Improving GPU performance for GooFit

Software engineering studies

Brad Hittle

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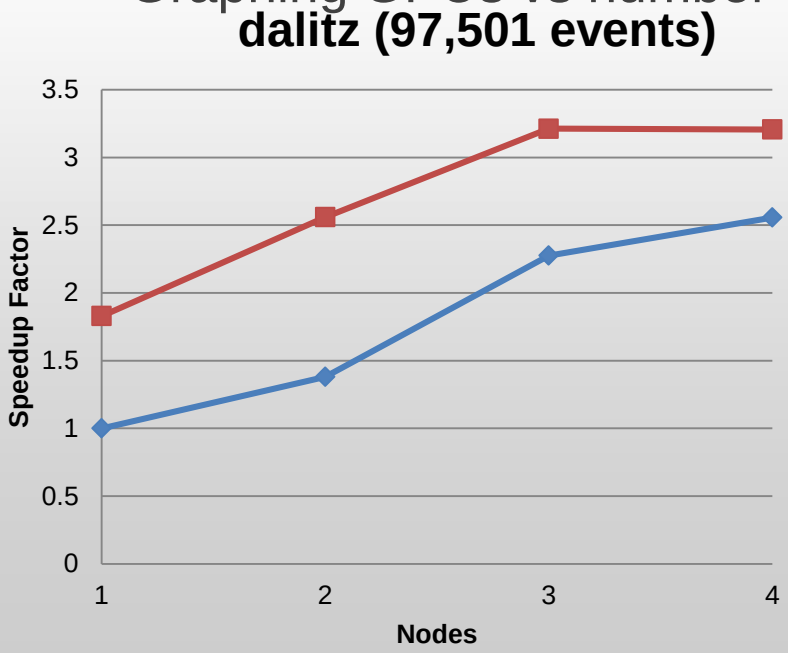
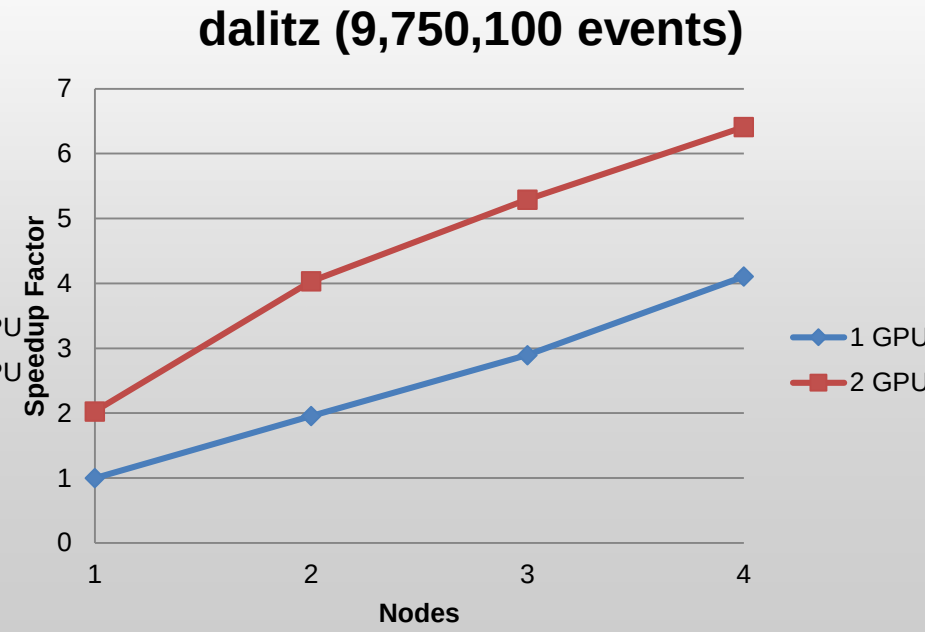
GooFit library

- Probability Density Function (PDF) fitting library
- GPUs for better performance
- Modifications to library for performance
  - Multiple GPU Improvements
  - Memory improvements
  - New PDFs in C++

