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Cover illustrations

Centre image: Trajectory of surface drifter 15371 in the vicinity of the Kuril Islands, western Pacific Ocean, for the period September 4 to December 3, 1993. The triangle denotes the start of the 90-day track. Squares denote 10-day positions along the trajectory. Depths are in meters.

Top left Image: Time series of the east-west component of surface current speed (u-component) as a function of time and water depth as the drifter advanced from the coast of Urup Island, through Friz Strait, and into the Sea of Okhotsk. The current variability was alternatively dominated by eddy-like features, wind-generated inertial motions, and regionally enhanced diurnal tidal currents.

Bottom left image: Wavelet (frequency-time domain) analysis for the clockwise rotary component of the current spectra. The graph highlights the timing and duration of episodic current events in the inertial, semidiurnal, and diurnal frequency bands as the drifter progressed from the open ocean through Friz Strait.

Illustrations taken from Thomson, R.E., P.H. LeBlond, and A.B. Rabinovich. 1997. Oceanic odyssey of a satellite-tracked drifter: North Pacific variability delineated by a single drifter trajectory. Journal of Oceanography, 53, 81-87.

DATA ANALYSIS METHODS IN PHYSICAL OCEANOGRAPHY

Second and Revised Edition

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Contents

Preface

Numerous books have been written on data analysis methods in the physical sciences over the past several decades. Most of these books lean heavily toward the theoretical aspects of data processing and few have been updated to include more modern techniques such as fractal analysis and rotary spectral decomposition. In writing this book we saw a clear need for a practical reference volume for earth and ocean sciences that brings established and modern techniques together under a single cover. The text is intended for students and established scientists alike. For the most part, graduate programs in oceanography have some form of methods course in which students learn about the measurement, calibration, processing and interpretation of geophysical data. The classes are intended to give the students needed experience in both the logistics of data collection and the practical problems of data processing and analysis. Because the class material generally is based on the experience of the faculty members giving the course, each class emphasizes different aspects of data collection and analysis. Formalism and presentation can differ widely. While it is valuable to learn from the first-hand experiences of the class instructor, it seemed to us important to have available a central reference text that could be used to provide some uniformity in the material being covered within the oceanographic community.

Many of the data analysis techniques most useful to oceanographers can be found in books and journals covering a wide variety of topics ranging from elementary statistics to wavelet transforms. Much of the technical information on these techniques is detailed in texts on numerical methods, time series analysis, and statistical techniques. In this book, we attempt to bring together many of the key data processing methods found in the literature, as well as add new information on data analysis techniques not readily available in older texts. We also provide, in Chapter 1, a description of most of the instruments used today in physical oceanography. Our hope is that the book will provide instructional material for students in the oceanographic sciences and serve as a general reference volume for those directly involved with oceanographic research.

The broad scope and rapidly evolving nature of oceanographic sciences has meant that it has not been possible for us to cover all existing or emerging data analysis methods. However, we trust that many of the methods and procedures outlined in the book will provide a basic understanding of the kinds of options available to the user for interpretation of data sets. Our intention is to describe general statistical and analytical methods that will be sufficiently fundamental to maintain a high level of utility over the years.

Finally, we believe that the analysis procedures discussed in this book apply to a wide readership in the geophysical sciences. As with oceanographers, this wider community of scientists would likely benefit from a central source of information that encompasses not only a description of the mathematical methods but also considers some of the practical aspects of data analyses. It is this synthesis between theoretical insight and the logistical limitations of real data measurement that is a primarily goal of this text.

William J. Emery and Richard E. Thomson
Boulder, Colorado and Sidney, BC

To our wives Dora Emery and Irma Thomson

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Many people have contributed to this book over the years that it has taken to write. The support and encouragement we received from our colleagues while we were drafting the manuscript is most gratefully acknowledged. Bill Emery began work on the book during a sabbatical year at the Institut für Meereskunde (IFM) in Kiel and is grateful for the hospitality of Drs Gerold Siedler, Wolfgang Kraus, Walter Zenk, Rolf Kasë, Juergen Willebrand, Juergen Kielman, and others. Additional progress was made at the University of British Columbia where Mrs Hiltrud Heckel aided in typing the handwritten text. Colleagues at the University of Colorado who helped with the book include Dr Robert Leben, who reviewed the text, contributed advice, text and figures, and Mr Dan Leatzow, who converted all of the initial text and figures to the Macintosh. The author would like to thank Mr Tom Kelecy for serving as the teaching assistant the first time that the material was presented in a course on "Engineering Data Analysis". Bill Emery also thanks the students who helped improve the book during the course on data analysis and the National Space and Aeronautics Administration (NASA) whose grant funding provided the laptop computer used in preparation of the manuscript. The author also thanks his family for tolerating the ever growing number of files labelled "dampo" on the family computer.

Rick Thomson independently began work on the book through the frustration of too much time spent looking for information on data analysis methods in the literature. There was clearly a need for a reference-type book that covers the wide range of analysis techniques commonly used by oceanographers and other geoscientists. Many of the ideas for the book originated with the author's studies as a research scientist within Fisheries and Oceans Canada, but work on the book was done strictly at home during evenings and weekends. Numerous conversations with Drs Dudley Chelton and Alexander Rabinovich helped maintain the author's enthusiasm for the project. The author wishes to thank his wife and two daughters (Justine and Karen) for enduring the constant tapping of the keyboard and hours of dark despair when it looked as if the book would never come to an end, and his parents (John and Irene) for encouraging an interest in science.

The authors would like to thank the colleagues and friends who took time from their research to review sections of the text or provide figures. There were others, far too numerous to mention, whose comments and words of advice added to the usefulness of the text. We are most grateful to Dudley Chelton of Oregon State University and Alexander Rabinovich of Moscow State University who spent considerable time criticizing the more mathematical chapters of the book. Dudley proved to be a most impressive reviewer and Sasha contributed several figures that significantly improved the section on time series analysis. George Pickard, Professor Emeritus of the University of British Columbia (UBC), and Susumu Tabata, Research Scientist Emeritus of the Institute of Ocean Sciences (IOS), provided thorough, and much appreciated, reviews of Chapters 1 and 2. We thank Andrew Bennett of Oregon State University for his comments on inverse methods in Chapter 4, Brenda Burd of Ecostat Research for reviewing the bootstrap method in Chapter 3, and Steve Mihaly for reviewing Appendix A. Contributions to the text were provided by Libe Washburn (University of California, Santa Barbara), Peter Schlussel (IFM), Patrick Cummins (IOS), and Mike Woodward (IOS). Figures or data were generously provided by Mark E. Geneau (Inter-Ocean Systems, Inc.), Gail Gabel (G.S. Gabel Associates), R. Lee Gordon (RD Instruments, Inc.), Diane Masson, Humfrey Melling, George Chase, John Love, and Tom Juhász (IOS), Jason Middleton and Greg Nippard (University of New South Wales), Doug Bennett (Sea-Bird Electronics, Inc.), Dan Schaas and Marcia Gracia (General Oceanics), Mayra Pazos (National Oceanic and Atmospheric Administration), Chris Garrett (University of Victoria), David Halpern (Jet Propulsion Laboratory), Phillip Richardson (Woods Hole Oceanographic Institution), Daniel Jamous (Massachusetts Institute of Technology), Paul Dragos (Battelle Ocean Sciences), Thomas Rossby (University of Rhode Island), Lynne Talley (Scripps), Adrian Dolling and Jane Eert (Channel Consulting), and Gary Hamilton (Intelex Research).

