Web-based Simulation for Contrast Transfer Function and Envelope Functions

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Abstract: We have implemented a Web-based simulation program for the contrast transfer function and envelope functions in Java and JavaScript. The simulation provides interactive controls of all the parameters in those functions. In addition to the predefined functions, users can easily define new functions that use any of the parameters in the preset functions. The most useful feature of this new simulation program is the convenient, universal accessibility through Web browsers on any computer platform that supports Java, such as Netscape and Internet Explorer.

Key words: contrast transfer function, envelope function, electron microscopy, simulation, Java applet, JavaScript

INTRODUCTION

Contrast of an electron micrograph is influenced by the contrast transfer function (CTF) (Erickson and Klug, 1970; Thon, 1971) and the envelope functions of the electron microscope (Chiu, 1978; Frank, 1969, 1973; Hanszen, 1971; Hanszen and Trepte, 1971; Wade and Frank, 1977). In order to plan the experimental conditions for data collection or to interpret the contrast of an electron micrograph, one needs to know the quantitative values of these functions for a given set of microscope parameters. There have been several versions of software written to simulate these functions (Ludtke et al., 1999; Zhou et al., 1996) but they are restricted to execution on specific computer platforms and display the results using specific graphic programs. This restriction has caused tremendous inconvenience to practicing electron microscopists and has hindered broader use of CTF/envelope functions for education and training purposes. We therefore have implemented a program for simulating CTF and envelope functions with convenience as the major goal. This new simulation program is accessible on almost any computer as it adopts the Web-based Java applet and JavaScript programming language. The graphical output of the simulations can be viewed in a Web page and can be printed. The parameters of these functions can be adjusted interactively with slider bars, updating the simulated function's plot instantaneously.

MATERIALS AND METHODS

The Web page (http://ncmi.bcm.tmc.edu/~wjiang/ctf) is designed to simulate the CTF and envelope functions. Two programming languages, Java and JavaScript, were adopted to realize the two major classes of functionalities. Java (http://java.sun.com/) is a general purpose programming language that has gained popularity in recent years and been adopted by the scientific research community as the preferred language for implementing Web-interfaced applica-
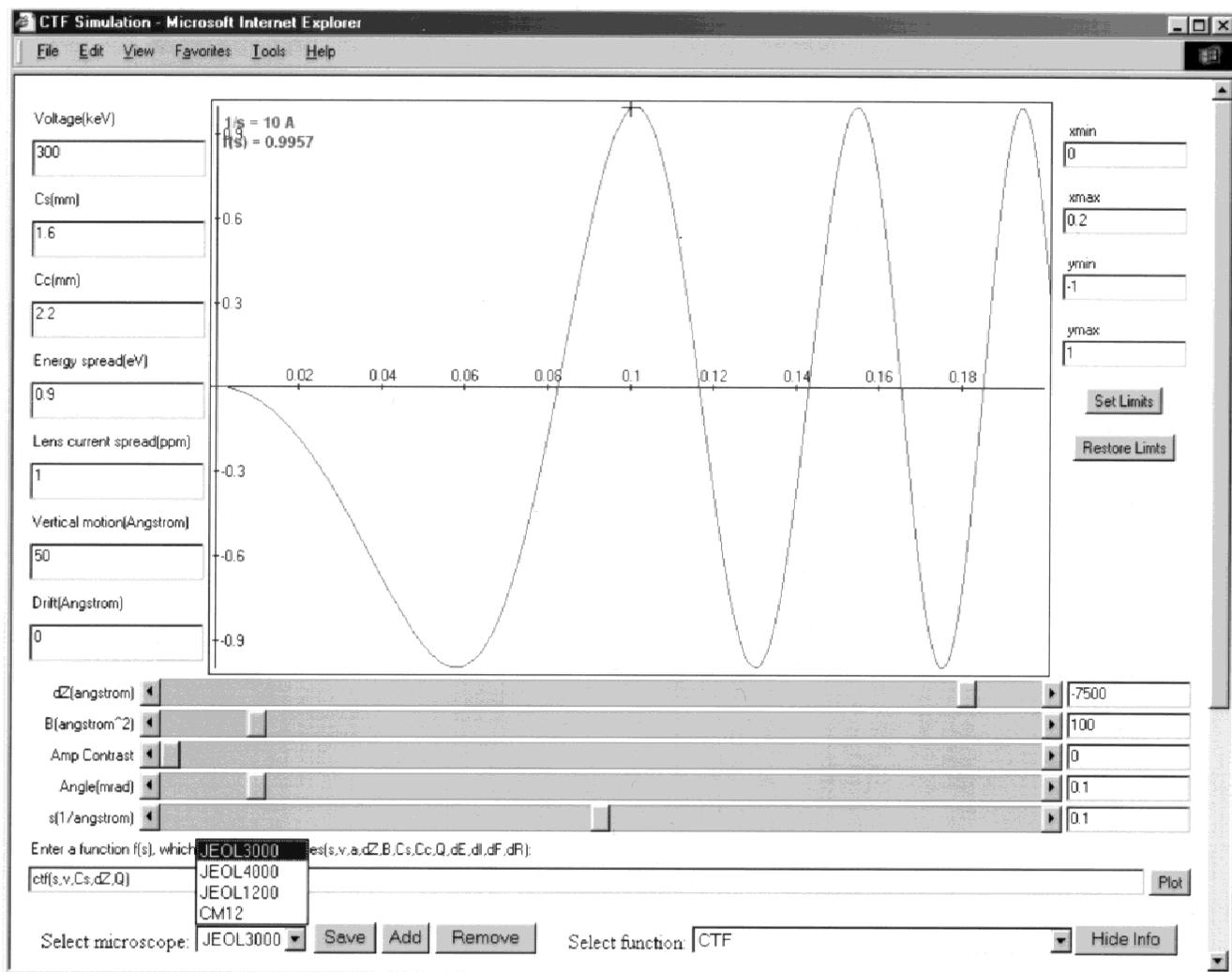
Figure 1. The Web page with the Java applet showing simulated contrast transfer function (CTF) plot. The marker on the curve and the text prompt for the coordinate are turned on. The microscope selector also shows the four preset microscopes.

