Microcalorimeter Spectroscopy at High Pulse Rates:
A Multi-Pulse Fitting Technique

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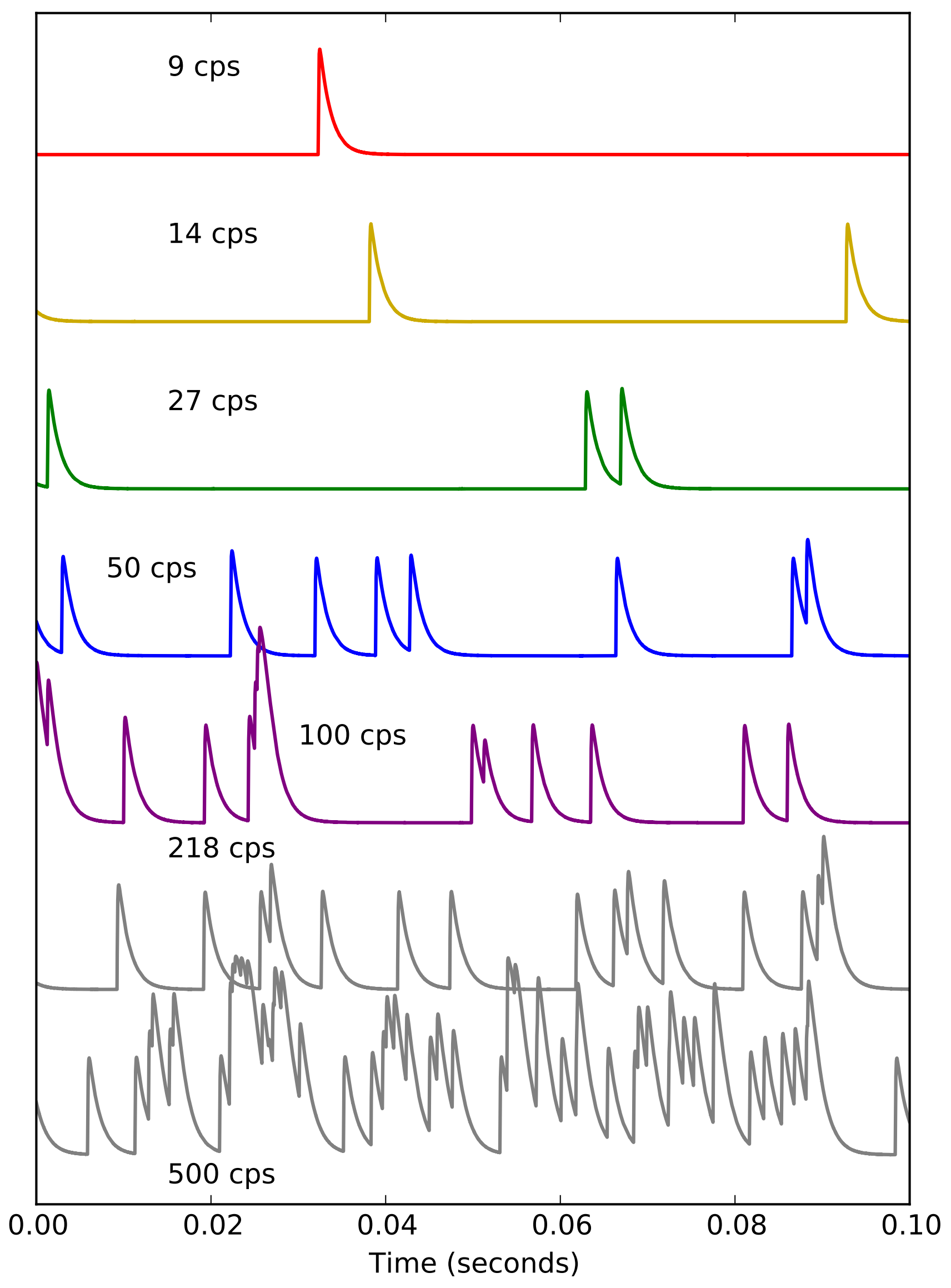
Motivation: pulses overlap in high-rate data

Central question: *Can pulse heights still be estimated from the data, even in the presence of some amount of pulse pile-up?*

