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FASTFLIGHTä, a Digital Signal Averager for Continuous High-Speed Data Acquisition with Electrospray Time-of-Flight Mass Spectrometers Coupled to Chromatographs

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Summary

- **Orders of Magnitude faster data acquisition compared to a Digital Oscilloscope**
- **>10 spectra/second to disk ... for >30 minutes**
- **2-GHz effective sampling rate (0.5-ns sampling interval)***
- **100 times higher data rate than a time digitizer for:**
  - **Better statistical accuracy**
  - **Lower detection limits**
- **End-of-scan dead time <1 μs (<1% idle time)**
- **Precision Enhancer* transforms the 8-bit ADC into a 12-bit ADC ... for 16 times greater dynamic range**
- **Record lengths up to 262,000 data points at 0.5, 1, or 2-ns sampling intervals for flight times up to 524 μs**
- **Sums up to 65,535 records in each spectrum for improved signal-to-noise ratios**
- **Real-time DSP data compression* reduces storage file size by more than a factor of 10**
- **Windows NT software provides data acquisition, control, display and analysis**

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* Patents pending

Synopsis

Feeding the output of a chromatograph to an Electrospray Time-of-Flight Mass Spectrometer (ES TOF-MS) requires ultra-high-speed data acquisition at the output of the TOF-MS. A chromatograph run typically lasts for 30 minutes, and contains multiple peaks, each having a width of the order of a few seconds. To identify the molecules in the various components of overlapping chromatograph peaks the TOF-MS must record a mass spectrum as frequently as every 0.1 second.

Flight times for the ionized molecules in the TOF-MS range from 1 to 100 μs, and peak widths are about 3 ns. Thus, digitization of the detector output requires 0.5-ns sampling intervals and record lengths of the order of 256 k sampling points.

The dominant source of error is caused by ion statistics. Therefore, circa 200 records must be summed or averaged every 100 ms to reduce the statistical error. This requires a data acquisition rate that is orders of magnitude beyond the capabilities of a digital oscilloscope.

As illustrated in Figures 1 and 2, the FASTFLIGHT™ Digital Signal Averager was specifically developed to accommodate the extreme data rates in the Chromatograph/TOF-MS application. The analog signal from the TOF-MS detector is amplified by a wideband preamplifier and then sampled at 2-ns intervals by an 8-bit ADC. A single record is formed by up to 262,000 samples following the Trigger Pulse. As each record is being acquired, the Averager Memory adds that record to the sum of the previous records. The dead time between records is <1 μs. When the last record in the spectrum is being added, the sum is written to the Output Buffer Memory for transfer to the supporting computer while the next spectrum is being acquired. Thus, the dead time between spectra is also <1 μs.

Uncompressed data rates are typically >5 MB/s and the file size from a 30-minute chromatograph is >10 GB. Consequently, data compression is required to reduce the data flow to fit the capacity of a state-of-the-art computer. The Digital Signal Processor accomplishes data compression (typically a factor of 14) by adaptively detecting peaks above the background fluctuations. It rejects background in favor of preserving the peaks in the stored spectra. Background points in the vicinity of peaks, and every 200th background point are preserved to allow background subtraction in the compressed spectra.

The sum of the peak areas in the TOF spectra is used to plot the live chromatograph spectrum in Figure 3. During acquisition, the TOF-MS spectrum for any point in the chromatograph can be displayed as in Figure 3. Display, control, data acquisition and analysis via a personal computer are implemented by software that runs under Windows NT.

In addition to controlling the input offset voltage, the 12-bit DAC in Figure 2 is used for the Precision Enhancer. At the end of each record, the DAC is pseudo-randomly stepped to a new value. The step size is 1/16 of the ADC LSB and the steps range over ±8 LSB. As a result the 8-bit resolution of the ADC is transformed to 12 bits when circa 256 records are summed. This improves the accuracy and dynamic range by a factor of 16.