Optimizations (Multi-GPU performance)

- Add Multiple GPUs using MPI [**GooFit 2.0+**]
- Each GPU gets portion of data
- Graphing GPUs vs number of workstations (**nodes**)

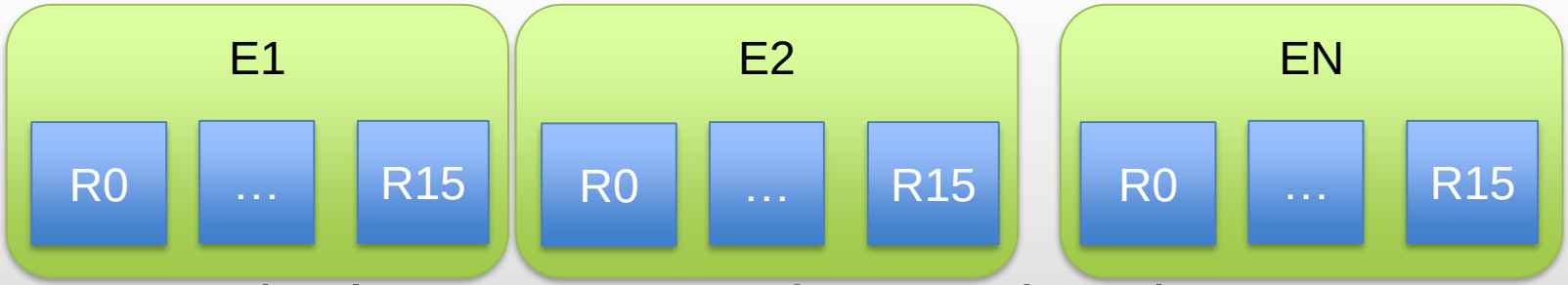




Intel Xeon x5650 (Westmere), 2x NVIDIA Tesla M2070 GPUs

Memory Cache Layout

- New memory layout for cached values, **[GooFit 2.0+]**
- Old method used a single array (**AoS**)



- New method uses 16 sets of arrays (**SoA**)

Over 25% improvement for *dalitz 9,750,100 events* over GooFit 1.0!

