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#### **Report Title**

Final Report: A Transitional Computational Platform to Migrate Parachute Simulation from Workstation to HPC

#### ABSTRACT

Supported by the DURIP grant W911NF-15-1-0403 for 'A Transitional Computational Platform to Migrate Parachute Simulation from Workstation to HPC', we purchased a parallel cluster from the Advanced Cluster Technologies, Inc.. This parallel cluster is named 'Intruder', after a type of sports parachute. It consists of one head node, 21 computing nodes (20 CPU (Central Processing Unit) nodes and 1 GPU (Graphic Processing Unit) node), connected with 56Gb/s InfiniBand and 1000MB/s Ethernet. Each node was populated with dual Eight-Core Intel E5-2630v3 'Haswell' 2.4GHz processors with different size of RAM (Random-access Memory) and Storage. The head node and compute node have 32GB of RAM for each, and the GPU node has 128GB of RAM. A 32TB of network file system using RAID6 (Redundant Array of Independent Disks) is installed in the head node, and is shared with other nodes. Each node also has a clone of the operation system on its local disk: 2TB SSD on head node, 1TB SATA drive on compute nodes, and 240GB SSD on GPU node. The parallel computing can be further accelerated by including the GPU node, which contains seven NVIDIA Tesla K40 GPUs with 12GB of RAM for each device.

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

TOTAL:

Number of Papers published in peer-reviewed journals:

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

Received Paper

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

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#### Names of Faculty Supported

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## Names of Under Graduate students supported

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#### **Student Metrics**

This section only applies to graduating undergraduates supported by this agreement in this reporting period	
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## Names of Personnel receiving masters degrees

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### Names of personnel receiving PHDs

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### Names of other research staff

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# **Scientific Progress**

#### Technical Report on the Transitional 'Intruder' Cluster

Supported by the DURIP grant W911NF-15-1-0403 for 'A Transitional Computational Platform to Migrate Parachute Simulation from Workstation to HPC', we purchased a parallel cluster from the Advanced Cluster Technologies, Inc. The parallel cluster is named 'Intruder' a type of sports parachute. It consists of one head node, 21 computing nodes (20 CPU (Central Processing Unit) nodes and 1 GPU (Graphic Processing Unit) node), connected with 56Gb/s InfiniBand and 1000MB/s Ethernet. Each node was populated with dual Eight-Core Intel E5-2630v3 'Haswell' 2.4GHz processors with different size of RAM (Random-access Memory) and Storage. The head node and compute node have 32GB of RAM for each, and the GPU node has 128GB of RAM. A 32TB of network file system using RAID6 (Redundant Array of Independent Disks) is installed in the head node, and is shared with other nodes. Each node also has a clone of the operation system on its local disk: 2TB SSD on head node, 1TB SATA drive on compute nodes, and 240GB SSD on GPU node. The parallel computing can be further accelerated by including the GPU node, which contains seven NVIDIA Tesla K40 GPUs with 12GB of RAM for each device. A hybrid computation utilizing both CPU and GPU has been performed on this platform. The detailed description of the hardware is summarized in Table 1 of the attached pdf file.

The software environment consists of the CentOS 6.7 operating system; the Intel OpenMPI compiler 1.8 for MPI-based applications; Sun Grid Engine 2011.11p1 as the job scheduler, PETSc3.6 with benchmark examples; FronTier with computational fluid dynamics applications. Benchmark tests have been performed within this environment, and the performance are compared with the workstation and Cray supercomputer.

We have carried out several experiments to investigate the impact of the computing platform on our main application: FronTier, which relies on a few parallel computing API (such as MPI, CUDA) and external packages (such as PETSc, HYPRE). In order to distinguish their impact of these external packages on FronTier, we created a few independent programs by including PETSc, MPI and CUDA separately. In the first test, a two dimensional Poisson equation was solved with PETSc using the KSP solver and HYPRE as the preconditioner. To test the strong scaling, we fix the domain size to be 4096X4096 while consecutively double the number of processors from 1 to 1024. The scaling results are summarized in Table 2 and illustrated by Figure 1 of the attached pdf file which and showed that the HPC has a wider range of linear scaling than "Intruder" cluster and workstation. The result also suggests that the speedup becomes slower when the machine is nearly fully occupied. We interpret this fact as an indicator of the limited bandwidth of the main memory which is substantially slower than the speed of the modern CPU. The second experiment is to test the weak scaling of FronTier by solving 2-D Riemann problem with MPI library. The base size for each processor is set to be 100X100, 200X200, 400X400 and 800X800. The efficiency is measured by T 1/T N, where N is the number of processors occupied. The results are displayed in Figure 2 and Table 3 in the attached pdf file, which implies that an efficiency over 50% can be achieved up to 256 cores when the base size is smaller than 400X400 while the efficiency decreases to 20% when the base size is 800X800\$. The third experiment tests the GPU acceleration on the cloth simulator. The GPU code is implemented with CUDA library, which is a parallel computing platform created by NVIDIA. We compare the computational time of solving spring model for different parachute types using or without using GPU device and calculate the speedup. As shown in Table 3 of the attached pdf file, using GPU device can achieve at least 16 times and up to 21 times speedup for cloth simulation.

