

RPPR Final Report
as of 20-Dec-2021

Agency Code: 21XD

Proposal Number: 75810MARIP

Agreement Number: W911NF-20-1-0065

INVESTIGATOR(S):

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Country: USA

DUNS Number: 076248616

EIN: 480680117

Report Date: 15-Jul-2021

Date Received: 20-Dec-2021

Final Report for Period Beginning 16-Apr-2020 and Ending 15-Apr-2021

Title: Graphics Processing Unit (GPU) Infrastructure for Massively Parallel Computing Research

Begin Performance Period: 16-Apr-2020

End Performance Period: 15-Apr-2021

Report Term: 0-Other

Submitted By: Suzanne Shontz

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Phone: (785) 864-8816

Distribution Statement: 1-Approved for public release; distribution is unlimited.

STEM Degrees: 5

STEM Participants: 15

Major Goals: The objective of this DURIP project is to acquire graphics processing unit (GPU) computing infrastructure to support research projects involving massive parallelism at the University of Kansas (KU). The acquired GPU infrastructure will leverage and extend existing KU infrastructure that is available to the researchers

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through the KU Advanced Computing Facility.

The GPU infrastructure will support general-purpose graphics processing unit (GPGPU) research in five DOD mission-critical thematic areas: computational fluid dynamics, nanostructured materials, machine learning, unstructured meshing, and materials chemistry. The proposed infrastructure will enhance the quality of research and research-related education that is currently supported by the Department of Defense, is under review at the Department of Defense, and establishment of novel research capabilities in areas of research of interest to the Department of Defense. The proposed infrastructure will enable several research projects including: large eddy simulation; optical interactions in nanostructured materials; modal decomposition, reduced-order modeling, and phase topology of complex flows; machine learning for unmanned aircraft systems (UAS) and parallel planning; parallel moving meshes; parallel high-order meshes; simulations of solid-liquid interfaces, gas separations, and gas expanded liquids.

Accomplishments: Please see the uploaded document which summarizes what was Accomplished Under Goals. This includes information on the equipment purchased, the quote for the equipment, and the research our team conducted on the GPU cluster.

Training Opportunities: The project allowed for 12 graduate students and 3 undergraduate students to be trained on the use of the GPU cluster during the reporting period. Students were trained in the areas of mesh generation for biomedical applications, machine learning models for control of unmanned aerial vehicles, GPU and GPU optimization for use on computational chemistry applications, optics simulations, and computational fluid dynamics methods for aerospace engineering applications.

Results Dissemination: Several journal and conference papers have been published based on results produced on the GPU cluster. In addition, several Ph.D. dissertations, master's theses, and master's project reports were published on research that was enabled by the GPU cluster.

Honors and Awards: Ezekiel Piskulich, a graduate student in the Brian Laird group, was awarded the 2021 KU Higuchi Dissertation Award for the top graduating Ph.D. candidate. He has also been chosen as one of three finalists for the 2022 Janukas Dissertation award from the Division of Chemical Physics of the American Physical Society. Dr. Piskulich was also chosen in 2020 as a participant in the Lindau Nobel Symposium.

Seth Martin, a graduate student in the Brian Laird Group, was awarded the 2021 Helen and Paul Gilles Award as the top advanced graduate student in Physical Chemistry at KU.

Protocol Activity Status:

Technology Transfer: Nothing to Report

PARTICIPANTS:

Participant Type: PD/PI

Participant: Suzanne Shontz

Person Months Worked: 1.00

Project Contribution:

National Academy Member: N

Funding Support:

Participant Type: Co PD/PI

Participant: Michael Branicky

Person Months Worked: 1.00

Project Contribution:

National Academy Member: N

Funding Support:

Participant Type: Co PD/PI

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Participant: Alessandro Salandrino
Person Months Worked: 1.00
Project Contribution:
National Academy Member: N

Funding Support:

Participant Type: Co PD/PI
Participant: ZJ Wang
Person Months Worked: 1.00
Project Contribution:
National Academy Member: N