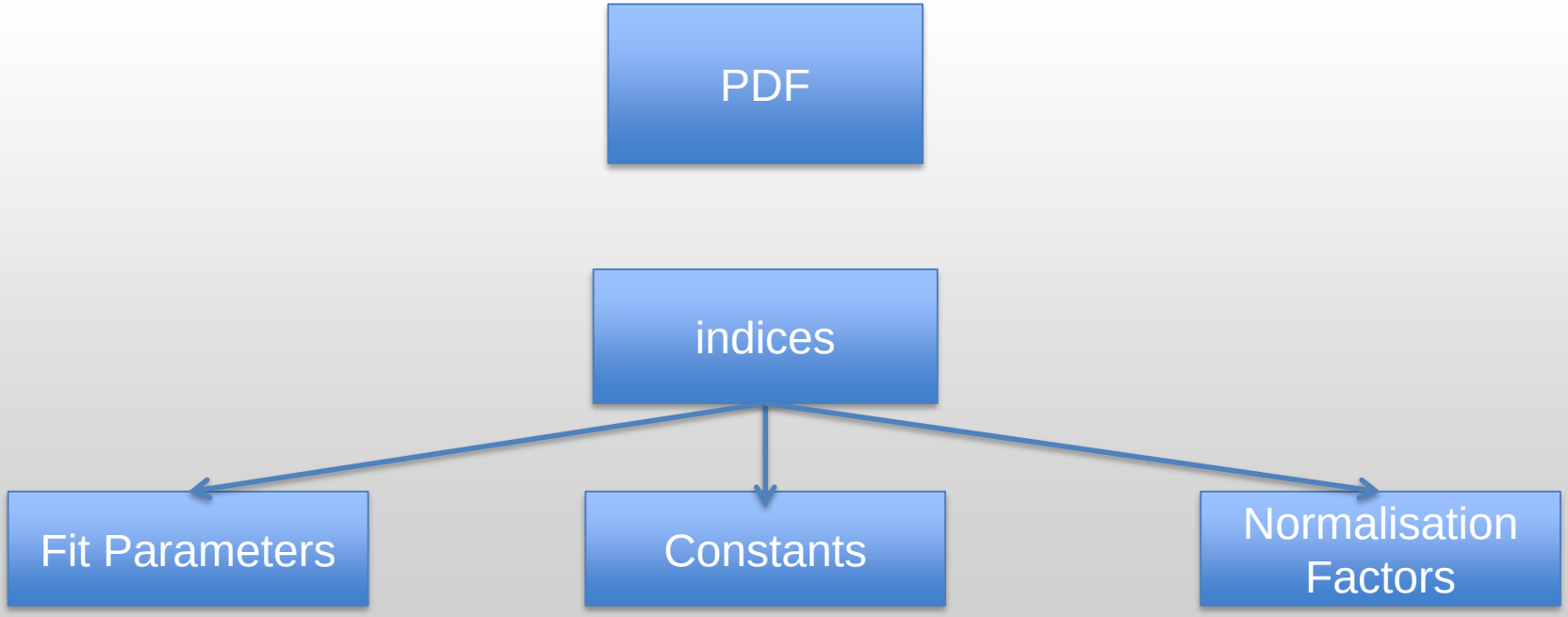
Memory Through Hardware Cache

- All GPU's have read-only cache for gaming
- Uses read-only cache instruction (ROC) [**GooFit 2.0+**]
  - Instruction requires new hardware (Kepler+)
- ROC used for parameters, constants, observable indices, normalisation factors. Unable to use on Observables.

dalitz	97,501 events	9,750,100 events
No ROC	2.27	161.7
ROC	2.09	137.1

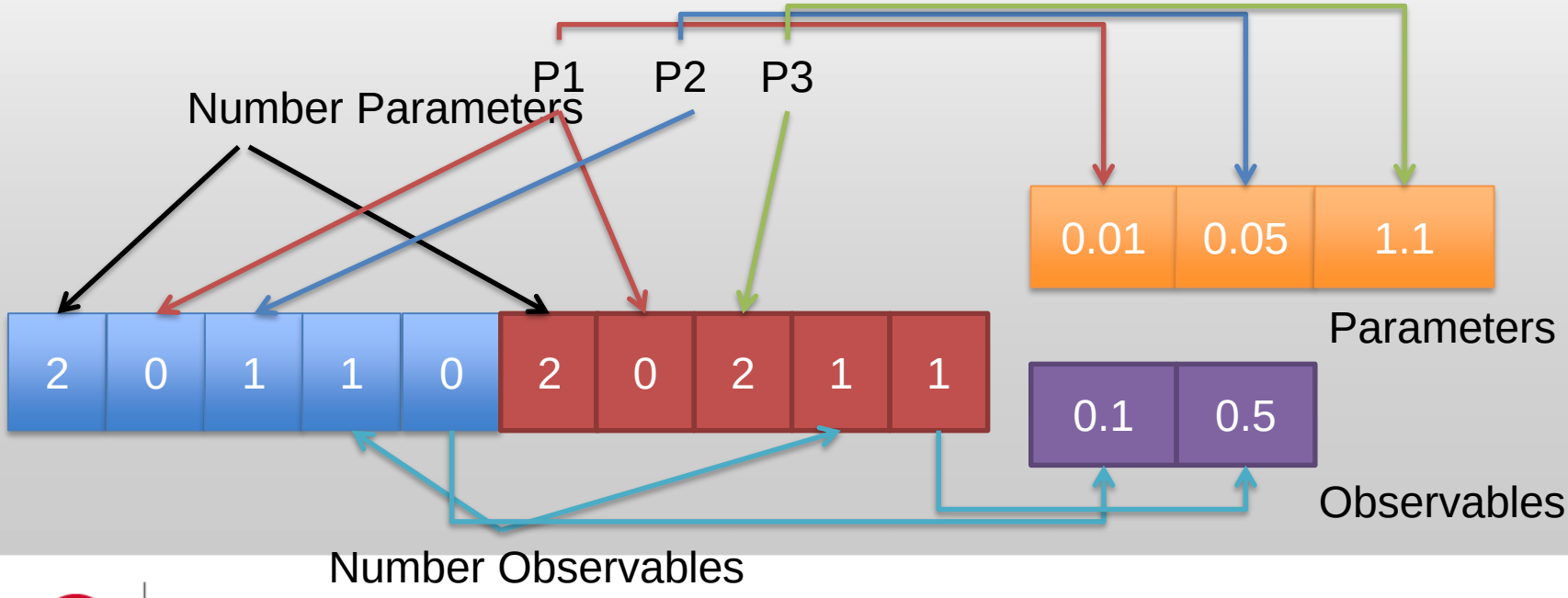
GooFit Indexing [1]

