pawl system. These parameters include:
1. Optimal distance between the pawl and ratchet teeth
2. Optimal ratio of surface area of the paddle to the feature size of the ratchet teeth
3. Identification of any non-linear relationships between the above parameters and the characteristics of the gas/fluid system being simulated (variances in atomic size/molecular weight, density, and temperature)
4. Production of simulation-based experimental results that can be used to develop parametric models for physical system design and optimization
The research task itself will require in total 1000 cpu hours. The nature of this simulation demands that each particle is simulated directly because any statistical assumptions could lead to inaccurate and misleading results. Because Simbody executes programs in O(N) time, the computational intensity is directly proportional to the number of particles in the system.

5) Provide an overall timeline for the CNMS tasks and describe how each facility/instrument that is checked on p. 2 will be used, including estimates of the number/quantities of samples, instrument time, CPU time, etc.

I will need an initial 100 NTI Computational Cluster cpu-hours, to run preliminary tests. Based upon the results from the initial simulations, the parameters will be updated using a Bayesian prediction model. This updating process and any consequent revision to the software should take less than two weeks. After the software is updated and recalibrated, an additional 900 cpu-hours would allow for refinement of the design based upon simulation results.

6) What is your team's specific experience and expertise relevant to this research project?

I have already developed a gas simulation that was used as an environment to facilitate the ratchet and pawl dynamics as a part of my Capstone project at Ensworth High School in Nashville. I have extensively researched the published literature on the Feynman ratchet(3-8) as a part of this Capstone and am familiar with the approaches taken by other researchers in the past. I earned the highest possible score on the Advanced Placement Computer Science Test (5) while only a freshman in high school and scored a 1520 on the SAT.

Literature cited above

[1] R. P. Feynman, R. B. Leighton, and M. Sands, The Feynman Lectures on Physics I Addison-Wesley, Reading, MA, 1963, Chap. 46.
[2] GitHub. "Simbody Project." https://github.com/simbody.
[3] Jianzhou Zheng, Xiao Zheng, ChiYung Yam, and GuanHua Chen, ""Computer simulation of Feynman's ratchet and pawl system," Phys. Rev. E 81, 061104 – Published 2 June 2010
[4] M. O. Magnasco and G. Stolovitzky, "Feynman's Ratchet and Pawl," Journal of Statistical Physics 93, 615 (1998).
[5] C. Van den Broeck, R. Kawai, and P. Meurs, "Microscopic Analysis of a Thermal Brownian Motor," Physics Review Letters 93, 090601 (2004).
[6] P. Skordos and W. Zurek, "Maxwell's demon, rectifiers, and the second law: Computer simulation of Smoluchowski's trapdoor," American Journal of Physics 60, 876 (1992).
[7] J. C. Maxwell, Theory of Heat Appleton, London, 1871.
[8] Bengt Nordén, "Ratchet device with broken friction symmetry" Applied Physics Letters 80, 2601 (2002).

Publication record

Trent Conley

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EDUCATION

Ensworth School **Nashville, TN**
Class of 2022 August 2020 – Present

- Cumulative GPA: 93.8/100 (including Q3 of 2021 school year)
- 1520 SAT: 790 Math, 730 Evidence-Based Reading and Writing

Menlo School **Atherton, CA**
Class of 2022 August 2018 – June 2020

- Cumulative GPA: 4.165 / 4.0
- Honor Roll: Highest Honors

EXTRACURRICULAR ACTIVITIES

Capstone **Nashville, TN**
Creator November 2020 – Present

- Conducting research to investigate the feasibility of a Brownian Ratchet
- If the simulation proves a Brownian Ratchets to work, a network of Brownian Ratchets has vast implications from having the ability to reverse global warming to significantly reducing the cost of energy around the world
- Developed a 2-D simulation of gas dynamic in Java, currently implementing a Brownian Ratchet

Computer Science Club at Ensworth **Nashville, TN**
Founder and Leader September 2020 – Present

- Created Computer Science Club at Ensworth
- Taught Python and Java to members, facilitating curiosity in Ensworth Students about Computer Science
- Recruited over a dozen students thus far

Computer Science Club at Menlo **Atherton, CA**
Co-Leader September 2019 – May 2020

- Worked with club members to solve USA Computing Olympiad problems
- Taught Python and Java to new members
- Recruited over 40 students

Cabaret Musical **Atherton, CA**
Lead September 2019 – November 2019

- Portrayed Clifford Bradshaw, an aspiring writer in the 1930s
- First musical in school history to be submitted for Rita Moreno Awards

Menlo Hacks **Atherton, CA**
Competitor March 2019

- Created Food4U, an iPhone application and website that connects homeless people in the Bay Area to local food distributers

Varsity Mock Trial Atherton, CA
Witness September 2018 – March 2019
- Awarded three Individual Outstanding Competitor Awards at NorCal Competition
- Won San Mateo County Championship
- Won California Mock Trial State Finals

Varsity Basketball **Atherton, CA**
Forward/Center November 2019 – March 2020
- WBAL champions
- Las Vegas Prep Tournament 2nd place

COMMUNITY SERVICE

Smash High **Nashville, TN**
Founder and President November 2020 – Present
- Founder and director of the first Smash High chapter in Tennessee
- Smash High is a non-profit organization that aids students in their pursuit of academic excellence
- Formed a team of five Ensworth Students to interview tutors and reach students in need

Peninsula Bridge **Atherton, CA**
Teacher June 2019 – July 2019
- Spearheaded development of Computer Science curriculum
- Created and taught an introductory course on Python to highly motivated low-income students
- Adapted course based on engagement and interest of students
- Taught daily for five weeks

Young Men's Service League **Atherton, CA**
Founding Member August 2018 – March 2020
- Vice President of Meetings
- Chair of Philanthropy
- Served local NGOs for more than 24 cumulative hours

WORK EXPERIENCE

Benetic Inc. **Nashville, TN**
Software Engineer September 2020 – Present
- Developed commercial software for a financial services technology company using Python and neural networks to automate the ingestion of government data filings in ERISA's 5500 database

Other Information

Computer:	*Fluent: Java, Python; Experience: C, C++, Swift, NodeJS*
Machine Learning:	*Developed iTurk, a neural net that returns the FEN of a given chessboard image*
Other:	*Interests include running, discus weightlifting, guitar, history, philosophy*