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Lastly, we would like to thank our colleagues who found and reported errors and omissions in the first printing of the book. Although the inevitable typos and mistakes are discouraging for the authors (and frustrating for the reader), it is better that we know about them so that they can be corrected in future printings and revisions. Our thanks to Brian Blanton (University of North Carolina), Mike Foreman (Institute of Ocean Sciences), Denis Gilbert (Institute Maurice-Lamontagne), Jack Harlan (NOAA, Boulder, Colorado), Clive Holden (Oceanographic Field Services, Pymbla, New South Wales), Frank Janssen (University of Hamburg), Masahisa Kubota (Tokai University), Robert Leben (University of Colorado), Rolf Lueck (University of Victoria), Andrew Slater (University of Colorado), and Roy Hourston (WeatherWorks Consulting, Victoria).

CHAPTER 1

Data Acquisition and Recording

1.1 INTRODUCTION

Physical oceanography is an evolving science in which the instruments, types of observations and methods of analysis have undergone considerable change over the last few decades. With most advances in oceanographic theory, instrumentation, and software, there have been significant advances in marine science. The advent of digital computers has revolutionized data collection procedures and the way that data are reduced and analyzed. No longer is the individual scientist personally familiar with each data point and its contribution to his or her study. Instrumentation and data collection are moving out of direct application by the scientist and into the hands of skilled technicians who are becoming increasingly more specialized in the operation and maintenance of equipment. New electronic instruments operate at data rates not possible with earlier mechanical devices and produce volumes of information that can only be handled by high-speed computers. Most modern data collection systems transmit sensor data directly to computer-based data acquisition systems where they are stored in digital format on some type of electronic medium such as a tape, hard-drive, or optical disk. High-speed analog-to-digital (AD) converters and digital-signal-processors (DSPs) are now used to convert voltage or current signals from sensors to digital values.

With the many technological advances taking place, it is important for oceanographers to be aware of both the capabilities and limitations of their sampling equipment. This requires a basic understanding of the sensors, the recording systems and the data-processing tools. If these are known and the experiment carefully planned, many problems commonly encountered during the processing stage can be avoided. We cannot overemphasize the need for thoughtful experimental planning and proper calibration of all oceanographic sensors. If instruments are not in near-optimal locations or the researcher is unsure of the values coming out of the machines, then it will be difficult to believe the results gathered in the field. To be truly reliable, instruments should be calibrated on a regular basis at intervals determined by use and the susceptibility of the sensor to drift. More specifically, the output from some instruments such as the piezoelectric pressure sensors and fixed pathlength transmissometers drift with time and need to be calibrated before and after each field deployment. For example, the zero point for the Paroscientific Digiquartz (0–10,000 psi) pressure sensors used in the Hawaii Ocean Time-series (HOT) at station "Aloha" 100 km north of Honolulu drifts about 4 dbar in three years. As a consequence, the sensors are calibrated about every six months against a Paroscientific laboratory standard, which is recalibrated periodically at special calibration facilities in the United States (Lukas, 1994). Our experience also shows that over-the-side field calibrations during oceanic surveys can be highly valuable. As we discuss in the following chapters, there are a number of fundamental requirements to be considered when planning the collection of field records, including such basic considerations as the sampling interval, sampling duration and sampling location.

It is the purpose of this chapter to review many of the standard instruments and measurement techniques used in physical oceanography in order to provide the reader with a common understanding of both the utility and limitations of the resulting measurements. The discussion is not intended to serve as a detailed "user's manual" nor as an "observer's handbook". Rather, our purpose is to describe the fundamentals of the instruments in order to give some insight into the data they collect. An understanding of the basic observational concepts, and their limitations, is a prerequisite for the development of methods, techniques and procedures used to analyze and interpret the data that are collected.

Rather than treat each measurement tool individually, we have attempted to group them into generic classes and to limit our discussion to common features of the particular instruments and associated techniques. Specific references to particular company products and the quotation of manufacturer's engineering specifications have been avoided whenever possible. Instead, we refer to published material addressing the measurement systems or the data recorded by them. Those studies which compare measurements made by similar instruments are particularly valuable.

The emphasis of the instrument review section is to give the reader a background in the collection of data in physical oceanography. For those readers interested in more complete information regarding a specific instrument or measurement technique, we refer to the references at the end of the book where we list the sources of the material quoted. We realize that, in terms of specific measurement systems, and their review, this text will be quickly dated as new and better systems evolve. Still, we hope that the general outline we present for accuracy, precision and data coverage will serve as a useful guide to the employment of newer instruments and methods.

1.2 BASIC SAMPLING REQUIREMENTS

A primary concern in most observational work is the accuracy of the measurement device, a common performance statistic for the instrument. Absolute accuracy requires frequent instrument calibration to detect and correct for any shifts in behavior. The inconvenience of frequent calibration often causes the scientist to substitute instrument precision as the measurement capability of an instrument. Unlike absolute accuracy, precision is a relative term and simply represents the ability of the instrument to repeat the observation without deviation. Absolute accuracy further requires that the observation be consistent in magnitude with some absolute reference standard. In most cases, the user must be satisfied with having good precision and repeatability of the measurement rather than having absolute measurement accuracy. Any instrument that fails to maintain its precision, fails to provide data that can be handled in any meaningful statistical fashion. The best instruments are those that provide both high precision and defensible absolute accuracy.

Digital instrument resolution is measured in bits, where a resolution of N bits means that the full range of the sensor is partitioned into 2^N equal segments ($N = 1, 2, \ldots$). For example, eight-bit resolution means that the specified full-scale range of the sensor, say $V = 10$ volts, is divided into $2^8 = 256$ increments, with a bit-resolution of $V/256 = 0.039$ volts. Whether the instrument can actually measure to a resolution or accuracy of $V/2^N$ units is another matter. The sensor range can always be divided into an increasing number of smaller increments but eventually one reaches a point where the value of each bit is buried in the noise level of the sensor.

1.2.1 Sampling interval

Assuming the instrument selected can produce reliable and useful data, the next highest priority sampling requirement is that the measurements be collected often enough in space and time to resolve the phenomena of interest. For example, in the days when oceanographers were only interested in the mean stratification of the world ocean, water property profiles from discrete-level hydrographic (bottle) casts were adequate to resolve the general vertical density structure. On the other hand, these same discrete-level profiles failed to resolve the detailed structure associated with interleaving and mixing processes that now are resolved by the rapid vertical sampling of modern conductivity–temperature–depth (CTD) profilers. The need for higher resolution assumes that the oceanographer has some prior knowledge of the process of interest. Often this prior knowledge has been collected with instruments incapable of resolving the true variability and may only be suggested by highly aliased (distorted) data collected using earlier techniques. In addition, theoretical studies may provide information on the scales that must be resolved by the measurement system.

