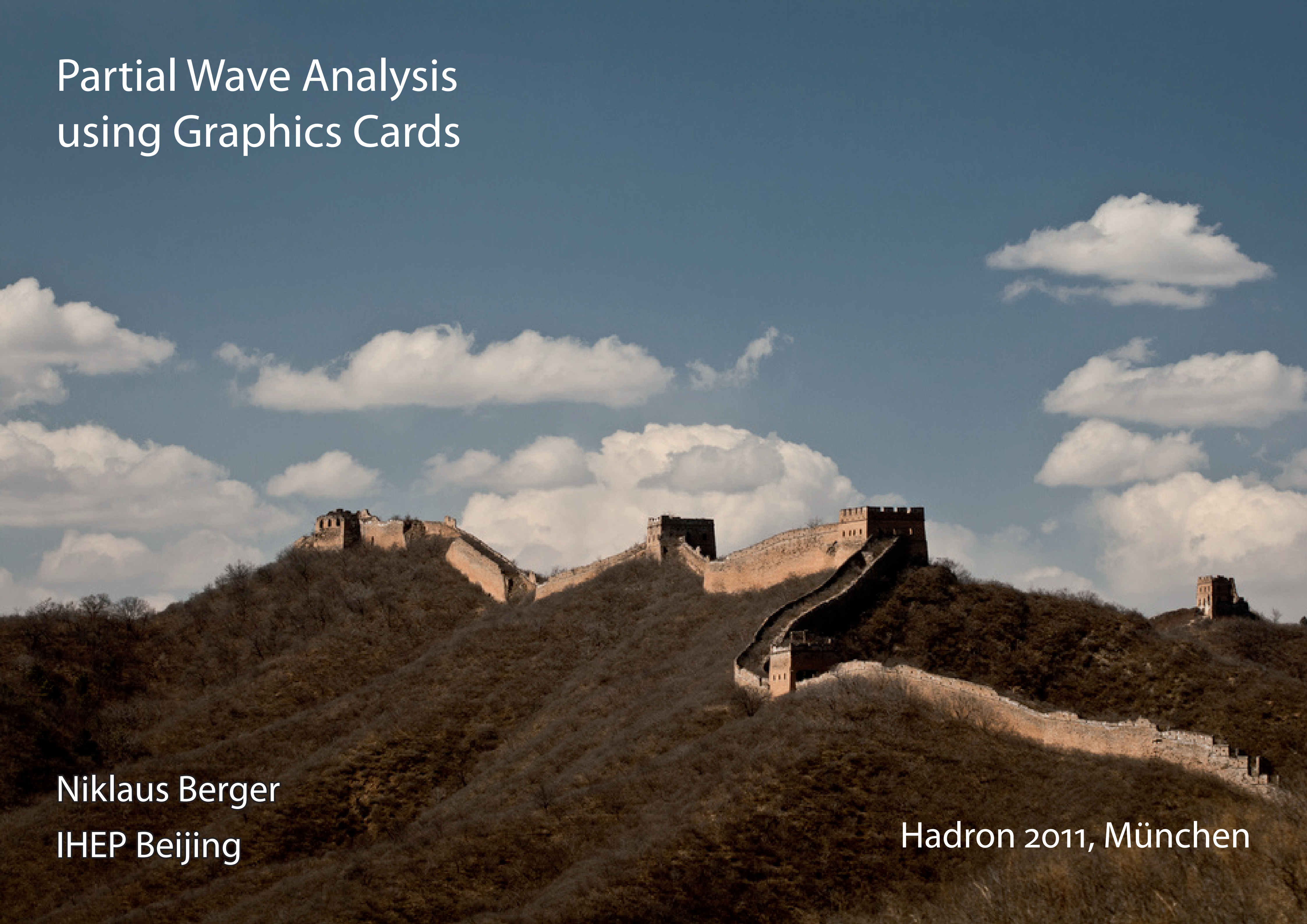


Partial Wave Analysis using Graphics Cards

Niklaus Berger

IHEP Beijing

Hadron 2011, München

The (computational) problem with partial wave analysis

$$\log \mathscr{L} \propto \sum_{i=1}^{n} \log\left(\sum_{\alpha,\alpha'} V_\alpha V^*_{\alpha'} A_\alpha(\Omega_i) A^*_{\alpha'}(\Omega_i)\right) - \sum_{\alpha,\alpha'} \log\left(V_\alpha V^*_{\alpha'} \left(\frac{1}{N^{gen}_{MC}} \sum_{i=1}^{N^{rec}_{MC}} A_\alpha(\Omega_i) A^*_{\alpha'}(\Omega_i)\right)\right)$$

A complex calculation
(repeated many times over)

+

lots of statistics at Babar, Belle, BES III, Compass, GlueX, Panda etc.

