

Computer Modern. I was willing to accept some variation in the pixel files, but as it turned out after I removed all the errors from the parameter files there were no differences in the pixel files either.

I had some trouble matching the .TFM files because of roundoff errors, particularly in fonts like CMSC, where some parameters are computed by modifying others. I solved this by using units of $\frac{1}{360}$ of a point rather than the standard $\frac{1}{36}$ of a point when I could do so without overflow, and by adding “fudge factors” to correct the remaining small differences.

I would like to distribute these files through the normal mechanism from Stanford, since I have received very good service from Maria Code, but I don't know how. I intended to research this problem before writing this article, but the deadline for this issue snuck up on me so I won't have time. Therefore, if anybody wants VMS Backup copies of all that I have described above—command files, alternative parameter files, and the resulting .TFM and pixel files for the DEC LN03—just write me and I'll send you a magnetic tape by return mail. If you can't read 6250 BPI tapes be sure to let me know, since that is my default density: it lets me use a smaller tape.

Editor's note: Arrangements are being made to include at least some of the files described above on the VAX/VMS distributions from Stanford and from Kellerman & Smith. The files have also been offered for inclusion on the VAX/Unix tape; this may take a bit more time to effect, since the algorithms must be translated to a Unix shell script, and VMS dependencies removed. Anyone wishing to volunteer to undertake a translation to Unix should communicate with Pierre MacKay or Barbara Beeton.

Output Devices

TEX and Macintosh – New Directions in Preview

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At SARA [1], the Academic Computing Services Amsterdam, the Macintosh application TEX Preview has been developed, a tool that you can use to view DVI files with a Macintosh microcomputer directly after running TEX on the host computer.

Why Preview

TEX is not an easy to use word processor, in fact TEX commands are quite error prone, so “debugging” a TEX document can be a rather tedious process. This is especially true if the DVI files are printed with an off-line typesetting machine. At SARA it may take as much as three days to get your DVI file printed. Clearly, it is very frustrating for the user to get (expensive) output with some typing errors or an entirely italic paragraph because there was a “}” missing.

Previewing of documents before actually typesetting them can be very useful to correct errors and to try things out. It saves you time, money and a lot of frustration if you can get a view of the results directly after running TEX.

Why Macintosh

To represent pages formatted by TEX with different fonts and styles you need a graphics device with very powerful graphics. As speed and cost are the main considerations, a graphics terminal and some kind of driver program on the host computer do not suffice. The previewing device must have these capabilities of its own. Therefore the Apple Macintosh was chosen for a TEX Preview facility. Macintosh is a microcomputer with very powerful graphics, different fonts, font sizes, styles, etc. Its excellent datacommunication facilities enable you to easily connect Macintosh to the host computer running TEX. You can use Macintosh as a terminal for editing the TEX input and for transferring the DVI file from the host computer to a Macintosh diskette for previewing.

TeX Preview

The goal of TeX Preview is not to be a substitute for a typesetter for printing the final copy. TeX Preview is a *tool* that you can use to display pages from a DVI file in a quite recognizable way. With TeX Preview you can:

- Check results directly after running TeX;
- See what an entire page looks like, its general appearance;
- View an enlarged part of the page, for viewing a formula for example;
- Check stylistic variations like italic, bold, slanted etc. and mathematical symbols.

As with most Macintosh applications, the operation of TeX Preview almost guides itself. Due to the consistent and intuitive Macintosh user interface you will know how to use TeX Preview if you know how to use any other Macintosh program.

TeX Preview displays information on screen in so called "windows". A window is a rectangular part of the screen where a program can display

text or graphics. Windows can overlap each other, but always there is one window the "frontmost" or "active" window. The advantage of using windows on a screen is that the total area to display information in is much larger than the area of the physical screen. Also, the information on screen can be logically grouped into specific windows. A window that is overlapped by another window, as in Figure 1, can be made the frontmost by pointing at it with the mouse and pressing the mouse button, see Figure 2.

