Performance Comparison of Two Virtual Machine Scenarios Using an HPC Application - A Case study Using Molecular Dynamics Simulations

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Outline

- Background
- Objectives
- Experimental setup
- Evaluation methodology
- Overall and detailed results
- Conclusion
- Future work

Background

- Virtualization is an increasing field of importance in HPC
  - Availability of low-overhead hypervisors, such as Xen
  - Added efficiency through full utilization of resources
  - Support for customized environments to fit application needs
  - Increased flexibility for high availability and fault tolerance
- While overheads are low, they still exist
  - Virtualization of hardware resources causes performance hit
  - Compute-bound applications experience a lower overhead
  - I/O-bound applications have a higher overhead
- Quantifying these overheads beyond pure wall clock time
  - Can help to understand their root causes
  - Can offer tunable solutions for adaptation to individual application needs

Objectives

- Investigate novel virtual machine (VM) configurations
  - To obtain a benefits vs. performance-loss tradeoff
  - To reduce the performance overhead of virtualization, while maintaining important benefits of virtualization
- Evaluate the difference between two VM configurations that perform the same work with different flexibility
  - 2 VMs per single-core node, 1 process per VM
  - 1 VM per single-core node, 2 processes per VM
- Since overheads are application depended, we focus on a specific scientific application
  - LAMMPS, a classical molecular dynamics code

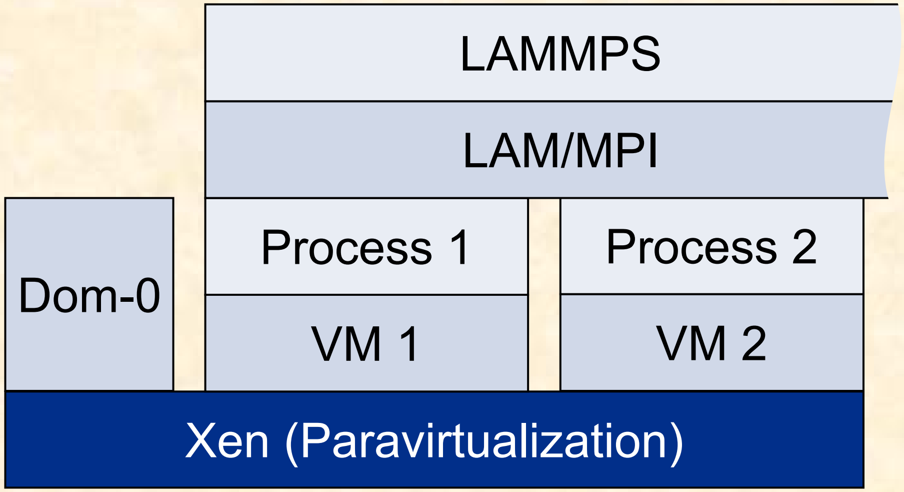
Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS)

- Parallel application that studies properties of particles over time
- Interaction through pair-wise forces using Newton’s law
- Widely used from material science to computational biology
- Most algorithms reduce cost from $O(n^2)$ to $O(n)$ through approximations
- Application setup:
  - LAMMPS protein benchmark: Rhodopsin protein in solvated lipid bilayer
  - 1,024,000 atoms, 100 timesteps

Input	Value
Atom style	full
Pair style	lj (Lennard-Jones potential)
Bond style	harmonic
Neighbor modify	Delay 5, every 1 second
Kspace style	pppm

