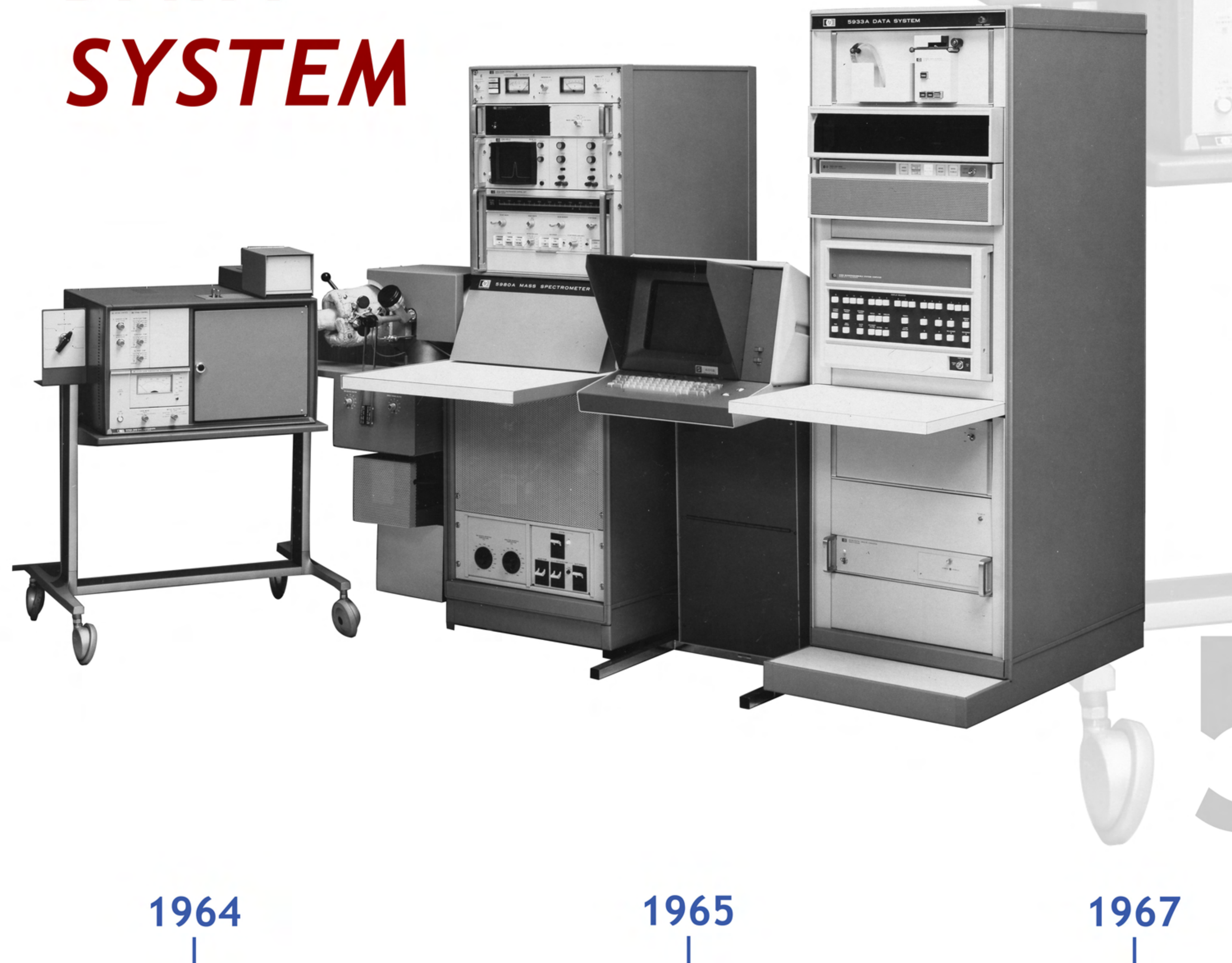
THE FIRST DATA CRUNCH CRISIS:

Prior to the introduction of combined GC/MS, mass spectral acquisition rates were typically on the order of tens of minutes per compound. The data, recorded on oscillographic chart paper, had to be manually mass marked and peak intensities had to be manually measured. These methods were impossibly slow for GC/MS analyses when literally dozens of mass spectra could be recorded in the time that it would take to record and analyze the spectrum from one compound by oscillographic recording techniques.