Funding Support:

Participant Type: Co PD/PI
Participant: Weizhang Huang
Person Months Worked: 1.00
Project Contribution:
National Academy Member: N

Funding Support:

Participant Type: Co PD/PI
Participant: Brian Laird
Person Months Worked: 1.00
Project Contribution:
National Academy Member: N

Funding Support:

International Collaboration:

GBR
DEU

ARTICLES:

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Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Adv. Aerodyn.
Publication Identifier Type: DOI Publication Identifier: <https://doi.org/10.1186/s42774-021-00071-0>
Volume: 3 Issue: 16 First Page #:
Date Submitted: 12/17/21 12:00AM Date Published: 6/22/21 5:00AM
Publication Location:
Article Title: Benchmark for scale-resolving simulation with curved walls: the Taylor Couette flow
Authors: Z.J. Wang, E. Jourdan
Keywords: CFD benchmark, Taylor-Couette flow, DNS data, hp-refinement study, high-order methods
Abstract: Flow between rotating concentric cylinders, or the Taylor Couette flow, has been studied extensively because of its rich physics, ranging from axisymmetric steady laminar flow, to fully developed turbulent flow. In the present study, we advocate the use of this problem as a benchmark case for scale-resolving simulation, such as large eddy simulation (LES) and direct numerical simulation (DNS). The problem is attractive because of its simple geometry, simple boundary conditions, and complex physics involving wall-shear induced and centrifugal instability. Unlike the well-known fully developed channel flow, this problem has a curved wall boundary, and it is unnecessary to add a source term to the governing equations to sustain the fully developed turbulent flow. A p-refinement study for $Re = 4000$ is performed first to establish DNS data. Finally, an hp-refinement study is performed to establish the relative accuracy and efficiency of high-order schemes of various accuracy.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: Y

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Journal of Physical Chemistry B
Publication Identifier Type: DOI Publication Identifier: 10.1021/acs.jpcc.1c05369
Volume: 125 Issue: 32 First Page #: 9341
Date Submitted: 12/17/21 12:00AM Date Published: 8/5/21 10:00AM
Publication Location:
Article Title: Molecular Simulations of Phase Equilibria and Transport Properties in a Model CO₂-Expanded Lithium Perchlorate Electrolyte
Authors: Zeke A. Piskulich, Brian B. Laird
Keywords: molecular dynamics simulations, diffusion, viscosity, lithium perchlorate electrolyte, CO₂-expanded acetonitrile
Abstract: Carbon-dioxide (CO₂)-expanded liquids, in which a significant mole fraction of CO₂ is dissolved into an organic solvent, have been of significant interest, especially as catalytic support media. Because the CO₂ mole fraction and density can be controlled over a significant range by changing the CO₂ partial pressure, the transport properties of these solvents are highly tunable. Recently, these liquids have garnered interest as potential electrolyte solutions for catalytic electrochemistry; however, little is currently known about the influence of the electrolyte on CO₂ expansion. In the present work, we use molecular-dynamics simulations to study diffusion and viscosity in a model lithium perchlorate electrolyte in CO₂-expanded acetonitrile. Our present results indicate that the electrolyte slows down diffusion of both CO₂ and MeCN, and that the slowed diffusion in the former is driven by the activation entropy, whereas slowed diffusion in the latter is driven by the activation energy.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: Y

CONFERENCE PAPERS:

Publication Type: Conference Paper or Presentation **Publication Status:** 1-Published
Conference Name: AIAA AVIATION 2021 Forum
Date Received: 17-Dec-2021 Conference Date: 02-Aug-2021 Date Published: 02-Aug-2021
Conference Location: Virtual Event
Paper Title: Relative Performance of High-Order over 2nd Order Schemes for Benchmark LES Problems
Authors: Z.J. Wang
Acknowledged Federal Support: Y