The Trigger Output is synchronized with the 2-ns clock in the digital signal averager, and is used to trigger the acceleration pulse in the ES TOF-MS. A single scan forms a record for 2-ns sampling. For 1-ns sampling, a first scan is completed with sampling at 2-ns intervals. Then the delay between the 2-ns clock and the Trigger Output is incremented by precisely 1 ns, and a second scan is taken. The results of the two scans are interlaced to form a complete record with 1-ns sample intervals. For 0.5-ns sampling, a 0.5-ns trigger offset is used and 4 scans are interlaced to

form a complete record. This provides an "effective" sampling rate of 2 GHz.

A thorough statistical analysis shows that "effective" 2-GHz sampling achieves the same information rate as "true" 2-GHz sampling for the ES TOF-MS application, but at a fraction of the cost.

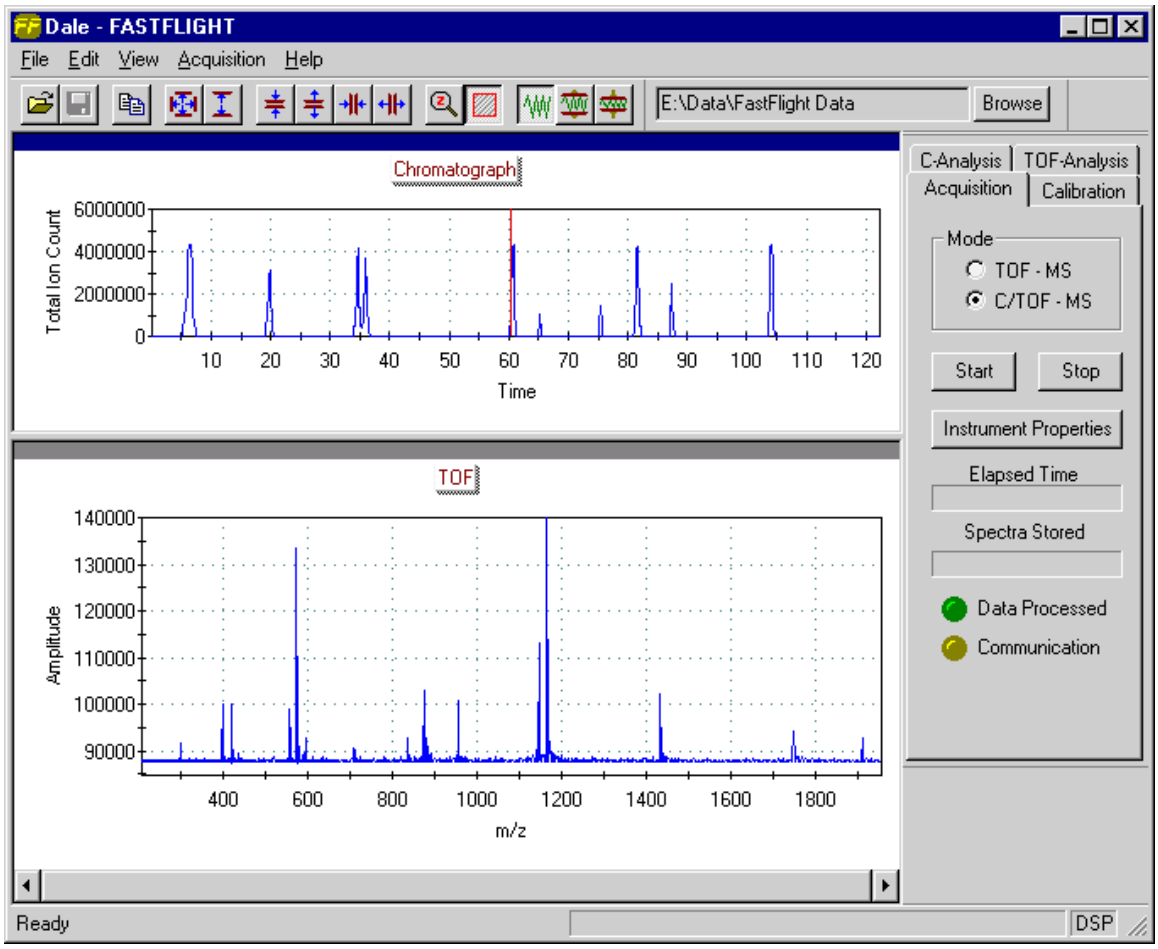

Figure 3. The Live Chromatograph and TOF-MS Display Provided by *FASTFLIGHTä* During Data Acquisition.