Clearly, data acquisition and processing by computer was necessary for the data rates from a GC/MS instrument. Hewlett Packard had already designed and produced a series of small computers beginning in 1966[8] and the application of their in-house expertise in computer technology helped them to move forward rapidly in the computerization of the QMF. As noted in the Application Note, they had devised computerized autotuning software for the HP 5985A in 1978.

Even with computers, the acquisition and processing of mass spectral data was a challenge. The computer hardware was slow and memory extremely limited by today's standards, so the problem of handling mass spectral data was right at the limit of the capabilities of the computational equipment of the day.

Enter the HP 5932A DATA SYSTEM



Hewlett Packard selected their HP 2100A computer to interface to the HP 5930A quadrupole mass filter and designated it as the HP 5932A Mass Spectrometer Data System.

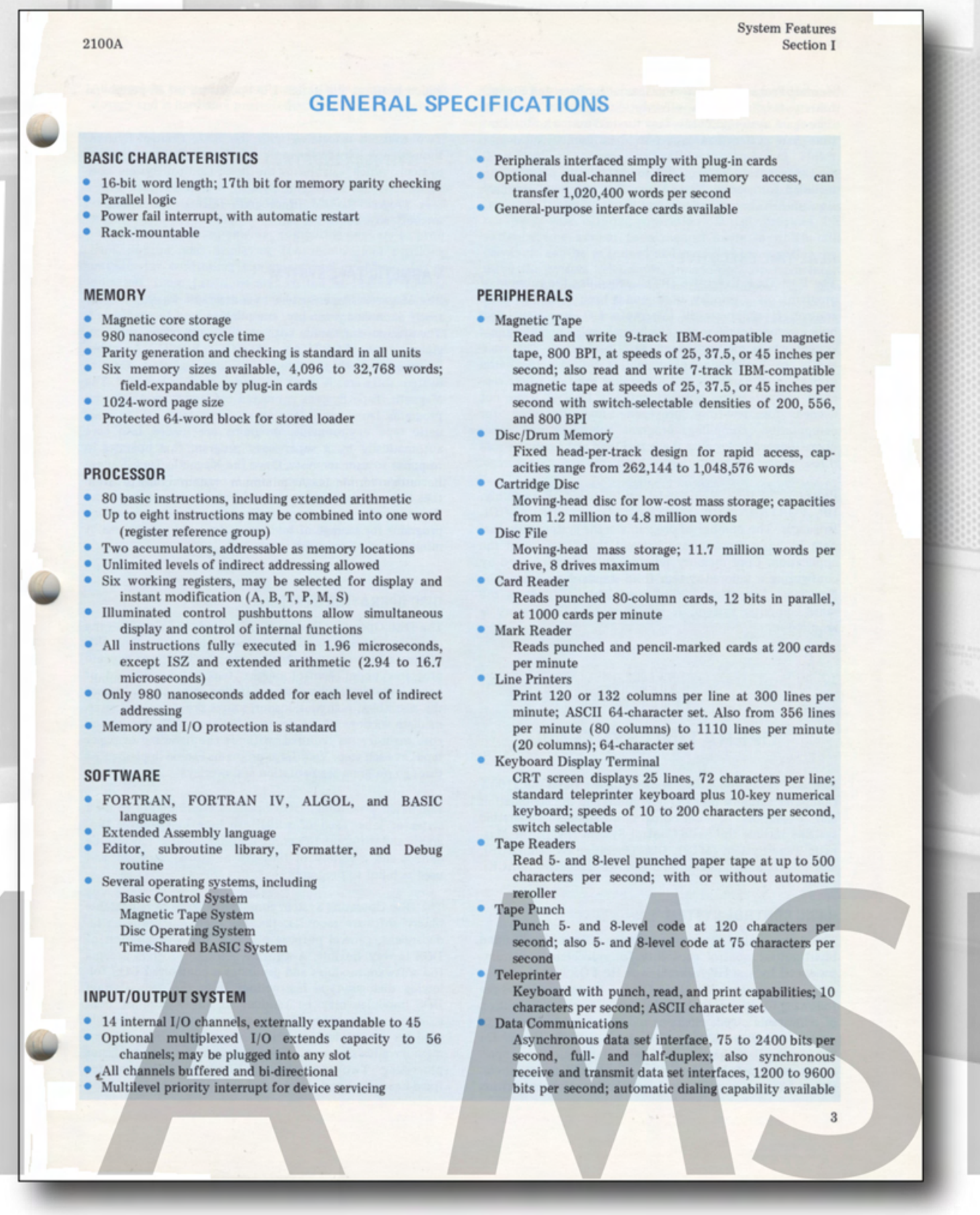
Evolution of HP2100A:

The HP2100A was preceded by Hewlett Packard's initial foray into the minicomputer market with the HP2116 series introduced in November of 1966. These machines were originally introduced as 'instrument controllers' rather than 'computers' since the founders of Hewlett Packard were on opposite sides of the fence with regard to the business decision to enter the minicomputer market. Bill Hewlett was against the venture while David Packard was for it.[10] Packard managed to prevail by the subterfuge of purchasing a small computer company, Data Systems Incorporated (DSI), and folding it into the Dymec Division of Hewlett Packard. However, Bill Hewlett had to sign off on the purchase and agreed to only after David Packard referred to DSI minicomputers as 'instrument controllers.'

The initial market entry, the HP2116A had a slot cage for the addition of 16 interface cards for connecting any of 20 HP metrology instruments, as well as a full complement of cards for all of the available I/O devices at the time. Interestingly, the 2116A was successful not only in the automated instrumentation market, but also in the business computer market; so much so that the HP2115A and 2114A were introduced minus the slot cage; since business users had no need for a wide variety of interface cards. These models were consequently smaller and less costly. These minicomputers used core memory and hardwired CPU.

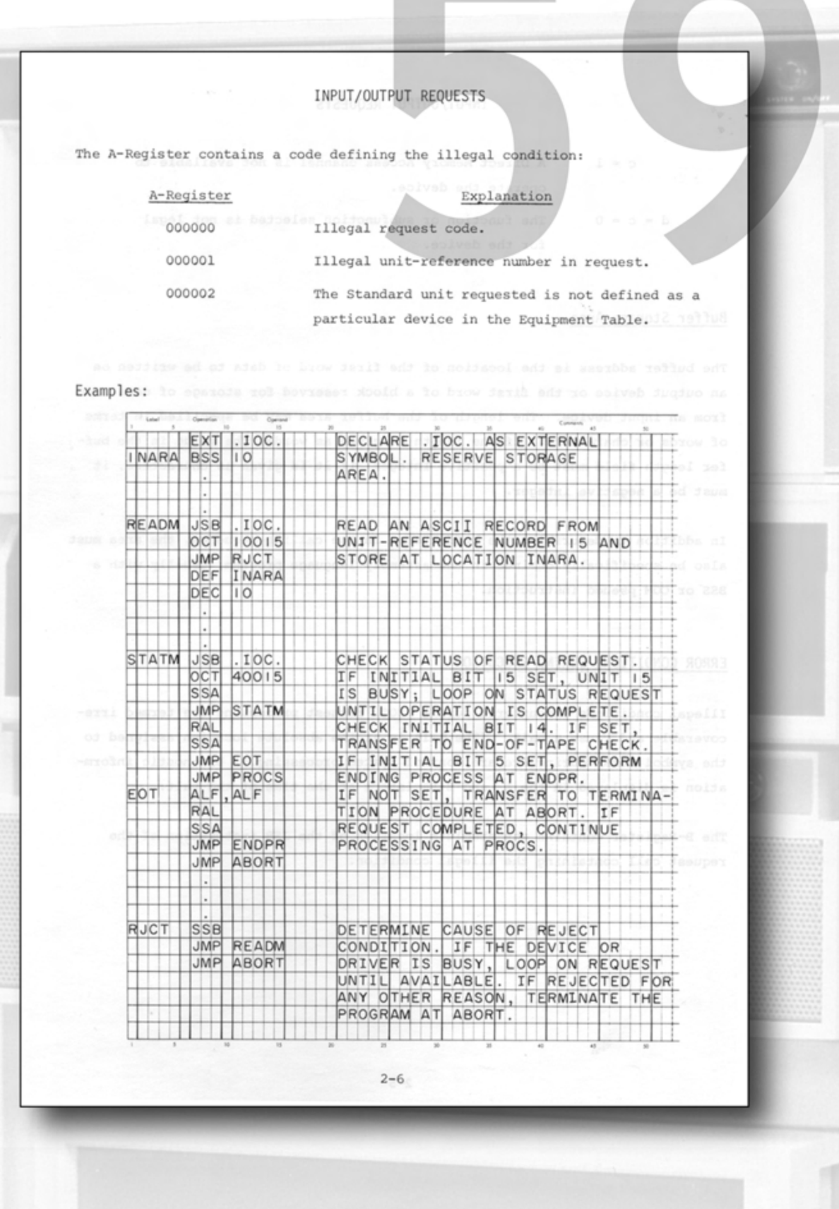
In 1970, Hewlett Packard produced an upgraded instrumentation controller, the HP2100 series. This machine still used core memory, but had a microprogrammable CPU. One of its earliest applications was the data system for the HP5930A mass spectrometer.

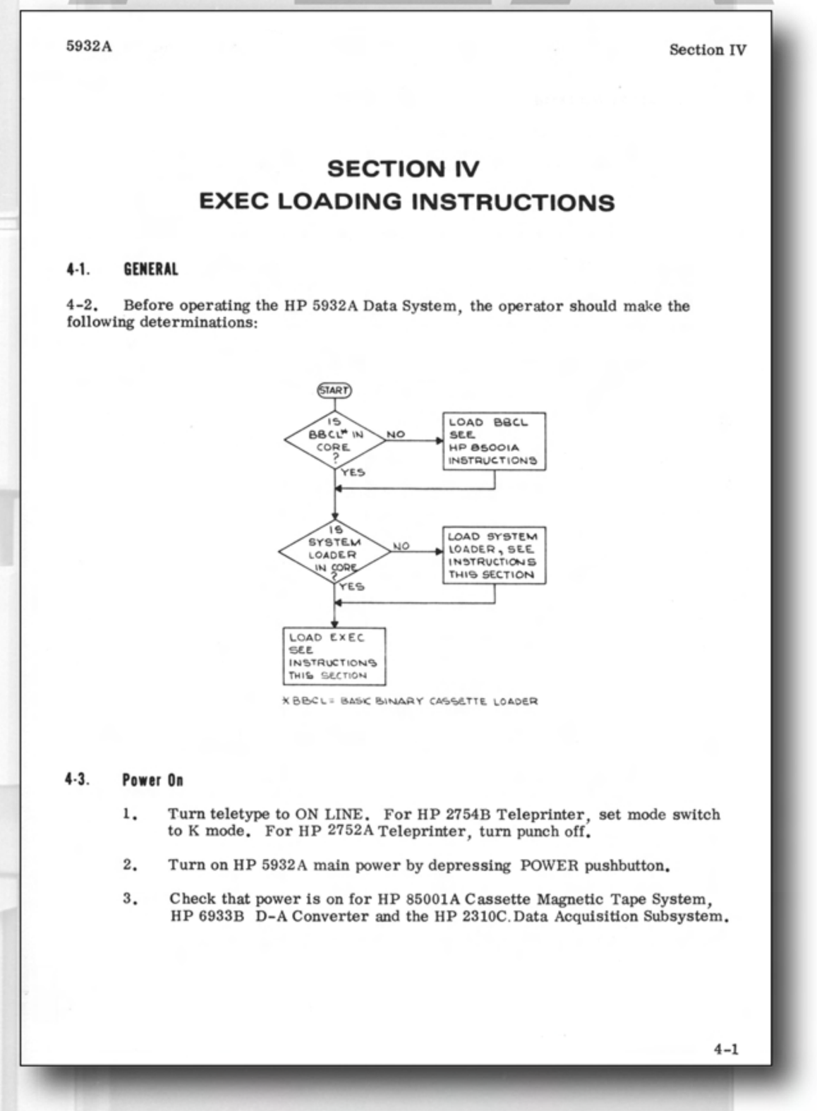
The specifications of the HP 2100A/HP 5932A Data System were amazingly archaic compared to modern equipment, but were state-of-the-art in the early '70s.



