Supplementary Information: Studying Effects of Meltdown and Spectre Patches on the Performance of HPC Applications Using Application Kernel Module of XDMoD

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Test Cluster Results

Table 1. Changes in selected metrics measured by **NAMD, NWChem and HPCC** on test cluster.

Nodes	Metric	Diff., %	Means are Diff.	Before Update			After Update			Units
				Mean	St.Dev.	N	Mean	St.Dev.	N	
Application: **NAMD**										
1	Wall Clock Time	3.3	Y	306.6	1.44	24	316.8	3.05	51	Second
1	Molecular Dynamics Simulation Performance	-3.5	Y	7.67E-10	7.11E-12	24	7.40E-10	1.45E-11	51	Second per Day
2	Wall Clock Time	6.9	Y	175.4	2.78	22	187.6	2.91	50	Second
2	Molecular Dynamics Simulation Performance	-6.6	Y	1.48E-09	5.60E-11	22	1.38E-09	8.39E-11	50	Second per Day
Application: **NWChem**										
1	Wall Clock Time	2.6	Y	77.8	1.91	23	79.8	1.13	54	Second
2	Wall Clock Time	11.4	Y	58.4	1.05	21	65.1	4.38	50	Second
Application: **HPCC**										
1	Wall Clock Time	2.2	Y	304.1	6.39	23	310.8	4.86	51	Second
1	Matrix Multiplication Floating-Point Performance	-1.2	Y	8,501.5	56.6	23	8,397.7	110.6	51	MFLOP per Second
1	Average STREAM 'Add' Memory Bandwidth	5.4	N	3,170.2	450.9	23	3,342.6	559.0	51	MByte per Second
1	Average STREAM 'Copy' Memory Bandwidth	3.6	N	4,357.3	495.8	23	4,513.0	579.3	51	MByte per Second
1	Average STREAM 'Scale' Memory Bandwidth	3.9	N	2,948.8	405.1	23	3,064.0	471.4	51	MByte per Second
1	Average STREAM 'Triad' Memory Bandwidth	9.0	N	3,290.7	501.0	23	3,586.5	689.2	51	MByte per Second
1	Fast Fourier Transform (FFTW) Floating-Point Performance	-5.6	N	7,925.9	555.2	23	7,479.6	1,528.8	51	MFLOP per Second
1	High Performance LINPACK Floating-Point Performance	-4.1	Y	61,832.2	1,237.0	23	59,315.6	1,278.7	51	MFLOP per Second
1	MPI Random Access	-23.2	Y	2.09	8.59E-02	23	1.61	3.61E-02	51	MUpdate / s
1	Parallel Matrix Transpose (PTRANS)	-11.8	N	3,032.1	437.4	23	2,673.0	846.0	51	Mbyte / s
2	Wall Clock Time	5.3	Y	345.1	5.41	22	363.4	8.16	50	Second
2	Matrix Multiplication (DGEMM) Floating-Point Performance	-1.9	Y	8,528.5	42.2	22	8,366.4	88.1	50	MFLOP per Second
2	Average STREAM 'Add' Memory Bandwidth	12.2	Y	3,124.5	291.4	22	3,504.7	590.6	50	MByte per Second
2	Average STREAM 'Copy' Memory Bandwidth	9.6	Y	4,349.7	316.1	22	4,766.1	584.4	50	MByte per Second
2	Average STREAM 'Scale' Memory Bandwidth	11.9	Y	2,917.9	308.6	22	3,264.7	553.2	50	MByte per Second
2	Average STREAM 'Triad' Memory Bandwidth	14.4	Y	3,214.6	328.5	22	3,678.2	651.3	50	MByte per Second
2	Fast Fourier Transform (FFTW) Floating-Point Performance	-6.7	N	12,343.7	634.6	22	11,519.4	1,714.7	50	MFLOP per Second
2	High Performance LINPACK Floating-Point Performance	-8.5	Y	1.22E+05	485.1	22	1.12E+05	2,784.2	50	MFLOP per Second
2	MPI Random Access	-53.9	Y	9.59	3.29E-01	22	4.42	2.83E-01	50	MUpdate / s
2	Parallel Matrix Transpose (PTRANS)	-10.3	Y	2,615.4	187.1	22	2,345.9	354.2	50	MByte / s

Table 2. Changes in selected metrics measured by **IMB** on test cluster.