For discrete digital data $x(t_i)$ measured at times t_i, the choice of the sampling increment Δt (or Δx in the case of spatial measurements) is the quantity of importance. In essence, we want to sample often enough that we can pick out the highest frequency component of interest in the time-series but not oversample so that we fill up the data storage file, use up all the battery power, or become swamped with a lot of unnecessary data. We might also want to sample at irregular intervals to avoid built-in bias in our sampling scheme. If the sampling interval is too large to resolve higher frequency components, it becomes necessary to suppress these components during sampling using a sensor whose response is limited to frequencies equal to that of the sampling frequency. As we discuss in our section on processing satellite-tracked drifter data, these lessons are often learned too late—after the buoys have been cast adrift in the sea.

The important aspect to keep in mind is that, for a given sampling interval Δt, the highest frequency we can hope to resolve is the *Nyquist* (or *folding*) *frequency*, f_N, defined as

$$f_N = 1/(2\Delta t) \tag{1.2.1}$$

We cannot resolve any higher frequencies than this. For example, if we sample every 10 h, the highest frequency we can hope to see in the data is $f_N = 0.05$ cph (cycles per hour). Equation (1.2.1) states the obvious—that it takes at least two sampling intervals (or three data points) to resolve a sinusoidal-type oscillation with period $1/f_N$ (Figure

1.2.1). In practice, we need to contend with noise and sampling errors so that it takes something like three or more sampling increments (i.e. $\geq$four data points) to accurately determine the highest observable frequency. Thus, f_N is an upper limit. The highest frequency we can resolve for a sampling of Δt = 10 h in Figure 1.2.1 is closer to $1/3\Delta t \approx 0.033$ cph.

An important consequence of (1.2.1) is the problem of *aliasing*. In particular, if there is considerable energy at frequencies $f > f_N$—which we obviously cannot resolve because of the Δt we picked—this energy gets folded back into the range of frequencies, $f < f_N$, which we are attempting to resolve. This unresolved energy doesn't disappear but gets redistributed within the frequency range of interest. What is worse is that the folded-back energy is disguised (or aliased) within frequency components different from those of its origin. We cannot distinguish this folded-back energy from that which actually belongs to the lower frequencies. Thus, we end up with erroneous (aliased) estimates of the spectral energy variance over the resolvable range of frequencies. An example of highly aliased data would be 13-h sampling of currents in a region having strong semidiurnal tidal currents. More will be said on this topic in Chapter 5.

As a general rule, one should plan a measurement program based on the frequencies and wavenumbers (estimated from the corresponding periods and wavelengths) of the parameters of interest over the study domain. This requirement then dictates the selection of the measurement tool or technique. If the instrument cannot sample rapidly enough to resolve the frequencies of concern it should not be used. It should be emphasized that the Nyquist frequency concept applies to both time and space and the Nyquist wavenumber is a valid means of determining the fundamental wavelength that must be sampled.

1.2.2 Sampling duration

The next concern is that one samples long enough to establish a statistically significant picture of the process being studied. For time-series measurements, this amounts to a requirement that the data be collected over a period sufficiently long that

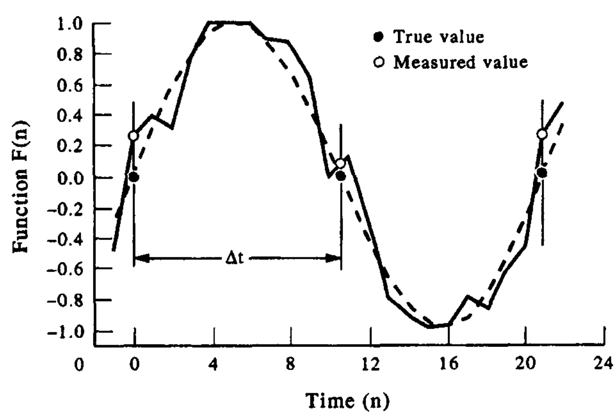

Figure 1.2.1. Plot of the function F(n) = *sin* $(2\pi n/20 + \phi)$ *where time is given by the integer* $n = -1, 0, ..., 24$. *The period* $2\Delta t = 1/f_N$ *is 20 units and* ϕ *is a random phase with a small magnitude in the range* ± 0.1. *Open circles denote measured points and solid points the curve F(n). Noise makes it necessary to use more than three data values to accurately define the oscillation period.*

repeated cycles of the phenomenon are observed. This also applies to spatial sampling where statistical considerations require a large enough sample to define multiple cycles of the process being studied. Again, the requirement places basic limitations on the instrument selected for use. If the equipment cannot continuously collect the data needed for the length of time required to resolve repeated cycles of the process, it is not well suited to the measurement required.

Consider the duration of the sampling at time step Δt. The longer we make the record the better we are to resolve different frequency components in the data. In the case of spatially separated data, Δx, resolution increases with increased spatial coverage of the data. It is the total record length $T = N\Delta t$ obtained for N data samples that: (1) determines the lowest frequency (the *fundamental frequency*)

$$f_o = 1/(N\Delta t) = 1/T \tag{1.2.2}$$

that can be extracted from the time-series record; (2) determines the frequency resolution or minimum difference in frequency $\Delta f = |f_2 - f_1| = 1/N\Delta t$ that can be resolved between adjoining frequency components, f_1 and f_2 (Figure 1.2.2); and (3) determines the amount of band averaging (averaging of adjacent frequency bands) that can be applied to enhance the statistical significance of individual spectral estimates. In Figure 1.2.2, the two separate waveforms of equal amplitude but different frequency produce a single spectrum. The two frequencies are well resolved for $\Delta f = 2/N\Delta t$ and $3/2N\Delta t$, just resolved for $\Delta f = 1/N\Delta t$, and not resolved for $\Delta f = 1/2N\Delta t$.

In theory, we should be able to resolve all frequency components, f, in the frequency range $f_o \leq f \leq f_N$, where f_N and f_o are defined by (1.2.1) and (1.2.2), respectively. Herein lies a classic sampling problem. In order to resolve the frequencies of interest in a time-series, we need to sample for a long time (T large) so that f_o covers the low end of the frequency spectrum and Δf is small (frequency resolution is high). At the same time, we would like to sample sufficiently rapidly (Δt small) so that f_N extends beyond all frequency components with significant spectral energy. Unfortunately, the longer and more rapidly we want to sample the more data we need to collect and store, the more time, effort and money we need to put into the sampling and the better resolution we require from our sensors.

Our ability to resolve frequency components follows from Rayleigh's criterion for the resolution of adjacent spectral peaks in light shone onto a diffraction grating. It states that two adjacent frequency components are just resolved when the peaks of the spectra are separated by frequency difference $\Delta f = f_o = 1/N\Delta t$ (Figure 1.2.2). For example, to separate the spectral peak associated with the lunar–solar semidiurnal tidal component M_2 (frequency = 0.08051 cph) from that of the solar semidiurnal tidal component S_2 (0.08333 cph), for which $\Delta f = 0.00282$ cph, requires $N = 355$ data points at a sampling interval $\Delta t = 1$ h or $N = 71$ data points at $\Delta t = 5$ h. Similarly, a total of 328 data values at 1-h sampling are needed to separate the two main diurnal constituents K_1 and O_1 ($\Delta f = 0.00305$ cph). Note that if f_N is the highest frequency we can measure and f_o is the limit of frequency resolution, then

$$f_N/f_o = (1/2\Delta t)/(1/N\Delta t) = N/2 \tag{1.2.3}$$

is the maximum number of Fourier components we can hope to estimate in any analysis.