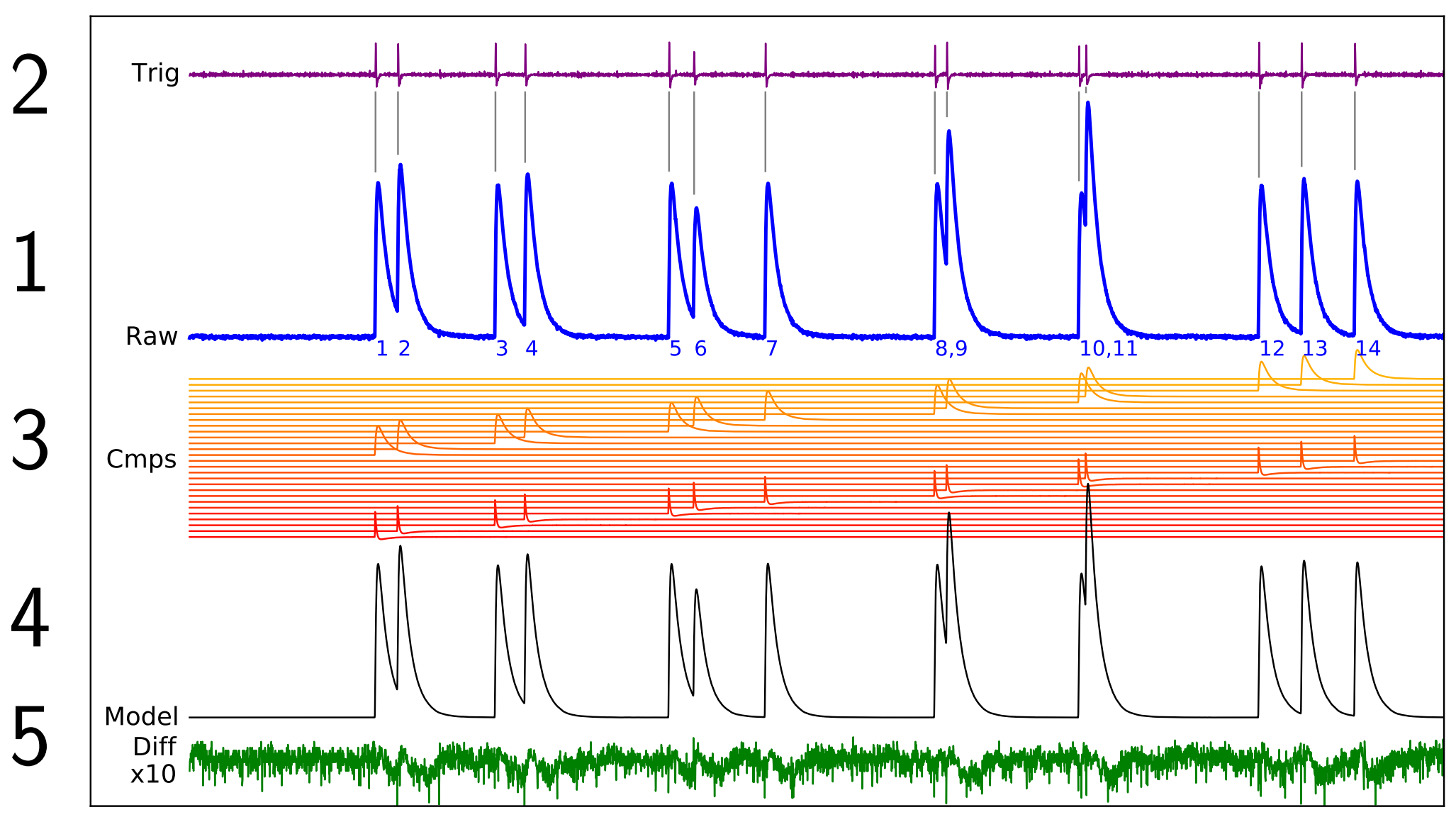


TES microcalorimeter data from one sensor, with a Mn fluorescence target at a variety of photon rates. Each trace lasts 100 ms. The data up to 100 cps are analyzed here.

Work shown here assumes perfect linearity of the sensors. Extensions for nonlinearity are part of our future plans.

Multi-pulse fitting concept

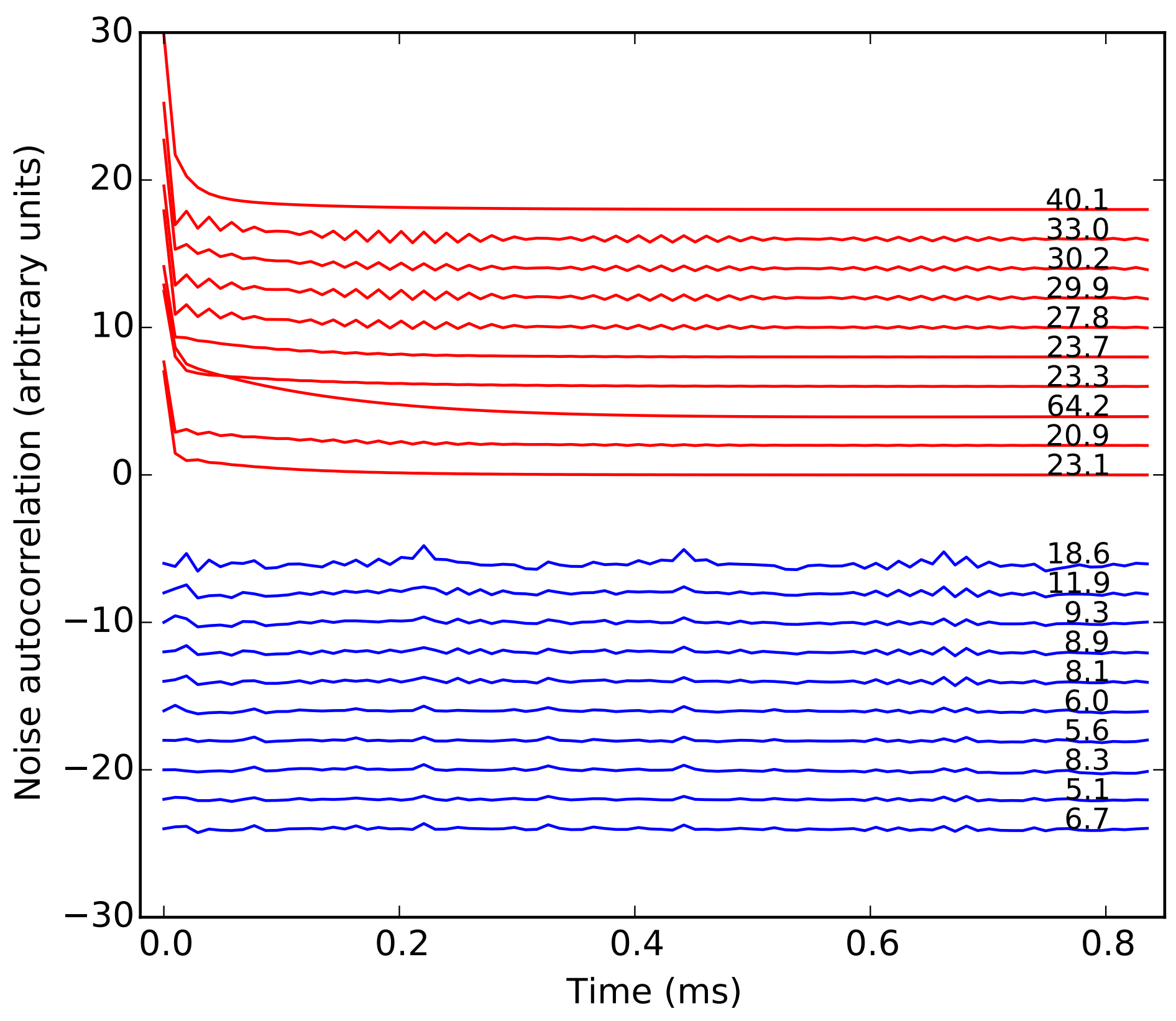
Conceptual steps in the fitting of multiple pulse heights from one data sequence.