Nodes	Metric	Diff., %	Means are Diff.	Before Update			After Update			Units
				Mean	St.Dev.	N	Mean	St.Dev.	N	
2	Wall Clock Time	4.1	Y	14.8	5.39E-01	21	15.4	1.47	50	Second
2	Max Exchange Bandwidth	0.3	N	3,898.9	36.0	21	3,911.1	63.3	50	MByte per Second
2	Max MPI-2 Bidirectional 'Get' Bandwidth (aggregate)	-0.6	N	1,990.3	43.1	21	1,979.2	54.9	50	MByte per Second
2	Max MPI-2 Bidirectional 'Get' Bandwidth (non-aggregate)	-2.8	Y	2,106.9	57.1	21	2,047.1	48.4	50	MByte per Second
2	Max MPI-2 Bidirectional 'Put' Bandwidth (aggregate)	0.5	N	2,048.0	65.1	21	2,057.7	30.1	50	MByte per Second
2	Max MPI-2 Bidirectional 'Put' Bandwidth (non-aggregate)	-1.7	Y	2,117.6	36.1	21	2,082.6	42.0	50	MByte per Second
2	Max MPI-2 Unidirectional 'Get' Bandwidth (aggregate)	-0.1	Y	3,099.1	14.5	21	3,095.5	8.67	50	MByte per Second
2	Max MPI-2 Unidirectional 'Get' Bandwidth (non-aggregate)	-0.8	Y	2,933.7	54.5	21	2,909.8	37.7	50	MByte per Second
2	Max MPI-2 Unidirectional 'Put' Bandwidth (aggregate)	0.0	N	3,123.7	6.18	21	3,122.8	7.73	50	MByte per Second
2	Max MPI-2 Unidirectional 'Put' Bandwidth (non-aggregate)	-1.0	Y	2,956.7	41.1	21	2,926.4	51.6	50	MByte per Second
2	Max PingPing Bandwidth	0.0	N	2,598.3	34.3	21	2,599.4	28.6	50	MByte per Second
2	Max PingPong Bandwidth	-0.1	Y	3,083.5	9.99	21	3,079.0	7.45	50	MByte per Second
2	Max SendRecv Bandwidth	-0.2	N	5,220.6	73.5	21	5,208.8	62.0	50	MByte per Second
2	Min AllGather Latency	1.4	Y	2.54E-06	5.12E-08	21	2.58E-06	6.22E-08	50	Second
2	Min AllGatherV Latency	-1.0	N	2.99E-06	1.16E-07	21	2.96E-06	7.21E-08	50	Second
2	Min AllReduce Latency	-2.2	Y	3.02E-06	1.22E-07	21	2.95E-06	7.40E-08	50	Second
2	Min AllToAll Latency	0.9	Y	2.53E-06	3.66E-08	21	2.55E-06	3.43E-08	50	Second
2	Min AllToAllV Latency	3.8	Y	3.21E-06	3.01E-08	21	3.33E-06	1.20E-07	50	Second
2	Min Barrier Latency	3.5	Y	2.41E-06	8.48E-08	21	2.49E-06	1.26E-07	50	Second
2	Min Broadcast Latency	-0.6	Y	2.40E-06	2.53E-08	21	2.39E-06	9.17E-08	50	Second
2	Min Gather Latency	-0.3	N	2.60E-06	9.05E-08	21	2.59E-06	3.40E-08	50	Second
2	Min GatherV Latency	1.0	N	2.44E-06	2.10E-08	21	2.46E-06	8.43E-08	50	Second
2	Min MPI-2 'Accumulate' Latency (aggregate)	0.1	N	1.00E-06	7.08E-08	21	1.01E-06	5.51E-08	50	Second
2	Min MPI-2 'Accumulate' Latency (non-aggregate)	1.5	N	6.29E-06	2.50E-07	21	6.38E-06	3.11E-07	50	Second
2	Min MPI-2 Window Creation Latency	0.3	N	2.44E-05	1.36E-07	21	2.45E-05	1.97E-07	50	Second
2	Min Reduce Latency	3.6	Y	2.74E-06	6.69E-08	21	2.84E-06	1.05E-07	50	Second
2	Min ReduceScatter Latency	1.0	N	1.65E-06	8.98E-08	21	1.67E-06	1.07E-07	50	Second
2	Min Scatter Latency	1.6	Y	2.58E-06	1.60E-08	21	2.63E-06	6.03E-08	50	Second
2	Min ScatterV Latency	0.1	N	2.54E-06	7.85E-08	21	2.54E-06	4.05E-08	50	Second

Table 3. Changes in selected metrics measured by **IOR** on test cluster.

Nodes	Metric	Diff., %	Means are Diff.	Before Update			After Update			Units
				Mean	St.Dev.	N	Mean	St.Dev.	N	
Application: **IOR** on local file system										
1	Wall Clock Time	3.7	Y	188.5	9.41	21	195.4	11.8	51	Second
1	HDF5 Collective N-to-1 Read Aggregate Throughput	-0.4	N	260.4	13.7	21	259.3	21.9	51	MByte per Second
1	HDF5 Collective N-to-1 Write Aggregate Throughput	-4.2	N	113.1	12.1	21	108.3	7.92	51	MByte per Second
1	HDF5 Independent N-to-1 Read Aggregate Throughput	-6.3	Y	163.7	21.7	21	153.4	20.7	51	MByte per Second
1	HDF5 Independent N-to-1 Write Aggregate Throughput	-3.0	N	166.1	26.7	21	161.2	23.0	51	MByte per Second
1	HDF5 N-to-N Read Aggregate Throughput	2.9	N	213.7	16.0	21	219.8	16.7	51	MByte per Second
1	HDF5 N-to-N Write Aggregate Throughput	1.0	N	220.3	21.2	21	222.4	25.2	50	MByte per Second
1	MPIIO Collective N-to-1 Read Aggregate Throughput	-2.2	N	270.0	8.86	21	264.0	30.0	51	MByte per Second
1	MPIIO Collective N-to-1 Write Aggregate Throughput	-7.5	N	230.8	38.9	21	213.6	41.2	51	MByte per Second
1	MPIIO Independent N-to-1 Read Aggregate Throughput	-0.2	N	155.1	17.3	21	154.8	15.4	51	MByte per Second
1	MPIIO Independent N-to-1 Write Aggregate Throughput	0.3	N	189.4	37.7	21	190.0	41.8	51	MByte per Second
1	MPIIO N-to-N Read Aggregate Throughput	1.1	N	216.7	9.06	21	219.1	10.6	51	MByte per Second
1	MPIIO N-to-N Write Aggregate Throughput	-7.2	N	262.3	47.7	21	243.5	43.0	51	MByte per Second
1	POSIX N-to-1 Read Aggregate Throughput	2.6	N	169.6	10.4	21	174.1	13.7	51	MByte per Second
1	POSIX N-to-1 Write Aggregate Throughput	-0.6	N	262.2	28.1	21	260.7	37.7	51	MByte per Second
1	POSIX N-to-N Read Aggregate Throughput	0.0	N	231.6	5.47	21	231.6	6.54	51	MByte per Second
1	POSIX N-to-N Write Aggregate Throughput	14.7	Y	233.2	43.7	21	267.6	35.2	51	MByte per Second
1	Parallel NetCDF Collective N-to-1 Read Aggregate Throughput	-0.2	N	236.1	11.9	21	235.5	13.0	51	MByte per Second
1	Parallel NetCDF Collective N-to-1 Write Aggregate Throughput	-1.2	N	197.8	14.7	21	195.5	19.7	51	MByte per Second
1	Parallel NetCDF Independent N-to-1 Read Aggregate Throughput	-1.2	N	227.3	6.42	21	224.6	9.70	50	MByte per Second
1	Parallel NetCDF Independent N-to-1 Write Aggregate Throughput	0.8	N	155.8	17.8	21	157.0	16.6	51	MByte per Second
2	Wall Clock Time	0.7	N	371.1	12.2	22	373.8	16.4	50	Second
2	HDF5 Collective N-to-1 Read Aggregate Throughput	0.3	N	186.9	7.19	22	187.5	14.7	50	MByte per Second
2	HDF5 Collective N-to-1 Write Aggregate Throughput	-6.8	Y	118.4	13.7	22	110.3	9.70	50	MByte per Second
2	HDF5 Independent N-to-1 Read Aggregate Throughput	-2.1	N	195.3	22.9	22	191.1	20.5	50	MByte per Second
2	HDF5 Independent N-to-1 Write Aggregate Throughput	-4.3	N	159.4	24.8	22	152.6	21.8	50	MByte per Second