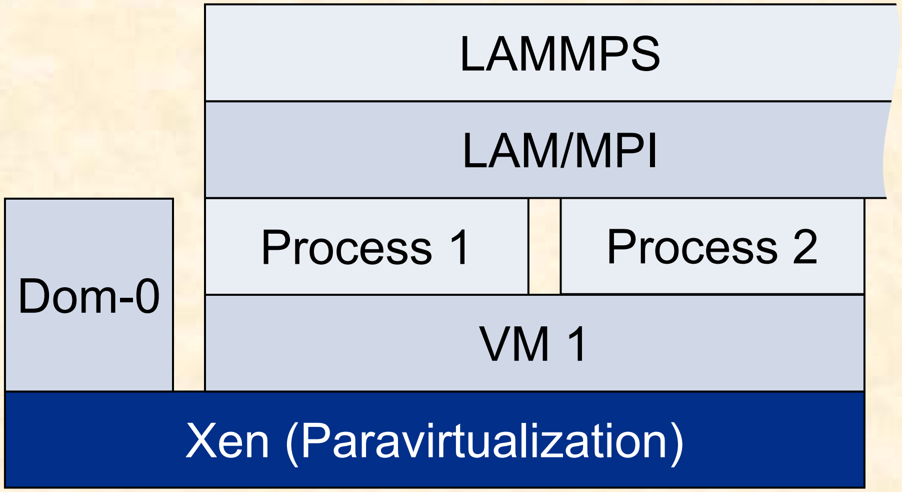
System Setup

Configuration 1



- **VM1 Resources = VM2 Resources**
- **Memory = 256 MB/VM**
- **Application memory = 231 MB/VM**
- **Total number of processes = 16**

Configuration 2



- **Memory = 512 MB/VM**
- **Application memory = 462 MB/VM**
- **Total number of processes = 16**

Physical node: Memory = 768MB, CPU = 2GHz, L2 Cache = 256kB, Local Root FS, NFS

Setup of 1 physical node is shown. This setup is replicated across 8 nodes.

Evaluation Methodology

- Compare VM configurations with the same application run
  - Total wall clock time
  - Detailed CPU, memory, system, and I/O metrics
- Collection of metrics with VMstat process in each VM
  - 1 second sample frequency
  - CPU metrics: User, system, idle, I/O wait, stolen time
  - Memory metrics: Swap, free, inactive, active
  - System metrics: Interrupts and context switches
  - I/O metrics: NFS disk I/O blocks sent and received

Overall Performance Difference

Configuration 1

Description	Wall clock time in sec
2 VMs per node, 1 process per VM	**1686**

- **Averaged over 5 runs**
- **Standard deviation: 3%**
- **2.4% slower**

Application phases	Wall clock time in %
Pair time	**45.33**
Bond time	**1.52**
Kspace time	**32.5**
Neighbor time	**7.05**
Communication time	**7.55**
Other time	**6.05**

Configuration 2

Description	Wall clock time in sec
1 VM per node, 2 processes per VM	**1646**

- **Averaged over 5 runs**
- **Standard deviation: 1.5%**
- **40 seconds faster**

Application phases	Wall clock time in %
Pair time	**46.05**
Bond time	**1.61**
Kspace time	**33.01**
Neighbor time	**7.12**
Communication time	**6.97**
Other time	**5.24**

CPU Metrics: VMstat Average Data

Configuration 1

Metric	VM1 in %	VM2 in %
User time	**27.4**	**26.4**
System time	**1**	**1.2**
I/O wait time	**4.1**	**4.5**
Idle time	**39.2**	**39.5**
Stolen time	**28.3**	**28.4**

Metric	Configuration 1 in %
User time	**53.8**
System time	**2.2**
I/O wait time	**2.6**
Idle time	**41.4**

Configuration 2

Metric	VM1 in %
User time	**63.9**
System time	**9**
I/O wait time	**0.7**
Idle time	**20.4**
Stolen time	**6**

Metric	Configuration 2 in %
User time	**63.9**
System time	**9**
I/O wait time	**0.7**
Idle time	**26.4**

CPU Metrics: XenTop Average Data

Configuration 1

Domain	CPU time in %
Dom-0	**15.4**
VM 1	**31.2**
VM 2	**31.2**
Idle	**22.2**

- **Total used CPU time: 77.8%**
- **More idle time**

Configuration 2

Domain	CPU time in %
Dom-0	**13**
VM 1	**74**
Idle	**13**

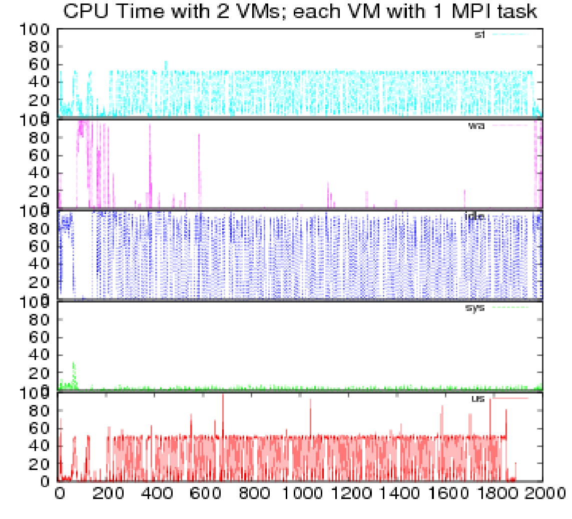
- **Total used CPU time: 87%**
- **Higher CPU utilization**