1. Raw data: 73 ms (5700 samples) from one TES observing NH_4NO_3 fluorescence at Brookhaven's U7A beamline in a 542 eV beam.
2. Linear filter to find arriving pulses (here, 15.6 pulses expected, 14 found).
3. A 29-component linear model: 1 constant offset (not shown), 14 pulse heights, and 14 dp/dt terms (linear-order corrections for arrival time).
4. Fit for the 29 components' amplitudes. Model the data as a sum of these 29 components.
5. The residual $(\mathrm{data} - \mathrm{model}) \times 10$.

Approximations of the noise autocorrelation

A full maximum-likelihood fit requires exactly solving a (potentially) very large noise autocorrelation matrix, an $O(N^3)$ operation for records of size N. This renders the procedure completely intractable.
Our approach: approximate the autocorrelation function $r(t)$ as the sum of a delta function $\delta(t)$ plus a small number M of exponential functions (possibly complex).
This model is equivalent to an *autoregressive moving-average* (ARMA) model of order (M, M).



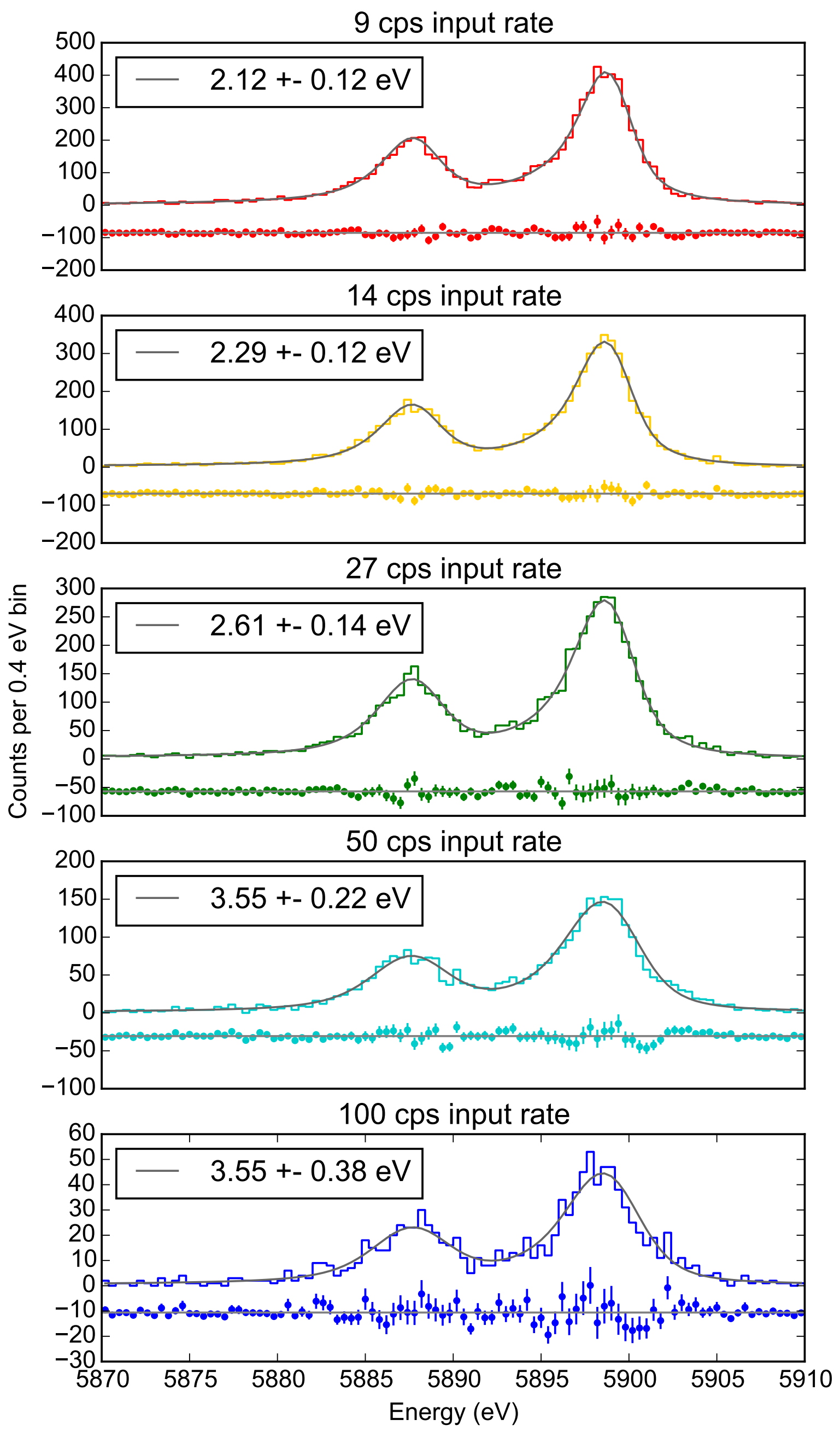
Top: ARMA(3,3) approximations to the noise autocorrelation of 10 TES detectors used in the NSLS experiment (last column of this poster).
Bottom: The difference between noise autocorrelation estimated from the data and the ARMA(3,3) model. All curves are labeled by the sum of the absolute deviation from zero.
Though the residual is only somewhat smaller than the noise itself, the approximation nevertheless allows for excellent inverse-noise-covariance weighting.