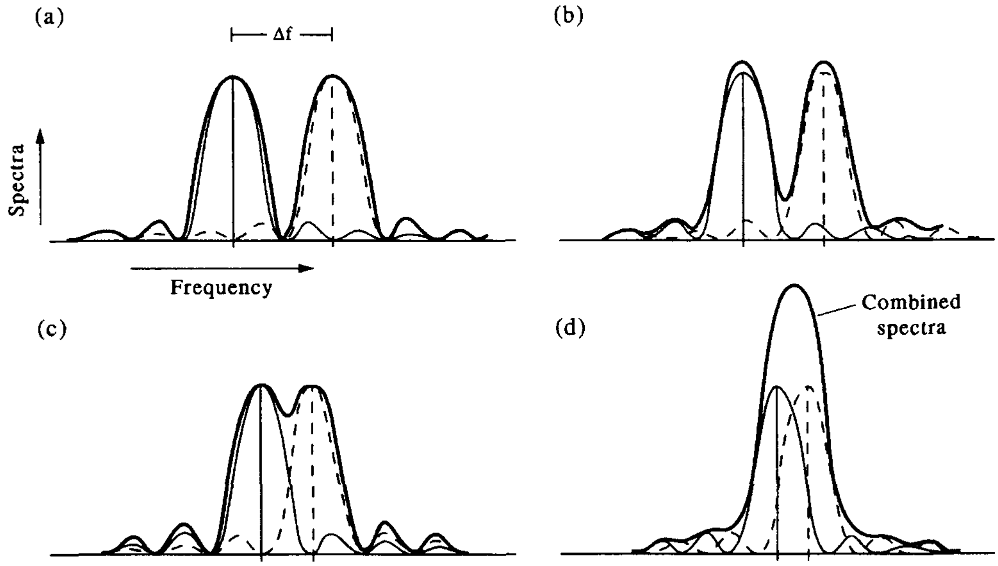

Figure 1.2.2. Spectral peaks of two separate waveforms of equal amplitude and frequencies f_1 and f_2 (dashed and thin line) together with the calculated spectrum (solid line). (a) and (b) are well-resolved spectra; (c) just resolved spectra; and (d) not resolved. Thick solid line is total spectrum for two underlying signals with slightly different peak frequencies.

1.2.3 Sampling accuracy

According to the two previous sections, we need to sample long and often if we hope to resolve the range of scales of interest in the variables we are measuring. It is intuitively obvious that we also need to sample as accurately as possible—with the degree of recording accuracy determined by the response characteristics of the sensors, the number of bits per data record (or parameter value) needed to raise measurement values above background noise, and the volume of data we can live with. There is no use attempting to sample the high or low ends of the spectrum if the instrument cannot respond rapidly or accurately enough to resolve changes in the parameter being measured. In addition, there are several approaches to this aspect of data sampling including the brute-force approach in which we measure as often as we can at the degree of accuracy available and then improve the statistical reliability of each data record through post-survey averaging, smoothing, and other manipulation.

1.2.4 Burst sampling versus continuous sampling

Regularly-spaced, digital time-series can be obtained in two different ways. The most common approach is to use a *continuous sampling mode*, in which the data are sampled at equally spaced intervals $t_k = t_o + k\Delta t$ from the start time t_o. Here, k is a positive integer. Regardless of whether the equally spaced data have undergone internal averaging or decimation using algorithms built into the machine, the output to the data storage file is a series of individual samples at times t_k. (Here, "decimation" is used in the loose sense of removing every nth data point, where n is any positive integer, and not in the sense of the ancient Roman technique of putting to death one in ten soldiers in a legion guilty of mutiny or other crime.) Alternatively, we can use a *burst sampling mode*, in which rapid sampling is undertaken over a relatively short time interval Δt_B or "burst" embedded within each regularly spaced time interval, Δt. That is, the data are sampled at high frequency for a short duration starting (or ending) at times t_k for which the burst duration $\Delta t_B \ll \Delta t$. The instrument "rests" between bursts.

There are advantages to the burst sampling scheme, especially in noisy (high frequency) environments where it may be necessary to average-out the noise to get at the frequencies of interest. Burst sampling works especially well when there is a "spectral gap" between fluctuations at the high and low ends of the spectrum. As an example, there is typically a spectral gap between surface gravity waves in the open ocean (periods of 1–20 s) and the 12-hourly motions that characterize semidiurnal tidal currents. Thus, if we wanted to measure surface tidal currents using the burst-mode option for our current meter, we could set the sampling to a 2-min burst every hour; this option would smooth out the high-frequency wave effects but provide sufficient numbers of velocity measurements to resolve the tidal motions. Burst sampling enables us to filter out the high-frequency noise and obtain an improved estimate of the variability hidden underneath the high-frequency fluctuations. In addition, we can examine the high-frequency variability by scrutinizing the burst sampled data. If we were to sample rapidly enough, we could estimate the surface gravity wave energy spectrum. Many oceanographic instruments use (or have provision for) a burst-sampling data collection mode. The "duty cycle" often used to collect positional data from satellite-tracked drifters is a cost-saving form of burst sampling in which all positional data within a 24-h period (about 10 satellite fixes) are collected only every third day. Tracking costs paid to Service Argos are reduced by a factor of three using the duty cycle. Problems arise when the length of each burst is too short to resolve energetic motions with periods comparable to the burst sample length. In the case of satellite-tracked drifters poleward of tropical latitudes, these problems are associated with highly energetic inertial motions whose periods $T = 1/(2\Omega \sin\theta)$ are comparable to the 24-h duration of the burst sample (here, $\Omega = 0.1161 \times 10^{-4}$ cycles per second is the earth's rate of rotation and $\theta \equiv$ latitude). Since 1992, it has been possible to improve resolution of high-frequency motions using a 1/3 duty cycle of 8 h "on" followed by 16 h "off". According to Bograd *et al.* (1999), even better resolution of high-frequency mid-latitude motions could be obtained using a duty cycle of 16 h "on" followed by 32 h "off".

1.2.5 Regularly versus irregularly sampled data

In certain respects, an irregular sampling in time or nonequidistant placement of instruments can be more effective than a more esthetically appealing uniform sampling. For example, unequal spacing permits a more statistically reliable resolution of oceanic spatial variability by increasing the number of quasi-independent estimates of the dominant wavelengths (wavenumbers). Since oceanographers are almost always faced with having fewer instruments than they require to resolve oceanic features, irregular spacing can also be used to increase the overall spatial coverage (fundamental wavenumber) while maintaining the small-scale instrument separation for Nyquist wavenumber estimates. The main concern is the lack of redundancy should certain key instruments fail, as often seems to happen. In this case, a quasi-regular spacing between locations is better. Prior knowledge of the scales of variability to expect is a definite plus in any experimental array design.

In a sense, the quasi-logarithmic vertical spacing adopted by oceanographers for bottle cast (hydrographic) sampling of 0, 10, 20, 30, 50, 75, 100, 125, 150 m, etc. represents a "spectral window" adaptation to the known physical–chemical structure of the ocean. Highest resolution is required near the surface where vertical changes are most rapid. Similarly, an uneven spatial arrangement of observations increases the number of quasi-independent estimates of the wavenumber spectrum. Digital data are most often sampled (or subsampled) at regularly-spaced time increments. Aside from the usual human propensity for order, the need for regularly-spaced data derives from the fact that most analysis methods have been developed for regular-spaced data. However, digital data do not necessarily need to be sampled at regularly-spaced time increments to give meaningful results, although some form of interpolation between values may eventually be required.