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Publication Type: Conference Paper or Presentation **Publication Status:** 1-Published
Conference Name: AIAA Scitech 2021 Forum
Date Received: 17-Dec-2021 Conference Date: 11-Jan-2021 Date Published: 11-Jan-2021
Conference Location: Virtual Event
Paper Title: A Matrix-free GMRES Algorithm on GPU Clusters for Implicit Large Eddy Simulation
Authors: Eduardo Jordan, Z.J. Wang
Acknowledged Federal Support: **Y**

DISSERTATIONS:

Publication Type: Thesis or Dissertation
Institution: University of Kansas
Date Received: 17-Dec-2021 Completion Date: 7/9/21 11:02PM
Title: Machine Learning for Aerospace Applications using the Blackbird Dataset
Authors: Patrick McNamee
Acknowledged Federal Support: **N**

Publication Type: Thesis or Dissertation
Institution: University of Kansas
Date Received: 17-Dec-2021 Completion Date: 5/14/21 5:00AM
Title: Beyond Arrhenius: Fluctuation Theory for Dynamics
Authors: Zeke A. Piskulich
Acknowledged Federal Support: **N**

Publication Type: Thesis or Dissertation
Institution: University of Kansas
Date Received: 18-Dec-2021 Completion Date: 5/11/21 6:45PM
Title: Acceleration Techniques for Industrial Large Eddy Simulation with High-Order Methods on CPU-GPU Clusters
Authors: Eduardo Jourdan de Araujo Jorge Filho
Acknowledged Federal Support: **N**

Publication Type: Thesis or Dissertation
Institution: University of Kansas
Date Received: 18-Dec-2021 Completion Date: 6/14/21 5:00AM
Title: Structure and Thermodynamics of Solid/Fluid Interfaces: Simulation and Theory
Authors: Seth C. Martin
Acknowledged Federal Support: **N**

Publication Type: Thesis or Dissertation
Institution: University of Kansas
Date Received: 18-Dec-2021 Completion Date: 8/27/21 10:46PM
Title: Mesh Adaptation Using Machine Learning
Authors: Justin Phommachanh
Acknowledged Federal Support: **N**

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Partners

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Co PD/PI:Zhaoquan (Charlie) Zheng -- Charlie was a member of our research team at the time the proposal was su

I certify that the information in the report is complete and accurate:

Signature: Suzanne M. Shontz

Signature Date: 12/20/21 3:08PM

Accomplished Under Goals:

Equipment: With our DURIP award from ARO, we purchased the following HPC system:

(15) Dell R740 Servers each with:

- (2) Intel Xeon Gold 6248, 2.5GHz, 20 Core
- 192GB 2933MT/s Memory
- (2) NVIDIA Tesla V100 16GB GPU
- Mellanox ConnectX-5 Single Port EDR Infiniband Card
- 1TB 7.2K RPM SATA Hard Drive
- 1GbE Network Interface Card
- Dual Power Supply, 2000W
- iDRAC Express

The cost of the equipment was as follows:

Dell R740 Server - \$15,771.03

Total - \$236,565.45.

Please see the end of this file for the attached quote of the equipment purchased.

An EDR Infiniband switch and cables along with networking equipment were purchased by the Center for Research Computing (CRC) at the University of Kansas (KU) for the necessary backend connections of the servers.

To acquire special end of fiscal year deal from Dell, the servers were purchased before grant money was transferred to the KU Center for Research (KUCR). Dell had given CRC a 90-day window to return the equipment if needed. The initial cost was placed on CRC's account. Servers were in storage for 60+ days until confirmation was given that a transfer was in route on March 23, 2020.

COVID-19 had shut down the KU campus in March 2020, and thus physical work on campus was restricted. CRC received permission to do non-remote work at the end of May 2020. Servers were installed and online on June 4, 2020.

Summary of Research Conducted on the GPU Cluster:

Suzanne Shontz: The Shontz group has used CPU cores on the GPU cluster in the development of our high-order curvilinear tetrahedral mesh generation method, which is a direct method based on an advancing front approach. In particular, the cluster was used to test the performance of the method and to generate several meshes of complex geometries including mechanical parts and cardiac anatomies (see Figure 1). The group's high-order mesh generation methods will be parallelized using the CPUs and GPUs available to us through the GPU cluster once a new graduate student is recruited to the group.

