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Final Report: Hybrid Computing Architectures as a Platform for Advanced Multi-scale Computational Methods

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5b. GRANT NUMBER

5c. PROGRAM ELEMENT NUMBER
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6. AUTHORS
Guglielmo Scovazzi

5d. PROJECT NUMBER

5e. TASK NUMBER

5f. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAMES AND ADDRESSES
Duke University
C/O Office of Research Support
2200 W. Main St., Ste. 710
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The views, opinions and/or findings contained in this report are those of the author(s) and should not contrued as an official Department of the Army position, policy or decision, unless so designated by other documentation.

14. ABSTRACT
The Mathematical Sciences Division of the Army Research Office (ARO) is sponsoring the PI through a grant W911NF1310452 titled “Continuous/Discontinuous Variational Multiscale Methods for Variable Density Flows.” Project W911NF1310452 aimed at developing algorithms and domain decomposition strategies for subsurface flows, using a multi-scale representation of the solution. By nature, these algorithms have the potential for performance enhancement on heterogeneous computational platforms, which combine conventional computational cores, mathematical co-processors, and GPUs.

15. SUBJECT TERMS
Computational subsurface modeling, multi scale methods, variational methods

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	15. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT	b. ABSTRACT	c. THIS PAGE			Guglielmo Scovazzi
UU	UU	UU	UU		19b. TELEPHONE NUMBER 919-660-5075

Report Title

Final Report: Hybrid Computing Architectures as a Platform for Advanced Multi-scale Computational Methods

ABSTRACT

The Mathematical Sciences Division of the Army Research Office (ARO) is sponsoring the PI through a grant W911NF1310452 titled "Continuous/Discontinuous Variational Multiscale Methods for Variable Density Flows." Project W911NF1310452 aimed at developing algorithms and domain decomposition strategies for subsurface flows, using a multi-scale representation of the solution. By nature, these algorithms have the potential for performance enhancement on heterogeneous computational platforms, which combine conventional computational cores, mathematical co-processors, and GPUs.

We then successfully obtained funding, on this DURIP grant (66829MARIP) to build a powerful computer cluster with heterogeneous computing nodes, large enough however to perform basic scalability tests. Work on this cluster was and is intended as a first step in the development of algorithms whose performance will be validated on DOD's large-scale heterogeneous computational platforms.

We started the prototyping of many new ideas on how to combine GPUs in combination with regular CPU nodes. Particularly we have started the development of a GPU-enabled compiler that can wrap around any C++ code to output GPU-capable code. This could be then incorporated in the PROTEUS computational framework of Dr. Chris Kees at USACE-Vicksburg.

Enter List of papers submitted or published that acknowledge ARO support from the start of the project to the date of this printing. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

Received		Paper
02/05/2017	1	Guoyin Wang, Guglielmo Scovazzi, Christopher E. Kees, Simone Rossi, Oriol Colomés, Alex Main. Dual-Scale Galerkin Methods for Darcy Flow, Journal of Computational Physics, ( ): . doi:
TOTAL:	**1**	

Number of Papers published in peer-reviewed journals:

(b) Papers published in non-peer-reviewed journals (N/A for none)

Received		Paper
TOTAL:		

Number of Papers published in non peer-reviewed journals:

(c) Presentations

Number of Presentations: 0.00

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received Paper

TOTAL:

Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received Paper

TOTAL:

Number of Peer-Reviewed Conference Proceeding publications (other than abstracts):

(d) Manuscripts

Received Paper

TOTAL:

Number of Manuscripts:

Books

Received Book

TOTAL:

Received	Book Chapter

TOTAL:

Patents Submitted

Patents Awarded

Awards

G. Scovazzi (2017) - Presidential Early Career Award for Scientists and Engineers (PECASE). The PECASE recognition is the highest honor bestowed by the United States government on science and engineering professionals in the early stages of their independent research careers.

Graduate Students

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Names of Post Doctorates

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Names of Faculty Supported

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Names of Under Graduate students supported

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period: 0.00

The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:..... 0.00

The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:..... 0.00

Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):..... 0.00

Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:..... 0.00

The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense 0.00

The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields:..... 0.00

Names of Personnel receiving masters degrees

NAME

Total Number:

Names of personnel receiving PHDs

NAME

Total Number:

Names of other research staff

NAME	PERCENT_SUPPORTED

FTE Equivalent:

Total Number:

Sub Contractors (DD882)

Inventions (DD882)

Scientific Progress

In early November 2015, through the present DURIP grant, the PI purchased "NIVOLET," a GPU-enabled high-performance computing cluster. The cluster was installed, tested and made operational by the end of November 2015, and a Duke press release acknowledging ARO support followed in early December:

http://pratt.duke.edu/about/news/nivolet-breaks-computing-records-pratt

We started the prototyping of many new ideas on how to combine GPU nodes in combination with regular CPU nodes. Particularly we have started the development of a GPU-enabled compiler that can wrap around any C++ code to output GPU-capable code. This could be then incorporated in the PROTEUS computational framework of Dr. Chris Kees at USACE-Vicksburg.