tions (Hadida-Hassan et al., 1999; Kisseberth et al., 1999). In this simulation Web page, a Java applet is implemented to provide the core function interpretation and plotting capabilities. The programming of the Java applet was based on *Java Components for Mathematics* (JCM) (http://math.hws.edu/javamath/), which provides reusable classes, the Java program building blocks, for function parsing and curve plotting. JavaScript is a client-side Web page scripting language (http://www.javascript.com/), which interacts easily with a Java applet and all aspects of a Web page. The other convenience features in this simulation Web page, such as function selector, function input buttons, storing microscope parameters, and the retrieval of curve data, are implemented using JavaScript. The combination of Java and JavaScript languages makes the core applet program-

ming and overall design of the Web page an easier process than if all functionalities had to be implemented using Java alone.

There are two functions needed in envelope functions that are not available in JCM: $\mathrm{sinc}(x)$ and $\mathrm{j}_0(x)$. Therefore, these functions are custom-defined as follows:

$$\mathrm{sinc}(x) = abs(x) < 10^{-5}?1:\frac{\sin(x)}{x}$$

$\mathrm{j}_0(x) =$
$(57568490574 + x*x*(-13362590354 + x*x*(651619640.7$
$+ x*x*(-11214424.2 + x*x*(77392.33017$
$+ x*x*(-184.9052456))))))/(57568490411$
$+ x*x*(1029532985 + x*x*(9494680.718$
$+ x*x*(59272.64853 + x*x*(267.8532712 + x*x*)))))$

Table 1. Definitions of Contrast Transfer Function and Various Envelope Functions[a]

$$\gamma(s) = 2\pi(\Delta Z\lambda s^2/2 - C_s\lambda^3 s^4/4)$$

$$CTF(s) = -(\sqrt{1 - Q^2}\sin(\gamma) + Q\cos(\gamma))$$

$$G_{sc}(s) = \exp(-\pi^2\alpha^2(C_s\lambda^2 s^3 - \Delta Zs)^2)$$

$$G_{tc}(s) = \exp\left(-\frac{\pi^2}{16\ln2}C_C^2\lambda^2\left(\frac{\Delta E}{E}\right)^2 s^4\right)$$

$$G_{ol}(s) = \exp\left(-\frac{\pi^2}{4\ln2}C_C^2\lambda^2\left(\frac{\Delta I}{I}\right)^2 s^4\right)$$