Table 3. (Continuation) Changes in selected metrics measured by **IOR** on test cluster.

Nodes	Metric	Diff., %	Means are Diff.	Before Update			After Update			Units
				Mean	St.Dev.	N	Mean	St.Dev.	N	
2	HDF5 N-to-N Read Aggregate Throughput	-0.2	N	244.6	13.5	22	244.2	11.3	50	MByte per Second
2	HDF5 N-to-N Write Aggregate Throughput	3.1	N	207.0	30.8	22	213.4	28.3	50	MByte per Second
2	MPIIO Collective N-to-1 Read Aggregate Throughput	2.4	Y	203.8	13.4	22	208.7	22.1	50	MByte per Second
2	MPIIO Collective N-to-1 Write Aggregate Throughput	-3.0	N	198.9	36.6	22	193.0	26.6	50	MByte per Second
2	MPIIO Independent N-to-1 Read Aggregate Throughput	-1.2	N	203.5	17.0	22	201.1	15.6	50	MByte per Second
2	MPIIO Independent N-to-1 Write Aggregate Throughput	-2.4	N	161.9	35.7	22	158.0	32.7	50	MByte per Second
2	MPIIO N-to-N Read Aggregate Throughput	-1.5	Y	262.2	7.73	22	258.3	9.17	50	MByte per Second
2	MPIIO N-to-N Write Aggregate Throughput	7.7	N	213.1	38.3	22	229.6	29.4	50	MByte per Second
2	POSIX N-to-1 Read Aggregate Throughput	0.6	N	201.9	9.31	22	203.0	12.7	50	MByte per Second
2	POSIX N-to-1 Write Aggregate Throughput	0.4	N	232.8	13.6	22	233.8	14.5	50	MByte per Second
2	POSIX N-to-N Read Aggregate Throughput	0.2	N	267.2	3.25	22	267.7	2.55	50	MByte per Second
2	POSIX N-to-N Write Aggregate Throughput	1.8	N	228.6	33.3	22	232.7	31.9	50	MByte per Second
2	Parallel NetCDF Collective N-to-1 Read Aggregate Throughput	-1.5	N	215.9	3.49	22	212.8	11.5	50	MByte per Second
2	Parallel NetCDF Collective N-to-1 Write Aggregate Throughput	3.8	N	167.6	19.2	22	173.9	22.7	50	MByte per Second
2	Parallel NetCDF Independent N-to-1 Read Aggregate Throughput	0.0	N	208.0	7.41	22	208.1	8.03	50	MByte per Second
2	Parallel NetCDF Independent N-to-1 Write Aggregate Throughput	3.6	N	151.4	20.9	22	156.9	21.9	50	MByte per Second
Application: **IOR** on local file system										
1	Wall Clock Time	2.0	N	462.8	16.4	12	471.8	19.1	50	Second
1	HDF5 Collective N-to-1 Read Aggregate Throughput	-0.7	Y	204.9	3.59	12	203.4	1.81	50	MByte per Second
1	HDF5 Collective N-to-1 Write Aggregate Throughput	-1.0	N	48.1	3.84	12	47.6	4.22	50	MByte per Second
1	HDF5 Independent N-to-1 Read Aggregate Throughput	-1.0	Y	2,605.3	62.1	12	2,579.8	39.0	50	MByte per Second
1	HDF5 Independent N-to-1 Write Aggregate Throughput	-2.9	N	29.0	2.05	12	28.2	1.81	50	MByte per Second
1	HDF5 N-to-N Read Aggregate Throughput	-2.2	Y	2,468.6	30.2	12	2,415.5	130.5	50	MByte per Second
1	HDF5 N-to-N Write Aggregate Throughput	-1.5	N	35.8	1.39	12	35.3	9.97E-01	50	MByte per Second
1	MPIIO Collective N-to-1 Read Aggregate Throughput	-1.3	Y	249.9	2.22	12	246.7	3.25	50	MByte per Second
1	MPIIO Collective N-to-1 Write Aggregate Throughput	-0.9	N	37.3	1.40	12	36.9	1.24	50	MByte per Second

Table 3. (Continuation) Changes in selected metrics measured by **IOR** on test cluster.