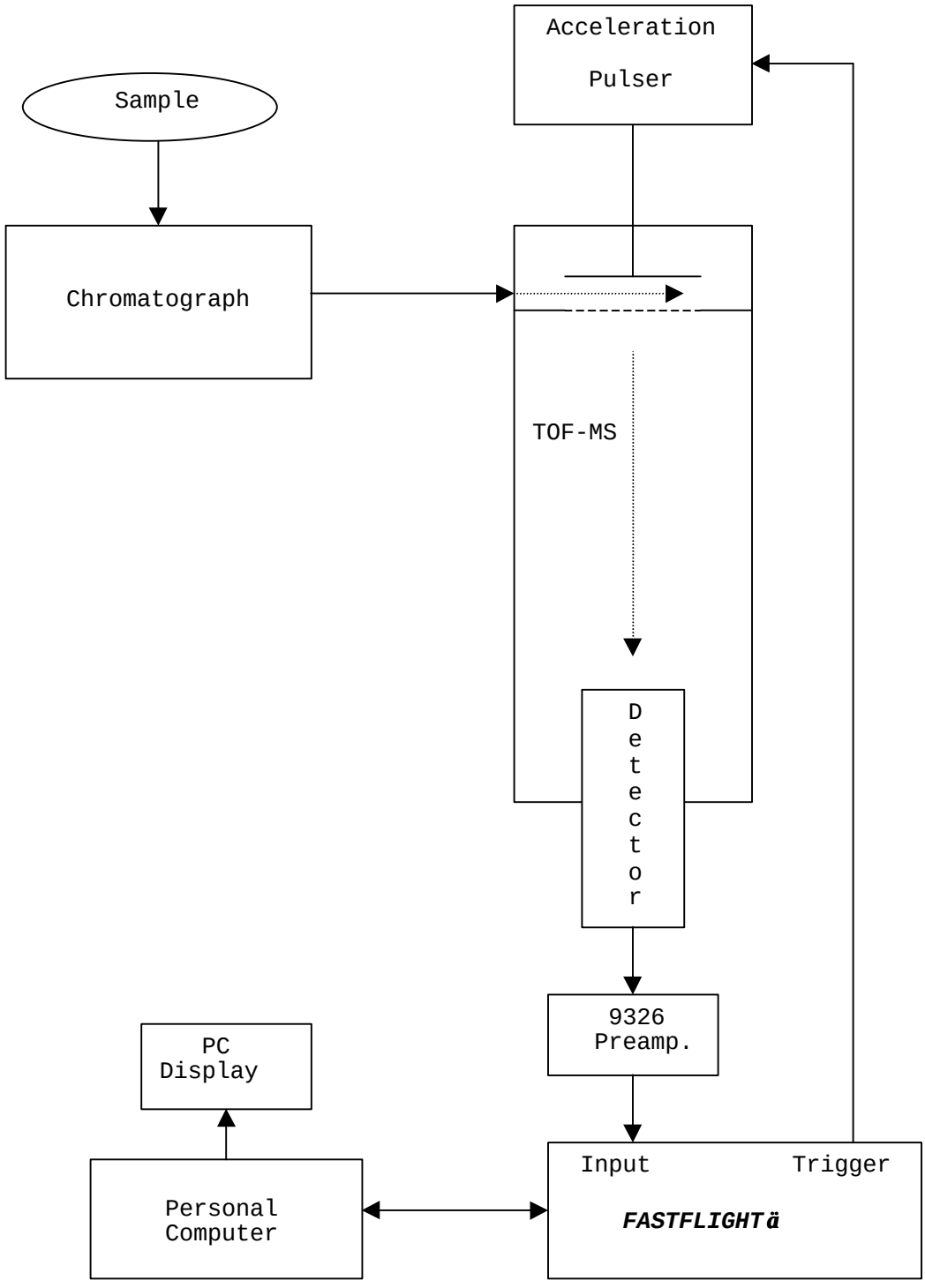

Figure 1. The *FASTFLIGHTä* Digital Signal Averager Applied to Data Acquisition with an Electrospray TOF-MS Receiving the Output of a Chromatograph.

