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Addendum to Glint Manual for GLint version 3.20:

This GLint software contains a number of new features as yet undocumented in the GLint operation manual. Whilst most are self-explanatory or simply improvements in presentation the following outlines particulary important additions.

1: Load dialog:

It is now possible to ignore a variable number of points from both the beginning and end of incoming kinetic data sets. This is useful for discarding any early mixing artifacts or removing excess timebase information.The skip points option has been extended to allow averaging of intermediate data rather than skipping.It is possible to introduce a time offset during loading to allow for dead-time correction when critical.

2: File formats:

In addition to loading APL kinetics, SVD files etc, 'DOS' filetype files containing space or tab delimited column data will also load when dragged into the main window. Such files MUST comprise the time course in seconds in the first column. A variable number of absorption/fluorescence columns (up to 40) can follow. Any leading header rows will be ignored providing they are character based and not numeric. Trailing rows MUST be removed. eg:

Column1	Column2	Column3	/ignored
.1	.5	.2	/time 1,abs11,abs21
.2	.4	.3	
.3	.3	.35	
...			
1.0	.05	.45	/time n,abs1n,abs2n

3: Tracking and fit range setting

On 2-D data displays the display dialog box now shows the numerical cursor position when the mouse pointer lies within the main display graph limits (when outside "——" is displayed). This can be used for obtaining useful estimates of data values from the display. When the Analysis dialog is displayed this cursor tracking is used to adjust the X-fitting range when required (providing the current 2D display is in signal vs time format). Two new editable fields display the X-start and X-stop fitting range in seconds. By default they display 0 and the current time-base limit respectively. To adjust the fitting X-start position point the mouse at the required position on the displayed trace (note tracking will be on and shown in the display dialog) and click the LEFT mouse button. The X-start parameter in the analysis dialog will be updated accordingly. To adjust the X-stop parameter, repeat this operation with the RIGHT mousebutton. Fitting will now carry out minimisation over only this time range. To reset the fit-range move the mouse just outside the graph boundary (still in the main window) and click the LEFT or RIGHT mouse button to reset the X-start and X-stop parameters respectively. This feature makes redundant the previous fit range setting method which involved reducing the displayed data using the group display feature in the spectra mode dialog box. It also makes the analysis of single kinetic traces more flexible (when the spectra mode display is not available).

4: Saving data

A single trace save facility is now availble. When a single kinetic trace is on display this will be saved (using the main menu SAVE option) in a format compatible with the SX17MV instrument software.

5: Comments

The comments dialog box is now a modeless dialog box which will remain on screen while other operations take place. New text will only be added to the main display when the OK button is pressed.

Peter King 1/6/94

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1.0 Introduction

This software is primarily intended for the analysis of time dependent spectra generated by the **Applied Photophysics BioSequential SX.17MV Stopped Flow Reaction Analyser**. It can, however, be used to analyse sets of data generated on other commercial spectrometers (eg the HP8452A diode array).

1.1 Application Summary:

The **GLint** application represents a major advance in the analysis capability available to scientists studying wavelength dependent reaction kinetics. The introduction of instrumentation capable of generating high quality sets of time dependent spectra comprising frequently many thousand individual absorbance (or fluorescence) measurements has prompted the development of an analysis system which can exploit this data fully and efficiently.

GLint allows the scientist to globally analyse the complete data set according to a proposed reaction scheme, providing a best fit parameter set which will accomodate all kinetic behaviour across the entire measured wavelength range.

The key feature of Global analysis is the optimisation of non-linear reaction parameters (rates) at all measured wavelengths simultaneously. Because individual rates contribute to each kinetic record to differing degrees over the measured wavelength range (depending on the spectral distribution of the reaction intermediates), analysis of all records globally reduces the correlation of these parameters, since events at all wavelengths contribute to the least squares minimisation procedure. This results directly in a more robust fit and the reliable identification of minor intermediates. In addition the identification of unknown species is supported by the availability of their calculated spectra.

1.2 Key numerical elements of GLint:

1.21: Singular value decomposition (SVD) of data sets

SVD of the original data matrix yields unbiased information about the minimum complexity of the underlying chemical system by providing a model free indication of the number of linearly independant components present. In doing so it outputs a reduced representation of the data matrix as an ordered set of basis spectra and corresponding time dependent amplitudes. Succesive pairs of these vectors approximate the independant components featuring in the original data in a least squares sense. Significantly only a subset of this output therefore need be used for subsequent model analysis. This application of SVD as a data reduction system is valuable in speeding up subsequent numerical calculations and substantially reduces the space occupied by the original data set both in memory and on disc.

1.22: Global optimisation of reaction parameters using the Marquardt-Levenberg algorithm

Either the original data set or the product of SVD may be analysed, exploiting the kinetic information at all wavelengths simultaneously. Separation of the non-linear (rates) and linear (amplitude) parameters is a crucial element of the method, substantially reducing the parameter space allowing reliable convergence of the fitting algorithm. Linear regression of best fit concentration profiles to the original data set yields the individual component spectra.

1.23: Fitting performed directly to reaction models using numerical integration

Fitting is conducted directly to concentration profiles generated by numerical integration. This allows fitting to arbitrary reaction mechanisms including simple decays and multi-step reactions including parallel reactions, second order reactions, equilibria etc. Models are entered using a simple reaction scheme editor. The user provides starting concentrations and rate estimates but has no need to refer to explicit rate equations or formulae. On completion residual plots of kinetics and spectra at all wavelengths and times illustrate the global accuracy of the selected model. To facilitate fitting of more complex schemes, which can possess more than a single least squares solution, the analysis allows the introduction of fixed (ie known) spectra and the locking of individual rate

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and equilibrium constants.

1.24: Simulation

To supplement analysis **GLint** includes a comprehensive simulation capability allowing the synthesis of artificial sets of time dependent spectra of arbitrary complexity. These data sets can then be analysed as a normal data set using the facilities described above. This simulation capability is invaluable for learning the systems capabilities, as well as providing an excellent tool for demonstrating and exploring the behaviour of spectrally active reaction mechanisms.

1.25: References

1. Henry E.R., Hofrichter J. Singular Value Decomposition: Application to Analysis of Experimental Data. Methods in Enzymology 1992 vol 210 p129 Academic Press.

2. Maeder M. Zuberbuhler A. Nonlinear Least-Squares Fitting of Multivariate Absorption Data. Anal Chem 1990 vol 62 p2220.

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2.0 Installation

The disc supplied contains one application, which can be viewed by clicking on the floppy disc icon on the icon bar.



It looks like this.

This file should be copied (dragged) to an appropriate location on the computer hard disc, ie to the root or other preferred directory.

3.0 Printer Drivers

If the software is supplied installed on the Applied Photophysics workstation together with a Canon Bubblejet printer the system will have been factory configured to automatically load the appropriate printer driver and no other action is necessary to enable hard copy output.

If this is not the case it is necessary to load the printer driver manually before attempting to use the print options within **GLint**. If you wish to install a particular driver for your own printer carry out the following steps (you may want to consult the RISC-OS user guide for a more detailed description, particularly if you are new to the windows interface).