- Indexing scheme up to **GooFit 2.1**



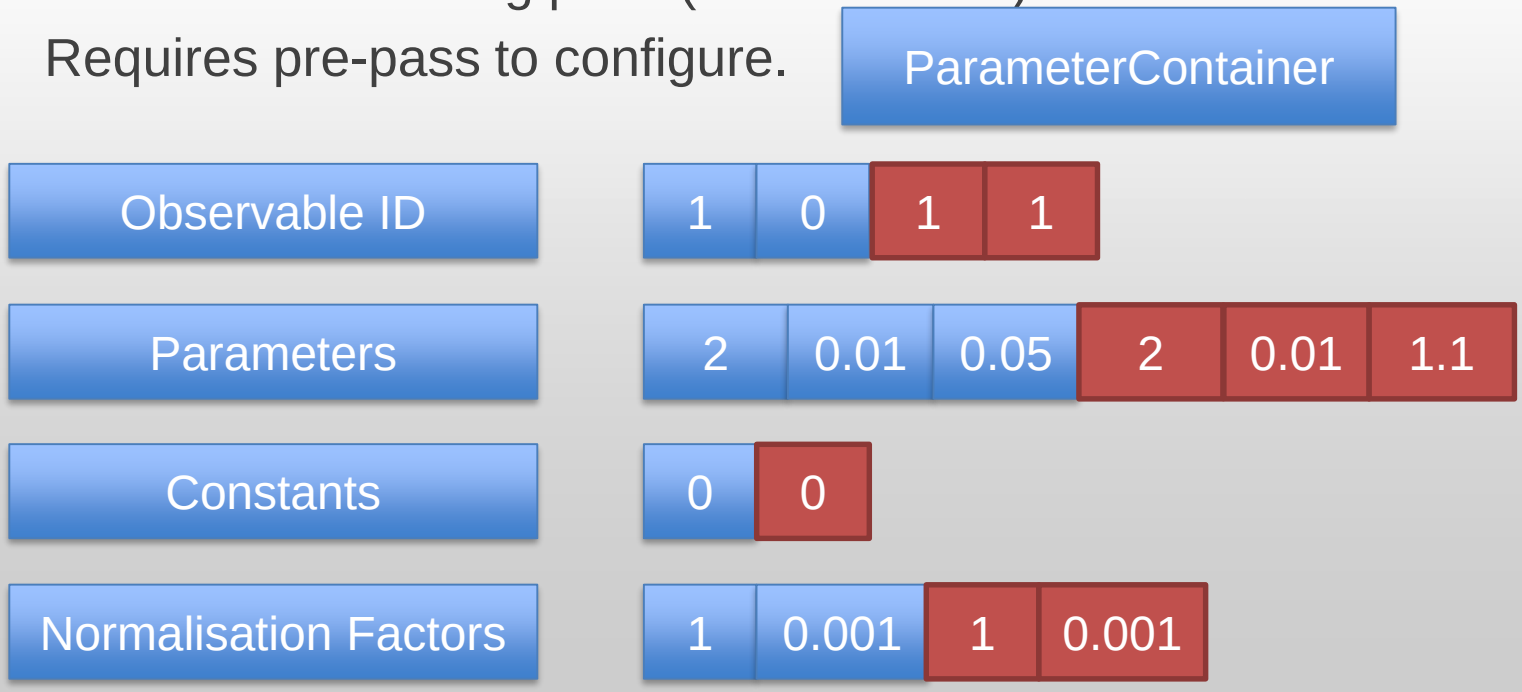
GooFit Indexing [2]