Due to the price reduction since we wrote the proposal, there is a fraction of fund left after the purchase of the cluster. We used the remaining fund to buy two workstations and three desktops to be used by graduate students in the research project, high school students in the HSAP program, and undergraduate students who are interested in our research.

## **Technology Transfer**

Recipient: Joseph Myers Army Research Office

#### ARO–DURIP: W911NF-15-1-0403

Award Report

A Transitional Computational Platform to Migrate Parachute Simulation from Workstation to HPC

> Principal Investigator: Xiaolin Li University at Stony Brook

Reporting Period: September 1, 2015 – August 31, 2016

> Recipient: Research Foundation University at Stony Brook Stony Brook, NY 11794-3366

Unexpended Funds: \$0.00 (0.0%) Exceeds 10% of available funds: No

# Technical Report on the Transitional "Intruder" Cluster

#### November 1, 2016

Supported by the DURIP grant W911NF-15-1-0403 for "A Transitional Computational Platform to Migrate Parachute Simulation from Workstation to HPC", we purchased a parallel cluster from the Advanced Cluster Technologies, Inc. The parallel cluster is named "Intruder", after a type of sports parachute. It consists of one head node, 21 computing nodes (20 CPU (Central Processing Unit) nodes and 1 GPU (Graphic Processing Unit) node), connected with 56Gb/s InfiniBand and 1000MB/s Ethernet. Each node was populated with dual Eight-Core Intel E5 - 2630v3 "Haswell" 2.4GHz processors with different size of RAM (Random-access Memory) and Storage. The head node and compute node have 32GB of RAM for each, and the GPU node has 128GB of RAM. A 32TB of network file system using RAID6 (Redundant Array of Independent Disks) is installed in the head node, and is shared with other nodes. Each node also has a clone of the operation system on its local disk: 2TB SSD on head node, 1TB SATA drive on compute nodes, and 240GB SSD on GPU node. The parallel computing can be further accelerated by including the GPU node, which contains seven NVIDIA Tesla K40 GPUs with 12GB of RAM for each device. A hybrid computation utilizing both CPU and GPU has been performed on this platform. The detailed description of the hardware is summarized in Table Table 1.

Node Type	CPU	RAM	Storage for data	Storage for OS	GPU
Head node	2x8-core Intel E5-2630v3	32 GB	32TB (RAID  6)	2TB (SSD)	none
CPU node	2x8-core Intel E5-2630v3	32 GB	none	1TB (SATA)	none
GPU node	2x8-core Intel E5-2630v3	128 GB	none	240 GB (SSD)	7 Tesla K40

Table 1: Summary of the hardware

The software environment consists of the CentOS 6.7 operating system; the Intel OpenMPI compiler 1.8 for MPI-based applications; Sun Grid Engine 2011.11p1 as the job scheduler, PETSc3.6 with benchmark examples; FronTier with computational fluid dynamics applications. Benchmark tests have been performed within this environment, and the performance are compared with the workstation and Cray supercomputer.

We have carried out several experiments to investigate the impact of the computing platform on our main application: FronTier, which relies on a few parallel computing API (such as MPI, CUDA) and external packages (such as PETSc, HYPRE). In order to distinguish their impact of these external packages on FronTier, we created a few independent programs by including PETSc, MPI and CUDA separately. In the first test, a two dimensional Poisson equation was solved with PETSc using the KSP solver and HYPRE as the preconditioner. To test the strong scaling, we fix the domain size to be 4096 × 4096 while consecutively double the number of processors from 1 to 1024. The scaling results are summarized in Table 2 and illustrated by Figure 1, and showed that the HPC has a wider range of linear scaling than "Intruder" cluster and workstation. The result also suggests that the speedup becomes slower when the machine is nearly fully occupied. We interpret this fact as an indicator of the limited bandwidth of the main memory which is substantially slower than the speed of the modern CPU. The second experiment is to test the weak scaling of FronTier by solving 2-D Riemann problem with MPI library. The base size for each processor is set to be  $100 \times 100$ ,  $200 \times 200$ ,  $400 \times 400$  and  $800 \times 800$ . The efficiency is measured by  $T_1/T_N$ , where N is the number of processors occupied. The results are displayed in Figure 2 and Table 3 which implies that an efficiency over 50% can be achieved up to 256 cores when the base size is smaller than  $400 \times 400$  while the efficiency decreases to 20% when the base size is  $800 \times 800$ . The third experiment tests the GPU acceleration on the cloth simulator. The GPU code is implemented with CUDA library, which is a parallel computing platform created by NVIDIA. We compare the computational time of solving spring model for different parachute types using or without using GPU device and calculate the speedup. As shown in Table 4, using GPU device can achieve at least 16 times and up to 21 times speedup for cloth simulation.