CPU Metrics: VMstat Sample Data

Configuration 1

Configuration 2

VM 1



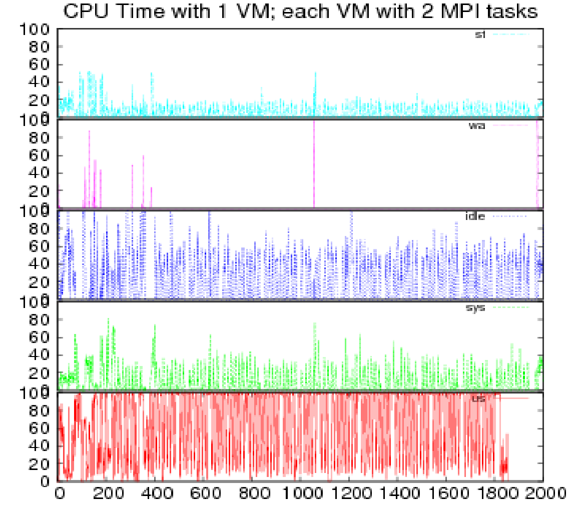
▶ Stolen time in % ◀

▶ I/O wait time in % ◀

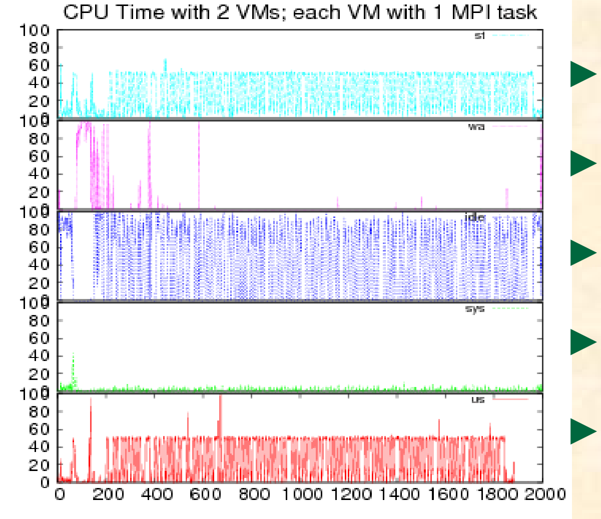
▶ Idle time in % ◀

▶ System time in % ◀

▶ User time in % ◀



VM 2



▶ Stolen time in %

▶ I/O wait time in %

▶ Idle time in %

▶ System time in %

▶ User time in %

- Wall clock difference is 2.4%, but user time difference is 19.2%
- Configuration 1:
  - Xen may not efficiently exploit idle time
  - More NFS pressure with 2VMs
- Configuration 2:
  - More context switches
  - Higher L2/TLB misses?

Memory Metrics: VMstat Average Data

Configuration 1

Metric	Per VM in %
Swap allocated	**20.1**
Free	**3**
Inactive	**18.7**
Active	**57.6**

- **Total available within a VM: 256.0 MB**
- **Used per VM: 285.6 MB**
- **Used by application process: 231.0 MB**

- **More used per VM due to resource management for 2 VMs on the same host**
- **Similar free amounts in both configs**

Configuration 2

Metric	Per VM in %
Swap allocated	**8.1**
Free	**3.9**
Inactive	**26.1**
Active	**61.8**

- **Total available within a VM: 512.0 MB**
- **Used per VM: 509.0 MB**
- **Used by application process: 462.0 MB**