1.2.6 Independent realizations

As we review the different instruments and methods, the reader should keep in mind the three basic concerns of accuracy/precision, resolution (spatial and temporal), and statistical significance (statistical sampling theory). A fundamental consideration in ensuring the statistical significance of a set of measurements is the need for independent realizations. If repeat measurements of a process are strongly correlated, they provide no new information and do not contribute to the statistical significance of the measurements. Often a subjective decision must be made on the question of statistical independence. While this concept has a formal definition, in practice it is often difficult to judge. A simple guide suggested here is that any suite of measurements that is highly correlated (in time or space) cannot be independent. At the same time, a group of measurements that is totally uncorrelated, must be independent. In the case of no correlation, the number of "degrees of freedom" is defined by the total number of measurements; for the case of perfect correlation, the redundancy of the data values reduces the degrees of freedom to one for scalar quantity and to two for a vector quantity. The degree of correlation in the data set provides a way of roughly estimating the number of degrees of freedom within a given suite of observations. While more precise methods will be presented later in this text, a simple linear relation between degrees of freedom and correlation often gives the practitioner a way to proceed without developing complex mathematical constructs.

As will be discussed in detail later, all of these sampling recommendations have statistical foundations and the guiding rules of probability and estimation can be carefully applied to determine the sampling requirements and dictate the appropriate measurement system. At the same time, these same statistical methods can be applied to existing data in order to better evaluate their ability to measure phenomena of interest. These comments are made to assist the reader in evaluating the potential of a particular instrument (or method) for the measurement of some desired variable.

1.3 TEMPERATURE

The measurement of temperature in the ocean uses conventional techniques except for deep observations where hydrostatic pressures are high and there is a need to protect the sensing system from ambient depth/temperature changes higher in the water column as the sensor is returned to the ship. Temperature is the ocean property that is easiest to measure accurately. Some of the ways in which ocean temperature can be measured are:

(a) Expansion of a liquid or a metal.
(b) Differential expansion of two metals (bimetallic strip).
(c) Vapor pressure of a liquid.
(d) Thermocouples.
(e) Change in electrical resistance.
(f) Infrared radiation from the sea surface.

In most of these sensing techniques, the temperature effect is very small and some form of amplification is necessary to make the temperature measurement detectable. Usually, the response is nearly linear with temperature so that only the first-order term is needed when converting the sensor measurement to temperature. However, in order to achieve high precision over large temperature ranges, second, third and even fourth order terms must sometimes be used to convert the measured variable to temperature.

1.3.1 Mercury thermometers

Of the above methods, (a), (e), and (f) have been the most widely used in physical oceanography. The most common type of the liquid expansion sensor is the mercury-in-glass thermometer. In their earliest oceanographic application, simple mercury thermometers were lowered into the ocean with hopes of measuring the temperature at great depths in the ocean. Two effects were soon noticed. First, thermometer housings with insufficient strength succumbed to the greater pressure in the ocean and were crushed. Second, the process of bringing an active thermometer through the oceanic vertical temperature gradient sufficiently altered the deeper readings that it was not possible to accurately measure the deeper temperatures. An early solution to this problem was the development of min–max thermometers that were capable of retaining the minimum and maximum temperatures encountered over the descent and ascent of the thermometer. This type of thermometer was widely used on the Challenger expedition of 1873–1876.

The real breakthrough in thermometry was the development of reversing thermometers, first introduced in London by Negretti and Zambra in 1874 (Sverdrup *et al.*, 1942, p. 349). The reversing thermometer contains a mechanism such that, when the thermometer is inverted, the mercury in the thermometer stem separates from the bulb reservoir and captures the temperature at the time of inversion. Subsequent temperature changes experienced by the thermometer have limited effects on the amount of mercury in the thermometer stem and can be accounted for when the temperature is read on board the observing ship. This "break-off" mechanism is based on the fact that more energy is required to create a gas-mercury interface (i.e. to break the mercury) than is needed to expand an interface that already exists. Thus, within the "pigtail" section of the reversing thermometer is a narrow region called the "break-off point", located near appendix C in Figure 1.3.1, where the mercury will break when the thermometer is inverted.

The accuracy of the reversing thermometer depends on the precision with which this break occurs. In good reversing thermometers this precision is better than 0.01°C. In standard mercury-in-glass thermometers, as well as in reversing thermometers, there are concerns other than the break point which affect the precision of the temperature measurement. These are:

(a) Linearity in the expansion coefficient of the liquid.
(b) The constancy of the bulb volume.

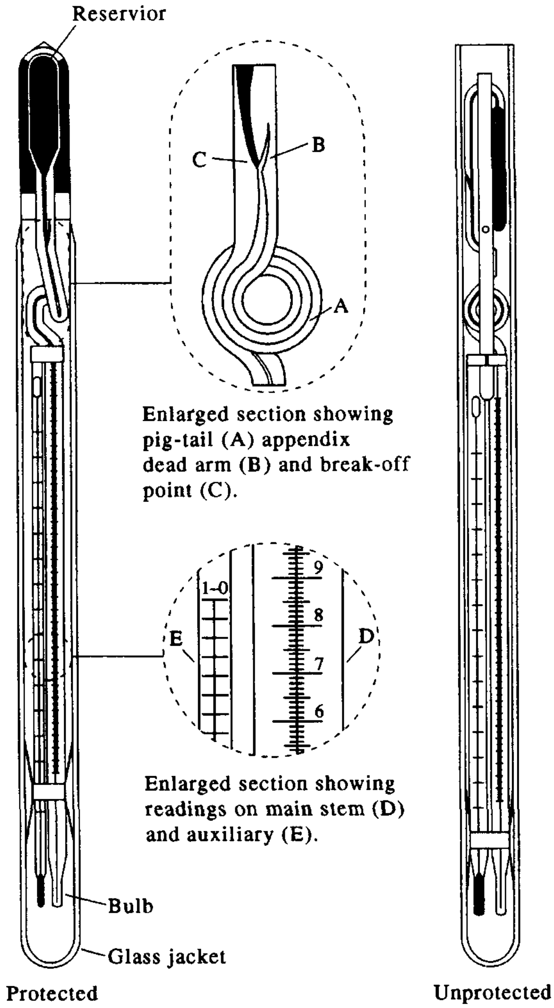

Figure 1.3.1. Details of a reversing mercury thermometer showing the"pigtail appendix".

(c) The uniformity of the capillary bore.
(d) The exposure of the thermometer stem to temperatures other than the bulb temperature.

Mercury expands in a near-linear manner with temperature. As a consequence, it has been the liquid used in most high precision, liquid–glass thermometers. Other liquids such as alcohol and toluene are used in precision thermometers only for very low temperature applications where the higher viscosity of mercury is a limitation. Expansion linearity is critical in the construction of the thermometer scale which would be difficult to engrave precisely if expansion were nonlinear.