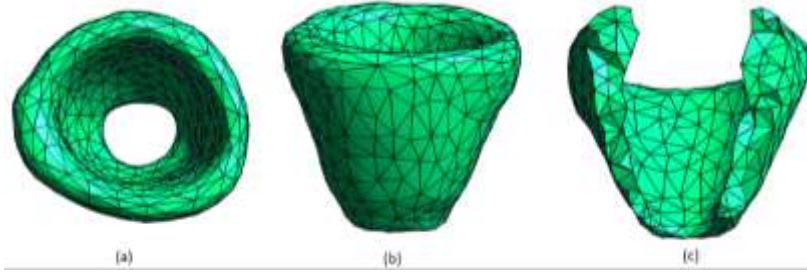


Figure 1: Second-order tetrahedral mesh of the left ventricle myocardium of a normal heart: (a) top view, (b) side view, and (c) cross-section.

Michael Branicky: The Branicky group used the open-source Blackbird Dataset to explore integration of machine learning (ML) models for control of unmanned aerial vehicles (UAVs). The Blackbird Dataset was overviewed to illustrate features and issues before investigating possible ML applications. Unsupervised learning models were used to determine flight-test partitions for training supervised Deep Neural Network (DNN) models for nonlinear dynamic inversion. The DNN models are used to determine appropriate model choices over several network parameters, including network layer depth, activation functions, epochs for training, and neural network regularization. The DURIP cluster was crucial to the completion of this work and was used extensively for DNN training. This work has been published as a Master's Project Report.

Weizhang Huang: This research group did not make use of the GPU cluster, as Dr. Huang did not recruit any new graduate or undergraduate students since the others graduated.

Brian Laird: Within the Laird group, the DURIP resources have been and are being used for several projects:

1) **Determination of the dependence of surface free energy on curvature for model systems:** To assess at a fundamental level the effect of surface curvature on surface and interfacial thermodynamics, we have been examining a model 2-d system (the hard-disk fluid) at a variety of curved walls. Currently, the GPU optimized molecular dynamics (MD) program HOOMD to perform simulations on hard-disk fluids in contact with elliptical and square walls to assess the dependence of surface thermodynamics on shape and evaluate against current geometrical theories (the so-called Morphometric Thermodynamics).

2) **Ion mobility and gas transport in CO₂-expanded organic electrolytes:** CO₂-expanded liquids, in which a significant mole fraction of CO₂ is dissolved into an organic solvent, have been of significant interest, especially as catalytic support media. Because the CO₂ mole fraction and density can be controlled over a significant range by changing the CO₂ partial pressure, the transport properties of these solvents are highly tunable. Recently, these liquids have garnered interest as potential electrolyte solutions for catalytic electrochemistry; however, little is currently known about the influence of the electrolyte on CO₂ we use MD simulations to study diffusion and viscosity in a model lithium perchlorate electrolyte in CO₂-expanded acetonitrile and demonstrate that these properties are highly dependent on the concentration of the electrolyte (See Figure 2). This work was published recently in J. Phys. Chem. B.

CO₂-Expanded Electrolytes

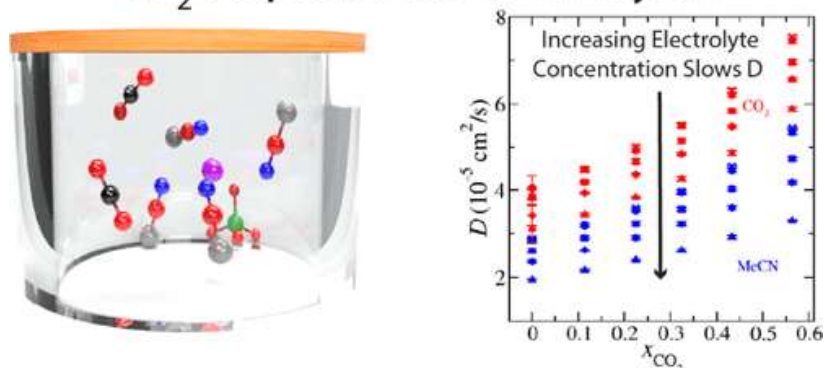


Figure 2: Dependence of CO₂ and acetonitrile (MeCN) diffusion on electrolyte concentration in CO₂-expanded acetonitrile/LiClO₄ electrolyte solutions.