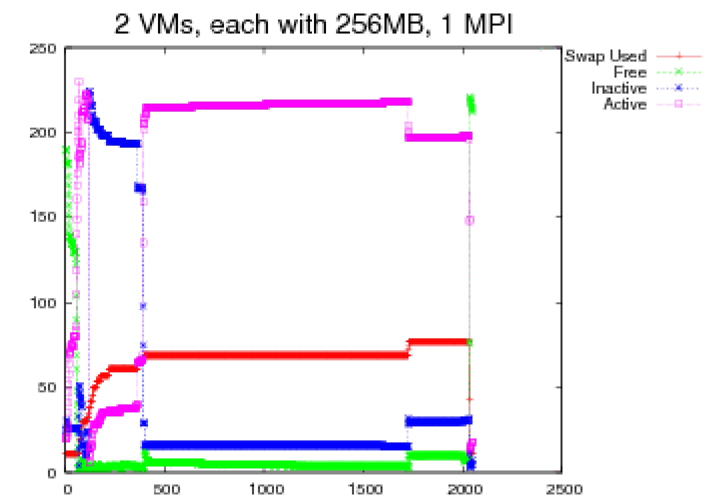
- **Less allocated swap, though not used!**
- **Remember, only 2.4% wall clock difference**

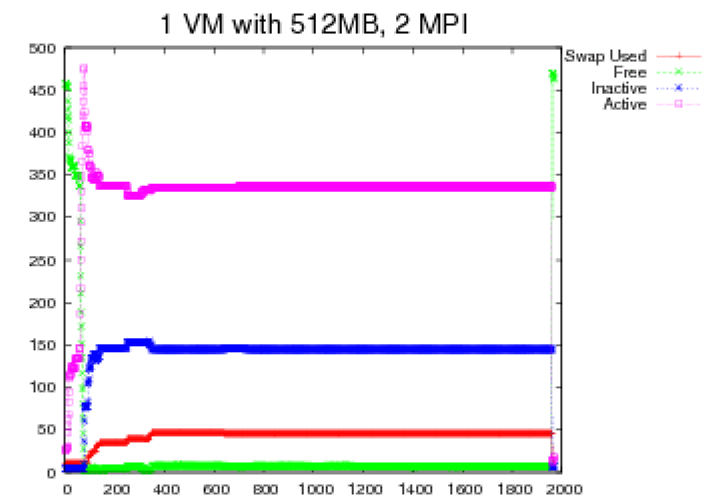
Memory Metrics: VMstat Sample Data

Configuration 1

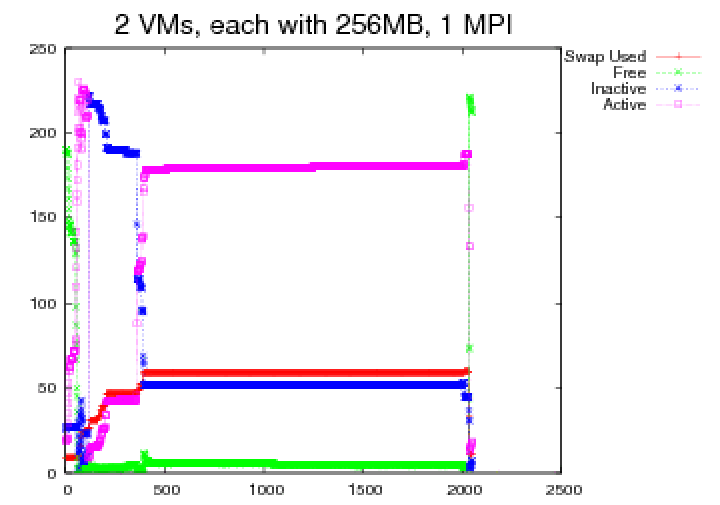
Configuration 2

VM 1





VM 2



I/O Metrics: VMstat Average Data

Configuration 1

Metric	
Disk I/O blocks sent/sec	65.5
Disk I/O blocks received/sec	51.5

Configuration 2

Metric	
Disk I/O blocks sent/sec	20
Disk I/O blocks received/sec	13.2

- Much higher I/O activity
- Remember, only 2.4% wall clock difference

- No aggregation of I/O requests/responses
- Increased I/O activity may be the cause for the increased memory usage per VM
- XenTop: Dom-0 CPU time was 15.4%