To install printer drivers manually double click on the !Printers application. This will be found either in the root directory or the App1 folder in the root directory. If it contains pre-installed drivers the names of the actively supported printers will appear on the icon bar. If your printer is not there you will need to install its driver by carrying out the following procedure.

A range of printer drivers for the majority of popular printers can be found in the Printers folder in the App2 directory on the hard drive. First select **Printer control** from the existing Printer icon menu on the icon bar. The menu is opened by pressing the middle mouse button while pointing at the icon. This will display a window showing the currently installed drivers. If this does not include your printer drag the required driver from the Printers folder (in App2) into this window to add it to the list. Select it with the left mouse button to highlight it. Next open the menu for the Printer control window (by pressing the middle mouse button) and select **Active**. An icon corresponding to the new model of printer you have installed should appear on the icon bar, indicating that printing is now enabled. Before running **GLint** re-open the !Printers icon menu and select **Save choices**. This will ensure the new driver is loaded and made active when the !Printers application is started on future occasions.

Always remember to run !Printers before attempting to print from GLint

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4.0 Getting Started

Double click on the !**GLint** icon and the application will be installed on the icon bar. On A5000 workstations the screen mode should automatically switch to high resolution (with Multisync monitors only).

To obtain a high resolution screen mode on 400 series workstations it is necessary to access the pallette menu (press the middle mouse button over the palette icon on the icon bar). Next move to the mode submenu and move the pointer to the bottom of the mode option list. A text entry caret should appear. Two new high resolution modes have been installed: 78 or 74. Type in one of these and press return. The new mode should now be displayed.
If you do not have a multisync monitor, such high resolution modes are not available. In this situation the best available mode for **GLint** is mode 16 which should be selected as above.

Click on the **GLint** "world" icon to open the application main window.

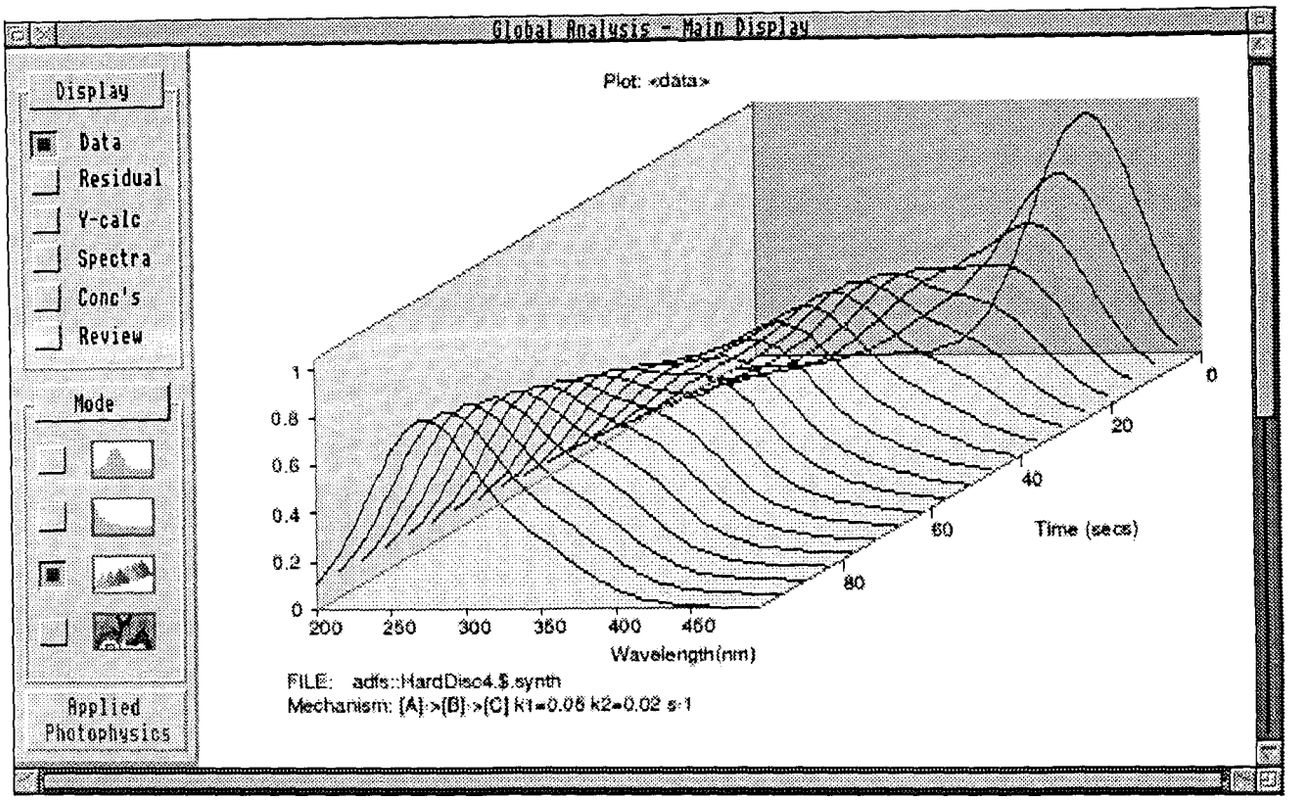


Fig.1 Main Display Window

The main window, seen above, is used for graphical presentation of data and fit results. The window will be blank since no data has yet been loaded or simulated. To generate some synthetic data press the middle mouse button over the window to open the main menu and select **Demo.** The screen will now show a three-D display of an artificial set of time dependent spectra (actually based on an A->B->C reaction model) which can be used for exploring many of the features of the **GLint** application.

There are three main ways in which the user interacts with the application: **icons, menus** and **dialogue boxes**. (Their attributes are described in detail in the RISC OS user guide.) The entire software is accessible through the options these features provide by simple selections with the mouse.
On the left hand side of the main window are a set of icon selected options for displaying experimental data and fit results in variety of formats. These are divided into two sections labelled **Display** and **Mode.**

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4.1 Main Window: Icons

The Display section determines the type of information to be displayed in the window.

"Data" displays either raw data (ie time dependent spectra), generated from a series of kinetic traces or data reconstituted from a previously saved SVD file.

"Residual" displays the residuals after a global fit has been performed.

"Y-Calc" displays the fitted data, i.e. the best fit modelled data calculated during global analysis.

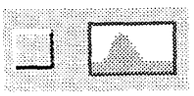
"Spectra" displays the start, intermediate and product spectra (following analysis).

"Conc's" displays the reactant, intermediate and product concentrations against time (folowing analysis).

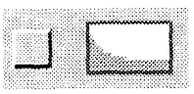
"Review" displays thumbnail sketches of the data, residuals, spectra and concentrations.

Note: prior to any analysis (as will be the case following Demo selection) only the **Data** option will be active. Other icons (with the exception of **Review**) in the Display section will produce blank screens at this stage.

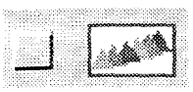
The mode section determines how the information is displayed in the window.



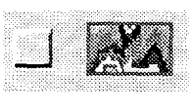
This Icon selects 2 dimensional spectral display and plots absorption against wavelength.



This Icon selects 2 dimensional kinetic display and plots absorption against time.