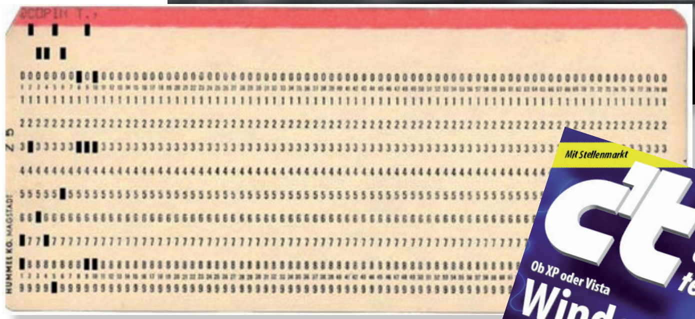
=

something potentially very slow

Four years ago...

- I moved to IHEP Beijing
- All I remembered about partial waves was an unpleasant theory exam
- People at IHEP were worried about a × 100 increase in statistics
- I did not know about partial waves, but new how to do things fast
- I happened to have just read a magazine article about computing on graphics processors

Photo: Andreas Rodler



Partial Wave Analysis as a Computational Problem

Splits into subtasks:

- Building a model
- Determining model parameters through a fit to the data
- Judge fit results

Iterate until satisfied

Tightly coupled with the physicist:
look at plots, adjust model and input parameters

From Model to Likelihood

Decay amplitudes:
Resonance and angular structure

Intensity (number of events)
at a phase-space point Ω

$$I(\Omega) = \left|\sum_\alpha V_\alpha A_\alpha(\Omega)\right|^2$$

Sum over partial waves

Production amplitudes:
Complex fit parameters

From Model to Likelihood

Decay amplitudes:
Resonance and angular structure

Intensity (number of events) at a phase-space point Ω

$$I(\Omega) = \left|\sum_\alpha V_\alpha A_\alpha(\Omega)\right|^2$$

Sum over partial waves

Production amplitudes:
Complex fit parameters

Likelihood,
given n data points at Ω_i

$$\mathscr{L} \propto \prod_{i=1}^{n} \frac{I(\Omega_i)}{\int \eta(\Omega) I(\Omega) d\Omega}$$

Normalisation integral over phase space

Product over data events

Detection efficiency

From Model to Likelihood

Likelihood, given n data points at Ω_i

$$\mathscr{L} \propto \prod_{i=1}^{n} \frac{I(\Omega_i)}{\int \eta(\Omega) I(\Omega) d\Omega}$$

Normalisation integral over phase space

Product over data events

Detection efficiency

Log likelihood

$$\log \mathscr{L} \propto \sum_{i=1}^{n} \log\left(\sum_{\alpha,\alpha'} V_\alpha V^*_{\alpha'} A_\alpha(\Omega_i) A^*_{\alpha'}(\Omega_i)\right) - \sum_{\alpha,\alpha'} \left(V_\alpha V^*_{\alpha'} \left(\frac{1}{N^{gen}_{MC}} \sum_{i=1}^{N^{rec}_{MC}} A_\alpha(\Omega_i) A^*_{\alpha'}(\Omega_i)\right)\right)$$

Sum over data events

Sum over partial waves

From Model to Likelihood: Fixed Amplitudes

Likelihood,
given n data points at Ω_i

$$\mathscr{L} \propto \prod_{i=1}^{n} \frac{I(\Omega_i)}{\int \eta(\Omega) I(\Omega) d\Omega}$$

Normalisation integral over phase space

Product over data events

Detection efficiency

Log likelihood

Independent of fit parameters: precalculate; memory $\mathcal{O}(N_{event} \times N^2_{wave})$

Independent of fit parameters: precalculate

$$\log \mathscr{L} \propto \sum_{i=1}^{n} \log\Big(\sum_{\alpha,\alpha'} V_\alpha V^*_{\alpha'} \overbrace{A_\alpha(\Omega_i) A^*_{\alpha'}(\Omega_i)}\Big) - \sum_{\alpha,\alpha'} \Big(V_\alpha V^*_{\alpha'} \overbrace{\Big(\frac{1}{N^{gen}_{MC}} \sum_{i=1}^{N^{rec}_{MC}} A_\alpha(\Omega_i) A^*_{\alpha'}(\Omega_i)\Big)}\Big)$$

Sum over data events

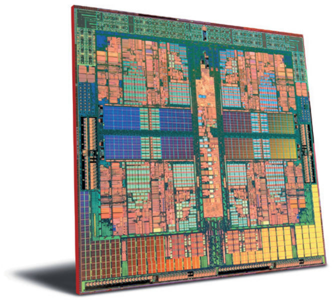
Sum over partial waves

Computationally intensive: $\mathcal{O}(N_{iteration} \times N_{event} \times N^2_{wave})$

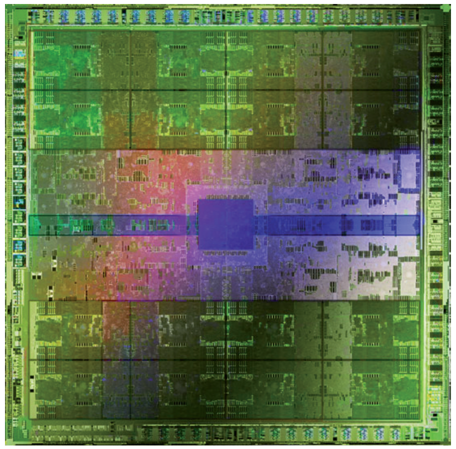
Normalisation integral as a sum over MC events
Summing only reconstructed events takes into account detection efficiency

Going parallel!