In a mercury thermometer, the volume of the bulb is equivalent to about 6000 stem-degrees Celsius. This is known as the "degree volume" and usually is considered to comprise the bulb plus the portion of the stem below the mark. If the thermometer is to retain its calibration, this volume must remain constant with a precision not commonly realized by the casual user. For a thermometer precision within ± 0.01°C, the bulb volume must remain constant within one part in 600,000. Glass does not have ideal mechanical properties and it is known to exhibit some plastic behavior and deform under sustained stress. Repeated exposure to high pressures may produce permanent deformation and a consequent shift in bulb volume. Therefore, precision can only be maintained by frequent laboratory calibration. Such shifts in bulb volume can be detected and corrected by the determination of the "ice point" (a slurry of water plus ice) which should be checked frequently if high accuracy is required. The procedure is more or less obvious but a few points should be considered. First the ice should be made from distilled water and the water–ice mixture should also be made from distilled water. The container should be insulated and at least 70% of the bath in contact with the thermometer should be chopped ice. The thermometer should be immersed for five or more minutes during which time the ice–water mixture should be stirred continuously. The control temperature of the bath can be taken by an accurate thermometer of known reliability. Comparison with the temperature of the reversing thermometer, after the known calibration characteristics have been accounted for, will give an estimate of any offsets inherent in the use of the reversing thermometer in question.

The uniformity of the capillary bore is critical to the accuracy of the mercury thermometer. In order to maintain the linearity of the temperature scale it is necessary to have a uniform capillary as well as a linear response liquid element. Small variations in the capillary can occur as a result of small differences in cooling during its construction or to inhomogeneities in the glass. Errors resulting from the variations in capillary bore can be corrected through calibration at known temperatures. The resulting corrections, including any effect of the change in bulb volume, are known as "index corrections". These remain constant relative to the ice point and, once determined, can be corrected for a shift in the ice point by addition or subtraction of a constant amount. With proper calibration and maintenance, most of the mechanical defects in the thermometer can be accounted for. Reversing thermometers are then capable of accuracies of $\pm 0.01°C$, as given earlier for the precision of the mercury break-point. This accuracy, of course, depends on the resolution of the temperature scale etched on the thermometer. For high accuracy in the typically weak vertical temperature gradients of the deep ocean, thermometers are etched with scale intervals between 0.1 and 0.2°C. Most reversing thermometers have scale intervals of 0.1°C.

The reliability and calibrated absolute accuracy of reversing thermometers continue to provide a standard temperature measurement against which all forms of electronic sensors are compared and evaluated. In this role as a calibration standard, reversing thermometers continue to be widely used. In addition, many oceanographers still believe that standard hydrographic stations made with sample bottles and reversing thermometers, provide the only reliable data. For these reasons, we briefly describe some of the fundamental problems that occur when using reversing thermometers. An understanding of these errors may also prove helpful in evaluating the accuracy of reversing thermometer data that are archived in the historical data file. The primary malfunction that occurs with a reversing thermometer is a failure of the mercury to break at the correct position. This failure is caused by the presence of gas (a bubble) somewhere within the mercury column. Normally all thermometers contain some gas within the mercury. As long as the gas bubble has sufficient mercury compressing it, the bubble volume is negligible, but if the bubble gets into the upper part of the capillary tube it expands and causes the mercury to break at the bubble rather than at the break-off point. The proper place for this resident gas is at the bulb end of the mercury; for this reason it is recommended that reversing thermometers always be stored and transported in the bulb-up (reservoir-down) position. Rough handling can be the cause of bubble formation higher up in the capillary tube. Bubbles lead to consistently offset temperatures and a record of the thermometer history can clearly indicate when such a malfunction has occurred. Again the practice of renewing, or at least checking, the thermometer calibration is essential to ensuring accurate temperature measurements. As with most oceanographic equipment, a thermometer with a detailed history is much more valuable than a new one without some prior use.

There are two basic types of reversing thermometers: (1) protected thermometers which are encased completely in a glass jacket and not exposed to the pressure of the water column; and (2) unprotected thermometers for which the glass jacket is open at one end so that the reservoir experiences the increase of pressure with ocean depth, leading to an apparent increase in the measured temperature. The increase in temperature with depth is due to the compression of the glass bulb, so that if the compressibility of the glass is known from the manufacturer, the pressure and hence the depth can be inferred from the temperature difference, $\Delta T = T_{\text{Unprotected}} - T_{\text{Protected}}$. The difference in thermometer readings, collected at the same depth, can be used to compute the depth to an accuracy of about 1% of the depth. This subject will be treated more completely in the section on depth/pressure measurement. We note here that the 1% accuracy for reversing thermometers exceeds the accuracy of 2–3% one normally expects from modern depth sounders.

Unless collected for a specific observational program or taken as calibrations for electronic measurement systems, reversing thermometer data are most commonly found in historical data archives. In such cases, the user is often unfamiliar with the precise history of the temperature data and thus cannot reconstruct the conditions under which the data were collected and edited. Under these conditions one generally assumes that the errors are of two types; either they are large offsets (such as errors in reading the thermometer) which are readily identifiable by comparison with other regional historical data, or they are small random errors due to a variety of sources and difficult to identify or separate from real physical oceanic variability. Parallax errors, which are one of the main causes of reading errors, are greatly reduced through use of an eye-piece magnifier. Identification and editing of these errors depends on the problem being studied and will be discussed in a later section on data processing.

1.3.2. The mechanical bathythermograph (MBT)

The MBT uses a liquid-in-metal thermometer to register temperature and a Bourdon tube sensor to measure pressure. The temperature sensing element is a fine copper tube nearly 17 m long filled with toluene (Figure 1.3.2). Temperature readings are recorded by a mechanical stylus which scratches a thin line on a coated glass slide. Although this instrument has largely been replaced by the expendable bathythermograph (XBT), the historical archives contain numerous temperature profiles collected using this device. It is, therefore, worthwhile to describe the instrument and the data it measures. Only the temperature measurement aspect of this device will be considered; the pressure/depth recording capability will be addressed in a latter section.

There are numerous limitations to the MBT. To begin with, it is restricted to depths less than 300 m. While the MBT was intended to be used with the ship underway, it is only really possible to use it successfully when the ship is traveling at no more than a

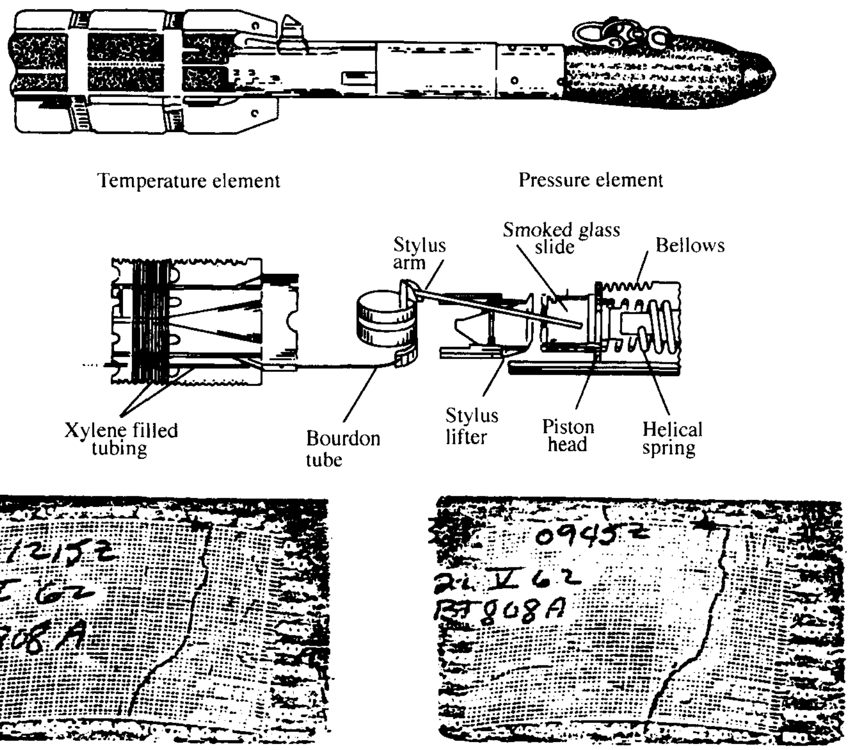

Figure 1.3.2. A bathythermograph showing its internal construction and sample BT slides.