This Icon selects 3 dimensional display and plots absorption against time against wavelength.



This Icon selects a contour plot and plots wavelength against time. It uses colour coding to indicate the absorption value.

The different display modes have a controlling dialog box associated with them which can be accessed by selecting Display.. in the main menu. The extra options provided are described in more detail in the Display section of this manual.

By default "Data" and "3-D" are selected. Clicking on the button icons selects the other modes and data types.

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5.0 Menu Options

As described earlier, pressing the middle mouse button over the main window reveals the **main menu**. When the main menu is opened selections can be made with either the left or right mouse key. If the left key is used the menu automatically closes, whilst using the right leaves the menu open which can be useful for immediate selection of a further menu item.Simple actions (such as Demo) are labelled by name only, whilst options follwed by '..' (eg Display..) will present a dialog box. Moving the mouse over arrows to the right of entries will produce submenus. Options which are currently invalid (eg Save when no data is loaded) are shown greyed out until they become available.

The main menu structure is as follows:

INFO..	Displays a dialog box containing application description
SAVE=>	Produces the Save submenu
COMMENTS=>	Produces the comment entry dialog box
PRINTOUT	Prints out the current display
DISPLAY..	Produces the display dialog box
ANALYSIS..	Produces the Analysis dialog box
LOAD..	Produces the Load dialog box
SVD=>	Either carries out SVD if clicked or => produces the SVD sub-menu
SIMULATE..	Produces the Simulation dialog box
DEMO	Synthesizes the demonstration data set
QUIT	Exits the application

The Save submenu:

DATA	Save the current data set in a single file (ASCII format)
SVD	Save the SVD output (8 most significant vectors only)
SPECTRA	Save the fitted spectra in a single file
CONC	Save the fitted concentration profiles in a single file
CSV	Save the current data in a single comma separated format suitable for reading into a spreadsheeet

The SVD submenu

CALCULATE	Calculate the SVD of the current data set
RECON U.S.V=>	Recombine the SVD output vectors to reconstitute the original data. Selecting => produces a dialog box in which the desired number of significant singular values for the calculation may be edited (this always defaults to 8)
SING. VALUES=>	Produces a dialog box listing the 8 most significant singular values
PRINT BASIS=>	Printout the SVD output vectors graphically, as displayed below the main display

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6.0 Data Loading & Filing

GLint is intended primarily for analysis of time dependent spectra produced on the SX.17MV by the point by point method. Data files produced by this technique comprise a number of separate kinetic records saved in ascii format, usually gathered in a group or directory on disc. The naming of such a set of records should comprise a name of up to 4 letters followed by unique and typically sequential run numbers separated from the name by an underbar.

To load this data open the directory window to display the multiple files. Select the first in the series (ie the one with the lowest run number) and drag it either into the **GLint** main window or to the !**GLint** icon on the icon bar. (ie click and hold down the left mouse button over the file icon and drag the pointer to the !**GLint** window, then release the button).

The entire series of files will be loaded and displayed according to the following rules:
No file is loaded with a run number lower than that dragged in first. If the file number sequence is not continuous, intervening gaps will be skipped over in search of further runs of the same name, up to a maximum run number of 100. The wavelength for a particular run is embedded in the file. If runs are found to be out of sequence they will be sorted automatically.

If no wavelength information is found or if the **Wavelength ignore** option in the **Load..** dialog box is selected (see below), then wavelengths are ignored and the kinetic runs are simply loaded and displayed as Absorbance vs time vs Run number. This allows single wavelength data to be loaded and analysed if required. (In such cases the fitted rates are valid but spectral information can be ignored).

When a set of kinetic files has been loaded it can be re-saved as a single file using the **Data** savebox which can be reached from the **Save** submenu. The savebox shows the existing pathname which is used if the OK icon is pressed. Edit the name and either click on OK or drag the file icon to the destination directory window (fig.2, below).

In addition it is possible to save the output of the SVD. This is also available from the **Save** submenu but only following SVD calculation.
A great benefit of saving the SVD output is the small space it occupies compared to the original data (typically a 5-10 fold improvement). It also means that SVD calculation can be skipped when the file is re-loaded.

To load either type of file simply drag it from its directory to the **GLint** main window or to the !**GLint** Icon. Existing data will be discarded and the new data displayed. Note that if an SVD file is loaded it is automatically expanded to 'regenerate' the original data (see section 9.0).

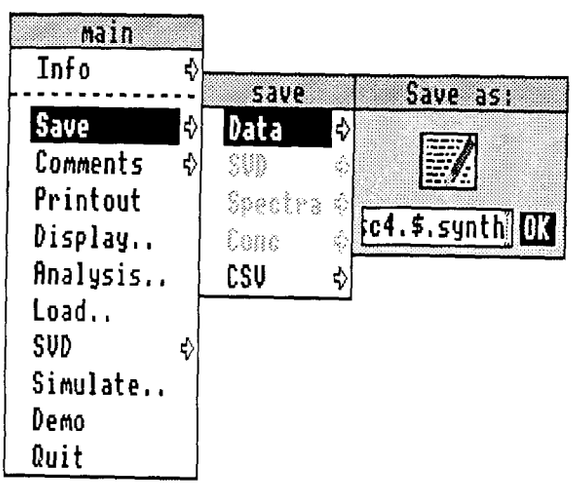


Fig. 2 Menu selections to save data

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6.1 Loading Options

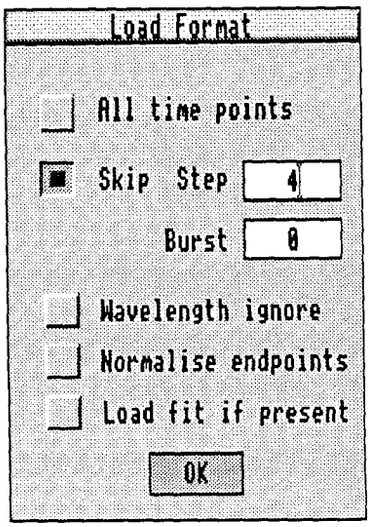


Fig. 3 Load Format Window

Clicking on the **Load..** option in the main menu brings up the load format dialog box (Fig.3). If **"All time points"** is selected, all of the time points in each kinetic trace are loaded at every wavelength. With kinetic data collected at very high time resolutions this can result in longer analysis times, particularly during preliminary investigation or when fitting simple models. The default is to **"skip"** through every fourth point in the kinetic trace, (ie to quarter the amount of information loaded.) This step size can be altered by the operator. The number in the box beside **"Burst"** indicates how many points will be kept together at the beginning of the kinetic traces. This ensures that fast phases at the beginning of traces are well defined. If **"Wavelength ignore"** is selected then traces are not scanned for their wavelengths but are loaded in the order of their suffix number (ie RUN_01, RUN_02, RUN_03 in that order). The wavelength axis is labelled in run numbers instead of in nanometers. If **"Normalise endpoints"** is selected then all of the kinetic traces are normalised to their endpoints prior to loading. This results in a set of difference spectra being produced (relative to the end point spectrum) which can then be analysed as normal. It should be noted that this, in effect, declares the final component species to be colourless which should be set in the analysis window prior to fitting. If **"Load fit"** is selected and the kinetic traces to be loaded have been analysed in the conventional **SX.17MV** software, then the best fit curve data will be loaded instead of the raw data. It is not intended that you should then proceed to analyses this data globally. This feature is included for data presentation and printout only.