Nodes	Metric	Diff., %	Means are Diff.	Before Update			After Update			Units
				Mean	St.Dev.	N	Mean	St.Dev.	N	
1	MPIIO Independent N-to-1 Read Aggregate Throughput	-3.3	Y	2,667.2	25.3	12	2,579.6	71.8	50	MByte per Second
1	MPIIO Independent N-to-1 Write Aggregate Throughput	-12.4	Y	67.0	7.77	12	58.7	10.0	50	MByte per Second
1	MPIIO N-to-N Read Aggregate Throughput	-2.8	Y	2,722.7	43.3	12	2,647.6	44.6	50	MByte per Second
1	MPIIO N-to-N Write Aggregate Throughput	1.7	N	37.1	2.23	12	37.8	3.48	50	MByte per Second
1	POSIX N-to-1 Read Aggregate Throughput	3.0	Y	2,819.7	489.9	12	2,903.1	40.0	50	MByte per Second
1	POSIX N-to-1 Write Aggregate Throughput	-0.3	N	1,148.2	53.3	12	1,145.1	45.1	50	MByte per Second
1	POSIX N-to-N Read Aggregate Throughput	-9.1	Y	2,727.7	32.3	12	2,480.9	356.1	50	MByte per Second
1	POSIX N-to-N Write Aggregate Throughput	-3.2	N	913.0	50.7	12	883.8	64.7	50	MByte per Second
1	Parallel NetCDF Collective N-to-1 Read Aggregate Throughput	-2.1	Y	2,574.1	97.0	12	2,521.1	114.5	50	MByte per Second
1	Parallel NetCDF Collective N-to-1 Write Aggregate Throughput	-4.0	N	800.7	93.7	12	768.4	149.1	50	MByte per Second
1	Parallel NetCDF Independent N-to-1 Read Aggregate Throughput	6.5	N	57.0	8.72	12	60.7	18.4	50	MByte per Second
1	Parallel NetCDF Independent N-to-1 Write Aggregate Throughput	-4.4	N	14.9	2.26	12	14.3	2.21	50	MByte per Second

Table 4. Changes in selected metrics measured by **MDTest** on test cluster.

Nodes	Metric	Diff., %	Means are Diff.	Before Update			After Update			Units
				Mean	St.Dev.	N	Mean	St.Dev.	N	
Application: **IOR** on local file system										
1	Wall Clock Time	22.9	Y	30.5	3.17	21	37.5	4.00	50	Second
1	Directory creation (single directory per process)	-9.6	Y	10,077.2	654.9	21	9,106.8	443.5	50	Operations/Second
1	Directory creation (single directory)	-11.2	Y	4,047.9	135.0	21	3,595.4	196.5	50	Operations/Second
1	Directory creation (single tree directory per process)	-12.2	Y	6,001.9	352.3	21	5,271.1	220.8	50	Operations/Second
1	Directory creation (single tree directory)	-15.2	Y	8,550.3	326.2	21	7,248.6	397.6	50	Operations/Second
1	Directory removal (single directory per process)	-12.0	Y	23,141.4	2,119.5	21	20,354.5	1,797.8	50	Operations/Second
1	Directory removal (single directory)	-17.7	Y	6,553.6	245.2	21	5,394.7	260.2	50	Operations/Second
1	Directory removal (single tree directory per process)	-14.3	Y	21,471.7	759.0	21	18,395.9	698.0	50	Operations/Second
1	Directory removal (single tree directory)	-16.0	Y	20,235.1	718.1	21	16,998.1	798.4	50	Operations/Second
1	Directory stat (single directory per process)	-15.6	Y	6.56E+05	2.20E+05	21	5.54E+05	1.62E+05	50	Operations/Second
1	Directory stat (single directory)	-16.1	Y	5.38E+05	2.01E+05	21	4.51E+05	1.39E+05	50	Operations/Second
1	Directory stat (single tree directory per process)	-14.0	Y	1.69E+05	32,922.1	21	1.45E+05	35,224.7	50	Operations/Second
1	Directory stat (single tree directory)	-14.2	N	1.90E+05	70,870.9	21	1.63E+05	64,240.9	50	Operations/Second
1	File creation (single directory per process)	-5.6	Y	11,511.4	973.1	21	10,867.9	884.6	50	Operations/Second
1	File creation (single directory)	-11.7	Y	3,653.2	116.8	21	3,225.5	165.6	50	Operations/Second
1	File creation (single tree directory per process)	-13.6	Y	6,915.2	363.9	21	5,971.9	382.0	50	Operations/Second
1	File creation (single tree directory)	-12.3	Y	8,093.8	313.4	21	7,098.2	365.6	50	Operations/Second
1	File read (single directory per process)	-12.6	Y	63,095.9	5,444.8	21	55,114.2	5,404.7	50	Operations/Second
1	File read (single directory)	-14.7	Y	48,885.8	2,314.8	21	41,685.9	2,402.5	50	Operations/Second
1	File read (single tree directory per process)	-10.9	Y	31,866.5	1,720.1	21	28,383.6	2,215.6	50	Operations/Second
1	File read (single tree directory)	-12.7	Y	32,764.4	1,957.9	21	28,589.8	2,149.2	50	Operations/Second
1	File removal (single directory per process)	-12.6	Y	20,091.9	1,302.4	21	17,565.3	1,159.7	50	Operations/Second
1	File removal (single directory)	-10.8	Y	3,052.8	102.3	21	2,722.0	112.6	50	Operations/Second
1	File removal (single tree directory per process)	-12.7	Y	19,059.2	994.7	21	16,629.6	932.2	50	Operations/Second
1	File removal (single tree directory)	-15.6	Y	13,335.3	672.5	21	11,253.3	528.7	50	Operations/Second
1	File stat (single directory per process)	-13.0	Y	6.59E+05	2.04E+05	21	5.74E+05	1.52E+05	50	Operations/Second

Table 4. (Continuation) Changes in selected metrics measured by **MDTest** on test cluster.