Acknowledgments

This work has been supported in part by the NIST Innovations in Measurement Science program, the NASA APRA program, by two NRC Postdoctoral Fellowships, and by a NIST ARRA Senior Fellowship.

Test Case 1: 5900 eV Manganese Kα lines

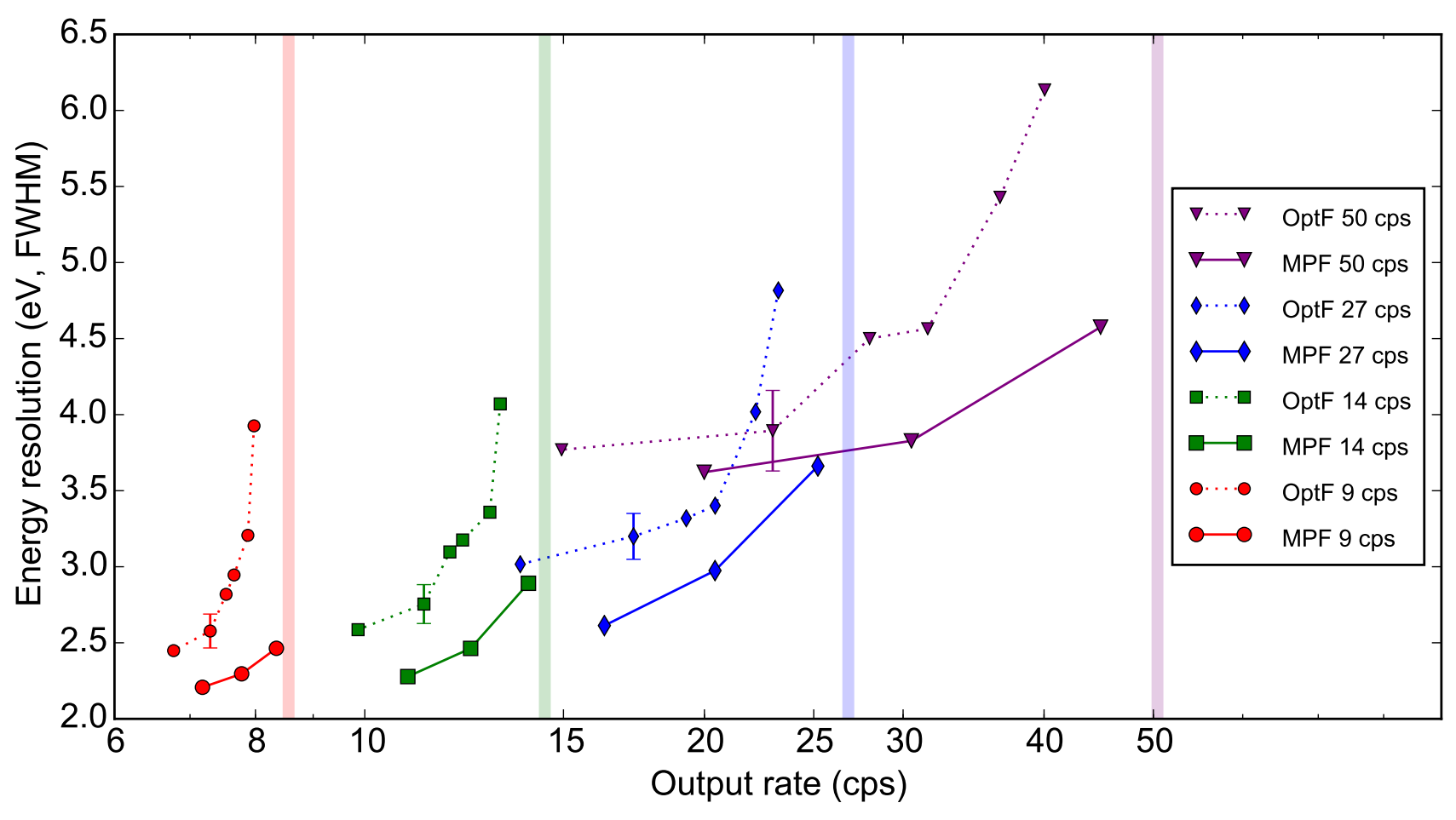
First test case: fluorescence of manganese at 5900 eV, produced at NIST with an x-ray tube source and observed with a single TES. The source was adjusted to produce photon rates between 9 and 100 counts per second.