Due to the price reduction since we wrote the proposal, there is a fraction of fund left after the purchase of the cluster. We used the remaining fund to buy two workstations and three desktops to be used by graduate students in the research project, high school students in the HSAP program, and undergraduate students who are interested in our research.

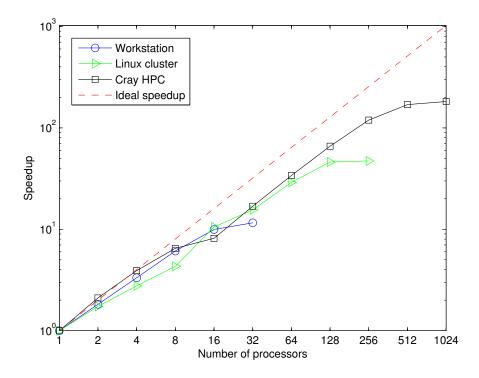


Figure 1: The figure displays the speedup of linear solver solving the 2-D Poisson equation with domain size  $(4096 \times 4096)$  on different machine: workstation, linux cluster and Cray supercomputer.

Number of processors	1	2	4	8	16	32	64	128	256	512	1024
Time on workstation (s)	136.80	88.61	48.45	27.71	16.99	14.59	-	-	-	-	-
Time on linux cluster (s)	129.10	87.59	54.86	37.06	15.14	10.28	5.77	3.62	3.70	-	-
Time on HPC (s)	78.06	56.63	31.53	20.90	17.67	9.98	5.34	3.05	1.082	1.31	1.22

Table 2: Computational time summary of strong scaling test on workstation, Linux cluster and CRAY HPC by solving the 2D Poisson equation.

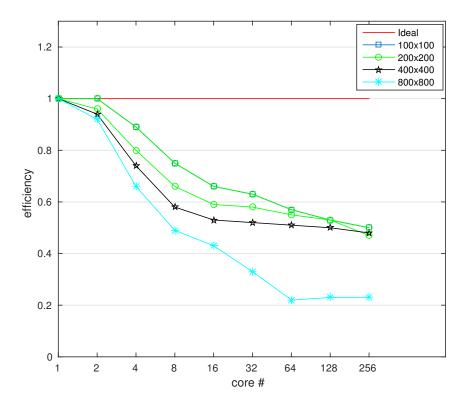


Figure 2: This figure shows the weak scaling test on 2d Riemann problem. The efficiency is calculated with  $T_1/T_N$ , where N is the number of processors used. The results implies that 50% efficiency has been achieved when mesh size per processor is smaller than 400 × 400.

Size per proc	num of procs	1	2	4	8	16	32	64	128	256
$100 \times 100$	time (s)	40	40	45	53	61	64	70	75	80
	efficiency	1.00	1.00	0.89	0.75	0.66	0.63	0.57	0.53	0.50
$200 \times 200$	time (s)	85	89	106	129	145	149	154	159	181
	efficiency	1.00	0.96	0.80	0.66	0.59	0.58	0.55	0.53	0.47
$400 \times 400$	time (s)	401	427	544	695	762	773	783	809	838
	efficiency	1.00	0.94	0.74	0.58	0.53	0.52	0.51	0.50	0.46
$800 \times 800$	time (s)	2081	2263	3161	4244	4839	6334	9282	8865	9114
	efficiency	1.00	0.92	0.66	0.49	0.43	0.33	0.22	0.23	0.23

Table 3: Weak scaling test on 2d Riemann problem by gradually increase the mesh size per processor through  $100 \times 100$ ,  $200 \times 200$ ,  $400 \times 400$ ,  $800 \times 800$ .

Parachute type	CPU/GPU	Time(s)	Avg time per step(s)	Speedup
C9	CPU	2805.85	3.39	1.00
	GPU	131.90	0.16	21.2
G11	CPU	5101.47	5.41	1.00
	GPU	243.18	0.26	20.81
Intruder	CPU	1252.65	2.00	1.00
	GPU	69.67	0.11	18.18
T10	CPU	5540.02	5.99	1.00
	GPU	282.74	0.36	16.64
T11	CPU	6791.9	5.12	1.00
	$\operatorname{GPU}$	352.07	0.29	17.66

Table 4: A comparison of computational time between different parachute type on CPU or GPU. The speedup is calculated based on the computing time by CPU.