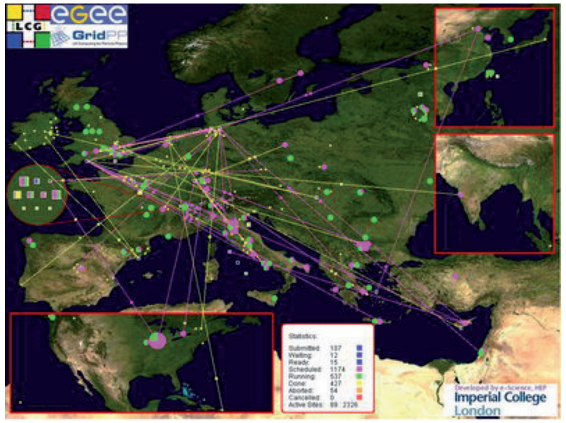
- Almost all our hardware is now parallel
- Almost all our software is not



- Almost all our problems are trivially parallel (events!)
- The solution to speed problems is obvious...



How to do parallel?

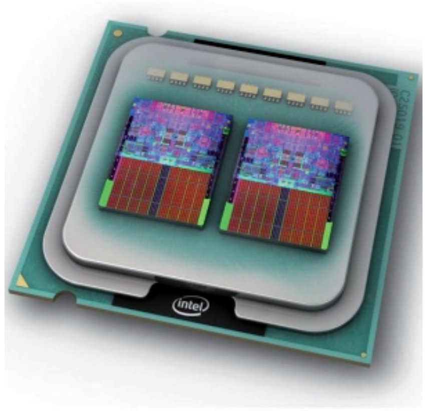


Grid

- Almost infinite power
- Very limited inter-process communication
- Very long latency

Farm/Cluster

- Lots of power
- Some inter-process communication
- Long latency (Network & Scheduling)



Multi-core CPU

- Finite power
- Very fast inter-process communication
- Almost no latency

Graphics Processor

- Almost infinite floating-point power
- Fast communication with CPU
- Short latency

Parallel PWA

PWA is embarassingly parallel:

- Exactly the same (relatively simple) calculation for each event
- Every event has its own data, only fit parameters are shared
- Use parallel hardware and make use of Single Instruction - Multiple Data (SIMD) capabilities
- Very strong here: Graphics processors (GPUs): Cheap and powerful hardware

Accessing the Power of GPUs

Programming for the GPU is less straightforward than for the CPU

- Early days: Use graphics interface (OpenGL) - translate problem to drawing a picture
- Vendor low-level frameworks: Nvidida CUDA and ATI CAL
- Vendor higher level framework: Brook+
- Independent commercial software: RapidMind
- Emerging standard: OpenCL

ATI Brook+

We started with using ATI Brook+

- Was the first to provide double precision
- Hardware with best performance/ price
- Very clean programming model, narrow interface

Had all of the early adopter problems

- Lots of bugs and limitations
- Small user base
- Mediocre support
- Uncertain future

Now discontinued by AMD/ATI,
we switched to OpenCL

OpenCL

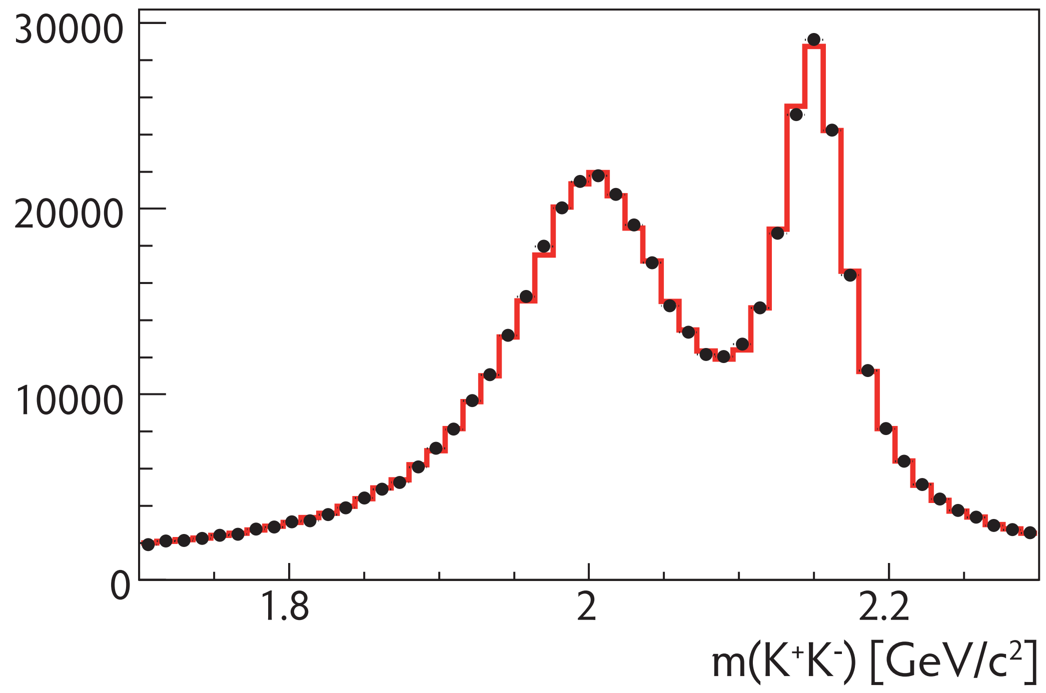
OpenCL is a vendor- and hardware independent standard for parallel computing (in principle...)