- 2 memory lookups
- Multiple PDFs cause random memory accesses
- Internal representation of two Gaussian PDFs



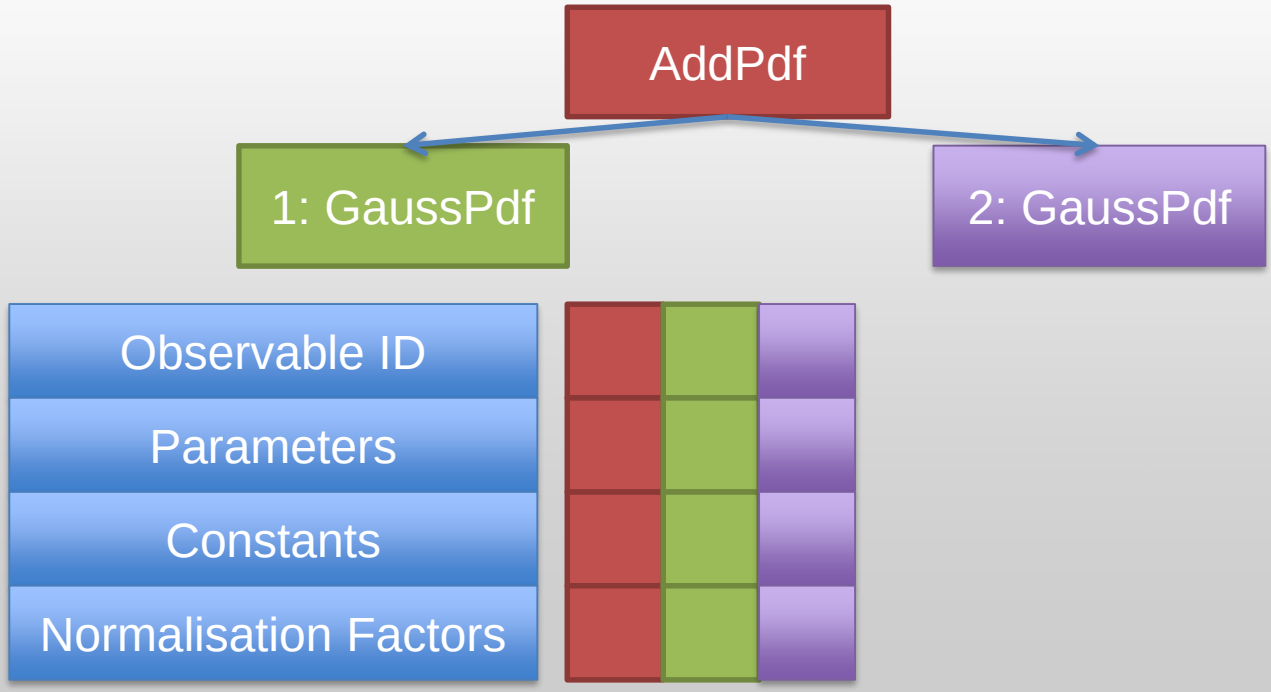
GooFit Indexing [3]

- **GooFit 2.2** scheme
- 4 separate arrays
- All constants floating point (cast constant)
- Requires pre-pass to configure.



GooFit Indexing [4]

- Arrays are populated in order.



GooFit Indexing [5]

- Reduce random memory accesses
- Reduce amount of memory accesses
- Simplified PDF model
  - Easier development and debugging of PDFs.