few knots. At higher speeds, it becomes impossible to retrieve the MBT without the risk of hitting the instrument against the ship. Higher speeds also make it difficult to properly estimate the depth of the probe from the amount of wire out. The temperature accuracy of the MBT is restricted by the inherent lower accuracy of the liquid-in-metal thermometer. Metal thermometers are also subject to permanent deformation. Since metal is more subject to changes at high temperatures than is glass it is possible to alter the performance of the MBT by continued exposure to higher temperatures (i.e. by leaving the probe out in the sun). The metal return spring of the temperature stylus is also a source of potential problems in that it is subject to hysteresis and creep. Hysteresis, in which the up-trace does not coincide with the down-trace, is especially prevalent when the temperature differences are small. Creep occurs when the metal is subjected to a constant loading for long periods. Thus, an MBT continuously used in the heat of the tropics may be found later to have a slight positive temperature error.

Most of the above errors can be detected and corrected for by frequent calibration of the MBT. Even with regular calibration it is doubtful that the stated precision of 0.1°F (0.06°C) can be attained. Here, the value is given in °F since most of the MBTs were produced with these temperature scales. When considering MBT data from the historical data files, it should be realized that these data were entered into the files by hand. The usual method was to produce an enlarged black-and-white photograph of the temperature trace using the nonlinear calibration grid unique to each instrument. Temperature values were then read off of these photographs and entered into the data file at the corresponding depths. The usual procedure was to record temperatures for a fixed depth interval (i.e. 5 or 10 m) rather than to select out inflection points that best described the temperature profile. The primary weakness of this procedure is the ease with which incorrect values can enter the data file through misreading the temperature trace or incorrectly entering the measured value. Usually these types of errors result in large differences with the neighboring values and can be easily identified. Care should be taken, however, to remove such values before applying objective methods to search for smaller random errors. It is also possible that data entry errors can occur in the entry of date, time and position of the temperature profile and tests should be made to detect these errors.

1.3.3. Resistance thermometers (expendable bathythermograph: XBT)

Since the electrical resistance of metals, and other materials, changes with temperature, these materials can be used as temperature sensors. The resistance (R) of most metals depends on temperature (T) and can be expressed as a polynomial

$$R = R(1 + aT + bT^2 + cT^3 + \dots) \tag{1.2.4}$$

where a, b, and c are constants. In practice, it is usually assumed that the response is linear over some limited temperature range and the proportionality can be given by the value of the coefficient a (called the temperature resistance coefficient). The most commonly used metals are copper, platinum, and nickel which have temperature coefficients of 0.0043, 0.0039, and 0.0066 $(^\circ\mathrm{C})^{-1}$, respectively. Of these, copper has the most linear response but its resistance is low so that a thermal element would require many turns of fine wire and would consequently be expensive to produce. Nickel has a very high resistance but deviates sharply from linearity. Platinum has a relatively high resistance level, is very stable and has a relatively linear behavior. For these reasons, platinum resistance thermometers have become a standard by which the international scale of temperature is defined. Platinum thermometers are also widely used as laboratory calibration standards and have accuracies of $\pm 0.001^\circ$C.

The semiconductors form another class of resistive materials used for temperature measurements. These are mixtures of oxides of metals such as nickel, cobalt, and manganese which are molded at high pressure followed by sintering (i.e. heating to incipient fusion). The types of semiconductors used for oceanographic measurements are commonly called thermistors. These thermistors have the advantages that: (1) the temperature resistance coefficient of $-0.05(^\circ\mathrm{C})^{-1}$ is about ten times as great as that for copper; and (2) the thermistors may be made with high resistance for a very small physical size.

The temperature coefficient of thermistors is negative which means that the resistance decreases as temperature increases. This temperature coefficient is not a constant except over very small temperature ranges; hence the change of resistance with temperature is not linear. Instead, the relationship between resistance and temperature is given by

$$R(T) = R_o \exp[\beta(T^{-1} - T_o^{-1})] \tag{1.2.5}$$

where $R_o = \beta/T^2$ is the conventional temperature coefficient of resistance, and T and T_o are two absolute temperatures (K) with the respective resistance values of $R(T)$ and

R_o. Thus, we have a relationship whereby temperature T can be computed from the measurement of resistance $R(T)$.

One of the most common uses of thermistors in oceanography is in expendable bathythermographs (XBTs). The XBT was developed to provide an upper ocean temperature profiling device that operated while the ship was underway. The crucial development was the concept of depth measurement using the elapsed time for the known fall rate of a "freely-falling" probe. To achieve "free-fall", independent of the ship's motion, the data transfer cable is constructed from fine copper wire with feed-spools in both the sensor probe and in the launching canister (Figure 1.3.3). The details of the depth measurement capability of the XBT will be discussed and evaluated in the section on depth/pressure measurements.

The XBT probes employ a thermistor placed in the nose of the probe as the temperature sensing element. According to the manufacturer (Sippican Corp.; Marion, Massachusetts, U.S.A.), the accuracy of this system is ±0.1°C. This figure is determined from the characteristics of a batch of semiconductor material which has known resistance–temperature (R–T) properties. To yield a given resistance at a standard temperature, the individual thermistors are precision-ground, with the XBT probe thermistors ground to yield 5000 Ω (Ω is the symbol for the unit of ohms) at 25°C (Georgi *et al.*, 1980). If the major source of XBT probe-to-probe variability can be attributed to imprecise grinding, then a single-point calibration should suffice to reduce this variability in the resultant temperatures. Such a calibration was carried out by Georgi *et al.* (1980) both at sea and in the laboratory.

To evaluate the effects of random errors on the calibration procedure, twelve probes were calibrated repeatedly. The mean differences between the measured and bath temperatures was ±0.045°C with a standard deviation of 0.01°C. For the overall calibration comparison, 18 cases of probes (12 probes per case) were examined. Six cases of T7s (good to 800 m and up to 30 knots) and two cases of T6s (good to 500 m and at less than 15 knots) were purchased new from Sippican while the remaining 10 cases of T4s (good to 500 m up to 30 knots) were acquired from a large pool of XBT probes manufactured in 1970 for the U.S. Navy. The overall average standard deviation for the probes was 0.023°C which then reduces to 0.021°C when consideration is made for the inherent variability of the calibration procedure.