- Gives you lots of detailed control and optimization options...
- ... at the cost of a very low level, hardware driver like interface
- No type safety, optimization depends on machine type
- For embarrassingly parallel tasks: use some higher level abstraction

GPUPWA at BES III

GPUPWA is our running framework

- Just done transition to OpenCL
- GPU based tensor manipulation
- Management of partial waves
- GPU based normalisation integrals
- GPU based likelihoods
- GPU based analytic gradients
- Interface to ROOT::Minuit2 fitters
- Projections and plots using ROOT

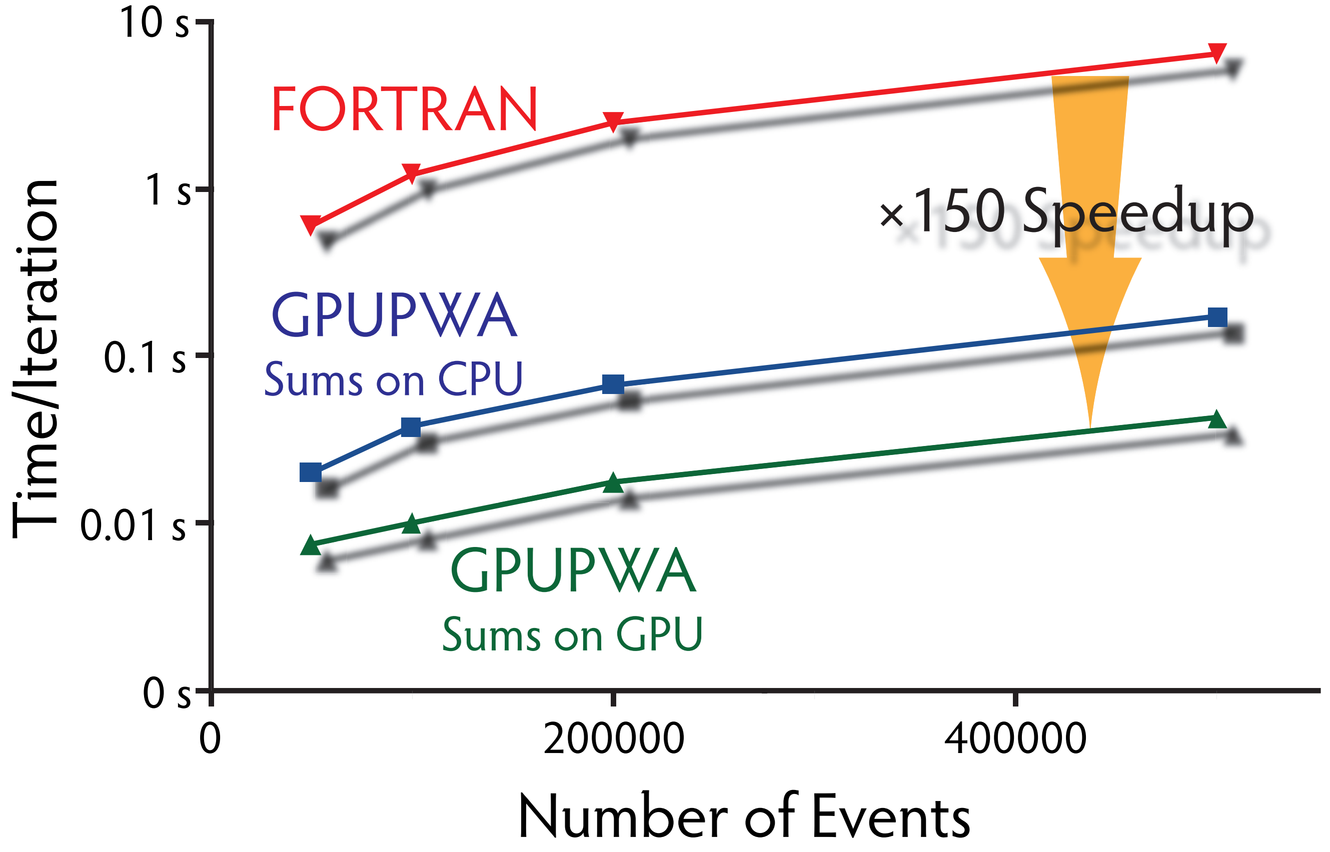


See: http://gpupwa.sourceforge.net

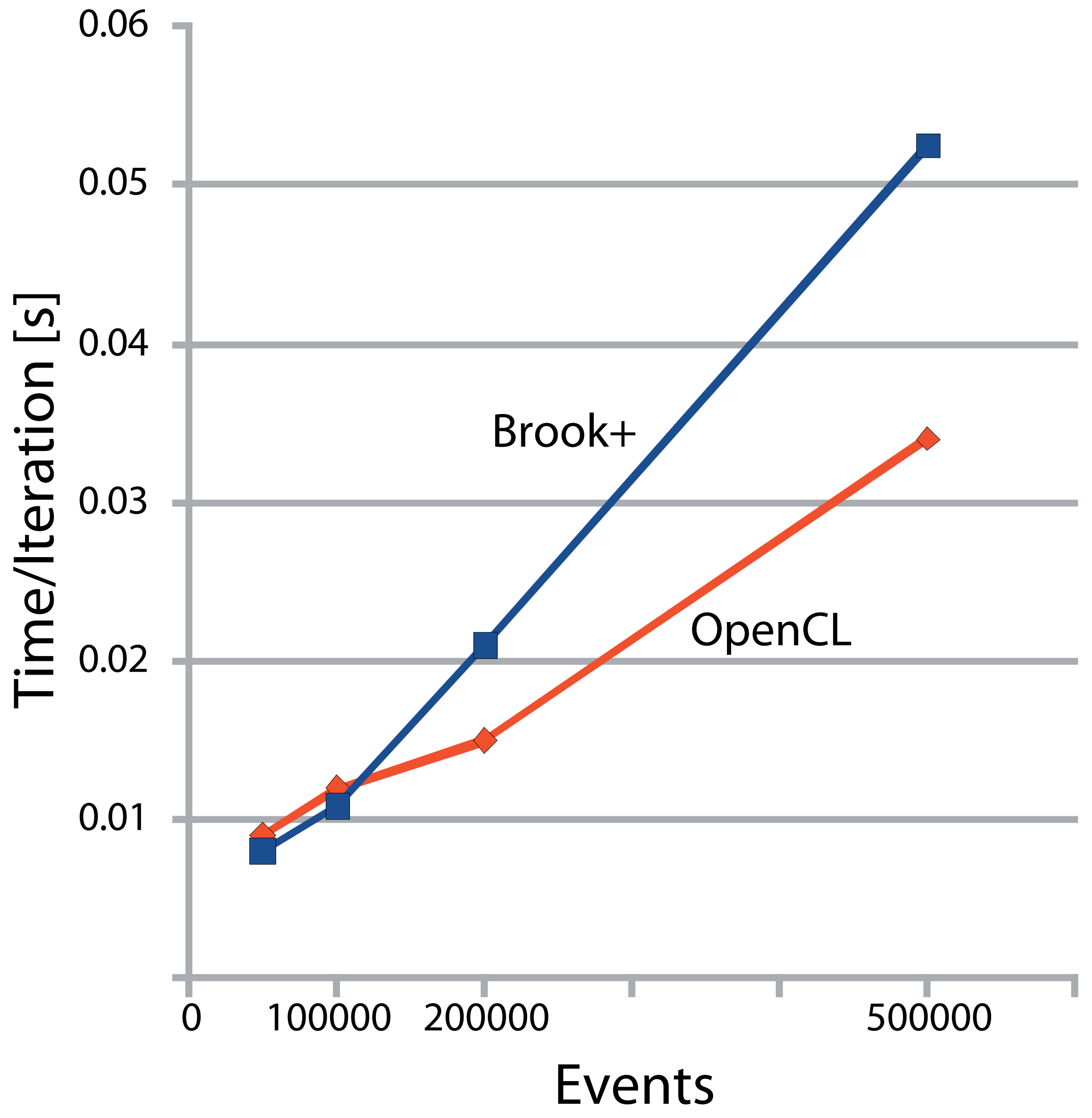
Performance (Brook+)

We use a toy model $J/\psi \rightarrow \gamma K^+K^-$ analysis for all performance studies