6.2 Loading Other Formats

As well as loading sets of kinetics files produced by the **SX.17MV**, sets of spectra or splines (generated by the slicing feature of the instrument control software: the **SX.17MV** application) can also be loaded. This facility is principally for presentation purposes only since the time resolution is only equal to the total number of spectra or spline files originally created, which is seldom equivalent to the time resolution of the original kinetic records from which they were derived.

In addition it is intended that **GLint** should accomodate time dependent spectra from other instruments. Currently spectra files (.WAV files) from the HP Diode array spectrophotometer (model HP 8452A) can be loaded with minor modification. All analysis capabilities of **GLint** can then be applied to this data.

We invite suggestions for other desired file compatibilities particularly if supplied with documentation of the particular format involved.

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7.0 Data Display

New data is initially displayed in 3-D mode or one of the 2-D modes if selected. Note that by default not all measured spectra are displayed since this can obscure the kinetic features and also slows the screen redraw time (see below). If a display doesn't appear check that the **Data** icon at the top left of the main window is selected.

Clicking on the **Mode** icons described in section 4.1 will provides the alternative available displays: absorbance vs wavelength, absorbance vs time, and wavelength vs time (contour plot).

Further control of the display can be achieved by selecting **Display..** in the main menu. This opens a dialog box showing the current display settings. These depend on the selected display mode. For 3-D display the dialog box appears as in Fig 4.

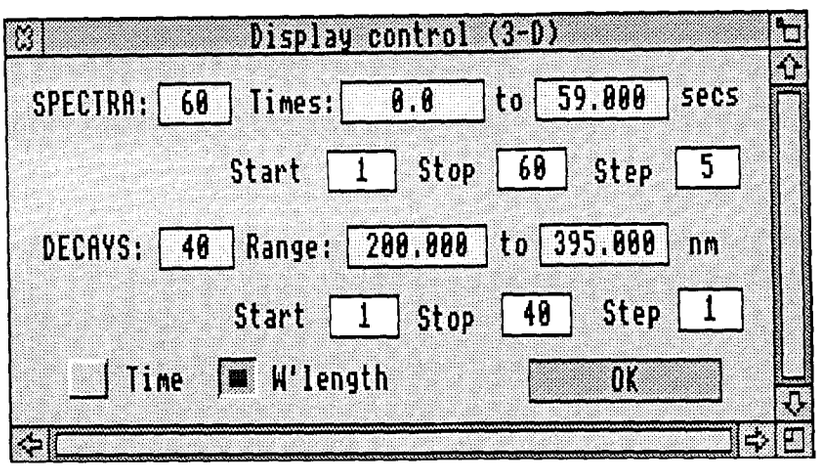


Fig. 4 Display Control Window for 3-D Display

The dialog box contains information on the total number of spectra and kinetic records (decays) in the current data set. In addition sets of editable text icons show values indicating the subset of the data which is currently on display. In the example (Fig.4) the data comprises 60 spectra measured at 40 wavelengths. Of the 60 spectra only every 5th is on display (for the reasons mentioned above). To change this distribution edit the start, stop and step icons as required.
Press OK to implement the change.

Note: When W'length is selected the data are presented as separate spectra. When Time is selected the data are shown as separate decays. In W'length format the wavelength start, stop and step indices (under 'Decays') are ignored and complete spectra are shown at the times selected by the 'Spectra' indices. Conversely, in Time format the reverse holds: the 'Spectra' indices are ignored and complete kinetic records at the wavelength indices selected under Decays are displayed. Experimentation will make these relationships clearer.

IMPORTANT: The 'Spectra' Start and Stop indices (ie the index used to select the first and last spectrum on display) are used during analysis to define the fitting range (ie time range) over which least squares regression is applied. This facility is important if any early artifacts (which are not uncommon in the first couple of milliseconds of stopped flow data) are apparent in the data. Since poor data at these times (typically below 1 or 2 msecs) will be disruptive when trying to fit fast early events, setting the start index to a spectrum beyond this region (say at 2msecs) will cause this corrupted region of data to be ignored.

In 2-D display modes the dialog box is slightly different, allowing data index adjustment in only one domain,

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wavelength or time (it should be noted that relevant indices set in any display mode are carried across to the newly selected mode). In addition it is also possible to switch from displaying a group of decays or spectra to displaying them individually. This is performed by selecting the **Single** icon button. Pressing the accompanying left and right arrows allows the user to flick through the individual traces. The current Y-axis text label is also displayed, and can be modified if required.
When viewing 2-D kinetic traces there are two special display options. **Isometric-X** can be used when the original data has been collected on a non-linear time-base (split time-base or log). This will display all measurements at equal intervals along the X-axis, rather than using their absolute time coordinate. This provides (visual) expansion of the more highly time resolved portions of the decay. Autoscale-Y expands individual curves in the Y-axis to fill the display.

IMPORTANT: In single trace mode, fitted curves (following analysis) are superimposed in red through the individual data curves. This provides the clearest facility for checking fit quality at all wavelengths and times individually.

7.1 Other Display Features

Below the graphical display are a number of comment lines. The first two comprise the data file path and, in single trace mode, an indication of the wavelength or time corresponding to the displayed trace.
Below these up to two lines of comments can be added by selecting the **Comment..** option in the main menu, These comments are automatically stored in the data files if saved to disc.

7.2 Printing

Selecting **Printout** from the main menu will print the current graphical display to your printer (see section 3.0).
Note that following analysis all printouts (excluding those in Review mode) include a complete description of the fitted model together with fitted rates and errors.

7.3 SVD output vector display

After SVD reduction of a data set a series of graphs is displayed below the principal display, which can be accessed using the scroll bars and main window size icon. These correspond to the first 8 columns (of US) and rows (of V) of the output of the decomposition (see section 10.0). They are included as they can aid in clarifying the principal components of the system under study. Note that the matrix product of US and V reconstitutes the original experimental data less the noise which is distributed in the lower order output vectors. See SVD submenu option **Recon U.S.V.**

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8.0 Data Reduction and Analysis