The windows on screen

In TeX Preview there are three windows for on-screen viewing of pages. With these windows you can:

- view entire pages on the Macintosh screen to get an overall impression of the layout of a page (Overview window);
- view an enlarged section of a page, for example to check a single formula or paragraph (Zoom window);

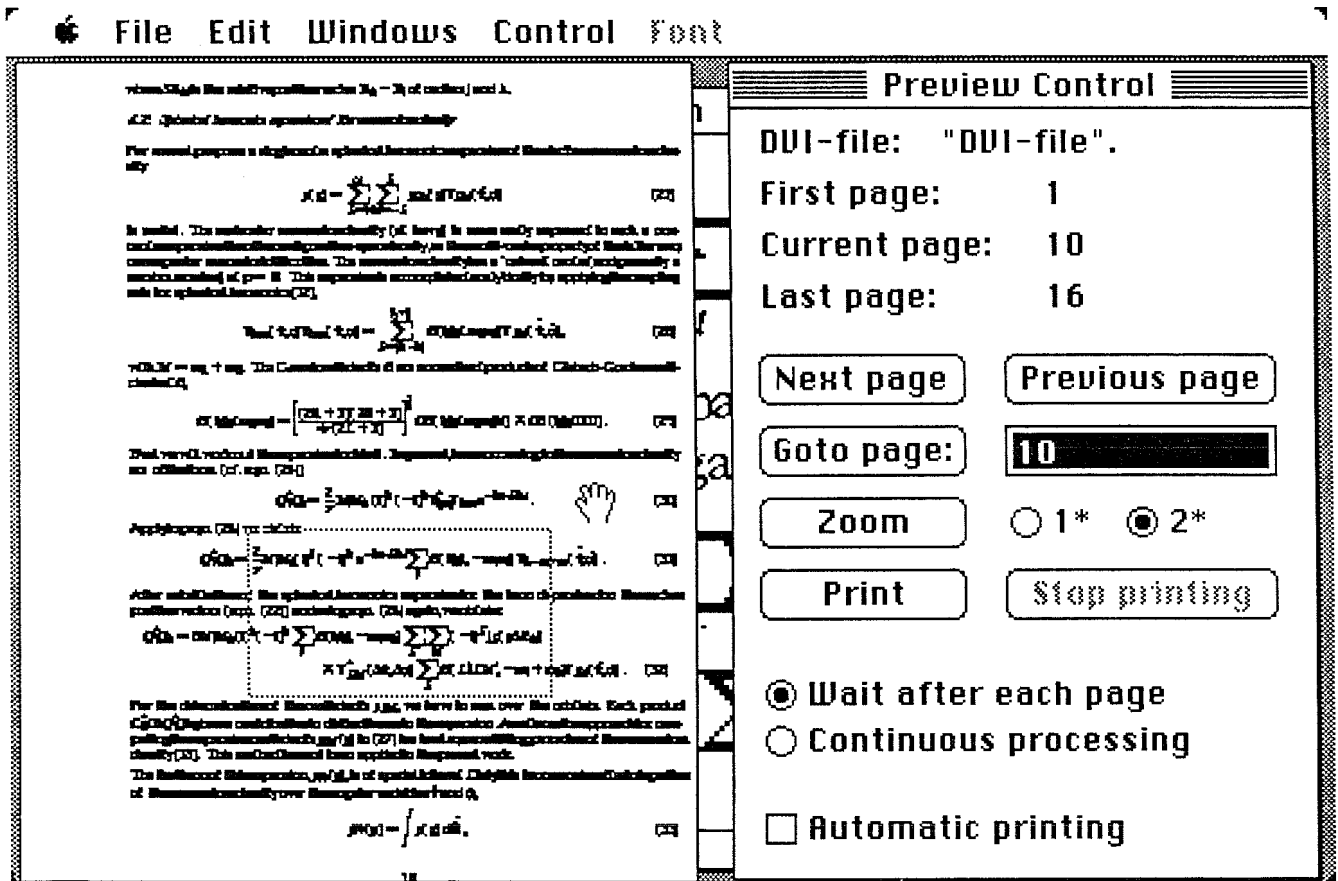


Figure 1. The Zoom window is the behindmost window

- issue commands by pressing buttons with the mouse (Preview Control window).

Overview

The Overview window displays the entire page. The page is reduced in size to fit on screen, see the leftmost window in Figure 1. The Overview window gives you an impression of the general layout of a page.

When the mouse is in the Overview window it changes from the arrow into a hand and a dotted rectangle appears. You can move this dotted rectangle with the mouse. The area inside the dotted rectangle can be viewed enlarged in the Zoom window. This process may remind you of "Show Page" in MacPaint, another Macintosh program.

Zoom

The Zoom window (see Figure 2) displays part of the page at its actual size, or at a size twice the actual size. This is useful to get a close view of a formula or paragraph. The Zoom window has two so called scrollbars with which you can scroll the window over the entire page. When T_EX Preview is just started the Zoom window lies behind the other windows (see Figure 1). To view part of the page enlarged you can get the Zoom window to the front, as is shown in Figure 2.