Nodes	Metric	Diff., %	Means are Diff.	Before Update			After Update			Units
				Mean	St.Dev.	N	Mean	St.Dev.	N	
1	File stat (single directory)	-14.8	Y	5.33E+05	1.89E+05	21	4.54E+05	1.21E+05	50	Operations/Second
1	File stat (single tree directory per process)	-17.8	Y	2.33E+05	82,709.0	21	1.91E+05	53,086.0	50	Operations/Second
1	File stat (single tree directory)	-19.2	Y	2.16E+05	70,999.6	21	1.74E+05	59,376.5	50	Operations/Second
1	Tree creation (single directory per process)	-9.6	Y	623.3	88.2	21	563.5	80.9	50	Operations/Second
1	Tree creation (single directory)	-11.7	Y	4,533.0	383.9	21	4,000.7	244.0	50	Operations/Second
1	Tree creation (single tree directory per process)	-11.2	Y	1,394.2	55.4	21	1,237.4	55.3	50	Operations/Second
1	Tree creation (single tree directory)	-18.2	Y	7,000.7	258.9	21	5,727.3	316.9	50	Operations/Second
1	Tree removal (single directory per process)	-7.6	Y	684.5	56.8	21	632.3	54.5	50	Operations/Second
1	Tree removal (single directory)	-12.8	Y	2,675.5	146.3	21	2,334.3	174.3	50	Operations/Second
1	Tree removal (single tree directory per process)	-17.2	Y	3,026.2	138.6	21	2,506.3	145.9	50	Operations/Second
1	Tree removal (single tree directory)	-20.5	Y	7,282.7	223.5	21	5,790.1	268.7	50	Operations/Second
2	Wall Clock Time	9.1	Y	166.7	3.60	23	181.9	2.92	50	Second
2	Directory creation (single directory per process)	-13.5	Y	17,579.0	903.1	23	15,202.8	1,420.8	50	Operations/Second
2	Directory creation (single directory)	-6.3	Y	205.7	21.2	23	192.8	14.1	50	Operations/Second
2	Directory creation (single tree directory per process)	-14.9	Y	11,290.7	830.1	23	9,604.3	685.3	50	Operations/Second
2	Directory creation (single tree directory)	-9.3	Y	4,299.0	238.0	23	3,900.7	346.7	50	Operations/Second
2	Directory removal (single directory per process)	-18.6	Y	44,863.2	2,049.4	23	36,517.6	5,190.1	50	Operations/Second
2	Directory removal (single directory)	-6.3	Y	165.6	6.87	23	155.2	7.44	50	Operations/Second
2	Directory removal (single tree directory per process)	-17.7	Y	38,972.6	2,303.5	23	32,070.6	3,274.8	50	Operations/Second
2	Directory removal (single tree directory)	-8.1	Y	3,265.5	292.3	23	3,002.5	269.9	50	Operations/Second
2	Directory stat (single directory per process)	-11.1	Y	1.13E+06	5.01E+05	23	1.00E+06	3.52E+05	50	Operations/Second
2	Directory stat (single directory)	-13.8	Y	99,839.9	51,901.6	23	86,016.3	65,695.7	50	Operations/Second
2	Directory stat (single tree directory per process)	-10.2	Y	2.52E+05	61,441.7	23	2.26E+05	56,220.0	50	Operations/Second
2	Directory stat (single tree directory)	-10.0	Y	28,149.5	1,859.8	23	25,336.0	2,306.4	50	Operations/Second
2	File creation (single directory per process)	-14.0	Y	24,602.9	1,239.1	23	21,165.3	2,428.8	50	Operations/Second
2	File creation (single directory)	-4.9	Y	147.7	4.61	23	140.5	4.71	50	Operations/Second

Table 4. (Continuation) Changes in selected metrics measured by **MDTest** on test cluster.