$$G_{lm}(s) = J_0(\pi\Delta f\lambda s^2)$$

$$G_{tm}(s) = \frac{\sin(\pi s\Delta r)}{\pi s\Delta r}$$

$$G_{au}(s) = \exp(-Bs^2)$$

[a]s, spatial frequency; λ, electron wavelength; C_s, spherical aberration coefficient; C_C, chromatic aberration coefficient; ΔZ, focus, positive for underfocus and negative for over-focus; γ, phase shift; Q, amplitude contrast; α, semi-illumination angle; E, electron energy; ΔE, electron energy spread; I, objective lens current; ΔI, variation of objective lens current; Δf, sample vertical motion amplitude; Δr, sample drift amplitude; B, amplitude decay factor; $CTF(s)$, contrast transfer function; $G_{sc}(s)$, spatial coherence amplitude decay; $G_{tc}(s)$, voltage temporal coherence amplitude decay; $G_{ol}(s)$, objective lens current stability amplitude decay; $G_{lm}(s)$, sample vertical motion amplitude decay; $G_{tm}(s)$, sample horizontal drift amplitude decay; $G_{au}(s)$, the Gaussian approximation of amplitude decay.

The sinc(x) function is necessary to prevent a zero-division error when $x = 0$. The Bessel function $j_0(x)$ is computed with polynomial fitting as shown in *Numerical Recipes* (Press et al., 1997).

RESULTS AND DISCUSSION

Functions of Choice

The simulation program is designed to compute the functions for CTF (Fig. 1) and its product with various combinations of different envelope functions, including spatial and temporal coherence, specimen vertical movement, and horizontal drift. The analytic forms of the functions are shown in Table 1 (Chiu, 1978; Erickson and Klug, 1970; Frank, 1969, 1973; Hanszen, 1971; Hanszen and Trepte, 1971; Thon, 1971; Wade and Frank, 1977). The function to be simulated can be selected through the pop-up function selector (Fig. 2) or created by the user. For instance, one can define a new function such as the square of the product of CTF and the envelope function for spatial coherence, as

shown in Figure 2. The custom function could also use the special input parameters for the CTF and envelope functions shown in the applet, as well as almost all the common mathematical functions including trigonometric, power, exponential, and square root. Detailed descriptions for the available functions/variables/constants can be found in the accompanying Web page.

In addition to the standard mathematical functions, aliases for the functions, which are specially defined in the context of electron microscope optics as in Table 1, can also be employed as user input in custom functions. However, in order to input these aliases as valid functions, the correct number and order of parameter variables have to be used. To relieve the burden of memorizing the correct syntax of these special CTF/envelope functions, a "calculator" type of input button array is provided at the lower left of the applet (Fig. 3), where each button provides the correct syntax for the corresponding CTF/envelope function. The user can just input the desired functions by clicking the corresponding button and the correct function symbols would be transferred to, and updated in, the function input/display area. For instance, the button labeled with "(. . .)**2" would turn the input function into its square form and adjust the plot of CTF/envelope functions in Y-axis scale to 0–1 automatically. This simplifies an otherwise multiple-step process into a single mouse click and is therefore a great convenience to the user.

Parameter Inputs

The upper-left input boxes are for voltage, spherical aberration coefficient, chromatic aberration coefficient, energy spread, specimen vertical motion, and horizontal drift (Figs. 1, 2). The other parameters (defocus, amplitude contrast, semi-illumination angle, and B decay factor as defined in Ludtke et al., 1999, and Saad et al., 2001) are in the form of sliders for easy interactive manipulation. Change in any parameter will be reflected in the plot immediately. All the parameters are in the most commonly used units as explained in the accompanying document Web page.