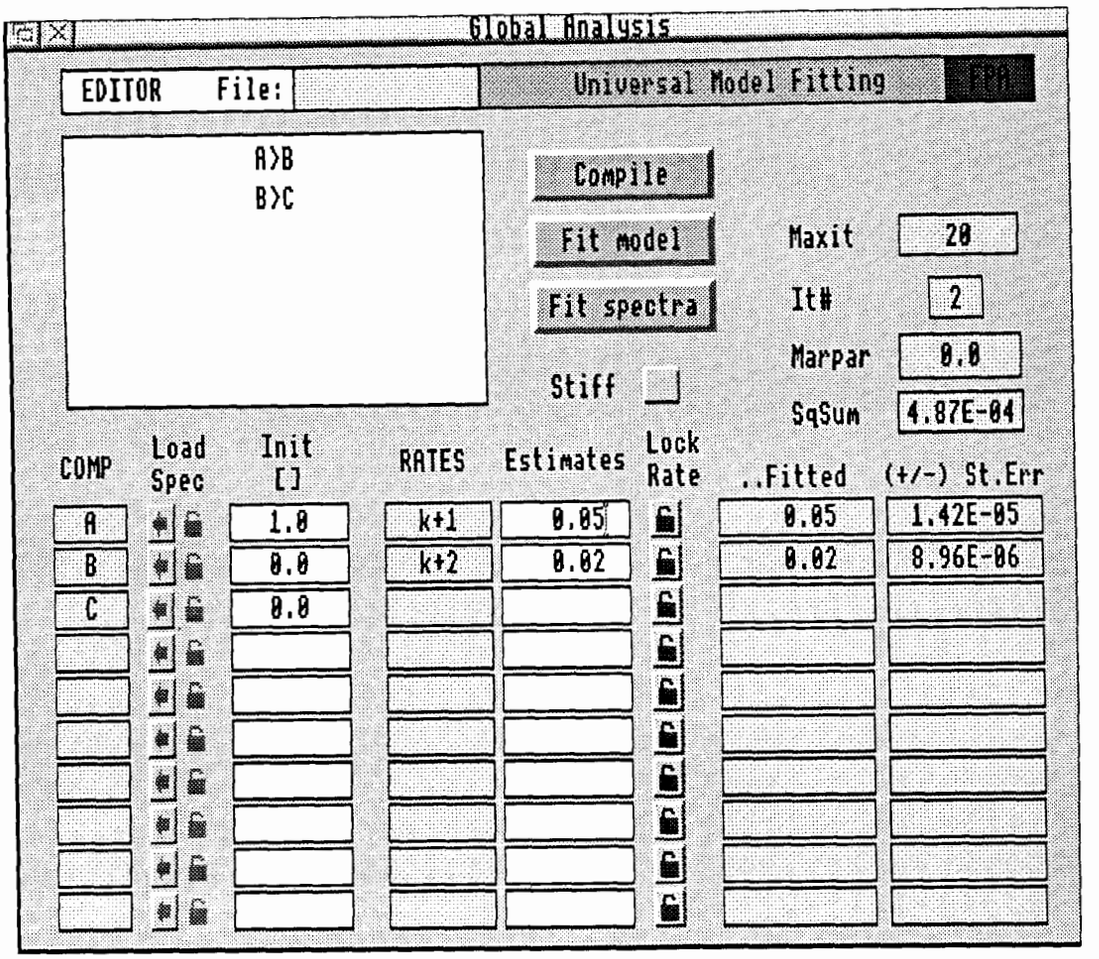


Fig. 5 Analysis Window

GLint provides a *unique* model fitting capability which may be accessed by selecting Analysis.. from the main menu. The dialog box shown in fig.5 appears.

The key feature of the analysis is the Global fitting of the entire data set to a supplied chemical reaction scheme.

Typically the data set to be analysed will have been reduced by SVD but this is not a requirement. Using the SVD result has a speed advantage for larger data sets since a subset of the output comprising the significant time dependent amplitudes is fitted rather than all the kinetic records at every measured wavelength (see section 9.0 for a discussion of the SVD reduction technique). By default 8 time vectors are fitted from the SVD output, therefore use of SVD reduced data for analysis is of benefit when the number of measured wavelengths exceeds this number. It should be emphasised that the result of the fit will not be affected either way.
Fitting a model to the data is performed in the following steps:

8.1 Model Entry

The top left of the analysis dialog contains a model entry box. To initiate entry click the left mouse button on the top line. A text caret will appear allowing normal typing and editing operations. Pressing <return> or the down arrow will move text entry to the next line.

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A reaction scheme is entered in terms of its reactants and products with forward and reverse conversions represented by the forward and reverse arrows respectively. The reaction model to be fitted must be broken down into lines each defining a single reaction step. For a two step consecutive scheme the following would be entered

A>B
B>C

A second order equilibrium would appear thus:

A+B<>C

Up to seven seperate steps are currently allowed. Mixed stoicheometries are allowed by prefixing the number to the relevant species (eg 3A+B>2C).
Note: It is not currently possible to have the same species name appearing more than once on a line. These are limitations in the current reaction scheme translator which will be resolved in future releases.

A+A>B	/Error/	Note however 2A>B is ok here
A>B+A	/Error/	

It is permissible to use multi-letter names for individual species but if species on either side of a step contain common letters then it is necessary to surround the names with [ ] brackets eg

[E]+[S]>[ES]
[ES]>[EP]
[EP]>[E]+[P]

Stoicheometries should preceed the opening bracket (eg 2[ES])

It is recommended that whenever possible unique single letter species names be used to prevent the risk of misinterpretation.

For the enzyme mechanism above use

E+S>B
B>C
C>E+P

8.2 Compilation

Once the model has been entered press the 'COMPILE' icon to the right of the model entry box. This causes translation of the scheme into a form understood by the program. At the same time the lower section of the dialog box is set up for parameter initialisation. Each species name is listed with a corresponding text insertion icon for its starting concentration. Similarly each rate specified in the scheme is listed with an index number corresponding to the step. Forward and reverse rates are distinguished using positive and negative indices respectively. For the model a+b<>c>d the rates would be listed k1, k-1 and k2. An estimate must be provided for each rate in the scheme in the corresponding text insertion icons prior to fitting.

8.3 Parameter Initialization

During fitting the starting concentrations and rates are used to generate intermediate concentration profiles according to the reaction model. These are then fitted to the original data in a linear regression step. This provides

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the overall residual which is the quantity iteratively minimised by the analysis. The fitting process involves optimisation of the rates by non-linear least squares such that the calculated concentration profiles yield the 'best fit' to the current data set. It is necessary to provide starting concentrations for all species in the compiled scheme as well as estimates of all listed rates. The accuracy required of the rate estimates is to a large extent dependent on the complexity of the scheme being modelled. These rates are then optimised by the global fitting algorithm. The initial concentrations provide the starting values for the numerical integration routines, and enable the subsequent calculation of true intermediate spectra. **It is crucial that non-zero concentration values are provided for the reactant species otherwise an 'Fit error' message will be reported.**

To enter values for a particular parameter click the mouse on the appropriate entry box. The cursor keys can be used to move between them.

Note: No visual distinction is made in the rate list between first (units:s-1) or second order ($M^{-1}s^{-1}$) rates since no units are displayed. If however the model contains a second order step then the corresponding rate for the combination is implicitly second order and should be supplied with a true second order estimate (units $M^{-1}s^{-1}$).

8.4 Fixing Spectra and Parameters

These two facilities are provided to constrain the fitting process. In some circumstances they are a requirement while in others they simply aid convergence.

Locking Rates:
To lock a rate simply click on its adjacent padlock icon.

Fixed Spectra:
Two options for 'fixing' spectra are provided. Known spectra for a species can be loaded from file or where appropriate a 'colourless' option selected.

In both cases the species in question should be selected by clicking on the arrow icon adjacent to its name (this will deselect any other).