The HP5932A featured a *'Basic Binary Cassette Loader'* that was essentially a primitive form of 'DOS'. This software was read into a protected portion of memory by means of switches on the computer control panel. Once in memory, the Basic Binary Cassette Loader took over the task of tape handling to load software for subsequent tasks into RAM.

All system software was on magnetic cassette and/or perforated paper tapes. Due to memory limitations, individual software programs were written in Assembler Language and tasks were run by swapping them in and out of RAM in serial order since the 8K of RAM was too small to perform more than one operation at a time.





The acquisition and processing of mass spectral data was a two-step task. "Scan" was used to acquire digital data from the mass spectrometer. This was probably the most demanding task for the data system as the mass spectrometer was on-line, controlling some basic instrument parameters, digitizing the data stream, determining peak centroids and areas in real-time, and writing the information to magnetic cassette tape.

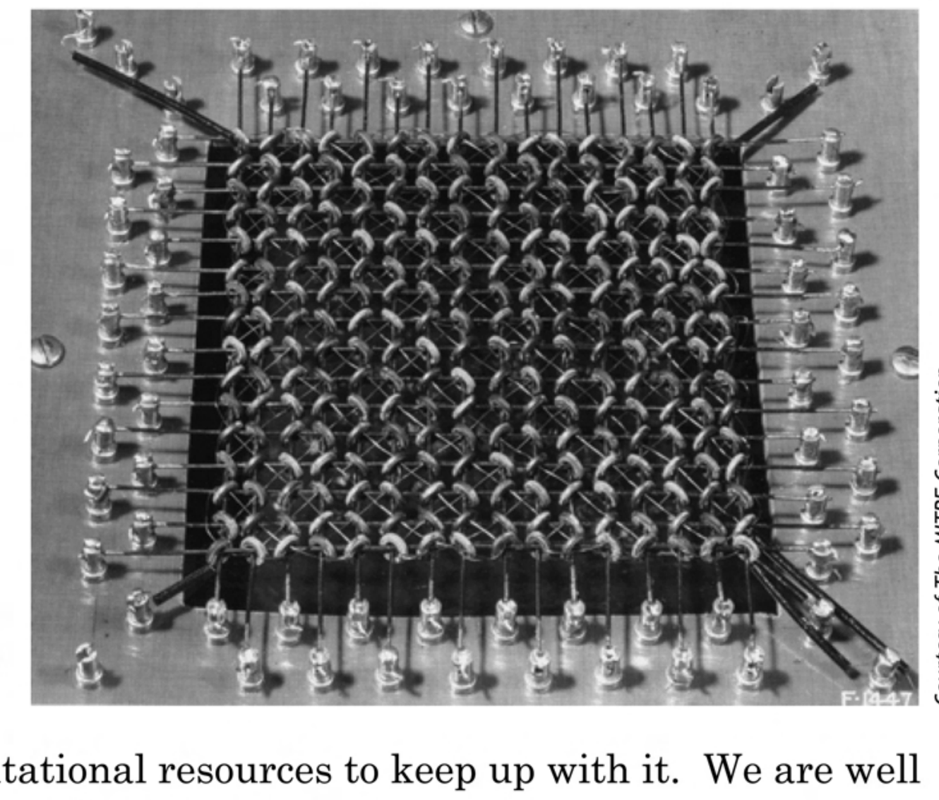
On-line Programs:
- Scan

Off-line Programs:
- Tabulate
- Plot
- Strip
- Search
- Synthesis