3) Construction and characterization of metal-doped amorphous silica surfaces: Metal-doped amorphous silica surfaces have significant application in heterogeneous catalysis. Successful modeling of these surfaces is made difficult by the large number of possible amorphous environments and the dearth of definitive experimental characterization. We are using the reactive force field ReaxFF to model these systems, but currently there are no parameters in this model to describe the interaction of dopant metals (such as chromium Cr and niobium Nb). We are using the GPUs purchased until this grant to implement genetic algorithm machine learning to optimize the force field for these metals relative to more accurate, but considerably more CPU intensive, density functional theory (DFT) calculations.

4) Simulation of gas adsorption and transport in fluoropolymers: We are currently using GPU-based MD simulation using the program LAMMPS to examine the adsorption and transport properties of gases (N₂, H₂, CO₂ and various refrigerants) in a series of candidate fluoropolymers.

Alessandro Salandrino: The equipment has been instrumental in carrying out some complex simulations for the current AFOSR-funded project FA9550-20-1-0046 “Parametric Resonances for Optical Limiting”.

The project’s goal is to a novel class of optical limiters able to protect equipment for the exposure to high optical intensity. The project investigates optical limiting applications of parametric resonances in nanostructured media constituted by metallic particles embedded in host materials with second-order optical nonlinearities.

High performance computing has proven highly beneficial in the analysis of such systems which is computationally demanding because it requires fine temporal and spatial discretization of large domains over long intervals. As an example, Fig. 3 shows the simulated temporal evolution of the polarization density associated with a high order parametric resonance of a silver sphere embedded in a 2-methyl-4-nitroaniline (MNA) host.

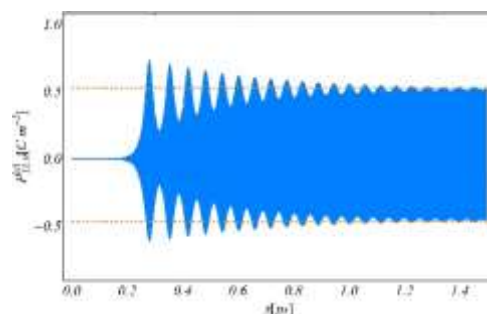


Figure 3 Temporal evolution of the polarization density amplitude of a Silver sphere immersed in a MNA background medium.

ZJ Wang: The GPU cluster has been used by the Wang group to develop and evaluate KU's high-order unstructured large eddy simulation solver, hpMusic, and perform large scale large eddy simulation (LES) for a variety of benchmark flow problems including the NASA Common Research Model high-lift configuration (CRM-HLC) from the 4th AIAA High-Lift Prediction Workshop. The implementation of the high-order flux-reconstruction method on GPUs has resulted in orders of magnitude reduction in computational time comparing with CPU clusters. For example, the speedup of a NVIDIA V100 over an Intel Xeon CPU is between 400-1500 depending on the element type and solution order. As a result, we have been able to compute LES of some very challenging flow problems which have contributed to the understanding of turbulent flow. One example is shown in Figure 4, which displays the vortex-dominated flow over the NASA CRM-HLC.