Mn Kα-line spectra computed using multi-pulse fitting, at five input photon rates. Each spectrum is shown as a histogram; the best-fit curve is the smooth gray curve; and the data-minus-fit residuals are shown (vertically offset for clarity) as points with error bars extending to $\pm\sqrt{N}$ to indicate the approximate range of consistency with the Poisson distribution of counts per bin.

Mn Kα resolution vs output rate

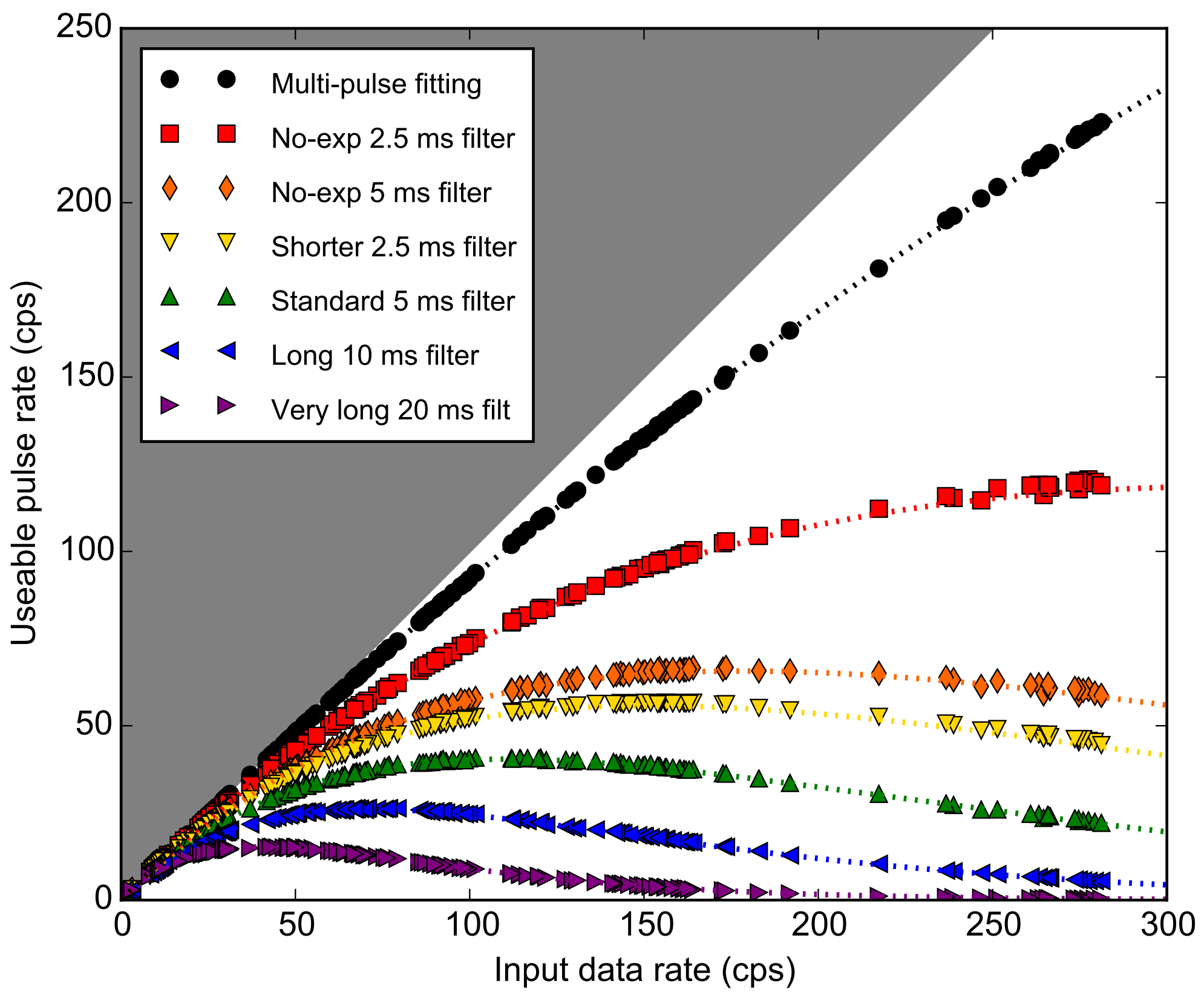
The energy resolution at 5900 eV at any given output rate is superior for the MPF method, compared with traditional optimal filtering. At any input photon rate (the 4 colors), various output rates can be selected by using a range of time-isolation cuts.



Incident photon rates of 9, 14, 27, and 50 counts per second are shown in different colors. The vertical shaded areas show the incident photon rates, which would indicate 100 % efficiency. The upper curves connected by dashed lines show results of the classic optimal filtering analysis; each point corresponds to a different filter and its appropriate pulse cuts. The lower curves connected by solid lines show the superior results from multi-pulse fitting to the same data. The three MPF points correspond to different selection cuts from most to least restrictive on pulse time-isolation.

