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Matrix Element Calculations on the GPU

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Based on arxiv:2106.06507

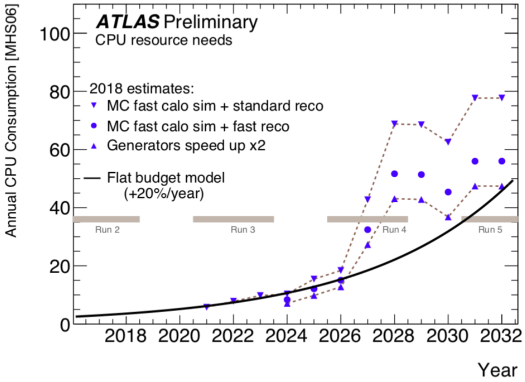
ML4Jets 2021

7 July 2021

FERMILAB-SLIDES-21-055-T

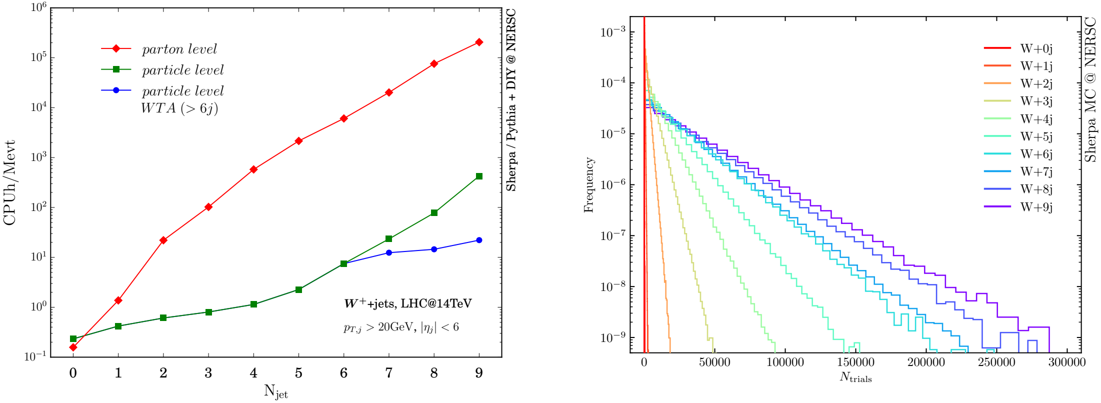
Motivation

- LHC requires large number of Monte Carlo events
- Due to CPU costs, MC statistics will become significant uncertainty



[ATLAS]

Motivation



[S. Höche, S. Prestel, H. Schulz, 1905.05120]

- Time to generate an event dominated by hard process not shower
- Large computational cost for unweighting at high multiplicity

ML Works to Reduce Cost

Phase Space Generation from Samples

- Requires a large sample before training
- GAN and VAE based [1707.0028, 1901.00875, 1901.05282, 1903.02433, 1907.03764, 1909.01359, 1909.04451, 1912.08824, 2008.06545, 2008.08558, etc.]

Phase Space Generation from Random Numbers

- Generates events as needed
- Normalizing flow based [2001.05478, 2001.05486, 2001.10028, 2104.04543]
- See talk from Timo Janßen from yesterday for more details

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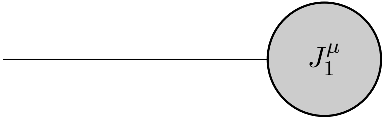
Both approaches will benefit from improved event generation time

Recursive Matrix Element Generation

Brends-Giele Recursion

- Reuse parts of calculation
- Most efficient for high multiplicity
- Reduces amplitude computations from $\mathcal{O}\left(n!\right)$ to $\mathcal{O}\left(3^n\right)$ for color-dressed and $\mathcal{O}\left(n^3\right)$ for color-ordered.
- $A(1,\ldots,n) = J_\mu(n)p_{1,n}^2 J^\mu(1,\ldots,n-1)$



[Nucl. Phys. B306(1988), 759]

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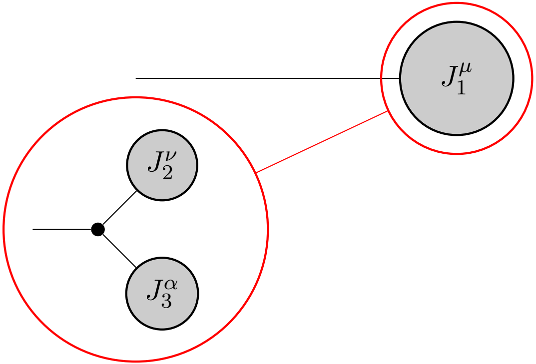