Due to the excellent performance of hpMusic on KU's V100 cluster, hpMusic was successfully ported to the nation's fastest supercomputer, Summit, from the Oak Ridge National Laboratory. Excellent performance was also achieved on Summit with up to 6000 V100s. DOE's INCITE program has selected KU's project entitled "Wall-resolved large eddy simulation of the NASA CRM high-lift configuration" for 2022 and awarded my group 590,000 Summit node hours. This project is instrumental in securing the INCITE award. Here is the announcement regarding the 2022 INCITE Awards:

<https://www.alcf.anl.gov/news/incite-program-awards-supercomputing-time-51-projects-advance-open-science> .

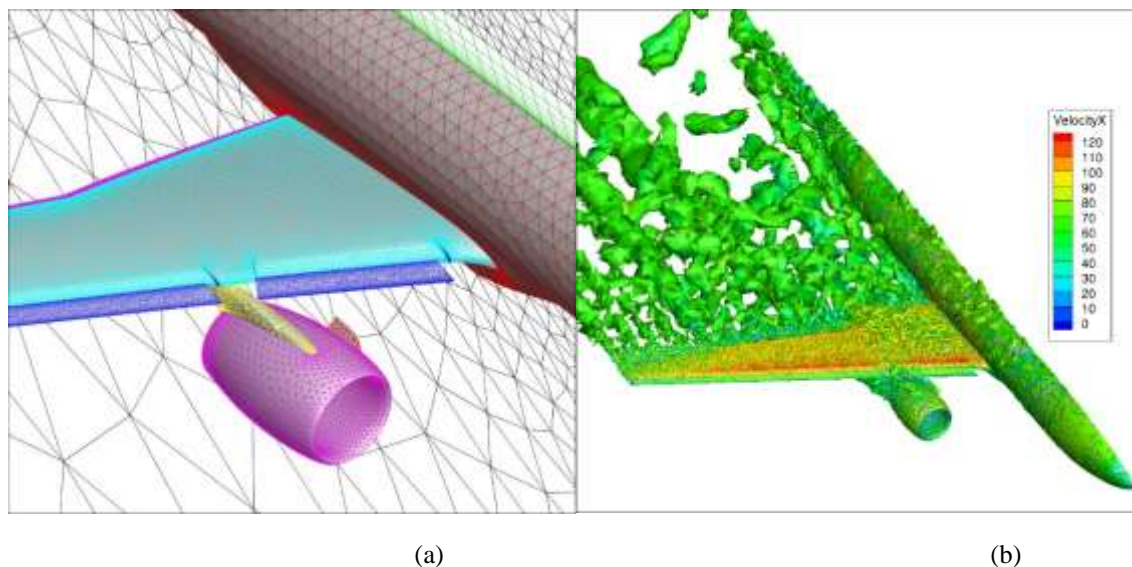


Figure 4. Large eddy simulation of flow over the NASA Common Research Model high-lift configuration. (a) Mesh and (b) iso-surfaces of the Q-criterion colored by streamwise velocity

Zhongquan (aka Charlie) Zheng: Charlie's group did not make use of the GPU cluster, as he moved to Utah State prior to the start of the grant and the acquisition of the GPU cluster.



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Quote No.	3000054142110.1	Sales Rep	Jordan Jackson
Total	\$236,565.45	Phone	(800) 456-3355, 80000
Customer #	138900542	Email	Jordan_Jackson@Dell.com
Quoted On	Jan. 21, 2020	Billing To	ACCTS PAYABLE UNIV OF KANSAS
Expires by	Jan. 30, 2020		KANSAS
Solution ID	12016478		UNIV OF KANSAS
Deal ID	18724248		1246 W CAMPUS RD RM 20
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Shipping Group

Shipping To	Shipping Method
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Product	Unit Price	Qty	Subtotal
PowerEdge R740 - [AMER_R740_12248]	\$15,771.03	15	\$236,565.45

Subtotal:	\$236,565.45
Shipping:	\$0.00
Non-Taxable Amount:	\$236,565.45
Taxable Amount:	\$0.00
Estimated Tax:	\$0.00
<hr/>	
Total:	\$236,565.45

Special lease pricing may be available for qualified customers and offers. Please contact your DFS Sales Representative for details.

