Vipul Harsh, Laxmikant Kale





#### Parallel sorting in the age of Exascale



- Charm N-body GrAvity solver
- Massive Cosmological N-body simulations
- Parallel sorting in every iteration





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- Charm N-body GrAvity solver
- Massive Cosmological N-body simulations
- Parallel sorting in every iteration

- Cosmology code based on Chombo
- Global sorting every step for load balance/locality







## Parallel sorting: Goals

- Load balance across processors
- Optimal data movement
- Generality: robustness to input distributions, duplicates
- Scalability and performance





## Parallel sorting: A basic template

- *p* processors, N/*p* keys in each processor
- Determine (p-1) splitter keys to partition keys into p buckets
- Send all keys to appropriate destination bucket processor
- Eg. Sample sort, Histogram sort





#### Existing algorithms: Parallel Sample sort

- Samples s keys from each processor
- Picks (*p*-1) splitters from *p x s* samples

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Problem: Too many samples required for good load balance

64 bit keys, p = 100,000 & 5% max load imbalance, sample size  $\approx 8 \text{ GB}$ 





#### Existing algorithms: Histogram sort A COMPARISON BASED PARALLEL SORTING ALGORITHM\*

- Pick s x p candidate keys
- Compute rank of each candidate key (histogram)
- Select splitters from the candidates





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- Pick s x p candidate keys
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- Select splitters from the candidates OR
- Refine the candidates and repeat
- Works quite well for large p
- But can take more iterations if input skewed





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- An adaptation of Histogram sort
- Sample before each histogramming round
  - Sample intelligently
  - Use results from previous rounds
  - Discard wasteful samples at source





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- HSS has sound theoretical guarantees
- Independent of input distribution
- Justifies why Histogram sort does well

































$\operatorname{Algorithm}$	Overall sample size	Overall sample size for $p = 10^5, \epsilon = 5\%$
Sample sort with regular sampling	$\mathcal{O}(rac{p^2}{\epsilon})$	$1600~\mathrm{GB}$
Sample sort with random sampling	$\mathcal{O}(rac{p\log N}{\epsilon^2})$	8.1 GB
HSS with one round	$\mathcal{O}(rac{p\log p}{\epsilon})$	184 MB
HSS with two rounds	$\mathcal{O}(p\sqrt{rac{\log p}{\epsilon}})$	24 MB
$\mathop{\mathrm{HSS}}\limits_{\mathrm{rounds}}$ with $k$	$\mathcal{O}(kp\sqrt[k]{rac{\log p}{\epsilon}})$	-
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64 bit keys, 5% load imbalance





## Number of histogram rounds

p (x 1000)	sample size/round (x p)	Number of rounds	Number of rounds (Theoretical)
4	5	4	8
8	5	4	8
16	5	4	8
32	5	4	8

Number of rounds hardly increases with  $p \rightarrow \log(\log p)$  complexity





## Optimizing for shared memory

- Modern machines are highly multicore
  - BG/Q: 64 hardware threads/node
  - Stampede KNL(2.0): 272 hardware threads/node
- How to take advantage of within-node parallelism?





## Final All-to-all data exchange

- In the final step, each processor sends a data message to every other processor
- $O(p^2)$  fine grained messages in the network





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- In the final step, each processor sends a data message to every other processor
- $O(p^2)$  fine grained messages in the network
- What if all messages having the same source, destination node are combined into one?
- Messages in the network:  $O(n^2)$ 
  - Two orders of magnitude less!





## What about splitting?...

- We really need splitting across nodes rather than individual processors
- (n-1) splitters needed instead of (p-1)
  - An order of magnitude less
  - Reduces sample size even more
- Add a final within node sorting step to the algorithm





#### Execution time breakdown



Very little time is spent on histogramming!

Weak Scaling experiments on BG/Q Mira with 1 million 8 byte keys and 4 byte payload per key on each processor, with 4 ranks/node





## Conclusion

- HSS combines sampling and histogramming to accomplish fast splitter determination
- HSS provides sound theoretical guarantees
- Most of the running time spent in local sorting & data exchange (unavoidable)





#### Future work

• Integration in HPC applications (e.g. ChaNGa)





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### Acknowledgements

- Edgar Solomnik
- Omkar Thakoor
- ALCF





# **Thank You!**





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# **Backup slides**





#### HSS: Computation/Communication complexity

Algorithm	Overall sample size	Overall sample size for $p = 10^5, \epsilon = 5\%$	Computation complexity	Communication complexity
Sample sort with regular sampling	$\mathcal{O}(rac{p^2}{\epsilon})$	1600 GB	$\mathcal{O}\left(\frac{N}{p}\log\frac{N}{p} + \frac{p^2}{\epsilon}\log p + \frac{N}{p}\log p\right)$	$\mathcal{O}\left(rac{p^2}{\epsilon} + p + rac{N}{p} ight)$
Sample sort with random sampling	$\mathcal{O}(rac{p\log N}{\epsilon^2})$	8.1 GB	$\mathcal{O}\left(\frac{N}{p}\log\frac{N}{p} + \frac{p\log N\log p}{\epsilon^2} + \frac{N}{p}\log p\right)$	$\mathcal{O}\left(rac{p\log N}{\epsilon^2} + p + rac{N}{p} ight)$
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HSS with two rounds	$\mathcal{O}(p\sqrt{rac{\log p}{\epsilon}})$	24 MB	$\mathcal{O}\left(\frac{N}{p}\log\frac{N}{p} + p\sqrt{\frac{\log p}{\epsilon}}\log N + \frac{N}{p}\log p\right)$	$\mathcal{O}\Big(p\sqrt{rac{\log p}{\epsilon}}+p+rac{N}{p}\Big)$
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HSS with $\mathcal{O}(\log \frac{\log p}{\epsilon})$ rounds	$\mathcal{O}(p\log rac{\log p}{\epsilon})$	10 MB	$\mathcal{O}\left(\frac{N}{p}\log\frac{N}{p} + p\log\frac{\log p}{\epsilon}\log N + \frac{N}{p}\log p\right)$	$\mathcal{O}\left(p\log rac{\log p}{\epsilon} + p + rac{N}{p} ight)$ (*



