A DISCRETIZATION SIZE AND STEP SIZE VARYING STRATEGY IN THE NUMERICAL SOLUTION OF 1–DIMENSIONAL SCHRÖDINGER'S EQUATION

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AUTHOR DECLARATION

I hereby declare that the work in this thesis is my own except for the quotations and summaries which have been duly acknowledged.

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STRATEGI PENGUBAHAN SIZE PENDISKRETAN DAN SIZE LANGKAH DALAM PELAKSANAAN BERPENDEKATAN PENYELESAIAN NUMERIK BAGI PERSAMAAN SCHRÖDINGER 1 – DIMENSI

OLEH

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2010

ABSTRAK

Dalam tesis ini kita memaparkan satu penyelesaian berangka persamaan Schrödinger 1-dimensi menggunakan berpendekatan kaedah garis (MOL) di mana kita diskretkan dimensi ruang menggunakan penghampiran beza terhingga untuk menghasilkan sistem masalah nilai awal hanya bergantung kepada dimensi masa. Kita kaji kesan mengubah saiz pendiskretan terhadap kejituan penyelesaian berbanding mengubah saiz langkah semasa mengkamirkan persamaan pembezaan yang terhasil. Kita juga masukkan penggunaan fungsi aturan simpson dalam MATLAB. Hasil kajian menunjukkan terdapat kebaikan jika keputusan yang betul diambil antara mengubah saiz pendisteretan atau saiz langkah dalam penyelesaian berangka sistem persamaan pembeza.

Katakunci: persamaan schrodinger, kaedah garis (MOL), beza terhingga, pendiskretan, persamaan schrodinger kubik tak linear.

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ABSTRACT

In this thesis we present a numerical solution of the 1-dimensional Schrödinger equation using the method of lines approach (MOL) where we discretize the spatial dimension using some finite difference approximation leaving the time dimension to be the only independent variable in the resulting system of initial value problems. We study the effect of changing the discretization size on the accuracy of the solution procedure versus changing the step size in the integration of the resulting differential equation. In the study we incorporate the use of Simpson's rule function in MATLAB. The results indicated that there are some advantages in deciding between the discretization sizes or step size in the numerical solution of differential equation as far as the computing time is concerned.

Keywords: Schrödinger equation, Method of lines (MOL), Finite difference Discretization, Nonlinear cubic Schrödinger equation.

تغير حجم القيم المنفصلة وإستراتيجية مرحلة الحجم في تطبيق معادلة سكرودينجر أحادية البعد

اعداد :

لاوال سعد (٣٠٩٠٠٠٣١)

٢٠١٠

ملخص البحث

في هذه الدراسة يتم طرح حل عددي لمعادلة سكرودينجر أحادية البعد (1-dimensional Schrödinger equation) باستخدام طريقة تقارب الخطوط (MOL)، حيث يتم تجزئة البعد او المدى الفضائي باستخدام تقريب الفرق المحدود (finite difference approximation) مع ترك مدى الوقت العامل الوحيد المستقل في نظام النتائج لمشاكل القيمة المبدئية. ترتكز هذه الدراسة على تأثير تغير حجم القيم المنفصلة على دقة عملية إيجاد الحل ضد تغير الحجم أثناء مرحلة التكامل للمعادلة التفاضلية الناتجة. يتم دمج استخدام دالة قانون سمبسون (Simpson's) في ماتلاب (MATLAB). النتائج بينت ان هناك بعض المزايا للإختيار المناسب و الصحيح بين تغير الحجم للقيم المنفصلة او تغير الحجم أثناء مرحلة التكامل لإيجاد الحل العددي للمعادلة التفاضلية.

كلمات دالة: معادلة سكرودينجر، طريقة تقارب الخطوط (MOL)، الفرق المحدود، القيم المنفصلة، معادلة سكرودينجر التكعيبية الغير خطية(NCSE).

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