Shipping Group Details

Shipping To

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 UNIV OF KANSAS
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 (785) 864-5800

Shipping Method

Standard Delivery

Description	SKU	Unit Price	Qty	Subtotal
PowerEdge R740 - [AMER_R740_12248]		\$15,771.03	15	\$236,565.45
Estimated delivery if purchased today: Feb. 25, 2020 Contract # 47AHA Customer Agreement # 13010074				
PowerEdge R740 Server	210-AKXJ	-	15	-
PowerEdge R740/R740XD Motherboard	329-BEIK	-	15	-
No Trusted Platform Module	461-AADZ	-	15	-
Chassis with up to 8 x 3.5" SAS/SATA Hard Drives for Software RAID	321-BCSP	-	15	-
PowerEdge R740 Shipping	340-BLKS	-	15	-
Module,Shipping Material,R740,NOCCC,Dell Americas Organization	340-CEEB	-	15	-
Intel Xeon Gold 6248 2.5G, 20C/40T, 10.4GT/s, 27.5M Cache, Turbo, HT (150W) DDR4-2933	338-BRVO	-	15	-
Intel Xeon Gold 6248 2.5G, 20C/40T, 10.4GT/s, 27.5M Cache, Turbo, HT (150W) DDR4-2933	338-BRVO	-	15	-
Additional Processor Selected	379-BDCO	-	15	-
HS Install Kit,GPU Config, EPS12V Cable	750-AAXX	-	15	-
2933MT/s RDIMMs	370-AEPP	-	15	-
Performance Optimized	370-AAIP	-	15	-
No RAID with Embedded SATA	780-BCDM	-	15	-
No Controller	405-AACD	-	15	-
No Operating System	619-ABVR	-	15	-
iDRAC Group Manager, Disabled	379-BCQY	-	15	-
iDRAC,Legacy Password	379-BCSG	-	15	-
Riser Config 4, 3x8, 4 x16 slots	330-BBHH	-	15	-
Broadcom 5720 Quad Port 1GbE BASE-T, rNDC	540-BBBW	-	15	-
No Internal Optical Drive	429-ABBJ	-	15	-
6 Performance Fans forR740/740XD	384-BBPZ	-	15	-
Dual, Hot-plug, Redundant Power Supply, 2000W, C19/C20 Power Cord Required for Use	450-AENU	-	15	-
PowerEdge 2U Standard Bezel	325-BCHU	-	15	-
Dell EMC Luggage Tag	350-BBKG	-	15	-

No Quick Sync	350-BBJV	-	15	-
Performance BIOS Settings	384-BBBL	-	15	-
ReadyRails Sliding Rails Without Cable Management Arm	770-BBBQ	-	15	-
No Systems Documentation, No OpenManage DVD Kit	631-AACK	-	15	-
US Order	332-1286	-	15	-
Declined Remote Consulting Service	973-2426	-	15	-
Basic Hardware Services: Business Hours (5x10) Next Business Day On-Site Hardware Warranty Repair, 3 Years	813-9118	-	15	-
Dell Hardware Limited Warranty Plus On-Site Service	813-9119	-	15	-
On-Site Installation Declined	900-9997	-	15	-
16GB RDIMM, 2933MT/s, Dual Rank	370-AEQF	-	180	-
1TB 7.2K RPM SATA 6Gbps 512n 3.5in Hot-plug Hard Drive	400-ASHH	-	15	-
No Media Required	421-5736	-	15	-
iDRAC9, Express	385-BBKS	-	15	-
Mellanox ConnectX-5 Single Port EDR VPI QSFP28 Infiniband Adapter, PCIe Full Height	540-BCDK	-	15	-
NVIDIA Tesla V100 16G Passive GPU	490-BEDZ	-	30	-
C19 to C20, PDU Style, 2.5M Power Cord	450-AEJI	-	30	-

Subtotal:	\$236,565.45
Shipping:	\$0.00
Estimated Tax:	\$0.00

Total: \$236,565.45

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