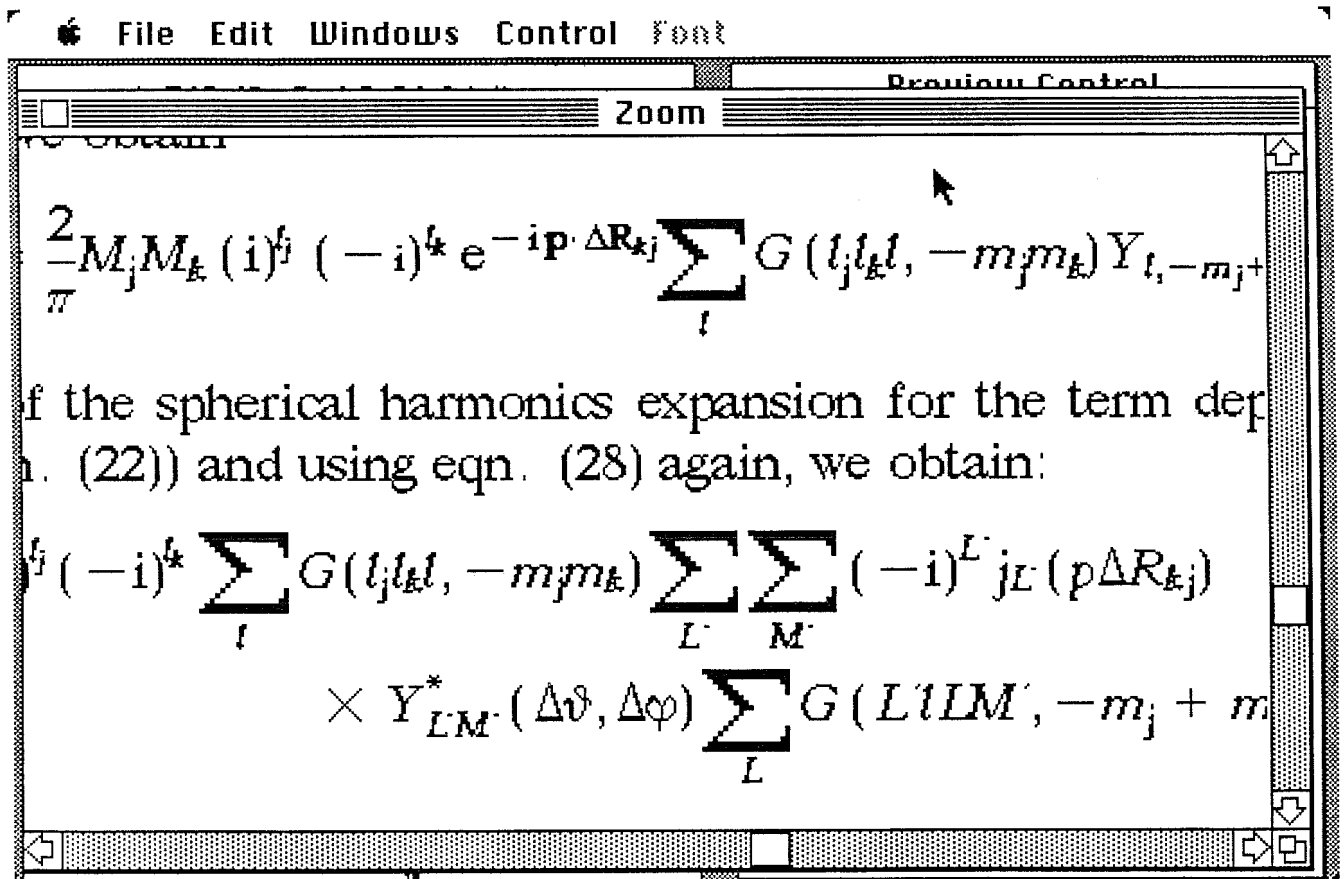


Figure 2. The Zoom window is now the frontmost

Preview Control

With the Preview Control window, the rightmost window in Figure 1, you control the operation of \TeX Preview. There are buttons to give commands and there are other controls to select certain options. The window also contains information on the current situation, for example the first, current and last page number etc. With the mouse you can "press" a button and the command with which the button is labeled is performed. For example if you "click" the "Next page" button \TeX Preview will display the next page from the DVI file.