GooFit Indexing [5]

- Performance between OMP/GPU versions
- Suspect cache related, requires further profiling OMP version

OMP=28	v2.0 (s)	v2.2 (s)
pipipi0DPFit toy 0 10	240.92	276.26
pipipi0DPFit toy 0 50	1092.2	1247.3
dalitz 9,750,100	151.9	230.54

-65%

GPU=Tesla P100	v2.0 (s)	v2.2 (s)
pipipi0DPFit toy 0 10	57.099	48.248
pipipi0DPFit toy 0 50	265.34	210.19
dalitz 9,750,100	112.86	85.132

+32%

Intel Xeon E5-2680 v4 (Broadwell), 1x NVIDIA Tesla P100

New PDF creation C++ [1]

- New PDF creation [**GooFit 2.2**], easier development and debugging
- Constructor
- recursiveSetIndices
- ‘Device’ function

New PDF creation C++ [2]

- 3 internal structures per PDF
  - Parameters
  - Observables
  - Constants
- registerParameter, registerConstant, registerObservable
- Once complete, `initialize();` from constructor

New PDF creation C++ [3]

```
GaussianPdf::GaussianPdf(std::string n,
        Observable _x,
        Variable mean,
        Variable sigma) : GooPdf(n, _x)
{
  int idx1 = registerParameter(mean);
  int idx2 = registerParameter(sigma);

  initialize();
}
```

New PDF creation C++ [4]

- Copy local information to global
- Copy current PDF, recursively call components
- Copy global structures to GPU

```
__host__ void GaussianPdf::recursiveSetIndices() {
 GET_FUNCTION_ADDR(ptr_to_Gaussian);
 host_function_table[num_device_functions]=host_fcn_ptr;
 functionIdx = num_device_functions++;
 populateArrays();
}
```

New PDF creation C++ [5]

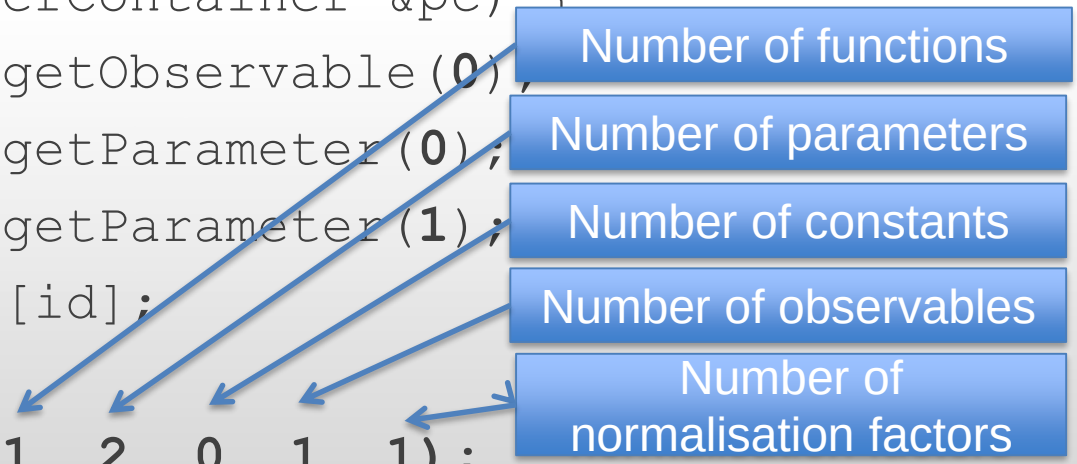
- ParameterContainer
  - Access values per PDF
  - Hide implementation details
- Two increment methods
  - **incrementIndex(# functions, # parameters, # constants, # observables, # normalisations);**
  - incrementIndex ();
- Constructor index == device index

New PDF creation C++ [6]

```
fptype device_Gaussian(fptype *evt,
                       ParameterContainer &pc) {
    int id       = pc.getObservable(0);
    fptype mean  = pc.getParameter(0);
    fptype sigma = pc.getParameter(1);
    fptype x     = evt[id];

    pc.incrementIndex(1, 2, 0, 1, 1);

    return exp(-0.5 * (x - mean) * (x - mean) /
               (sigma * sigma));
}
```



Future improvements

- [**GooFit 2.3+**]
- SoA-style observable data access
- Reducing register count per GPU kernel