To load a previously scanned spectrum, open the directory viewer containing the known spectrum file. This will have been collected using the SCAN facility in the !**SX17MV** application. Note that it must have the same wavelength resolution as the data set to be analysed.
It is then necessary to append the scan file with the species concentration in the cell at the time of the scan. This is used by **GLint** to translate the scan into an array of molar extinction coefficients for each measured wavelength. To do this double click on the scan file which will load it into the text editor !Edit.
Important: The concentration must first be multiplied by the ratio of cell pathlengths ($L_{spectra}/L_{scan}$) if they differ.
The value should then be typed below the final pair of points in the scan file followed by <return>. Any additional file information beyond this value should be removed. The file can then be re-saved by clicking on SAVE in the !Edit main menu.

Example: if the spectrum for a species X was taken with 10uM X in the observation cell and the time dependent spectra set are collected after initiating a reaction of X with Y in the cell with the same pathlength then 10e-6 should be added to the X spectrum file. If however the cell pathlength is changed from 1cm to 0.2cm between scan and spectra set 10e-6 x 1/0.2 = 50e-6 should be added to the file.
Note: if no concentration term is found at the end of a scan file a value of 1.0 is used by default.
To load the scan for the selected intermediate simply drag the scan file icon over the analysis dialog and release it. The padlock icon for the selected species will be highlighted indicating that the fixed spectrum has been loaded.

In the case where an intermediate is known to be colourless over the measured wavelength range, click the middle mouse button over the analysis dialog (which will open the analysis menu) and select 'SET COLORLESS'.

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In all cases to cancel a fixed spectrum click on the appropriate highlighted padlock to clear it.

8.5 Minimisation

Once the model has been compiled and the starting parameters supplied (together with any fixed spectra) rate optimisation is is initiated by clicking the FIT RATES icon. During minimisation the mouse pointer is replaced by an hourglass 'busy' icon
A non-linear Marquardt-Levenberg algorithm is used which iteratively attempts to improve the non-linear parameters (rates) to minimise the sum of the squares of the residuals of a theoretical data set calculated from those parameters and the real observed data (termed the SqSum). The iteration number is updated in the display together with the current SqSum. In addition the current Marquardt factor (MarPar) is displayed. This is an internal weighting parameter used by the algorithm to modify its technique of minimisation. In difficult cases it will be seen to increase by factors of ten at a time then decrease as a valid least squares minimum is approached (ref xxx). The final step of a successful minimisation is always conducted with a Marquardt factor of zero, since this yields the correct standard errors for each fitted parameter.

If convergence is not achieved (signified by a SqSum improvement of less than 0.1%) the minimisation stops by default after 20 iterations. The number of iterations performed must be checked to ensure that convergence has indeed been achieved rather than default termination (this is often indicated by a non-zero Marquardt factor). This is most easily ensured by accepting completion only when total iterations number less than 20.

To halt the minimisation process after the current iteration press 'ESC' once.

When fitting is complete the optimised rates are listed together with their standard errors. It is now possible to view the **Y-calc** (the modelled best fit data set), **residual**, calculated **spectra** and **concentration** profile displays (by choosing the appropriate icon in the main display window). In the 2D display modes (ie Absorbance vs time or Absorbance vs wavelength) the individual modelled curves are superimposed in red over the original data when the **Single** icon is selected in the display control dialog box (accessed from the main display menu option: **Display..**).

Any display can be printed by selecting the **Printout** option in the main display menu. Printouts are accompanied by a listing of the fitted model and optimised reaction parameters.

Error Conditions:
Occasionally an error will occur within the algorithm signified by an 'Fit Error' message. The two most common causes for this are:

1. A reactant concentration has been accidently left at zero.

2. A model has been incorrectly entered which translates into an impossible set of equations for integration.

If the fitting appears to have 'locked up' ie the hourgalss icon remains but nothing seems to be happening, this will almost certainly be due to an attempt to fit a 'stiff' model (or one that has become stiff) with the non-stiff integration method (see below). The only option is to press 'ESC' and wait for the current iteration to complete. Then select 'Stiff' and continue.

8.6 Convergence Problems

It is important to appreciate that convergence is not necessarily garanteed. Minimisation to a unique set of parameters requires either that changing a parameter affects the overall residual and that the effect of changing one parameter on the residual is not compensated by a change in another.

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The minimisation procedure can, and should be, repeated with alternative models as required (starting with the simplest), by repeating the cycle of model entry, parameter initialisation and minimisation. In particular, with more complex schemes, the identification of a satisfactory model may take several attempts and stepwise refinement.

In some cases there may not be sufficient information in the data to succesfully fit to an elaborate model even though there is other evidence for it. This situation can for example occur when the observed spectral changes accompany only slow events in a proposed mechanism, but fast events such as ligand binding equilibria are known to precede them. To include the fast part of the mechanism (unless its rates are fixed) in the fitting may well cause problems, since it is poorly characterised.

Wherever possible always start with a simple model and build on a succesful fit. Look for areas where the residuals are poor and consider adding an appropriate step to account for the behaviour. Where possible fix rates and spectra since this serves to constrain the fit and in many cases will enable convergence which might otherwise not occur.

8.7 Model Validity

Convergence of a fit means that a least square minimum for that model to the data has been found. The most informative guage to the goodness of fit is the residual plot (available from the icon in the main display window). Any systematic deviations (as opposed to random noise) apparent here indicate that either a genuine spectral event has been missed (or rather not accounted for) or that an instrumental artifact is corrupting the data. Hopefully the contribution of the latter will be minimal or of an obvious form (spikes or other abrupt deviations).
The second assesment of fit validity can be made by inspecting the calculated spectra. If a model is satisfactory in terms of the residual plots then it must be accompanied by calculated spectra which make chemical sense in terms of shape and sign. An incorrect model may well produce reasonable residuals but bizarre or negative going extinction spectra. This can also arise, even with a correct model, when calculated rates are assigned to individual steps in the wrong order (try modelling the system: A>B>C with rates 10s-1 and 1s-1). Also remember as schemes become more complex the first mechanism which fits the data well may not be unique. This has to be judged on the basis of knowledge of the chemistry and evidence from other experiments and conditions.

8.8 Constraining the Fit - Locking Rates and Fixing Spectra

It is not possible to describe every situation where either a fixed rate or spectrum will be needed but the following illustrate two examples:

Data Model: A+B>C or A+B<>C

The spectrum of either A or B must be supplied (unless one is colorless - see below). This is because there are an infinite number of solutions for the spectra of A and B calculated by linear regression. This will prevent fit convergence unless one or other is supplied.

Data Model A<>B

By itself this is an unrealistic model, but illustrates the general problem of separating individual rates from equilibria. In this case the data can be fitted with the model A>B since the transition occurs with an observed monotonic rate $k_{obs} = k_1 + k_{-1}$. The fit to A>B will converge yielding k_{obs} and good residuals but produce incorrect spectra. Attempting to fit to the model A<>B will produce an arbitrary solution (note the fit will converge) for k_1 and k_{-1} though in all cases they will add up to the constant and unique k_{obs}. This system can only be solved by fixing correctly one or other of the two rate constants.
Both these examples illustrate the problem that arises when there are too many variable parameters free to account for the observed data. The only way to obtain the unique and hopefully correct solution is to apply appropriate constraints either by supplying fixed spectra or locking rates.