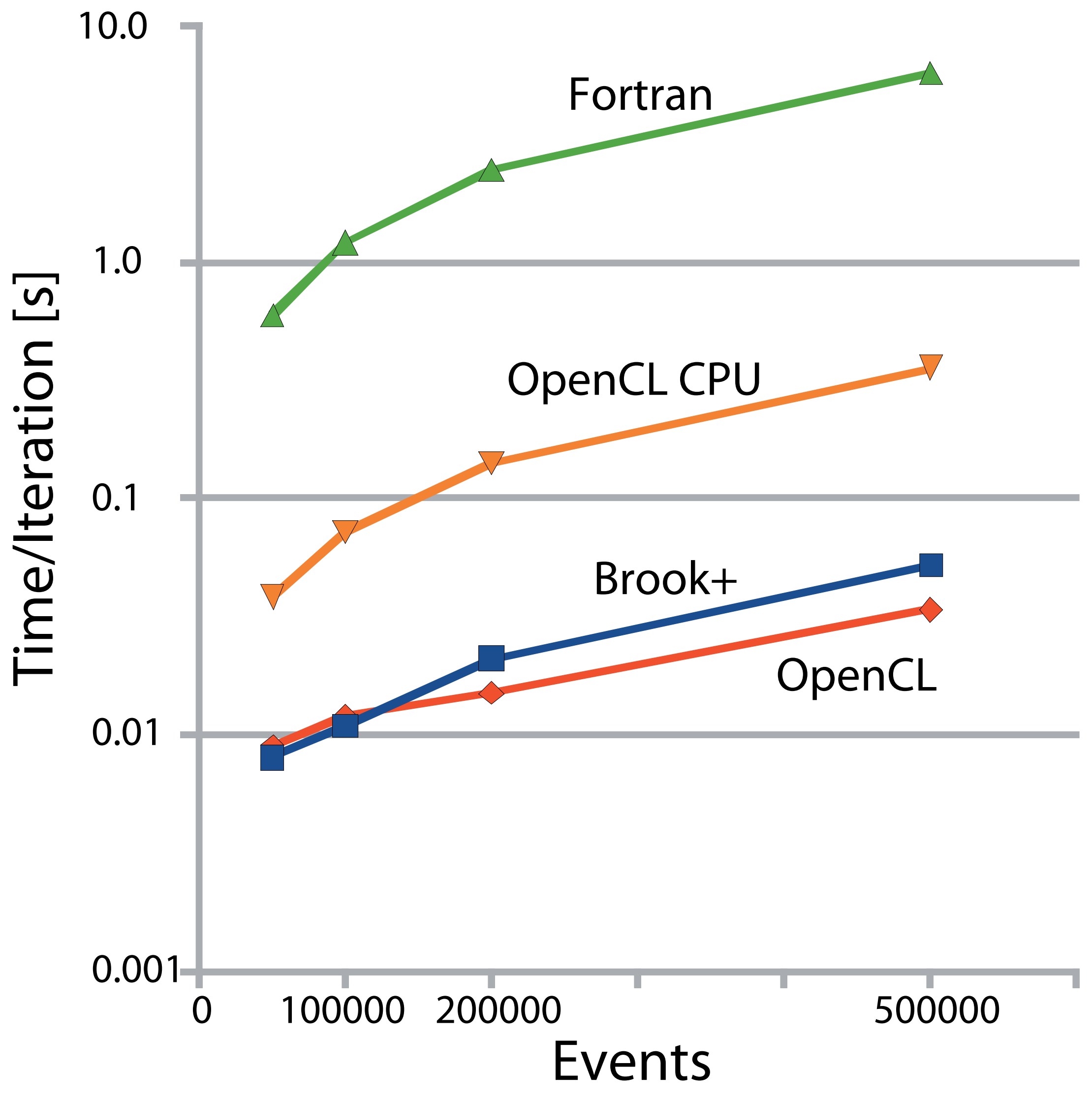
Using an Intel Core 2 Quad 2.4 GHz workstation with 2 GB of RAM and an ATI Radeon 4870 GPU with 512 MB of RAM for measurements



Performance (OpenCL)



Performance (CPU/GPU)



Indiana framework (Cleo-c, BES III and GlueX)

Following a presentation by M. Shepherd; work done by M. Shepherd, R. Mitchell and H. Matevosyan, Indiana University

Using a cluster with message passing interface (MPI)

- High-level inter-process communication; "easy" to code and debug
- Perform likelihood calculation in parallel; each node with a subset of data and MC
- Use Open MPI implementation of MPI2 (www.open-mpi.org)
- Scales well over multiple cores, with fast network also over small cluster

Calculation on GPUs using Nvidias CUDA (also on a cluster)

- Need more than hundred-fold parallel tasks: amplitude calculation at event level
- Some cost for copying data to and from GPU
- Small fraction of code (large, expensive loops) ported to GPU
- Coding/debugging somewhat challenging

Speed benchmarks

- Tested with a $\gamma p \to \pi^+\pi^+\pi^- n$ analysis with 5 $\pi^+\pi^+\pi^-$ resonances and one floating Breit-Wigner mass
- Amplitudes and log likelihoods are done on the GPU(s), the rest on the CPU(s)
- CPU parallelizaition handled by MPI