- Total number of block sent/received similar for both configurations

- Aggregation of requests/responses possible

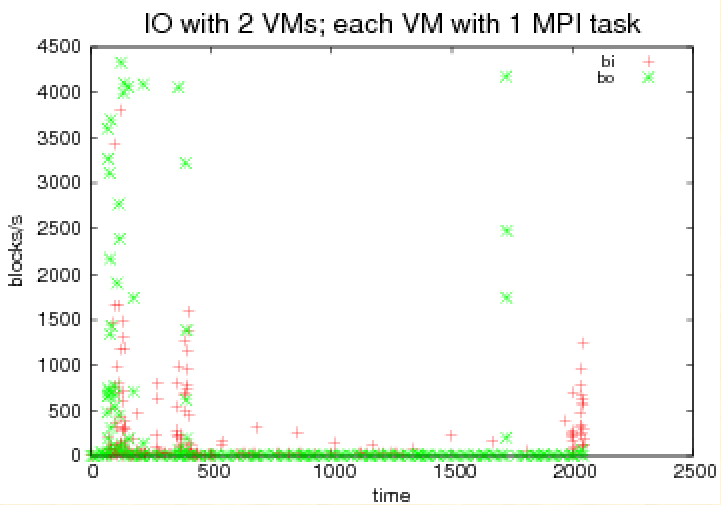
- XenTop: Dom-0 CPU time was 13.4%

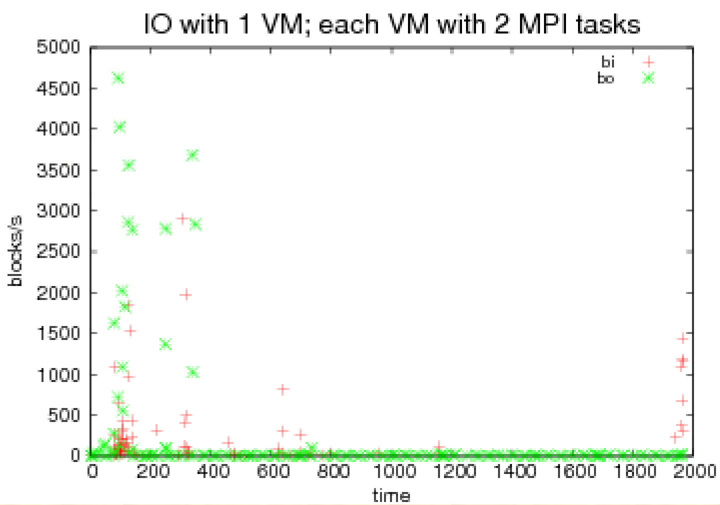
I/O Metrics: VMstat Sample Data

Configuration 1

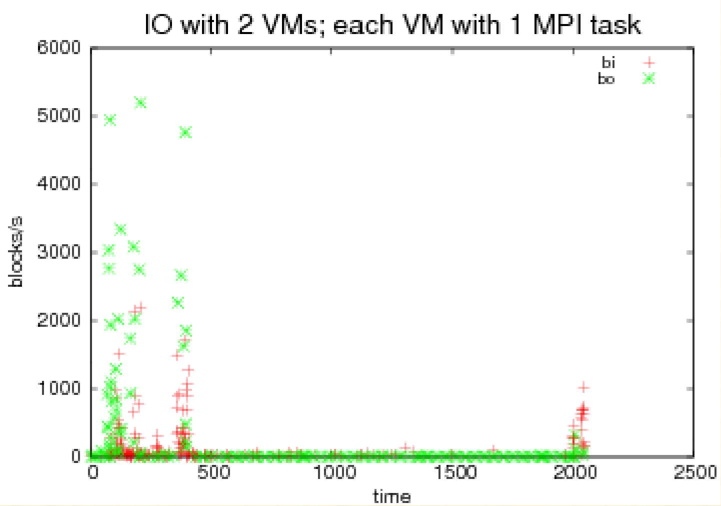
Configuration 2

VM 1





VM 2



System Metrics: VMstat Average Data

Configuration 1

Metric	
Number of interrupts/sec	**1403.8**
Number of context switches/sec	**1332.8**

Configuration 2

Metric	
Number of interrupts/sec	**1357.5**
Number of context switches/sec	**1698.1**

