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14. ABSTRACT

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RPPR Final Report
as of 24-Apr-2019

Agency Code:

Proposal Number: 68472CHRIP **Agreement Number: W911NF-16-1-0167**

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Report Date: 17-Jul-2018 Date Received: 14-Jan-2019
Final Report for Period Beginning 18-Apr-2016 and Ending 17-Apr-2018

Title: Acquistion of Computer Cluster for First-Principles Predictions of Structure and Properties of Cocrystals

Begin Performance Period: 18-Apr-2016 **End Performance Period:** 17-Apr-2018
Report Term: 0-Other

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STEM Degrees: 0 **STEM Participants:** 0

Major Goals: The goal of this project was an acquisition of a computer cluster to enable computations needed for the ARO MURI project “Theory and Experiment of Cocrystals: Principles, Synthesis, and Properties” that investigates cocrystals of energetic, ferroelectric, and nonlinear optical materials. The main role of the University of Delaware (UD) group in this project is to perform first-principles computational predictions of structure and properties of such materials prior to their cocrystallization and analyze trends in crystallized materials at atomistic level. While significant computational resources are available at the DoD High- Performance Computing (HPC) centers, the current security regulations make it practically impossible to get access to these centers for foreign citizens (except for one machine, the heavily used open system copper). Therefore, the UD group needed a reasonably powerful local computer cluster.

Accomplishments: A significant effort has been invested into purchasing an optimal cluster for our group. Initially, our plan was to become a participant in the UD Community Cluster. A third such cluster was in the planning stage when the proposal leading to the DURIP grant was written. The costs of community clusters are shared in such a way that UD covers the costs all the racks, cabling, and network, while users are charged only the actual costs for the node. In addition to no costs for the infrastructure, the nodes are highly discounted and therefore users are able to maximize the computational power from a given amount of grant support leading to savings up to 50%. The purchase of the UD Community Cluster was delayed several times which resulted in the request for a non-cost extension of this grant beyond the initial one-year period. However, extensive negotiations of the PI with the UD Information Technology personnel did not succeed. UD decided to purchase a cluster with nodes of minimal expandability (in fact, these nodes are half of the size of typical current cluster nodes). This made the UD nodes not a good choice for us since the nodes could not accommodate a sufficient amount of local disk space, which is critical for the work we do. The PI then negotiated individually with several vendors and was able to get discounts resulting in savings similar to those offered by the UD Community Cluster. All vendors provided access to clusters with various configurations including Intel vs. AMD processors and hard vs. SSD drives of various types. Our codes have been tested on this hardware, so that the final choice of hardware has indeed been optimal for the type of calculations that our group does. The best offer came from Dell and the cluster was bought in December 2017 and installed in March 2018. The whole amount granted was spent on the cluster. The configuration purchased is as follows:

1. PowerEdge R640 head node with 2 Xeon Gold 6130 2.1 G 16-core processors, 64 GB memory, 1 TB disk drive
2. 22 PowerEdge R640 compute nodes, each node with 2 Xeon Gold 6130 2.1 G 16-core processors (32 cores per node), 192 GB memory, and 6.7 TB of SSD disk space in 7-way RAID configuration
3. PowerEdge R740XD network attached storage node with 2 Intel Xeon Silver 4114 2.2 G 10-core processors,

64 GB memory, and 48 TB hard disk space
4. S4148 backbone 10 Gb Base-T communication network including network switch and a network card in each node
5. 42U rack with AP8641 power supply

The highlights of this cluster are large number of cores (756) per amount of funds and the very fast solid-state disk (SSD) space. With increased numbers of fast cores available, hard disks are not able to read and write data fast enough. Our SSD disks are not only a few times faster than the best hard disks, but are 7-way stripped, i.e., each chunk of data is split into 7 parts which are written/read at the same time, each part to a different disk.

The cluster has performed as expected and computational power of our group has increased by about a factor of ten. Thanks to the very broad disk IO bandwidth (about 3.5 TB/s), our jobs are not slowed down by disk access and we can run efficiently even 32 simultaneous jobs per node.

Training Opportunities: Nothing to Report

Results Dissemination: Nothing to Report

Honors and Awards: Nothing to Report

Protocol Activity Status:

Technology Transfer: Nothing to Report

PARTICIPANTS:

Participant Type: PD/PI
Participant: Krzysztof Szalewicz
Person Months Worked: 1.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Final report on W911NF1610167 grant: "Acquisition of Computer Cluster for First-Principles Predictions of Structure and Properties of Cocrystals"

I. MAJOR GOALS

The goal of this project was an acquisition of a computer cluster to enable computations needed for the ARO MURI project "Theory and Experiment of Cocrystals: Principles, Synthesis, and Properties" that investigates cocrystals of energetic, ferroelectric, and nonlinear optical materials. The main role of the University of Delaware (UD) group in this project is to perform first-principles computational predictions of structure and properties of such materials prior to their cocrystallization and analyze trends in crystallized materials at atomistic level. While significant computational resources are available at the DoD High-Performance Computing (HPC) centers, the current security regulations make it practically impossible to get access to these centers for foreign citizens (except for one machine, the heavily used open system copper). Therefore, the UD group needed a reasonably powerful local computer cluster.

II. ACCOMPLISHED TASKS

A significant effort was invested into purchasing an optimal cluster for our group. Initially, our plan was to become a participant in the UD Community Cluster. A third such cluster was in the planning stage when the proposal leading to the DURIP grant was written. The costs of community clusters are shared in such a way that UD covers the costs all the racks, cabling, and network, while users are charged only the actual costs for the node. In addition to no costs for the infrastructure, the nodes are highly discounted and therefore users are able to maximize the computational power from a given amount of grant support leading to savings up to 50%. The purchase of the UD Community Cluster was delayed several times which resulted in the request for a non-cost extension of this grant beyond the initial one-year period. However, extensive negotiations of the PI with the UD Information Technology personnel did not succeed. UD decided to purchase a cluster with nodes of minimal expandability (in fact, these nodes are half of the size of typical current cluster nodes). This made the UD nodes not a good choice for us since the nodes could not accommodate a sufficient amount of local disk space which is critical for the work we do. The PI then negotiated individually with several vendors and was able to get discounts resulting in savings similar to those offered by the UD Community Cluster. All vendors provided access to clusters with various configurations including Intel vs. AMD processors and hard vs. SSD drives of various types. Our codes have been tested on this hardware, so that the final choice of hardware has indeed been optimal for the type of calculations that our group does. The best offer came from Dell and the cluster was bought in December 2017 and installed in March 2018. The whole amount granted was spent on the cluster. The configuration purchased is as follows:

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