As different microscopes have different characteristic parameters, a microscope selector has been implemented to let the user input the parameters for a particular microscope simply by selecting the corresponding microscope from the available microscope list. Four microscopes and their corresponding parameters are provided as default available options: JEOL 1200, JEOL 4000, JEOL 3000, and Philips CM12. For other microscopes not included in the default
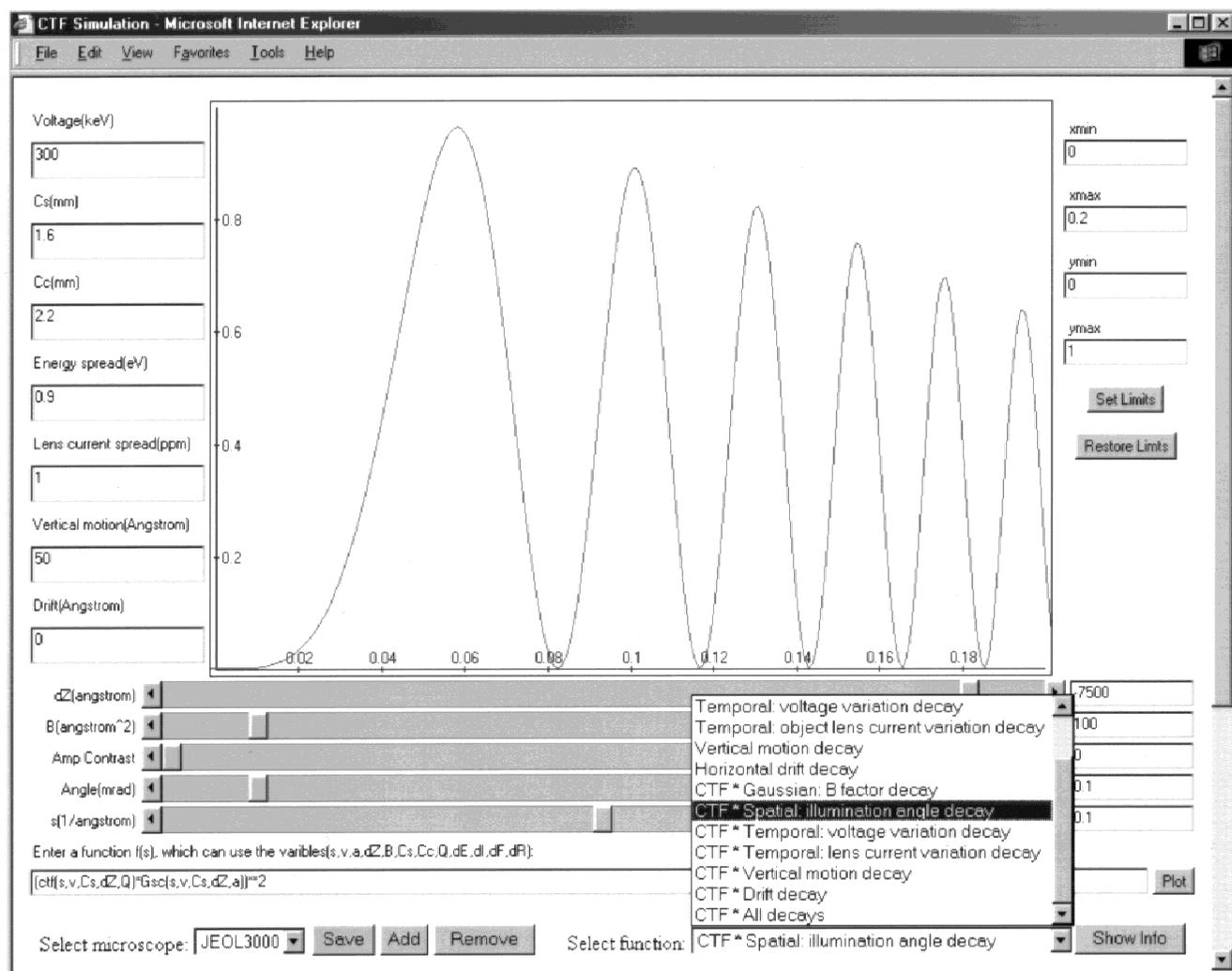
Figure 2. The Java applet is shown with the plot of the square of the product of CTF and the envelope function for spatial coherence as defined by the user. The marker on the curve and the text prompt for the coordinate are turned off. The function selector also shows part of the 14 predefined CTF and envelope functions.

option list, a flexible mechanism was implemented to let the user add/delete/modify/save the parameters and tailor the option list to their own microscopes. The user would then be able to easily recall the stored information from the microscope selector (Fig. 1). Information storage employs "cookie" technology (http://www.cookiecentral.com/) and stays effective for 1 year. If the user has not accessed the CTF simulation Web page after a year, the stored custom information is automatically deleted.

Display

The plot of the simulated function is shown in the upper center of the applet (Figs. 1, 2). The X-axis represents spatial frequency in 1/Å while the Y-axis is the value of the simulated function. A crosshair marker shows on the curve at the corresponding X-coordinate, and a text prompt in the upper-left corner of the plot displays the corresponding real space resolution in Å for the marker position. The crosshair and text prompt can be toggled on and off by clicking the button labeled "Hide Info".