- Reconstruct
- Duplicate
- Print
- Edit

Once the mass spectral data acquisition phase was complete, off-line programs were loaded to read the data tapes, tabulate and plot data, perform background subtraction of one spectrum from another, and perform searches to identify analyte mass spectra by comparison with library spectra. "Synthesis" permitted the creation and management of mass spectral libraries and "Reconstruct" provided a means to create reconstructed ion current plots, 'mass chromatograms.'

RAM Limitations

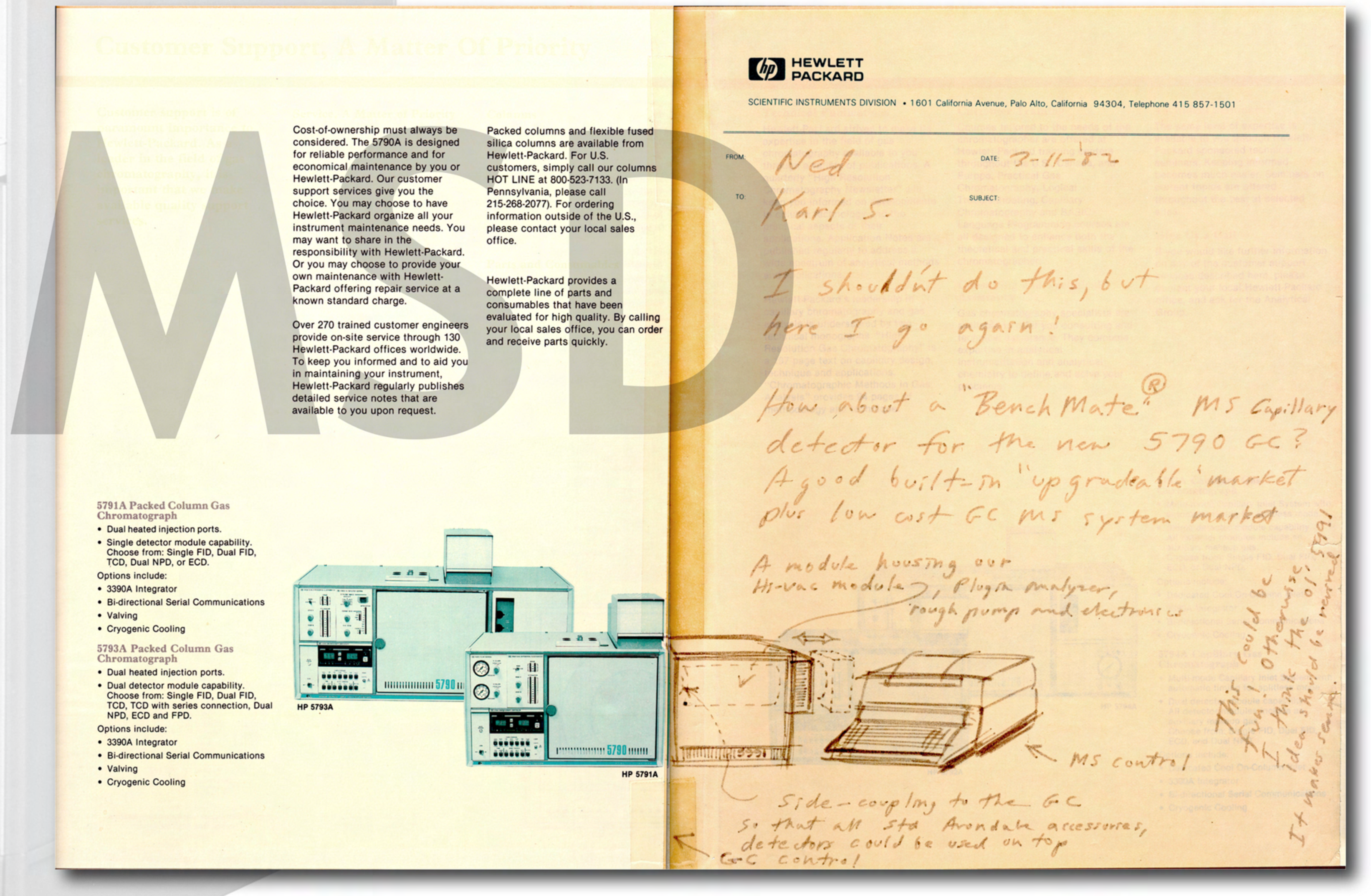
One of the most limiting aspects of minicomputers in the mid '60s to mid '70s was the issue of random access memory, RAM, sometimes called core memory. Core memory technology was bulky, slow, and expen$ive.[11] 8K of core memory was standard; although systems could be configured up to 32K, provided you had enough money. The HP series of computers were based on 16 bit words and one word of core memory cost in the neighborhood of a dollar in the mid '60s. Prices had decreased in the late '70s to 30 to 40¢ a word. Even at these reduced prices, half a meg of memory would cost in the range of $180,000! Needless to say, programming was extremely efficient.