Nodes	Metric	Diff., %	Means are Diff.	Before Update			After Update			Units
				Mean	St.Dev.	N	Mean	St.Dev.	N	
2	File creation (single tree directory per process)	-15.8	Y	13,230.6	887.4	23	11,146.1	973.1	50	Operations/Second
2	File creation (single tree directory)	-7.8	Y	2,250.1	107.6	23	2,074.2	150.6	50	Operations/Second
2	File read (single directory per process)	-14.4	Y	1.09E+05	11,905.2	23	93,507.3	14,652.9	50	Operations/Second
2	File read (single directory)	-26.3	Y	83,715.1	9,200.7	23	61,661.4	8,887.8	50	Operations/Second
2	File read (single tree directory per process)	-14.4	Y	61,208.9	5,284.2	23	52,369.5	6,751.7	50	Operations/Second
2	File read (single tree directory)	-24.3	Y	59,445.9	2,900.6	23	44,976.3	4,910.6	50	Operations/Second
2	File removal (single directory per process)	-15.6	Y	39,263.6	2,159.3	23	33,139.5	3,247.3	50	Operations/Second
2	File removal (single directory)	-4.6	Y	206.3	7.66	23	196.7	6.77	50	Operations/Second
2	File removal (single tree directory per process)	-14.4	Y	36,028.4	2,620.9	23	30,857.0	3,300.8	50	Operations/Second
2	File removal (single tree directory)	-10.4	Y	1,618.6	124.6	23	1,449.6	98.2	50	Operations/Second
2	File stat (single directory per process)	-8.8	Y	1.17E+06	5.10E+05	23	1.07E+06	3.25E+05	50	Operations/Second
2	File stat (single directory)	15.8	N	7.55E+05	4.30E+05	23	8.75E+05	3.34E+05	50	Operations/Second
2	File stat (single tree directory per process)	-12.7	Y	3.00E+05	83,769.0	23	2.61E+05	69,033.6	50	Operations/Second
2	File stat (single tree directory)	-9.7	Y	21,943.9	1,619.0	23	19,817.7	1,312.3	50	Operations/Second
2	Tree creation (single directory per process)	-8.9	Y	70.9	4.54	23	64.7	6.10	50	Operations/Second
2	Tree creation (single directory)	-14.7	Y	5,180.4	515.3	23	4,418.9	409.7	50	Operations/Second
2	Tree creation (single tree directory per process)	-10.8	Y	532.5	33.5	23	475.2	37.2	50	Operations/Second
2	Tree creation (single tree directory)	-14.3	Y	6,350.4	305.6	23	5,440.7	551.7	50	Operations/Second
2	Tree removal (single directory per process)	-6.6	Y	17.5	8.76E-01	23	16.3	7.97E-01	50	Operations/Second
2	Tree removal (single directory)	-10.2	Y	261.1	40.3	23	234.5	33.5	50	Operations/Second
2	Tree removal (single tree directory per process)	-11.8	Y	597.7	54.5	23	527.2	47.5	50	Operations/Second
2	Tree removal (single tree directory)	-3.7	N	929.5	225.3	23	895.0	214.0	50	Operations/Second
Application: **MDTest** on local file system										
1	Wall Clock Time	68.0	Y	3.75	6.22E-01	12	6.30	2.40	50	Second
1	Directory creation (single directory per process)	6.0	Y	1.04E+05	1,788.6	12	1.10E+05	6,223.7	50	Operations/Second
1	Directory creation (single directory)	-6.2	N	38,409.5	3,125.0	12	36,034.1	3,534.2	50	Operations/Second

Table 4. (Continuation) Changes in selected metrics measured by **MDTest** on test cluster.

Nodes	Metric	Diff., %	Means are Diff.	Before Update			After Update			Units
				Mean	St.Dev.	N	Mean	St.Dev.	N	
1	Directory creation (single tree directory per process)	16.1	Y	1.10E+05	8,266.4	12	1.28E+05	8,801.2	50	Operations/Second
1	Directory creation (single tree directory)	2.8	N	1.04E+05	7,435.5	12	1.07E+05	7,777.9	50	Operations/Second
1	Directory removal (single directory per process)	6.7	Y	1.08E+05	6,988.4	12	1.15E+05	8,970.1	50	Operations/Second
1	Directory removal (single directory)	-12.1	Y	49,212.9	1,723.6	12	43,254.9	4,700.9	50	Operations/Second
1	Directory removal (single tree directory per process)	0.2	N	1.40E+05	5,187.4	12	1.40E+05	6,201.6	50	Operations/Second
1	Directory removal (single tree directory)	-10.5	Y	1.30E+05	3,695.4	12	1.16E+05	10,654.1	50	Operations/Second
1	Directory stat (single directory per process)	-29.9	Y	1.77E+06	1.23E+05	12	1.24E+06	1.37E+05	50	Operations/Second
1	Directory stat (single directory)	-29.2	Y	1.89E+06	1.77E+05	12	1.34E+06	1.39E+05	50	Operations/Second
1	Directory stat (single tree directory per process)	-26.4	Y	1.88E+06	46,500.6	12	1.39E+06	49,826.7	50	Operations/Second
1	Directory stat (single tree directory)	-25.4	Y	1.92E+06	57,201.5	12	1.43E+06	44,995.9	50	Operations/Second
1	File creation (single directory per process)	-27.6	Y	2.41E+05	94,038.8	12	1.75E+05	13,963.9	50	Operations/Second
1	File creation (single directory)	0.2	Y	73,822.2	1,875.7	12	73,964.7	21,028.1	50	Operations/Second
1	File creation (single tree directory per process)	-1.5	N	2.03E+05	17,884.4	12	2.00E+05	11,253.3	50	Operations/Second
1	File creation (single tree directory)	-11.4	Y	1.79E+05	14,521.2	12	1.58E+05	14,441.9	50	Operations/Second
1	File read (single directory per process)	-31.5	Y	1.40E+06	1.61E+05	12	9.61E+05	1.10E+05	50	Operations/Second
1	File read (single directory)	-27.2	Y	1.38E+06	99,843.8	12	1.01E+06	99,375.9	50	Operations/Second
1	File read (single tree directory per process)	-24.5	Y	1.38E+06	22,204.6	12	1.04E+06	23,656.5	50	Operations/Second
1	File read (single tree directory)	-25.0	Y	1.39E+06	30,950.2	12	1.04E+06	25,861.7	50	Operations/Second
1	File removal (single directory per process)	-8.0	Y	2.00E+05	11,634.5	12	1.84E+05	17,439.9	50	Operations/Second
1	File removal (single directory)	-6.4	Y	1.32E+05	5,415.1	12	1.24E+05	16,267.7	50	Operations/Second
1	File removal (single tree directory per process)	-7.9	Y	2.10E+05	3,755.7	12	1.93E+05	11,090.9	50	Operations/Second
1	File removal (single tree directory)	-8.8	Y	2.08E+05	7,989.9	12	1.89E+05	15,568.0	50	Operations/Second
1	File stat (single directory per process)	-30.6	Y	1.78E+06	1.36E+05	12	1.24E+06	1.11E+05	50	Operations/Second
1	File stat (single directory)	-29.7	Y	1.89E+06	1.94E+05	12	1.33E+06	1.51E+05	50	Operations/Second
1	File stat (single tree directory per process)	-26.1	Y	1.91E+06	49,643.8	12	1.41E+06	32,775.7	50	Operations/Second

Table 4. (Continuation) Changes in selected metrics measured by **MDTest** on test cluster.