Conclusions

- Multi-GPU support [**GooFit 2.0+**]
  - Large events, 1 GPU 4 workstations [**4x speedup**]
- Memory optimizations
  - Changed **AoS** to **SoA** memory layout [**25% improvement, GooFit 2.0+**]
  - Utilized read only cache [**20% improvement, GooFit 2.0+**]
  - New indexing [**32% improvement, GooFit 2.2+**]
- Simplified PDF creation [**GooFit 2.2+**]
  - GPU improvement, readability & debugging
  - Degraded performance for OMP

Memory layout matters

Questions, Feedback?

Brad Hittle

bhittle@osc.edu

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Optimizations (Improved if/else condition)

- Current code:

```
EXEC_TARGET bool inDalitz (fptype m12, fptype m13, fptype bigM, fptype dm1,
fptype dm2, fptype dm3) {
  if (m12 < POW(dm1 + dm2, 2)) return false;
  if (m12 > POW(bigM - dm3, 2)) return false;
  // Calculate energies of 1 and 3 particles in m12 rest frame.
  fptype e1star = 0.5 * (m12 - dm2*dm2 + dm1*dm1) / SQRT(m12);
  fptype e3star = 0.5 * (bigM*bigM - m12 - dm3*dm3) / SQRT(m12);
  // Bounds for m13 at this value of m12.
  fptype minimum = POW(e1star + e3star, 2) - POW(SQRT(e1star*e1star -
dm1*dm1) + SQRT(e3star*e3star - dm3*dm3), 2);
  if (m13 < minimum) return false;
  fptype maximum = POW(e1star + e3star, 2) - POW(SQRT(e1star*e1star -
dm1*dm1) - SQRT(e3star*e3star - dm3*dm3), 2);
  if (m13 > maximum) return false;

  return true;
}
```

Optimizations (Improved if/else condition) [2]

- [**GooFit 2.0+**]
- GPU's have no branch-prediction.
- Referred to as *Divergent threads* when some take the 'if' path and others take the 'else' path
- Each warp executes the 'if' portion of the if/else with some threads stalling, then the 'else' portion executes similarly if needed.
- Wasted cycles waiting for if/else portions to complete per warp if there are divergent threads.
- Depending on situation, computing both sides is more efficient than handling if/else
- Improved by 21%

Optimizations (Improved if/else condition) [3]

```
EXEC_TARGET bool inDalitz (fptype m12, fptype m13, fptype bigM, fptype dm1, fptype dm2, fptype dm3) {
  bool dm1_dm2 = (m12 < POW(dm1 + dm2, 2)) ? true : false;
  bool bigM_dm3 = (m12 > POW(bigM - dm3, 2)) ? true : false;
  // Calculate energies of 1 and 3 particles in m12 rest frame.
  fptype e1star = 0.5 * (m12 - dm2*dm2 + dm1*dm1) / SQRT(m12);
  fptype e3star = 0.5 * (bigM*bigM - m12 - dm3*dm3) / SQRT(m12);
  // Bounds for m13 at this value of m12.
  fptype minimum = POW(e1star + e3star, 2) - POW(SQRT(e1star*e1star - dm1*dm1) + SQRT(e3star*e3star - dm3*dm3), 2);
  bool m13_minimum = (m13 < minimum) ? true : false;
  fptype maximum = POW(e1star + e3star, 2) - POW(SQRT(e1star*e1star - dm1*dm1) - SQRT(e3star*e3star - dm3*dm3), 2);
  bool m13_maximum = (m13 > maximum) ? true : false;

  return dm1_dm2 && bigM_dm3 && m13_minimum && m13_maximum;
```

GPU Grid size [1]

- [**GooFit 2.0+**]
- (**Group size**, **Group size**)
  - Determines GPU threads/block distribution
  - Thrust has fixed distribution
- Override for runtime performance; unique per PDF

dalitz	97, 501 events	9,750,100 events
ruby (128, 7)	2.09892	137.133
ruby (544, 7)	1.66221	110.333