About fonts

\TeX formats text for a specific output device. This output device can be a photo typesetter or for instance a laserprinter. A typesetter or laserprinter prints text using its built-in fonts.

\TeX knows of the output device the dimensions of each character within each font. As these fonts are somewhat different for each typesetter, the DVI file which \TeX creates contains device *dependent* information, or better said *font* dependent information. Only the format of the DVI file is device independent.

The names of the fonts \TeX used when formatting the text are stored in the DVI file, so the program which actually prints the DVI file on a typesetter or laserprinter knows which fonts to use. This is, of course, also the case for \TeX Preview. To be able to generate typesetter-like output \TeX Preview must have access to typesetter-like Macintosh fonts.

\TeX Preview reads the DVI file and decides which Macintosh font to use for the font used by \TeX . For this purpose a "font mapping" has been implemented in \TeX Preview. The font mapping tells \TeX Preview which Macintosh font to use for a font used by \TeX . You may have to modify the font mapping to get \TeX Preview use the corresponding fonts.

\TeX Preview has the following fonts built-in:

- cmr-7 Times Roman like font, 7pt
- cmr-10 Times Roman like font, 10pt
- cmti-10 Times Roman Italic like font, 10pt
- cmsy-10 Mathematical symbol font, 10pt
- cmmi-10 Mathematical symbol font, 10pt
- cmex-10 Mathematical symbol extension font, 10pt

If one of these fonts is requested at another size the font is scaled to that size from an existing size.

Printing

Besides viewing pages from the DVI file on screen you can also print pages with the ImageWriter matrix printer or with the LaserWriter laser printer. Printing is one of the best ways of previewing, as you can view the entire page at its actual size, and at a resolution much higher than the resolution of the screen. The only disadvantage is that printing is much slower than viewing pages on the screen. You can print one page at a time, print the entire DVI file, or you can specify a range of pages to be printed.

For previewing DVI files from an existing \TeX the ImageWriter matrix printer is the best choice as you can print the different fonts with the ImageWriter just like you can see them on the screen. The LaserWriter is less suited for previewing as you cannot alter the LaserWriter fonts. Also the LaserWriter fonts have a different layout than the \TeX fonts, this is especially the case for the math fonts.

Printing with the ImageWriter offers the highest resolution available in a stand alone Macintosh system. The ImageWriter has a high resolution mode, which is used when high quality printing, of 144 pixels per inch. The Macintosh screen has half this resolution: 72 pixels per inch. At a resolution of 144 pixels per inch you can make a reasonably good resemblance of the fonts of your typesetter. Figures 3 and 5 are sample pages from the typesetter (a Harris 7500), Figures 4 and 6 are the corresponding pages printed with \TeX Preview and the ImageWriter matrix printer. [Editor's note: Figures 3-6 have been reduced to 70%.]

Using the LaserWriter

\TeX formats your text with knowledge of the dimensions of the fonts of the printing device. The LaserWriter has, at this moment, four fonts stored in the LaserWriter in ROM: Times, Helvetica, Courier and a Symbol font. So, to take full advantage of the LaserWriter's capabilities, you will have to feed \TeX with the font definitions of these LaserWriter fonts for proper formatting. For previewing you can, of course, use the LaserWriter, but special symbols like integrals and sum signs will not be printed correctly without adapting your \TeX .

Configuration

\TeX Preview will work with 128K, 512K and Macintosh/XL systems. However, printing with a 128K system is very slow. If you want to print pages a 512K Macintosh is recommended.

Apart from the fundamental approximations, the method is implemented with a very efficient computational scheme. First, the Diophantine integration method [25] is used for the calculation of the Fock-matrix elements. Second, a single centered (at all nuclei) charge density fit is applied for the calculation of both Coulomb and Exchange potentials in the Fock operator. This implies a more complicated use of a computer program package applying the HFS method compared to the (standard) Hartree-Fock program packages.

In the HFS package point group symmetry is applied for the construction of atomic or molecular orbitals from the primitive basisfunction sets. Additionally a molecular wavefunction can be built up from fragment orbitals rather than from basisfunctions. Although these two ways of describing the wavefunction are numerically equivalent, the analysis of the molecular orbitals will be more straightforward if this is done in terms of significant fragment orbitals. Throughout this study computation of molecular orbitals will be performed in a basis of fragment orbitals. Such a basis set can be any truncated set of the fragment orbitals, provided that the occupied orbitals are available. If no virtual fragment orbitals are included in the overall molecular basis we speak of a 'minimal-basis' wavefunction, which is assumed to be more suitable for interpretation than the one obtained by using a single primitive basisfunction for each atomic orbital. The latter wavefunction we will refer to as a single- ζ wavefunction.