Nodes	Metric	Diff., %	Means are Diff.	Before Update			After Update			Units
				Mean	St.Dev.	N	Mean	St.Dev.	N	
1	File stat (single tree directory)	-26.2	Y	1.92E+06	51,711.8	12	1.41E+06	26,961.3	50	Operations/Second
1	Tree creation (single directory per process)	-6.9	Y	3,278.2	304.8	12	3,052.7	239.1	50	Operations/Second
1	Tree creation (single directory)	0.1	N	21,033.8	5,823.8	12	21,055.5	5,146.7	50	Operations/Second
1	Tree creation (single tree directory per process)	-2.7	N	9,688.4	586.0	12	9,426.6	867.8	50	Operations/Second
1	Tree creation (single tree directory)	7.0	Y	33,237.8	3,985.5	12	35,553.1	3,029.0	50	Operations/Second
1	Tree removal (single directory per process)	-4.6	Y	2,866.2	98.7	12	2,733.1	259.9	50	Operations/Second
1	Tree removal (single directory)	-12.0	Y	5,730.9	959.9	12	5,042.0	1,136.1	50	Operations/Second
1	Tree removal (single tree directory per process)	-8.1	Y	14,300.0	818.4	12	13,141.2	1,396.9	50	Operations/Second
1	Tree removal (single tree directory)	-11.8	Y	23,226.3	788.7	12	20,494.3	2,007.1	50	Operations/Second

Performance Cluster Results

Table 5. Changes in selected metrics measured by **NAMD, NWChem** and **GAMESS** on test cluster.

Nodes	Metric	Diff., %	Means are Diff.	Before Update			After Update			Units
				Mean	St.Dev.	N	Mean	St.Dev.	N	
Application: **NAMD**										
1	Wall Clock Time	3.1	Y	308.6	2.94	22	318.1	4.42	102	Second
1	Molecular Dynamics Simulation Performance	-3.3	Y	7.61E-10	9.17E-12	22	7.35E-10	1.86E-11	102	Second per Day
2	Wall Clock Time	5.7	Y	179.5	3.93	17	189.8	3.98	67	Second
2	Molecular Dynamics Simulation Performance	-5.0	Y	1.44E-09	5.04E-11	17	1.37E-09	8.03E-11	67	Second per Day
4	Wall Clock Time	11.3	Y	106.1	1.93	11	118.1	4.05	44	Second
4	Molecular Dynamics Simulation Performance	-10.7	Y	2.72E-09	1.96E-10	11	2.43E-09	2.65E-10	44	Second per Day
8	Wall Clock Time	15.0	Y	76.2	1.42	7	87.6	3.34	35	Second
8	Molecular Dynamics Simulation Performance	-20.3	Y	4.56E-09	3.14E-10	7	3.63E-09	4.53E-10	35	Second per Day
Application: **NWChem**										
1	Wall Clock Time	4.1	Y	78.0	1.08	25	81.2	1.88	83	Second
2	Wall Clock Time	9.8	Y	60.5	1.63	20	66.5	3.33	84	Second
4	Wall Clock Time	21.6	Y	41.0	1.23	14	49.8	8.61	79	Second
8	Wall Clock Time	27.2	Y	32.2	2.30	15	40.9	4.37	102	Second
Application: **GAMESS**										
1	Wall Clock Time	1.0	Y	286.4	1.75	23	289.4	1.88	73	Second
1	Time Spent in MP2 Energy Calculation	0.1	N	124.7	9.33E-01	23	124.8	6.71E-01	73	Second
1	Time Spent in Restricted Hartree-Fock Calculation	0.3	Y	155.1	6.81E-01	23	155.5	7.11E-01	73	Second
2	Wall Clock Time	5.7	Y	171.7	43.1	19	181.5	55.5	50	Second
2	Time Spent in MP2 Energy Calculation	0.4	N	63.6	5.96E-01	19	63.8	7.44E-01	50	Second
2	Time Spent in Restricted Hartree-Fock Calculation	7.6	N	97.8	43.3	19	105.2	55.4	50	Second
4	Wall Clock Time	-6.7	Y	102.7	46.5	16	95.8	18.1	38	Second
4	Time Spent in MP2 Energy Calculation	0.1	Y	32.1	4.17E-01	16	32.2	1.97	38	Second
4	Time Spent in Restricted Hartree-Fock Calculation	-17.9	N	59.5	46.4	16	48.9	16.0	38	Second
8	Wall Clock Time	-35.7	N	104.9	122.2	16	67.4	38.1	26	Second
8	Time Spent in MP2 Energy Calculation	-1.5	Y	18.1	4.26	16	17.9	2.49	26	Second
8	Time Spent in Restricted Hartree-Fock Calculation	-28.9	N	47.3	47.3	16	33.6	36.8	26	Second

Table 6. Changes in selected metrics measured by **ENZO** on test cluster.