The limits of display for both X- and Y-axis can be varied to facilitate viewing convenience. In the upper-right portion of the display, the entries are inputs for setting the X–Y axis limits, as well as buttons for resetting the default limits for X (0–0.1) and Y (0–1 or, −1–1 depending on the function plotted). The user can also zoom the plot in or out by clicking in the plot area (left click for zooming in,
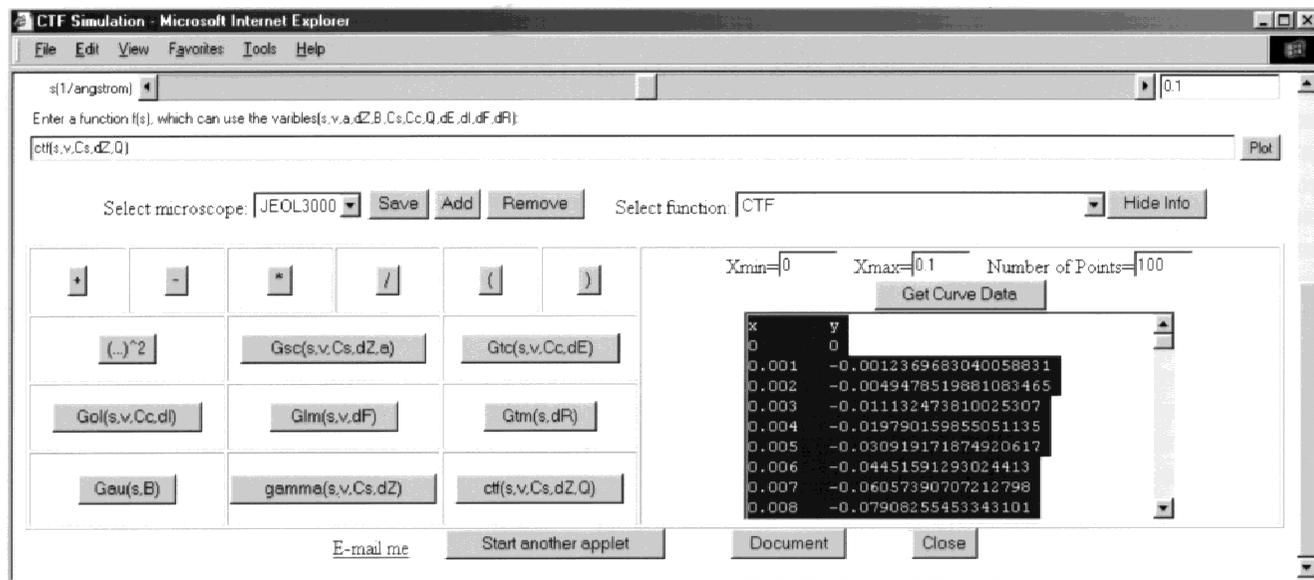
Figure 3. The "calculator-like" function input buttons are shown on the left, while the data retrieval area is shown on the right in the function-simulation Web page. In the data text box, the X,Y data are shown in a two-column format. They can be selected and copied to the input for other high-quality plot programs.

and shift–left click for zooming out). Furthermore, the applet size, and thus the plot area size, is adjustable by fitting to the Web browser window size.

While the graphic plot of the curve is fast and convenient, it is not intended for publishable, high-quality plots. To provide a means for high-quality graphing, a special section was implemented, located in the lower right-hand corner, just under the function selector (Fig. 3). Included are the input controls for minimal and maximal X-coordinates, and the number of sampling points wanted. A single click on the button labeled with "Get Curve Data" fills the text area with the X-coordinates and the corresponding Y-values in two columns, which then can be copied to any preferred graphing software for high-quality plots.

Conclusions

We have developed a new CTF and envelope function simulation Web site for convenient access and flexible options of the simulated functions and the parameters. The Web interface has overcome the daunting specific platform requirement, software downloading, installation, and configuration of available CTF simulation programs. This simulation has a practical utility in facilitating the choice of the appropriate parameters in a microscopy experiment, as well as in understanding the effects of these functions on an image contrast in transmission electron microscopy.

Acknowledgments

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