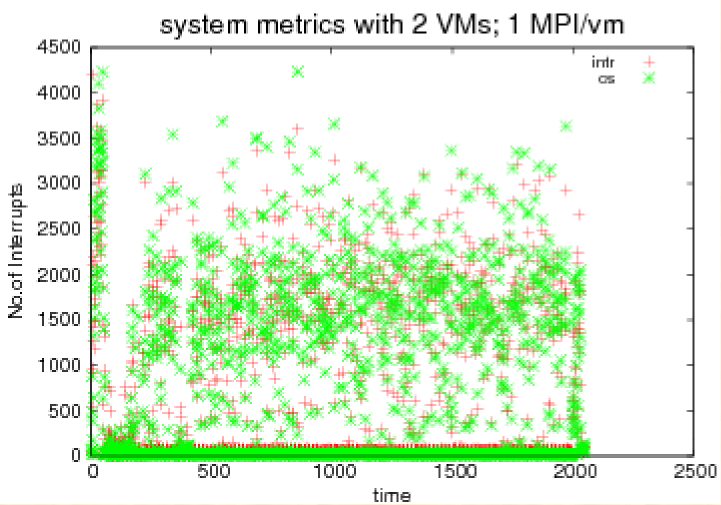
- **22% more context switches**
- **Probably higher L2/TLB misses**
- **May explain higher contribution to user and system utilization**

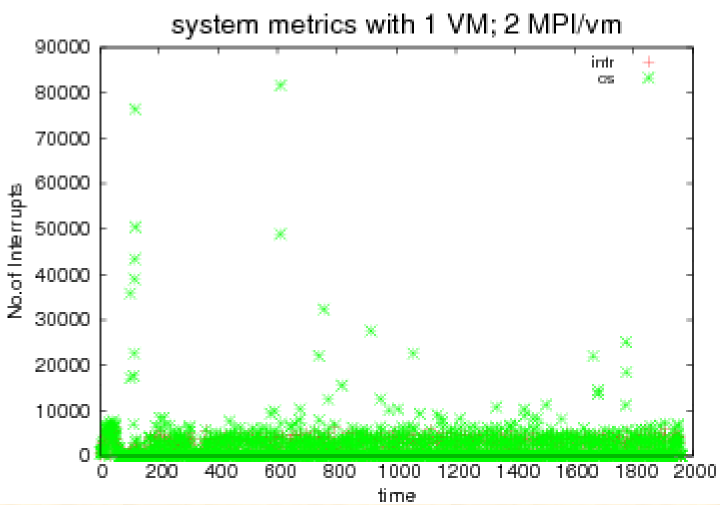
System Metrics: VMstat Sample Data

Configuration 1

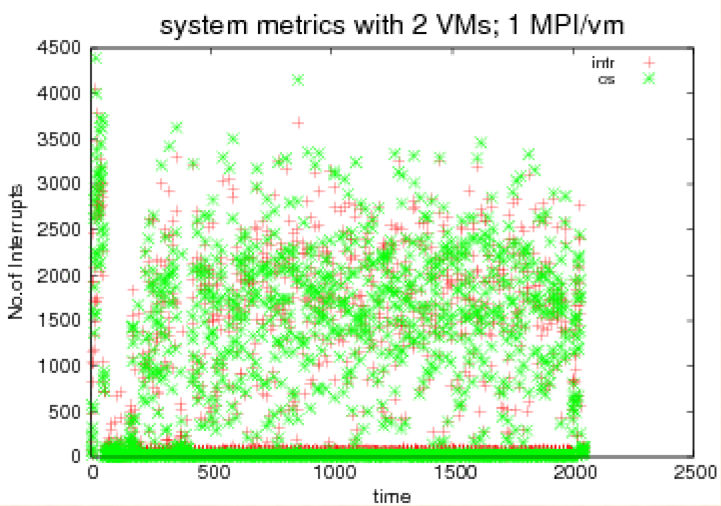
Configuration 2

VM 1





VM 2



Conclusion

- 8 VMs with 2 processes each is slightly more efficient than 16 VMs with 1 process each
- Overall performance difference is only 2.4%
- This study sheds light on how VM configurations impact an HPC application
- The investigation shows how Xen in configuration 1 and Linux in configuration 2 manage resources differently

Future Work

- Compare more VM configurations with and without hardware virtualization support
- Use tools such as Xenoprof along with VMstat and XenTop
- Study more, different HPC applications
- Study and quantify the effects of flexibility offered by various VM configurations

Questions?