Multi-pulse fitting is very photon-efficient

The per-sensor rate of usable photons in the nylon data (test case 2) as a function of the total rate of photons. The multi-pulse fitting method makes much more efficient use of photons than optimal filtering does at 100+ photons per second.



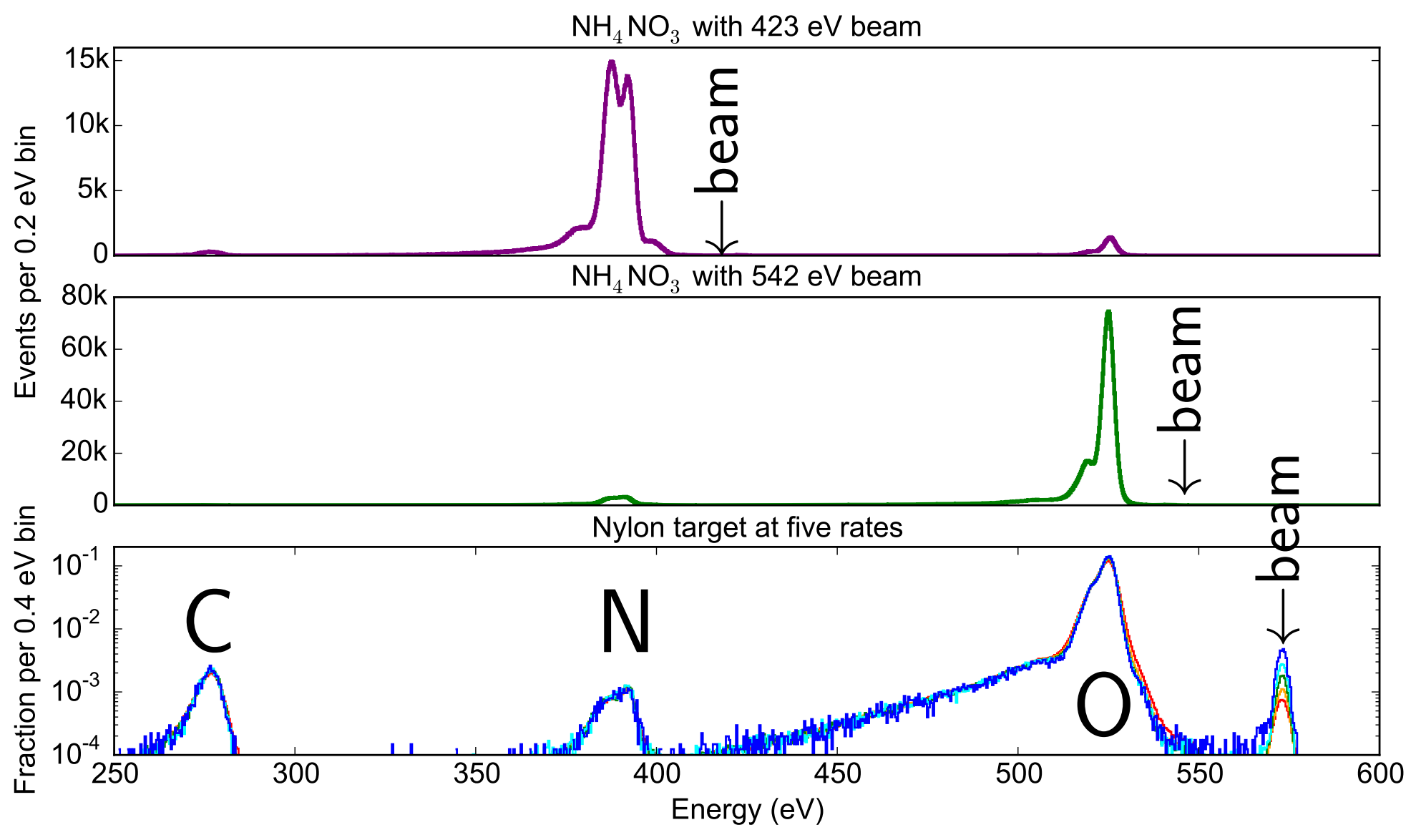
Each color/marker shape corresponds to a different analysis. The black circles represent the multi-pulse fitting. There are approximately 200 circles: one for each of the 40 working TESs at each of five different fluorescence photon rates. The other six marker shapes correspond to a traditional analysis using optimal filters of various fixed lengths. Each of these analyses has a corresponding "veto window": a pulse has to be cut if another photon arrives during its veto window. The lines represent the theoretical usable rate re^{-rw}, where r is the raw photon rate and w is the duration of the relevant veto window (r and w are given, not fit). The gray shading (upper left) indicates efficiency exceeding 100%.

Further Information

This work will appear in *Astrophysical Journal Supplement Series* in 2015 and can be found at `http://arxiv.org/abs/1503.05989`

Test Case 2: 390 eV Nitrogen x-rays (NSLS)

Second test case: fluorescence of nitrogen at 390 eV, observed with a 45-sensor TES spectrometer at the National Synchrotron Light Source beamline U7A, Brookhaven National Laboratory in Upton, New York.
We use the unique 2-peaked shape of the nitrogen K line from NH_4NO_3 to assess energy resolution at 390 eV. We use the Gaussian scattered beam line at 573 eV to study resolution as a function of photon rate.