As already noted above, the basis sets always consist of Slater type functions. This might be particularly important for the momentum-space electron density discussed in later chapters: the position and momentum space representations are inversely weighted, a diffuse orbital in one representation is contracted in the other representation and vice versa. Because the wavefunctions are always evaluated in the position-space representation of the Schrodinger equation, the amplitude at high r is important for the amplitude at low p , being of primary importance in momentum space studies.

In many parts of this work the bond energy plays an important role. This energy is always calculated with the Transition-State method as developed by Ziegler and Rauk [26], which has been implemented along with the HFS program.

5.3. Practical use and some results

The topics discussed in the previous section are of a methodological nature but do have some implications on the practical use of the HFS computer program package. Generally molecular orbital calculations within the HFS scheme are performed within the so-called frozen core orbital approximation. Hence a basis set is extended with one STO for each core orbital to provide orthogonalization among core and valence orbitals. So three basis sets are needed for most atoms, viz. the valence set, the core set (including expansion coefficients for the core orbitals) and a fitfunction set. By now the core sets are standardized and optimized valence sets are available for all atoms [27] in single- ζ , double- ζ and triple- ζ quality. The choice of fitfunctions is less obvious. In most cases a selection is made out of basisfunction products using criteria of overlap (in order to avoid near-dependency) and the position of the maxima in the fitfunctions. Recently new investigations have been initiated to obtain a better standard and general quality of automatically generated (even tempered) fitfunction sets. The core-potentials are computed with a numerical $X\alpha$ method and must be available for each atom during a run of the program. The numerical integration method requires three user specified parameters for each atom in the calculation: the halfwidth and an exponent for the distribution sphere, and the fraction of the total number of integration points for the molecule. The integration method introduces a not exactly known amount of numerical noise which may become evident under different circumstances, such as the influence of the initial guess wavefunction, or the route along which the bond energy is computed. These effects may be caused by e.g. local minima in the SCF surface or errors in potentials due to the electron density fit. A very careful study

where $\Delta\mathbf{R}_{kj}$ is the relative position vector $\mathbf{R}_k - \mathbf{R}_j$ of centers j and k .

6.2. Spherical harmonics expansion of the momentum density

For several purposes a single center spherical harmonics expansion of the electron momentum density

$$\rho(\mathbf{p}) = \sum_{L=0}^{\infty} \sum_{M=-L}^L \rho_{LM}(p) Y_{LM}(\hat{\vartheta}, \hat{\varphi}) \quad (27)$$

is useful. The molecular momentum density (at low p) is more easily expressed in such a one-centre expansion than the configuration-space density, as the multi-centre property of the latter may cause greater numerical difficulties. The momentum density has a 'natural' centre (and generally a maximum value) at $\mathbf{p} = \mathbf{0}$. This expansion is accomplished analytically by applying the coupling rule for spherical harmonics [32],

$$Y_{l_1 m_1}(\vartheta, \varphi) Y_{l_2 m_2}(\vartheta, \varphi) = \sum_{L=|l_1-l_2|}^{l_1+l_2} G(l_1 l_2 L m_1 m_2) Y_{LM}(\hat{\vartheta}, \hat{\varphi}), \quad (28)$$

with $M = m_1 + m_2$. The Gaunt coefficients G are normalized products of Clebsch-Gordan coefficients CG ,

$$G(l_1 l_2 L m_1 m_2) = \left[\frac{(2l_1 + 1)(2l_2 + 1)}{4\pi(2L + 1)} \right]^{1/2} CG(l_1 l_2 L m_1 m_2 M) \times CG(l_1 l_2 L 0 0). \quad (29)$$

Next we will work out the expansion in detail. In general, terms occurring in the momentum density are of the form (cf. eqn. (26))

$$Q_j^* Q_k = \frac{2}{\pi} M_j M_k (i)^{l_j} (-i)^{l_k} Y_{l_j m_j}^* Y_{l_k m_k} e^{-i\mathbf{p} \cdot \Delta\mathbf{R}_{kj}}. \quad (30)$$

Applying eqn. (28) we obtain

$$Q_j^* Q_k = \frac{2}{\pi} M_j M_k (i)^{l_j} (-i)^{l_k} e^{-i\mathbf{p} \cdot \Delta\mathbf{R}_{kj}} \sum_l G(l_j l_k l, -m_j m_k) Y_{l, -m_j + m_k}(\hat{\vartheta}, \hat{\varphi}). \quad (31)$$