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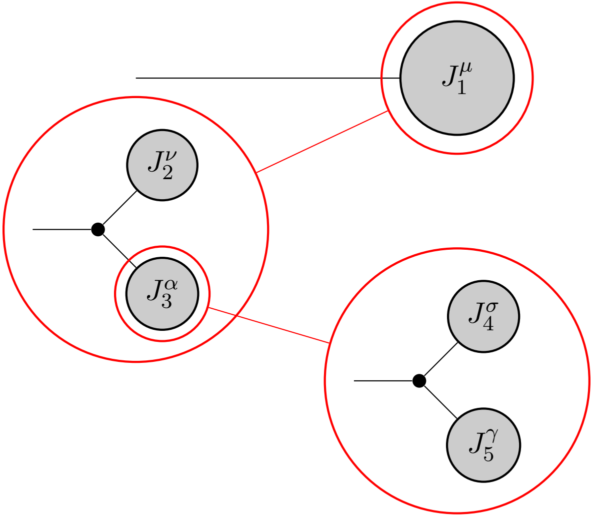

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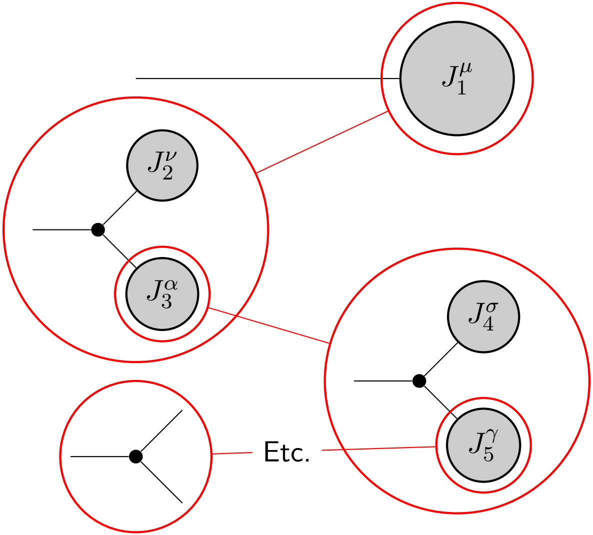
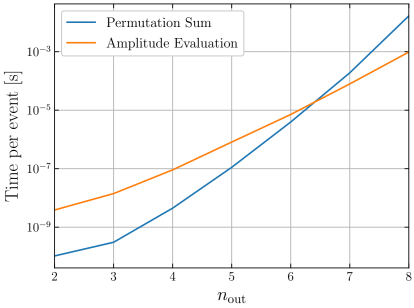


Color-Ordered vs. Color-Dressed



Scaling for Color-Ordered calculations

Color-Ordered (CO):

- Requires $(n-2)!^2$ color coefficients given by: $C_{\vec{\sigma}\vec{\sigma}'} = \sum_{a_1 \ldots a_n} (F^{a_{\sigma_2}} \ldots F^{a_{\sigma_{n-1}}})_{a_1 a_n} (F^{a_{\sigma'_2}} \ldots F^{a_{\sigma'_{n-1}}})^*_{a_1 a_n}$
- Need to sum over all permutations to obtain full amplitude

Color-Dressed (CD):

- Color summed at each vertex. No need to sum over permutations
- Can sample color to Monte-Carlo the color sum
- Need to store color information of the gluons at each vertex

Why a GPU Implementation?

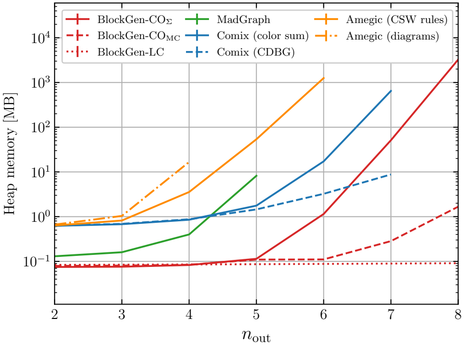
Next-Gen Supercomputer Aurora:

[https://alcf.anl.gov/aurora]

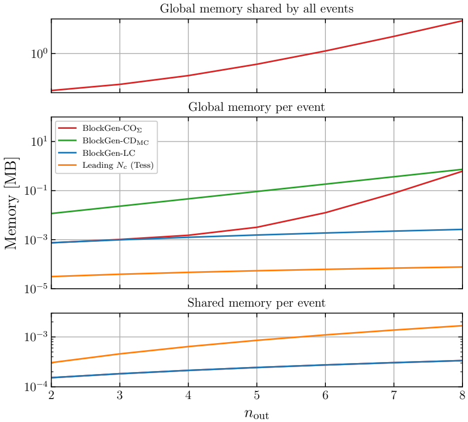
- Event generation is trivially parallelizable
- Aurora Compute Nodes:
  - 2 Intel Xeon processors
  - 6 Xeon arch-based GPUs
  - Unified Memory
- Take advantage of modern supercomputer setups
- ML is already on GPUs, only missing piece is event generation

