A Computer Program to Extract the Continuous and Discrete Relaxation Spectra from Dynamic Viscoelastic Measurements

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Abstract:
We describe and implement an efficient, open-source, multi-platform computer program ReSpect to infer the continuous and discrete relaxation spectra from dynamic moduli measurements obtained by small-angle oscillatory shear experiments. We employ nonlinear Tikhonov regularization and the Levenberg-Marquardt method to extract the continuous relaxation spectrum. To obtain the discrete relaxation spectrum, we introduce a novel algorithm that exploits the continuous spectrum to position the modes. It uses a simple criterion which balances accuracy and conditioning of the resulting least-squares problem to determine a parsimonious number of modes. The end result is an easy-to-use, and easy-to-extend program, which can be used from the command-line or from a graphical user interface to override some of the default algorithmic choices.

Zusammenfassung:
Ziel der vorliegenden Untersuchung ist die Implementierung eines effizienten, open-source und multi-platform Computerprogramms ReSpect zur Bestimmung von kontinuierlichen und diskreten Relaxationsspektren aus dynamischen Modulmessungen, die aus kleinwinkligen oszillatorischen Schubexperimenten stammen. Die nichtlineare Tikhonov-Regularisierung sowie die Levenberg-Marquardt-Methode werden eingesetzt, um das kontinuierliche Relaxationsspektrum zu bestimmen. Dafür wird ein neuer Algorithmus eingesetzt, der auf dem kontinuierlichen Spektrum beruht, um die Positionierung der Modi anzugeben. Es wird ein einfaches Kriterium verwendet, welches einen Kompromiss zwischen Genauigkeit und Konditionierung des resultierenden Problems der kleinsten Quadrate darstellt, mit dem Ziel die genaue Anzahl an Modi zu bestimmen. Ein leicht zu bedienendes sowie erweiterbares Programm wird erstellt, welches direkt entweder von einer Befehlszeile oder von der graphischen Schnittstelle aus, einfach einige Default-Werte des Algorithmus' überschreiben kann.

Résumé:
Nous décrivons et implémentons un programme efficace, d'accès libre, multi-plateforme, appelé ReSpect, afin d'extraire les spectres de relaxation continu et discret des mesures de modules dynamiques obtenues avec des expériences de cisaillement dynamique de petite amplitude. Nous employons la régularisation non linéaire de Tikhonov et la méthode de Levenberg-Marquardt afin d'extraire le spectre de relaxation continu. Afin d'obtenir le spectre de relaxation discret, nous introduisons un nouvel algorithme qui exploite le spectre continu pour positionner les modes. Il utilise un critère simple qui balance la précision et le conditionnement du problème de moindres carrés résultant, afin de déterminer un nombre parcimonieux de modes. Le résultat final est un programme facile d'utilisation et d'extension facile, qui peut être utilisé à partir du « command-line » ou d'une interface graphique afin de surpasser certains des choix algorithmiques par défaut.

Key words: relaxation spectrum, linear rheology, continuous spectra, discrete spectra

ReSpect software available for free download from:
http://www.mathworks.com/matlabcentral/fileexchange/40458-respect

1 INTRODUCTION

In linear rheology, the continuous relaxation spectrum (CRS), $h(\tau)$, is a quantity of vital importance, for once it is known, it is straightforward to compute all other material functions [1, 2]. Unfortunately, it cannot be measured directly; instead, it has to be inferred indirectly, most commonly, from small amplitude oscillatory shear experiments. These experiments yield the frequency-dependent dynamic moduli, $G^*(\omega) = G'(\omega) + iG''(\omega)$, where $G'(\omega)$ and $G''(\omega)$ are the storage and loss modulus, respectively, and ω is the frequency of deformation. The resulting problem of deducing $h(\tau)$ from $G^*(\omega)$ has a long and rich history [2–10]. Mathematically, $h(\tau)$ and $G^*(\omega)$ are related by:

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squares problem to obtain the discrete spectrum. After determining N_{opt} using a heuristic which tries to balance conditioning and accuracy, the function PlotMaxwellModes does some basic plotting.

There are only two functions that are shared by contSpec and discSpec, viz. kernel and SetParameters. All the data files (with suffix '.dat'), except the input file Gst.dat, are results of computation written by the software. Other than specgui.m, the other files related to the GUI are specgui.fig, which sets the basic background, and updateplot which updates plots in the figure window of the GUI, when the user selects a new or different plot.

6.2 EXAMPLE

Using the default settings, we call the function:
>> contSpec(): If the function is called without any input arguments, it reads the parameters from the file SetParameters. Alternatively, it is possible to call the function by specifying the parameters (contSpec(par)), in which case the settings in the file SetParameters are not used. contSpec computes $H_{\lambda C}(\tau)$, writes it to the file H.dat, and displays it graphically. It also computes the corresponding $G^*(\omega)$, writes it to the file Gfit.dat, and displays the fit with the input data graphically. It writes the range of λ sampled, with the corresponding ρ and η in the file rho-eta.dat.
>> discSpec(): Like contSpec, it reads parameters from the file SetParameters, when called without any input arguments. discSpec also computes the corresponding $G^*(\omega)$, writes it to the file Gfitd.dat, and displays the fit with the input data graphically. It writes the range of N sampled and the corresponding error and condition numbers in the file Nopt.dat.

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