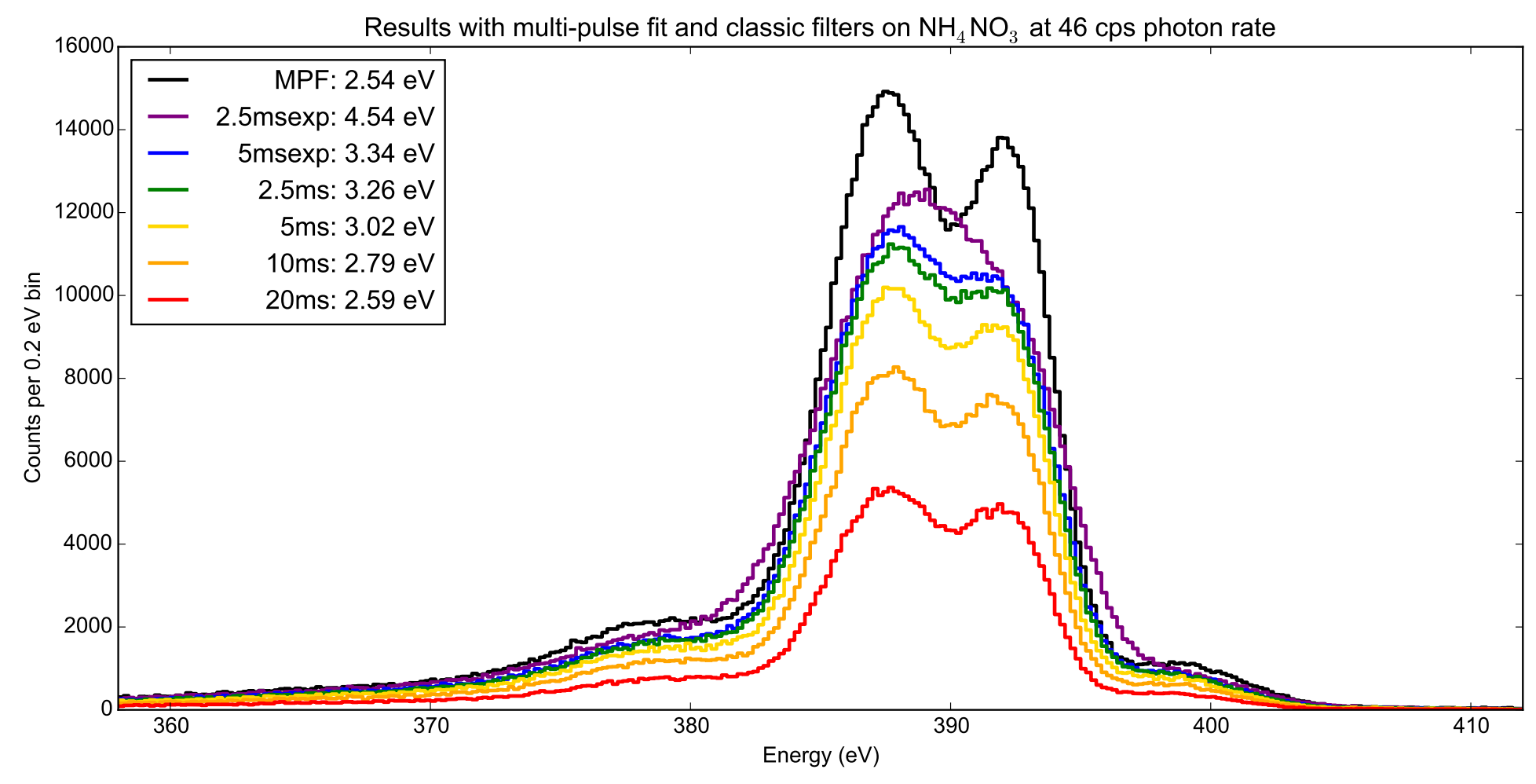


X-ray energy spectra from 7 different low-energy observations at NSLS.
Top: fluorescent emission from NH_4NO_3 featuring the 2-peaked nitrogen K line.
Center: same target but with incident beam energy now above the oxygen K edge.
Bottom: Nylon target at 5 different intensities (10 to 280 counts per second per TES). The width of the scattered beam peak at 573 eV is used to estimated the energy resolution at very high pulse rates.

These spectra all employ multi-pulse fitting to estimate pulse heights. These are converted to energy using a weakly nonlinear function, selected by requiring the C, N, and O fluorescence K lines and the scattered beam peak to fall at their known locations.