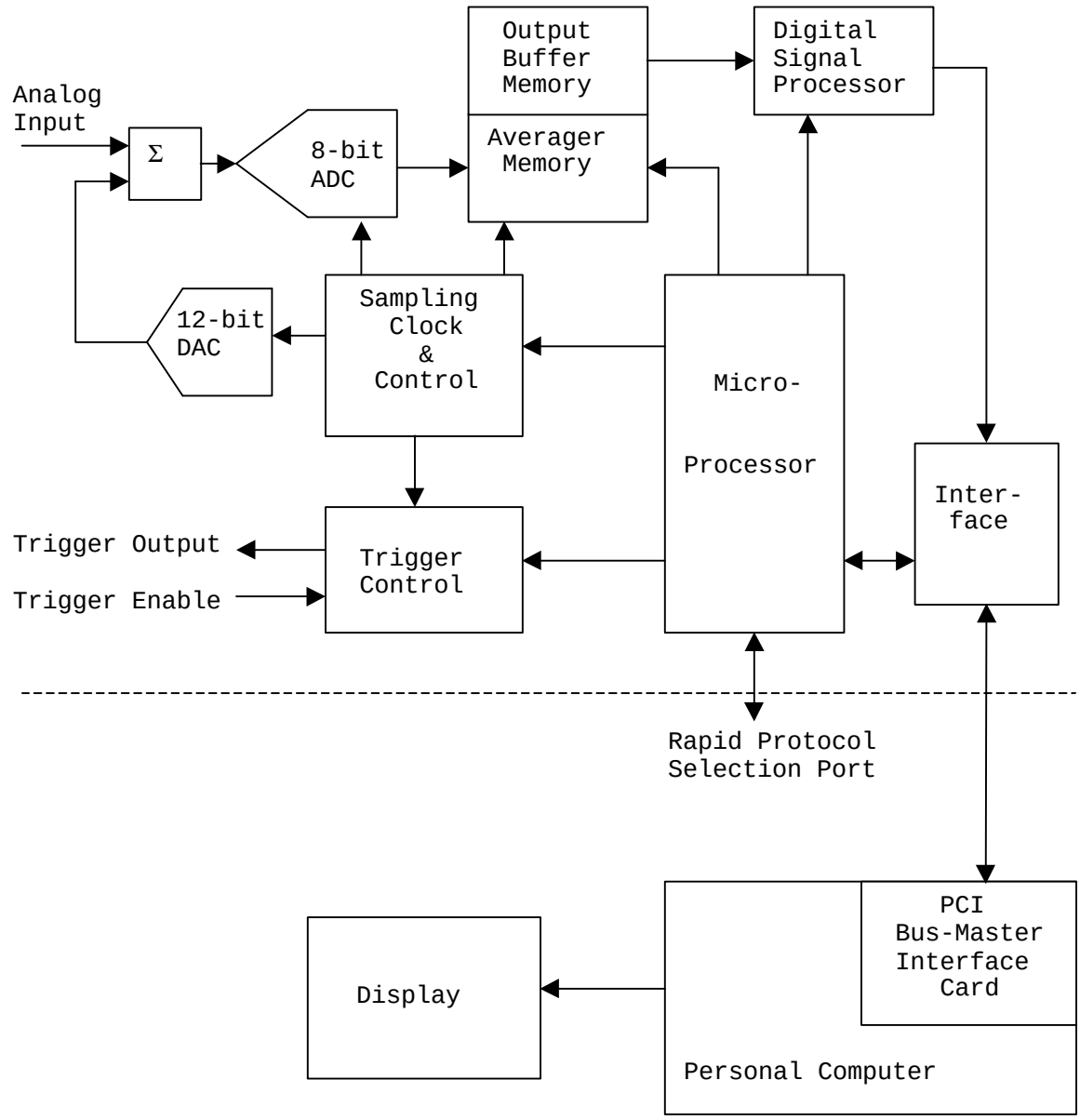

Figure 2. Schematic Diagram of the *FASTFLIGHTä* Functions.