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8.9 Using the Stiff Option

The **Stiff** option should be selected when a system to be modelled contains time dependent events which differ by more than (roughly) 3 orders of magnitude (1000 fold difference between the slowest and the fastest). **Stiff** invokes a specialised routine to handle the numerical integration calculations during fitting since the normal routine becomes extremely slow under such circumstances. It is not selected by default since for non 'stiff' scenarios the standard integration routine is much quicker. The only danger when it is not selected is that rates may become widely separated during the fitting process leading to a non-stiff system becoming stiff. This problem should be avoidable with reasonable anticipation and preparation.

Example A>B>C (first order rates)

	k_1	k_2	ratio
Non Stiff:	10	1	10/1 = 10
	10000	1000	10000/1000 = 10
	.001	.1	.001/1 = .001
	k_1	k_2	
Stiff:	10	.001	10/.001 = 1e4
	10000	1	10000/1 = 1e4
	100	.001	100/.001 = 1e5

For second order steps it is less obvious when a system is stiff since the concentration of species combines with the second order rate to give a measure of the overall speed of the event (which can then be compared to first order rates). Thus if A+B>C with a second order rate of $1e^7 M^{-1}s^{-1}$ but the concentration of A and B are 1uM each then the speed of the change to relate to first order steps can be calculated as $1e^7 x\ 1e^{-6}$ (or the greater reactant concentration) = 10 s^{-1}.

Example A+B>C>D Ao=$1e^{-5}$, Bo=$1e^{-6}$

	$k_1(M^{-1}s^{-1})$	k_2	ratio
Non-Stiff:	$1e^6$	1	$1e^6$ x $1e^{-5}$(Ao) / 1 = 10
	$1e^8$	100	1000 / 100 = 10
Stiff:	$1e^8$	.01	1000 / .01 = $1e^5$
	$1e^4$	1000	.1 / 1000 = $1e^{-4}$

The anticipation of stiff systems may be overlooked: if in doubt select it!

8.10 Fit Spectra

The FIT SPECTRA icon can be selected at any time when a compiled model and parameter set is present. It simply carries out a linear regression fit of the concentration profiles defined by the current model and displayed rates (from the estimate column) to the current data set. This is exactly the same as the final step that takes place automatically after minimisation (above) and yields the best fit extinction spectra and residual plots etc. The difference is that the currently displayed rate or concentration values are used ie there is no requirement that the rates are the best fit values. Therefore it is possible to modify these parameters eg swap the order of rates, adjust a rate up or down etc, and see the effect on the subsequent residuals and spectra.

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9.0 Simulation

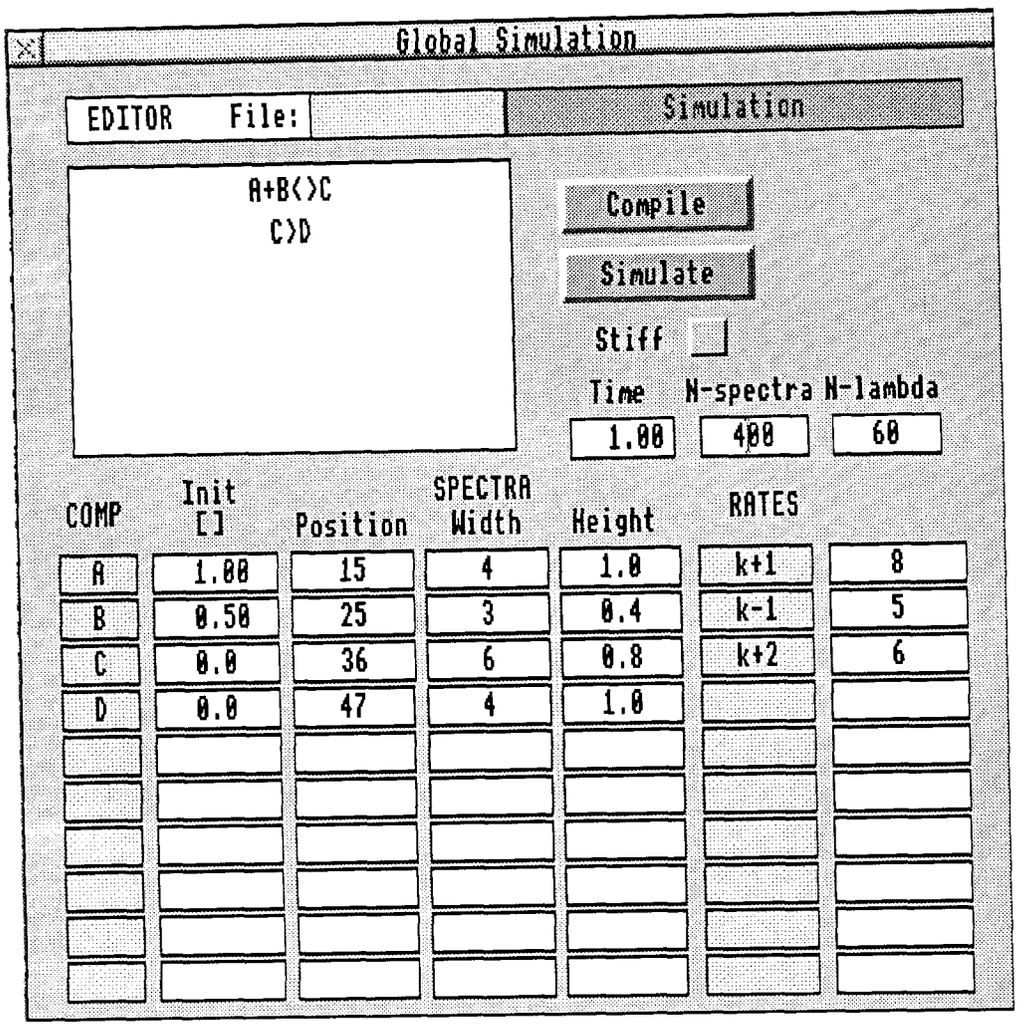


Fig. 6 Simulation Window

In addition to the global analysis facilities described in section 8, **GLint** provides an extremely powerful data simulation facility. This allows the creation of artificial sets of time dependent spectra (including added noise) for experimentation and analysis. These are synthesized according to reaction models and spectral characteristics provided by the user. The data can then be analysed as if it had been collected during an experiment.

This tool is invaluable for learning the behaviour of the data analysis facilities with respect to different data sets of varying complexity. ie if a data set is synthesised according to a particular model does that mean it can be fitted directly to the same model without locking rates or spectra? It also allows the user to get a feel for how chemical mechanisms behave and account for observed spectral characteristics (eg isosbestic points).

When SIMULATION is selected from the Main menu the dialog box shown in fig.6 appears. It bears several similarities to the analysis dialog box, the major difference being the array of input icons for setting up the spectral characteristics of the individual species.

The first step for simulation is model entry. This is carried out in the same way as described for analysis (section 8).

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Once complete select the COMPILE icon to translate the scheme and set up the dialog box for individual parameter entry.