Fit Configuration	Time per fit iteration (milliseconds)
Single CPU	268
Single CPU + 1 GPU	47
CPU Master + 4 (CPU + GPU)	14
CPU Master + 11 CPU Workers	27

Time for 10^6 Amplitude Computations (ms)

Amplitude	CPU	GPU*
Breit-Wigner	800	8
Ang. Dist. (D-functions)	15,000	87

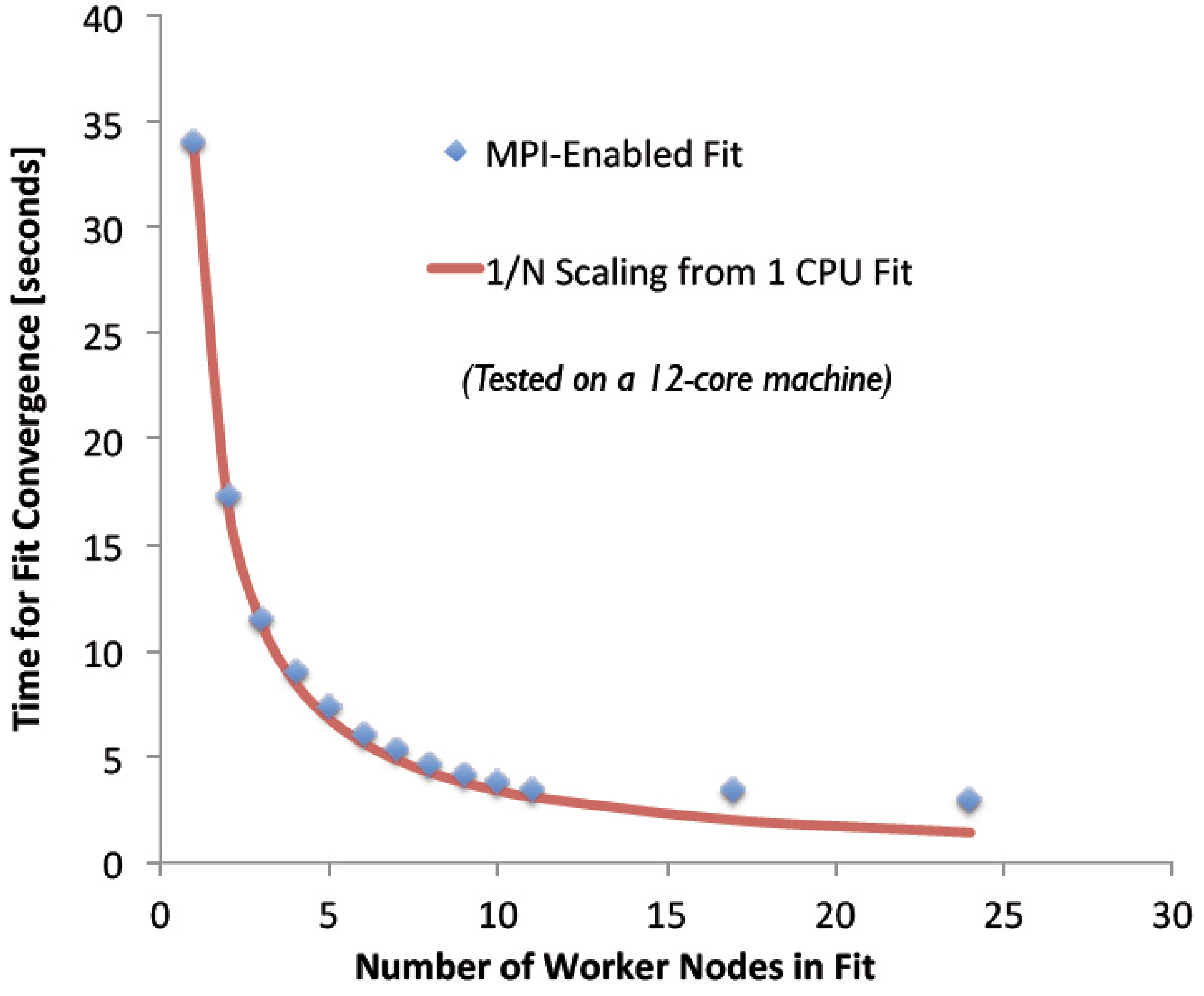
* includes time to copy result from GPU memory

Preliminary conclusions:

- MPI paralellization is efficient
- It is difficult to use the full power of GPUs