Courtesy of The MITRE Corporation

Clearly, computing hardware and software have become more sophisticated and powerful since the period when the HP5932A GC/MS/DS was a viable product. The acquisition, processing, and analysis of mass spectral data at even higher scan speeds are routine with today's computational resources. Nevertheless, with increased emphasis on a wide variety of "-omic" applications, the amount of data that can be acquired in a short period of time is once again outpacing the ability of computational resources to keep up with it. We are well into The Second Data Crunch Crisis in Mass Spectrometry.

The HP-way in action This product concept, generated from a hand-drawn sketch, was one of the most successful GC/MS instruments in the world.



5972A

5973A MSD

5992A

5970A MSD

5971A MSD

1964
IBM introduces System/360 mainframe computer

DEC introduces the PDP-8, a 12 bit computer that is generally considered to be the first 'minicomputer'

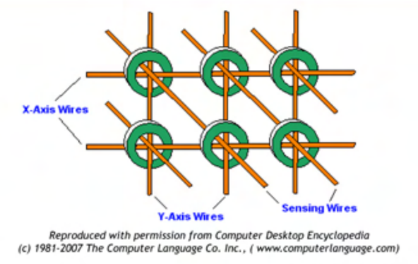
HP purchases DSI and folds it into DYMEC Division where the first HP minicomputer design is initiated, the HP2116A

ENIAC patent granted

1965
HP enters the analytical instrumentation field with the acquisition of GC manufacturer F&M Scientific Corporation of Avondale, Pennsylvania.

1967
HP introduces first derivative of HP2116A, the 2115A

1968
HP introduces second derivative of HP2116A, the 2114A



1970
HP introduces the HP2100A minicomputer for instrumentation control

HP enters the mass spectrometry market by establishing its Scientific Instrument Division in Palo Alto, California

1971
HP5930A analytical mass spectrometer based on dodecapole technology introduced

1976
HP5992 first benchtop GC/MS with hyperbolic rods

1980
HP GC/MS used at Lake Placid Olympic Games for drug testing

1982
HP5970 Mass Selective Detector introduced

1989
Wolfgang Paul and Hans G. Dehmelt receive the Nobel Prize "for the development of the ion trap technique"

1998
Compaq acquires DEC

1999
HP spins off instrument operations into Agilent and expands its computer business

2001
HP and Compaq merge