Memory Requirements

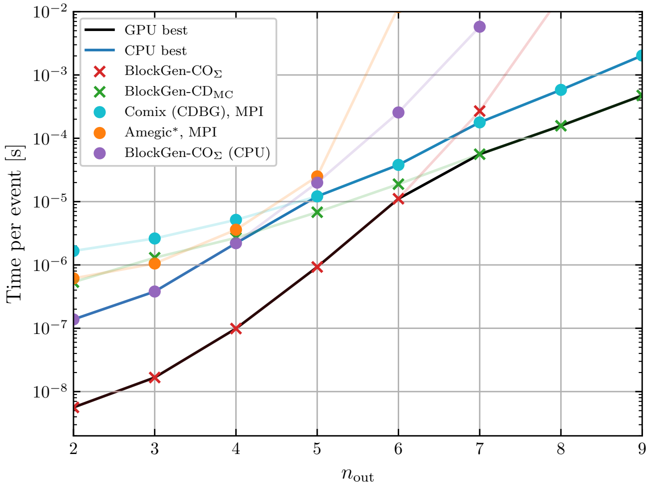
CPU Memory



GPU Memory

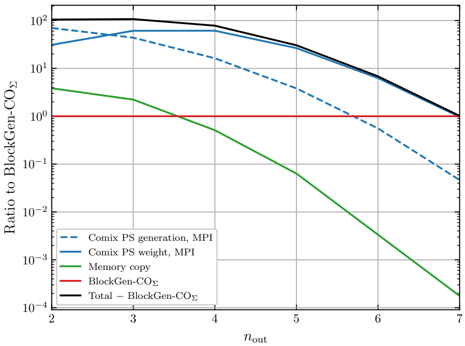


Timings



- CPU:
  Intel® Xeon®
  E5-2650 v2 8-core
  (2.60 GHz, 20 MB cache).
- GPU: NVIDIA V100
- CPUs are run with MPI with 16 threads to supply realistic chip-to-chip comparison

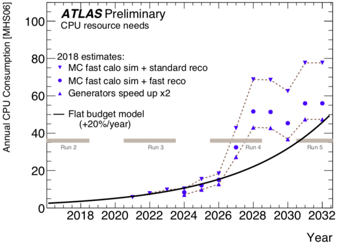
Future Steps



- Implement quarks and massive vector Bosons
- Develop hybrid calculation approach
- GPU Phase Space generator
  - Generate PS with cuts on CPU
  - Calculate PS weight and ME on GPU
  - Need to ensure memory transfer is not the bottleneck

Conclusions

Cost of Event Generation:



- Matrix elements most expensive

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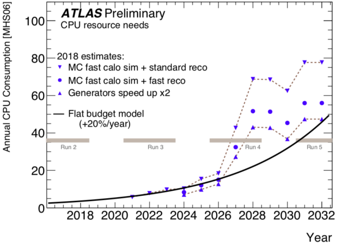

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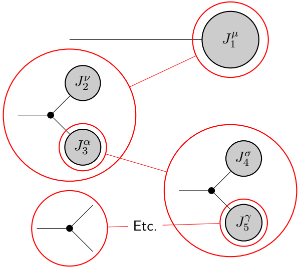
Brends-Giele:

- Optimal generation
- Event generation trivially parallelizable



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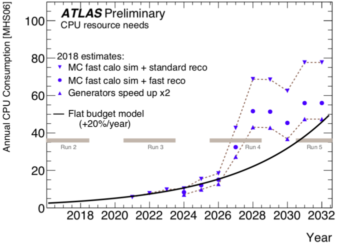

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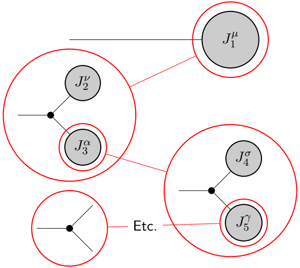
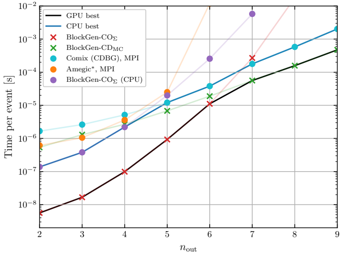


Results:



- Speedup of approximately a factor of 10
- BlockGen-CO$_\Sigma$ is best for $n_{out} < 7$