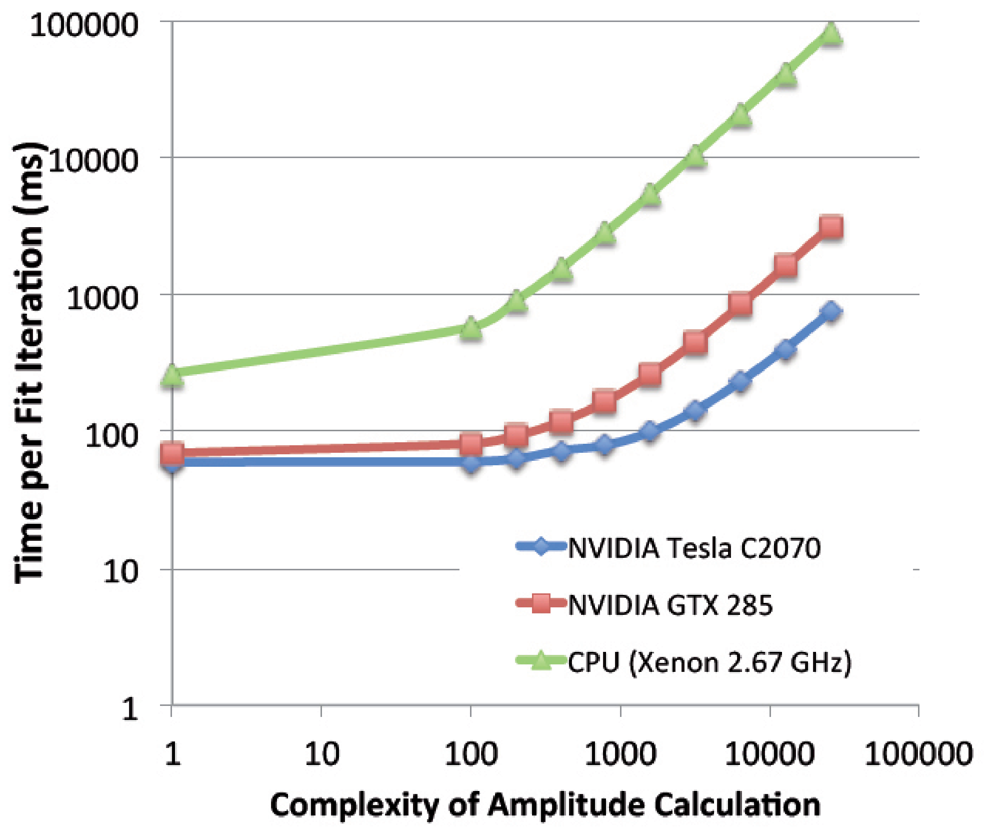
Multi-CPU scaling

- MPI allows very efficient parallelization of likelihood computation
- Only parameters and partial sums need to be exchanged between nodes
- User never needs to write MPI calls - all taken care of behind the scenes
- Fast and easy solution for multi-core systems



Compute-intensive amplitudes on the GPU

- Same fit with one change: Compute π in the Breit-Wigner using the first *n* terms of the arctan Taylor-expansion
- Now the fit time is dominated by the computational complexity of the amplitude
- More compute intensive amplitudes, i.e. more sophisticated models, are an excellent match for GPU accelerated fitting



Real two orders of magnitude speed gain for single Tesla C2070 with compute intensive amplitudes!

AmpTools

- Independent of the experiment and the particular physics process the amplitude analysis fit (i.e. construction of the likelihood) is pretty much the same
- This suggests it is possible to write a general software package that does all the "heavy lifting" — especially regarding parallel computing
- The user provides code for two types of C++ objects:
  - A recipe for calculating amplitudes, e.g., Breit-Wigner function -- no built-in physics!
  - A mechanism to read data into the framework
- The user specifies how many amplitudes, what types, arguments, free parameters, etc., via a configuration file (limits recompiling between fits)
- Library has been used/developed at Indiana U. over the past several years -- has provided a unified approach for several analyses the group is working on
- They are now trying to make available for general use:
  amptools.sourceforge.net
  (although, at this stage, documentation/examples are under development)

Speed is not the problem...

- We are fast enough, if we actually use our hardware
- This requires some work (which is however well invested...)
- This requires moving beyond FORTRAN (to some sort of C...)
- This will allow us to focus on the real problems...

Fitting in the dark...

In partial wave analysis, we perform fits with 20 (40, 60, more...) free parameters

- We will never know, whether we found the global minimum
- We can tell if a wave-set is “sufficient”, but can we know it is “right”?
- Can we even judge the goodness of fit? (“Badness” is easy...)
- We know that there must be multiple solutions...
- There is detector resolution

On the technical side:

- Could we get minimisers working with complex numbers?
- Could we get more control over the minimizers?
- Could we get a high level language building on OpenCL?

Which results will be believed?

- However "wrong" the analysis, people will usually believe quantum numbers if there is a bump in the mass spectrum

- However "right" the analysis, people will usually not believe in a new resonance if there is no bump, especially if it is exotic

Summary

- PWA profits from massively parallel computing on GPUs
- We have created a software framework to harness this power - speedups of two orders of magnitude
- User base at BES is growing, development continues
- OpenCL (and beyond) is the way to go
- Interesting work also ongoing at Indiana University - including multiple nodes via MPI and here in Munich

- PWA has fundamental problems because of fits with too(?) many free parameters
- With GlueX (JLAB) and PANDA (FAIR), big new PWA facilities are on the horizon — what can we do?