For any simulation it is possible to define the required number of time points (N-spectra) and the number of wavelengths (N-lambda) in the entry icons provided. This determines the overall number of absorption measurements synthesized. The default settings are N-spectra=100 and N-lambda=60. This will simulate data with 100 absorption values per kinetic run at each of 60 wavelengths (6000 values in all). Note that the 'wavelength' range starts from 1 and runs to N-lambda (ie the displayed wavelength for synthetic data sets merely represents an index rather than a realistic wavelength).

It is also necessary to enter the desired time course (in seconds) of the simulation which will of course depend on the rates of the model to be simulated. Absorption values will be synthesized at intervals of Time/N-Spectra seconds.

The desired starting concentrations and rates can now be entered alongside their labels (below the model entry box). Note that the **Stiff** selection icon for simulating models with widely differing rates (section 8.0).

Remember to provide finite concentrations for all reactants.

It is then necessary to type in values for spectra calculation. Each spectrum (for each species) has one gaussian peak, characterised by its peak POSITION, its WIDTH and its HEIGHT.

POSITION: a floating point value between 1 and N-lambda.

WIDTH: a floating point value chosen according to the total number of wavelengths.This provides the spread of each peak. The smaller the value (minimum 1) the narrower the peak. For an Nlam of 60 a WIDTH value of 5 will produce sensible individual spectra.

HEIGHT: any floating point number. This will be the relative peak height for each component. 1.0 is good value to start with!
Important: To set up a colourless species type in 0 (zero) for its height parameter. Its peak position and width parameters will be ignored.

Having set up and compiled the model and entered all the parameters press SIMULATE. After a few seconds the synthesized data will be displayed in the main window. Any data previously loaded or simulated will be discarded. If an error is displayed this will almost certainly be due to incorrect parameter entry, which can easily be corrected.

Once the simulated data has been displayed proceed with SVD or analysis exactly as if this were a real data set loaded from file.

Note: If the Analysis dialog is chosen while the Simulation dialog is on display, the latter will be automatically closed and vice-versa. In addition the model plus concentration and rate parameters, used for the simulation will automatically be transferred to the analysis dialog.

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10.0 Singular Value Decomposition

The singular value decomposition (SVD) algorithm is an integral feature of **GLint**.

When applied to a data matrix Y (Time x Wavelength) containing a set of time dependant spectra the result is a set of output matrices comprising ordered sets of **basis spectra** and **time dependent amplitudes**, together with corresponding weighting factors known as **singular values**.

The relationship of the input to output matrices is as follows:

$$Y = U.S.V^T$$

The time dependent amplitudes are present in the column vectors of U whilst the basis spectra occupy the row vectors of V. S is a diagonal matrix containing the singular values. It should be noted that within U there are available as many time-dependent amplitude vectors as there are individual wavelengths defining the number of columns in Y.
The important feature of the decomposition is that only a subset of the paired vectors, together with their corresponding singular value (which acts as a weighting term), need be used to reconstruct the features of Y when Y contains measurements on sytems comprising only relatively few (with respect to the number of wavelengths) independent components. In other words multiplying together only the first N vector pairs and singular values will provide the best N component reconstruction of the data matrix Y in a least squares sense. Increasing N beyond the number of underlying components causes vectors to be included which reconstitute nothing but noise present in the original data.
This separation brought about by SVD of the data into its underlying linearly independent components provides the basis for its usefulness in **GLint** analysis and data compression.

10.1 Component Prediction

Once SVD has been performed it is possible to inspect both the output vectors and the singular values. The first eight vector pairs are displayed below the main display screen with time dependent amplitudes (actually pre-multiplied by their corresponding singular value) above basis spectra. To view this display scroll the main display. The singular values are listed in a dialog box available in the SVD submenu (off the main menu). Typically the singular values will fall from the first and largest value down (through intermediate values) to a minimum threshold which plateaus out (eg 3.4, 0.8, .25, .0011, 0010, .0010, .0010...). **The number of significant singular values (SSV) can be used as a model free indication of the number of linearly independent components present in the original data.** In a chemical system these linearly independent components reflect the contribution of independent absorbing species. The plateau amplitude is representitive of the background noise level. The SSV's have corresponding spectral and time vectors displayed graphically. It should be clear that only the vectors corresponding to the SSVs contain significant features which will be reflected in the reconstructed data.

10.2 Analysis

All the time dependent information inherent in the original data is contained in the significant time dependent amplitude vectors from matrix U. This can be used to considerably improve the performance of the global analysis since only these vectors (premultiplied by their corresponding weighting singular value), rather than every original kinetic curve, need be globally fitted to obtain the optimised rates for a reaction model. Since there are typically far fewer significant time dependent amplitude vectors than measured wavelengths this both speeds up the minimisation process and reduces the number of amplitude parameters that need to be calculated at each step. Once the minimisation phase is completed the resulting best fit concentration decays need only be fitted to the original data once to calculate the corresponding amplitudes for the original data matrix, yielding the individual component spectra.

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10.3 Data Compression and Filtering

A useful by-product of SVD is the reduction of the data into a form which separates its significant components from noise. Since only the vector pairs corresponding to the SSV's reconstruct the events of interest in the data matrix, only these are required for storage purposes. Therefore a datafile originally comprising say 1000 time points at each of 50 wavelengths, 50000 points in all, can be replaced by a file comprising, if we assume 4 SSV's, 4 x 1000 (time dependent amplitudes) + 4 x 50 (basis spectra) + 4 (singular values) = 4204 points, a space reduction factor of more than 10. When reloaded from archive the original data set can be simply reconstructed (minus the noise) by matrix multiplication according to the relationship above.

10.4 GLint Analysis and the SVD

When the SVD of a data set has been calculated data analysis automatically uses the SVD output time vectors for regression analysis rather than the original kinetic curves at every wavelength. Currently the first 8 vectors are used regardless of the number of independent components actually contributing to the data. Strictly speaking this may well be more than are required for simple systems. The alternative is to allow the operator to choose the number of significant singular values to pre-determine the number of time vectors to use. This however has the danger of the user actually removing component information from the transformed data before fitting takes place, which means the final residuals as calculated with respect to the real data are incorrect (ie not the true least squares). By removing this option it is felt that the user is prevented from making potentially hazardous assumptions about data complexity, and not taking into account minor components.

The effect of using selected time vectors can however be explored by using the Recon U.S.V menu option and selecting the number of required significant singular values to be used (from the Recon U.S.V. dialog box) in reconstituting a data set after its (original) SVD has been calculated. A new data set is generated comprising the components corresponding to only the selected singular values (between 1 and 8). This can then be saved and manipulated as if it were a set of real measurements. This provides an indirect means of removing lower order time vectors prior to analysis and allows the user to exlore the behaviour of the SVD algorithm and its influence when employed for data reduction.

Note: the use of 8 singular values and time vectors implies an upper limit on model complexity of 8 independent absorbing species. This is to some extent an arbitrary value and if necessary can easily be increased on request. Difficulties in minimisation with more complicated schemes do however suggest that it is unlikely that many more components could be effectively fitted with real absorption or fluorescence measurements, and that the vast majority of systems will be adequately defined by this limit. Any comments on this feature are welcome.

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