MPF has higher throughput and better resolution than any standard optimal filter

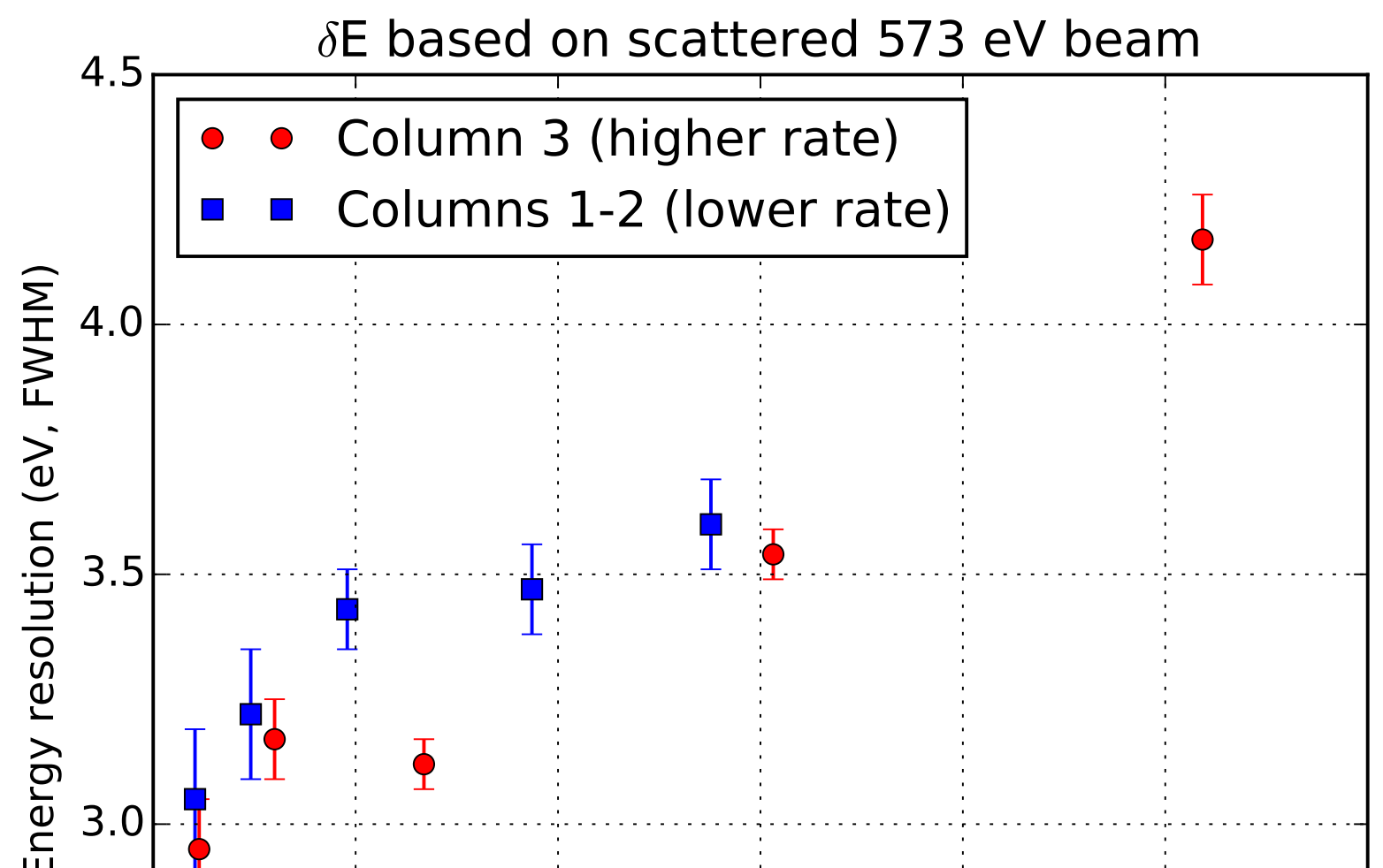
Optimal filters allow one to choose longer records, achieving higher resolution at the cost of being more sensitive to pileup. Here six optimal filters (colors) show that the increased throughput comes at a resolution cost (the purple curve does not resolve the two N peaks). The MPF spectrum (black) has the best resolution *and* the highest throughput.



The 2-peaked nitrogen K x-ray fluorescence line emitted by a NH_4NO_3 target illuminated by a 423 eV probe beam. The seven spectra correspond to the same 1,038,000 photons analyzed in seven different ways. The six lower spectra were generated by standard optimal filter analysis, with six different choices of filter. The top spectrum is the result of multi-pulse fitting of the same data. The legend gives the estimated energy resolution (FWHM of Gaussian broadening). The MPF analysis achieves energy resolution as good as the longest standard optimal filter's, while also making use of more pulses than even the shortest, lowest-resolution constrained optimal filter.

MPF energy resolution still good at 260 cps

The energy resolution at 573 eV deteriorates very little (from 3.0 to 3.5 eV) at photon rates up to 150 cps and is still only 4.2 eV even at 262 cps, even though multi-pulse fitting accepts 80 % of all photons at that rate.



Estimated energy resolution at 573 eV based on multi-pulse fitting analysis of the Nylon target data, as a function of the incident photon rate (per sensor). The energy resolution reported is the estimated FWHM of the best-fit Gaussian to the scattered-beam peak. The fit is performed with photons between 568 eV and 578 eV; a linear trend is included in the fit to allow for background photons. Multiplexer Column 3 is handled separately from the others, because—for geometric reasons—the photon rates observed in Column 3 are substantially higher.

Future extensions and plans

Future prospects depend on adapting this technique to accommodate nonlinearity in the sensors without increased scaling of computational resources. Steps in this direction might include:

1. Fit for only *one* pulse height at a time, but use the framework of multi-pulse fitting to allow fitting the longest possible sequence available for that pulse.
2. The DC ("baseline") level varies slowly. Use Bayesian priors so that past estimates of the DC level can influence future ones.
3. Model pulses as the sum of several linear components, not just one. Use MPF to estimate the amplitude of *all* components. Then a non-linear procedure can be used to convert these to energy.
4. Model noise-whitened pulses as sum of decaying exponentials. This would greatly speed up computation, supposing a good exponential-only basis can be found.
5. We need a very robust method for approximating any reasonable, observed noise as an ARMA(p, p) process noise.

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Low Temperature Detectors 16, 2015 Grenoble, France