Nodes	Metric	Diff., %	Means are Diff.	Before Update			After Update			Units
				Mean	St.Dev.	N	Mean	St.Dev.	N	
1	Wall Clock Time	2.1	Y	4,863.7	106.7	21	4,964.2	100.8	57	Second
1	All Data Group Write Time	1.7	N	61.2	2.15	21	62.2	3.64	57	Second
1	All Grid Level 00 Calculation Time	1.3	Y	869.1	25.6	21	880.0	13.8	57	Second
1	All Grid Level 01 Calculation Time	2.3	Y	844.3	21.0	21	863.4	24.2	57	Second
1	All Grid Level 02 Calculation Time	2.0	Y	2,874.4	106.0	21	2,932.3	84.3	57	Second
1	Boundary Conditions Setting Time	2.8	Y	234.1	8.98	21	240.6	6.70	57	Second
1	Communication Transpose Time	31.0	Y	8.13	1.13	21	10.7	1.98	57	Second
1	Gravitational Potential Field Computing Time	4.1	Y	162.3	4.14	21	168.9	4.86	57	Second
1	Grid Hierarchy Rebuilding Time	5.5	Y	109.6	8.13	21	115.6	6.75	57	Second
1	Hydro Equations Solving Time	1.0	Y	833.1	8.43	21	841.6	9.71	57	Second
1	Poisson Equation Solving Time	3.6	Y	240.5	4.50	21	249.2	7.67	57	Second
1	Total Time Spent in Cycles	2.1	Y	4,859.0	106.6	21	4,959.7	100.8	57	Second
2	Wall Clock Time	7.9	Y	3,378.6	120.0	22	3,644.8	144.6	44	Second
2	All Data Group Write Time	2.0	N	34.0	2.16	22	34.7	3.80	44	Second
2	All Grid Level 00 Calculation Time	5.7	Y	431.9	4.66	22	456.6	5.86	44	Second
2	All Grid Level 01 Calculation Time	4.5	Y	462.5	10.7	22	483.4	12.0	44	Second
2	All Grid Level 02 Calculation Time	8.6	Y	2,312.5	115.0	22	2,511.2	135.3	44	Second
2	Boundary Conditions Setting Time	9.5	Y	128.8	3.06	22	141.0	3.79	44	Second
2	Communication Transpose Time	139.6	Y	6.89	1.01	22	16.5	2.80	44	Second
2	Gravitational Potential Field Computing Time	27.9	Y	41.2	1.08	22	52.6	2.70	44	Second
2	Grid Hierarchy Rebuilding Time	14.0	Y	76.7	2.59	22	87.4	3.72	44	Second
2	Hydro Equations Solving Time	0.9	Y	413.5	1.90	22	417.2	1.72	44	Second
2	Poisson Equation Solving Time	9.1	Y	128.9	1.80	22	140.6	3.88	44	Second
2	Total Time Spent in Cycles	7.9	Y	3,376.6	119.9	22	3,642.8	144.6	44	Second
4	Wall Clock Time	11.2	Y	2,305.2	229.5	17	2,562.6	216.2	37	Second
4	All Data Group Write Time	3.4	N	21.8	2.51	17	22.5	3.12	37	Second
4	All Grid Level 00 Calculation Time	11.4	Y	191.8	17.4	17	213.5	11.0	37	Second
4	All Grid Level 01 Calculation Time	12.1	Y	238.3	5.10	17	267.0	8.71	37	Second
4	All Grid Level 02 Calculation Time	10.2	Y	1,756.7	219.6	17	1,936.6	210.3	37	Second
4	Boundary Conditions Setting Time	16.6	Y	72.0	3.16	17	83.9	3.97	37	Second
4	Communication Transpose Time	126.3	Y	6.25	1.12	17	14.2	8.03	37	Second
4	Gravitational Potential Field Computing Time	69.2	Y	11.6	1.90	17	19.7	8.10	37	Second
4	Grid Hierarchy Rebuilding Time	25.6	Y	53.7	3.47	17	67.4	4.97	37	Second
4	Hydro Equations Solving Time	0.7	Y	204.7	1.83	17	206.2	1.61	37	Second
4	Poisson Equation Solving Time	18.5	Y	70.8	1.45	17	84.0	4.14	37	Second
4	Total Time Spent in Cycles	11.2	Y	2,304.4	229.5	17	2,561.5	216.2	37	Second
8	Wall Clock Time	27.8	Y	1,893.6	101.6	12	2,419.2	388.7	27	Second
8	All Data Group Write Time	34.1	N	18.5	1.54	12	24.8	28.1	27	Second
8	All Grid Level 00 Calculation Time	38.6	Y	109.5	6.74	12	151.8	24.9	27	Second
8	All Grid Level 01 Calculation Time	27.4	Y	151.6	6.13	12	193.1	17.0	27	Second
8	All Grid Level 02 Calculation Time	26.0	Y	1,528.2	95.9	12	1,925.3	357.4	27	Second
8	Boundary Conditions Setting Time	31.8	Y	45.6	2.41	12	60.1	5.02	27	Second
8	Communication Transpose Time	111.6	Y	16.7	2.73	12	35.3	20.6	27	Second
8	Gravitational Potential Field Computing Time	101.6	Y	18.5	2.80	12	37.2	20.7	27	Second
8	Grid Hierarchy Rebuilding Time	38.3	Y	47.4	3.44	12	65.5	5.95	27	Second

Table 6. (Continuation) Changes in selected metrics measured by **ENZO** on test cluster.

Nodes	Metric	Diff., %	Means are Diff.	Before Update			After Update			Units
				Mean	St.Dev.	N	Mean	St.Dev.	N	
8	Hydro Equations Solving Time	0.5	N	109.0	1.53	12	109.5	1.37	27	Second
8	Poisson Equation Solving Time	35.5	Y	45.4	1.85	12	61.5	7.24	27	Second
8	Total Time Spent in Cycles	27.7	Y	1,892.5	101.6	12	2,417.6	388.6	27	Second