We have started profiling and optimization of some prototype codes for GPU applications. In general, we observe 50-fold acceleration of the computing performance in dense linear algebra calculations, and we also observed that the new C++/GPU compiler is rather simple to use for new code developers that are going the PI team. We hope to report soon on the integration of this work wit the PROTEUS framework of Chris Kees at the Army Corps of Engineers in Vicksburg (MS).

Included in attachment is the invoice from the vendor for the purchase and installation fees.

Technology Transfer

We are currently working on the development of a new C++ compiler that seamlessly enables GPU integration and can be transferred to any code. This has the potential to be transferred to any ARO-related computational programs and software developed by ARO and related research institutional partners.

Silicon Mechanics
22029 23rd Dr SE
Bothell, WA 98021-4410
(425) 424-0000

Quote

Date	Quote #	Confirmation #
08 / 11 / 2015	294706	162118277

Please note that due to unusually high volatility in memory and storage component prices in recent months, Silicon Mechanics quotes are now valid for 14 calendar days from date of issue.

Bill To:	Ship To:
Accounts Payable Duke University 324 Blackwell St. Washington Bldg., Ste 800 Box 104131 Durham, NC 27708 ron.stubbs@duke.edu	Stelian Iges, PO#4550255861 Duke University 118A Civil Engineering Hudson Hall 100 Science Drive Durham, NC 27708 ron.stubbs@duke.edu

Description	Duke Cluster - Army Funding
Notes	

Quantity	Description	Price Each	Amount
1	**ITEM** Qty 32: Rackform R352.v5 "GPU Node, Passively Cooled GPUs Only" NOTE: For more than 8 DIMMs, or multiple GPUs, please select 2 CPUs CPU: 2 x Intel Xeon E5-2670v3, 2.3 GHz (12-Core, HT, 30MB Cache, 120W) 22nm RAM: 64GB (8 x 8GB DDR4-2133 ECC Registered 1R 1.2V DIMMs) Operating at 2133 MT/s Max NIC: Intel i350 Dual-Port RJ45 Gigabit Ethernet Controller Management: IPMI 2.0 & KVM with Dedicated LAN - Integrated Integrated Drive Controller: 10 Ports 6Gb/s SATA3 via Intel C612 Chipset PCIe 3.0 x16 - 1: No Item Selected PCIe 3.0 x16 - 2: No Item Selected PCIe 3.0 x16 - 3: No Item Selected LP PCIe 3.0 x8 (x16): Mellanox ConnectX-3 VPI FDR InfiniBand and 40/56GbE Network Adapter, Single-Port QSFP, PCIe 3.0 x8 Hot-Swap Drives: 1 x 120GB Intel DC S3510 Series MLC (6Gb/s, 0.3 DWPD) 2.5" SATA SSD NOTE: No Item Selected RAID Configuration: JBOD: Stand-Alone Disks Power Supply: Redundant (1+1) 1000/1600W Power Supply with PMBus - 80 PLUS Platinum Certified Rail Kit: No Item Selected OS: No Item Selected Management SW: Supermicro Update Manager (SUM) Out-of-Band Management Software NOTE: For full warranty and service terms, please visit our warranty page. Standard Warranty: 3 Year Silicon Mechanics Standard Warranty NOTE: Advanced Parts Replacement service covers the cross shipping of replacement parts. Advanced Parts Replacement: 3 Year Advanced Parts Replacement NOTE: Expanded Services begin on the same day as the warranty term and run concurrent to the Standard Warranty. Expanded Services: No Item Selected NOTE: No Item Selected Notes: OS: Install RHEL 7.1 - Duke has license and will register after delivery	197470.00	197470.00

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Accounts Payable Duke University 324 Blackwell St. Washington Bldg., Ste 800 Box 104131 Durham, NC 27708 ron.stubbs@duke.edu	Stelian Iges, PO#4550255861 Duke University 118A Civil Engineering Hudson Hall 100 Science Drive Durham, NC 27708 ron.stubbs@duke.edu

Quantity	Description	Price Each	Amount
	SUM: YES Qty 13: NVIDIA Tesla K40m GPU, 12GB GDDR5, 235W, PCIe 3.0 x16 - Passive Cooling - CUDA Center of Excellence		

Subtotal	197,470.00
Sales Tax (7.5%)	14810.26
Total	USD 212,280.26

Orders shipped to WA, CA, CO, GA, NC, OH, and TX are subject to the appropriate tax rate. The quoted tax amount is subject to change.

Subject to Silicon Mechanics' Warranty Terms and Conditions - http://www.siliconmechanics.com/terms-and-conditions.php