After substitution of the spherical harmonics expansion for the term dependend on the nuclear position vectors (eqn. (22)) and using eqn. (28) again, we obtain:

$$Q_j^* Q_k = 8M_j M_k (i)^{l_j} (-i)^{l_k} \sum_l G(l_j l_k l, -m_j m_k) \sum_{L'} \sum_{M'} (-i)^{L'} Y_{L'M'}(\mathbf{p} \Delta\mathbf{R}_{kj}) \times Y_{L'M'}^*(\Delta\vartheta, \Delta\varphi) \sum_L G(L' l L M', -m_j + m_k) Y_{LM}(\hat{\vartheta}, \hat{\varphi}). \quad (32)$$

For the determination of the coefficients ρ_{LM} , we have to sum over the orbitals. Each product $C_{ij}^* C_{ik} Q_j^* Q_k$ gives a contribution to distinct terms in the expansion. An alternative approach for computing the expansion coefficients $\rho_{LM}(p)$ in (27) is a least squares fitting procedure of the momentum density [33]. This method has not been applied in the present work.

The first term of this expansion, $\rho_{00}(p)$, is of special interest. Only this term remains after integration of the momentum density over the angular variables $\hat{\vartheta}$ and $\hat{\varphi}$,

$$\rho_{00}(p) = \int \rho(\mathbf{p}) d\hat{\Omega}, \quad (33)$$

Down-loading DVI files

For previewing of a DVI file this DVI file has to be transferred from the host computer to a Macintosh diskette. \TeX Preview reads a DVI file from the diskette and displays the pages.

There is a large number of very good terminal emulators available for Macintosh. Most of these packages also have a file transfer facility built-in, which makes it very easy to transfer the DVI files from the host computer to Macintosh. Two common terminal emulators that offer error free file transfer with the popular XMODEM protocol are VersaTerm [2] and MacTerminal [3]. Also, there are special programs for file transfer. A very common program is called Kermit [4].

Both XMODEM and Kermit use an error correcting protocol to ensure that errors during the file transfer are detected and corrected. For file transfer with an error correcting protocol you always need two programs, one on the computer where the to be transferred file is, and one on the computer the file is to be transferred to. These two programs "talk" to each other, one program sends the data, the other receives the data. The sending program adds some extra information so that the receiving program can detect errors in the transfer. If an error occurs the receiving program "asks" the sending program to retransmit the part where the error occurred.

The XMODEM protocol is implemented in many terminal emulators. On the host computer there must also be a program to support the XMODEM protocol. For UNIX systems these are two public domain programs called MacPut and MacGet [5] (both written in "C"). Kermit is also available for a wide range of machines (from microcomputers to mainframes), including Macintosh. Kermit for Macintosh is a stand alone program with a VT100 terminal emulator built-in.

Availability of \TeX Preview

\TeX Preview is available in two versions: for \TeX -80 and \TeX -82. The package is directly available from SARA, at a price of Dfl 300 (which is ca US\$ 110 at the current exchange rate). It includes one diskette and a user's guide. The disk contains the \TeX Preview program and some utility programs. With one of these utilities, called "TeXSetScrap", you can put Macintosh pictures created with for example MacPaint or MacDraw into your \TeX document, using *standard* \TeX . (No \special command needed.)

If you are interested in obtaining the program then please contact us at one of the addresses listed below. We will then send you an order form.

References

1 SARA is the computing centre of the University of Amsterdam (UvA), the Free University (VU) and the Centre for Mathematics (CWI, formerly called MC). SARA is a foundation maintaining computing facilities for its founders. SARA's computing facilities include:

- General service on two Cyber 170/750 mainframes;
- Supercomputer service on a Cyber 205;
- Front-end service for the Cyber 205 on a Cyber 825;
- IBM 4381 service for the universities administrations;
- Electronic mail services (EARN/BitNet) on a VAX 750.

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2 VersaTerm supports VT100, Tektronix 4010 and Data General D200 terminals. It is distributed by Peripherals Computers & Supplies, Inc., 2232 Perkiomen Avenue, Mt. Penn, PA 19606.

3 MacTerminal is available from Apple dealers.

4 Kermit was developed by Frank da Cruz at Columbia University. Kermit is available through user groups or directly from Columbia University.

5 MacPut and MacGet were written in "C" by Dave Johson at Brown, and have been maintained (at New York University) by David Spector.