A separate investigation was made of the R–T relationship by studying the response characteristics for nine probes. The conclusion was that the R–T differences ranged from +0.011°C to −0.014°C which then means that the measured relationships were within ±0.014°C of the published relationship and that the calculation of new coefficients, following Steinhart and Hart (1968), is not warranted. Moreover the final conclusions of Georgi *et al.* (1980) suggest an overall accuracy for XBT thermistors of ±0.06°C at the 95% confidence level and that the consistency between thermistors is sufficiently high that individual probe calibration is not needed for this accuracy level.

Another method of evaluating the performance of the XBT system is to compare XBT temperature profiles with those taken at the same time with an higher accuracy profiler such as a CTD system. Such comparisons are discussed by Heinmiller *et al.* (1983) for data collected in both the Atlantic and the Pacific using calibrated CTD systems. In these comparisons, it is always a problem to achieve true synopticity in the data collection since the XBT probe falls much faster than the recommended drop rate for a CTD probe. Most of the earlier comparisons between XBT and CTD profiles (Flierl and Robinson, 1977; Seaver and Kuleshov, 1982) were carried out using XBT temperature profiles collected between CTD stations separated by 30 km. For the

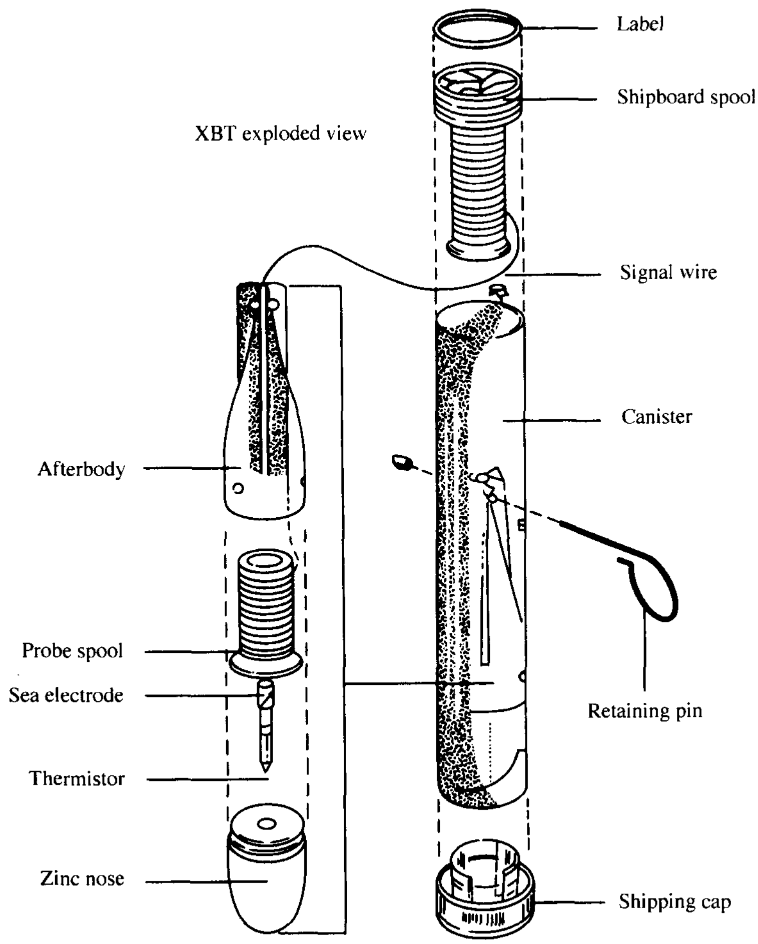

Figure 1.3.3. Exploded view of a Sippican Oceanographic Inc. XBT showing spool and canister.

purposes of intercomparison, it is better for the XBT and CTD profiles to be collected as simultaneously as possible.

The primary error discussed by Heinmiller *et al.* (1983) is that in the measurement of depth rather than temperature. There were, however, significant differences between temperatures measured at depths where the vertical temperature gradient was small and the depth error should make little or no contribution. Here, the XBT temperatures were found to be systematically higher than those recorded by the CTD. Sample comparisons were divided by probe type and experiment. The T4 probes (as defined above) yielded a mean XBT-CTD difference of about 0.19°C while the T7s (defined above) had a lower mean temperature difference of 0.13°C. Corresponding standard deviations of the temperature differences were 0.23°C, for the T4s, and 0.11°C for the T7s. Taken together, these statistics suggest an XBT accuracy less than the ±0.1°C given by the manufacturer and far less than the 0.06°C reported by Georgi *et al.* (1980) from their calibrations.

From these divergent results, it is difficult to decide where the true XBT temperature accuracy lies. Since the Heinmiller *et al.* (1983) comparisons were made *in situ* there are many sources of error that could contribute to the larger temperature differences. Even though most of the CTD casts were made with calibrated instruments, errors in operational procedures during collection and archival could add significant errors to the resultant data. Also, it is not easy to find segments of temperature profiles with no vertical temperature gradient and therefore it is difficult to ignore the effect of the depth measurement error on the temperature trace. It seems fair to conclude that the laboratory calibrations represent the ideal accuracy possible with the XBT system (i.e. better than ±0.1°C). In the field, however, one must expect other influences that will reduce the accuracy of the XBT measurements and an overall accuracy slightly more than ±0.1°C is perhaps realistic. Some of the sources of these errors can be easily detected, such as an insulation failure in the copper wire which results in single step offsets in the resulting temperature profile. Other possible temperature error sources are interference due to shipboard radio transmission (which shows up as high frequency noise in the vertical temperature profile) or problems with the recording system. Hopefully, these problems are detected before the data are archived in historical data files.

In closing this section we comment that, until recently, most XBT data were digitized by hand. The disadvantage of this procedure is that chart paper recording doesn't fully realize the potential digital accuracy of the sensing system and that the opportunities for operator recording errors are considerable. Again, some care should be exercised in editing out these large errors which usually result from the incorrect hand recording of temperature, date, time or position. It is becoming increasingly popular to use digital XBT recording systems which improve the accuracy of the recording and eliminate the possibility of incorrectly entering the temperature trace. Such systems are described, for example, in Stegen *et al.* (1975) and Emery *et al.* (1986). Today, essentially all research XBT data are collected with digital systems, while the analog systems are predominantly used by various international navies.

1.3.4 Salinity/conductivity–temperature–depth profilers

Resistance thermometers are widely used on continuous profilers designed to replace the earlier hydrographic profiles collected using a series of sampling bottles. The new *in situ* electronic instruments continuously sample the water temperature, providing much higher resolution information on the ocean's vertical and horizontal temperature structure. Since density also depends on salinity, electronic sensors were developed to measure salinity *in situ* and were incorporated into the profiling system. As discussed by Baker (1981), an early electronic profiling system for temperature and salinity was described by Jacobsen (1948). The system was limited to 400 m and used separate supporting and data transfer cables. Next, a system called the STD (salinity–temperature–depth) profiler was developed by Hamon and Brown in the mid-1950s (Hamon, 1955; Hamon and Brown, 1958). The evolution of the conductivity measurement, used to derive salinity, will be discussed in the section on salinity. This evolution led to the introduction of the conductivity–temperature–depth (CTD) profiling system (Brown, 1974). This name change identified improvements not only in the conductivity sensor but also in the temperature sensing system designed to overcome the mismatch in the response times of the temperature and conductivity sensors. This mismatch often resulted in erroneous salinity spikes in the earlier STD systems (Dantzler, 1974).