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An Efficient Replacement for Schrödinger's Partial Differential Equation

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Abstract:- The classical finite difference method for solving time-dependent partial differential equations has become quite tedious and requires the use of off-the-shelf algorithms such as those in MATLAB. The treatment by finite difference method then solution of the n resulting first order algebraic equations is quite difficult since the underlying matrix is singular. We propose an alternative revolutionary statistical technique using Bmatrix chains, which are a product of the Cairo techniques. This technique is valid for both classical macroscopic physics such as the heat diffusion equation and modern microscopic quantum mechanics such as Schrödinger's PDE. He completely neglects partial differential equations as if they never existed. The numerical results of the proposed numerical statistical method show stability, accuracy and superiority over conventional PDE methods.

I. INTRODUCTION

There are two completely different languages for approaching the subject of time-dependent physical phenomena (in both classical macroscopic physics and modern microscopic quantum mechanics) investigating the temporal evolution of energy density field in geometrical space (x,y,z), resulting in two different approaches A and B:

A-classical theory where the energy density field U(x,y,z,t) is represented via a partial differential equation relating the time derivative of U to its space derivatives.

This theory is valid both for classical physics situations describing physical phenomena at the macroscopic scale such as the heat diffusion equation and for quantum mechanics situations described by the Schrödinger equation.

Here, time t is considered as an external controller.

The normal procedure to solve this PDE numerically is to advance through the following three consecutive step procedure:

- Discretize the relevant space of the system into n equidistant free nodes. The accuracy of the solution increases as n increases.

- Apply the variable separation method,

U(x,y,z,t)=X(x) . Y(y). Z(z). f(t)

Obtain four ordinary differential equations.

- The third step consists of applying finite difference methods (FDM) to the above-mentioned ordinary differential equations subject to Dirichlet boundary conditions (or any other suitable boundary condition BC) to obtain three sets of algebraic equations of the first order of n variables corresponding to the n free nodes in addition to an algebraic equation of initial condition (called initial value problem), where (U(x,y,z,t=0) is presupposed everywhere, for l temporal evolution of U.

The fundamental flaw of the method of partial differential equations is that it must be supplemented by the natural conditions of stability and symmetry. **In other words, the PDE and the boundary conditions are not autonomous**.

B- Modern numerical statistical theory known as Bmatrix chains, which is a product of the Cairo techniques (valid for both classical macroscopic physics such as the heat diffusion equation and modern microscopic quantum mechanics such as the Schrödinger's PDE) suggests a different approach that completely neglects partial differential equations. as if they never existed.

Note that particle physics is fundamentally different from wave mechanics because they both have a different physical nature.

The nature of particles is described or modelled as being small and confined to a point in space, while a particle wave is something that propagates and extends almost into infinite free space. Additionally, particles collide and scatter while matter waves refract, diffract, and interfere in a process called superposition. They add or cancel each other in superpositions.

The question arises how can Bmatrix chains describe the seemingly opposite nature via the same matrix?

The answer lies in how to specifically define the boundary conditions in both cases.

We assume that if the boundary conditions in Bmatrix chains are Dirichlet or similar, they then describe a microscopic or macroscopic particle. On the other hand, assuming that the boundary condition extends to infinity, the chains of the B matrix describe the mechanics of wave particles.

Note that Bmatrix chains operate in 4D unit space x-t where time t is woven into geometric space.

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Here the real time t is completely lost and is replaced by N dt where dt is the time step and N the number of iterations.

The Bmatrix chains are well defined [1,2,3,4] and have been successfully applied to the solution of the Laplace and Poisson PDE solution, the heat diffusion PDE, the Schrödinger equation as well as to double and triple digital integration.

An introductory prerequisite to numerical methods can be found in reference 5.

It is worth mentioning that the Cairo technical approach is not entirely new and has been effectively applied to a wide area of physical situations since its birth in 2020.

We emphasize once again that the Cairo technical approach does not require iteration of the MATLAB algorithm or any other conventional mathematical method! Again, the question of why the Bmatrix on-chain approach is widely successful while the PDE approach fails?

We assume that the answer is that Bmatrix chains are in some way a branch of the so-called stabilization methods since Bmatrix chains are intrinsically autonomous or autonomous in the sense that they have maximum possible symmetry and maximum possible stability.

II. THEORY

❖ We explain the theory in two consecutive steps:

In step A we explain how strings from matrix B can replace the time-dependent PDE of classical physics, then in step B we extend this treatment to explain how strings from matrix B can replace the time-independent Schrödinger PDE.

A-Classical Physics PDE

The importance of finding a powerful numerical solution for the Laplacian matrix A in the Laplace and Poisson partial differential equations is obvious.

Here again, the classic numerical procedure for solving the Laplace partial differential equation is based on the discretization of the 1D, 2D, 3D geometric space into n equidistant free nodes then on the use of the FDM finite difference method supplemented by Dirichlet boundary conditions. (vector b) to obtain a system of algebraic equations of order n first in the matrix form A,

$$A \cdot U(x,y,z,t) = b \quad \ldots\ldots (1)$$

The solution to the above equation is,

$$U(x,y,z,t) = A^{-1}.b \quad \ldots\ldots (2)$$

which is often quite complicated since the matrix A is singular.

It is worth mentioning that common numerical iteration methods such as Gaussian elimination and Gauss-Seidel methods are complicated and require the use of ready-made algorithms such as those in MATLAB or PYTHON ..etc .

We assume that there exists another SIMPLE statistical numerical solution expressed by:

$$\mathbf{A^{-1}=(I-A)^{-1}=A^0+A+A+A^2+....+A^N \quad \ldots\ldots (3)}$$

Where $A^0=I$ and N is the number of iterations or time steps dt.

Equation 1 actually introduces a revolutionary technique!

Note that the numerical solution of equation 3 is quite simple via the calculation of the first terms (Normally the first 12 terms will suffice) of the infinite matrix series 3 or equivalently via the expression,

$$A^{-1}=1/(I-A) \ldots\ldots (4)$$

Equation 4 is valid for a sufficiently large number N.

It is obvious that when the matrix A is singular then the matrix I-A is not singular and can be inverted.

B-Schrodinger PDE in quantum mechanics

We suppose,

a- the starting point is to replace the complex PDE for the complex wave function Ψ (probability amplitude) by a real PDE for Ψ^2.

The PDE for Ψ^2 which is the probability density of finding the quantum particle in the volume element x-t dx dy dz dt is assumed exactly equal to the energy density of the quantum particles.

b- Therefore, the solution of the Bmatrix chain follows the same procedure of solving the heat diffusion equation explained above in the last question:

How to invert a 2D and 3D Laplacian matrix without using MATLAB iteration or any other conventional mathematical method?

c-Follow the three steps explained in section A, then a final step is to take the square root of the solution for Ψ^2 as the solution for Ψ itself.

In order not to worry too much about the details of the theory, let us move directly to the illustrative applications and their numerical results.

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III. NUMERICAL RESULTS

Case A:

Two dimensions heat diffusion equation 9 equidistant free nodes with Dirichlet boundary conditions as shown in Fig.1

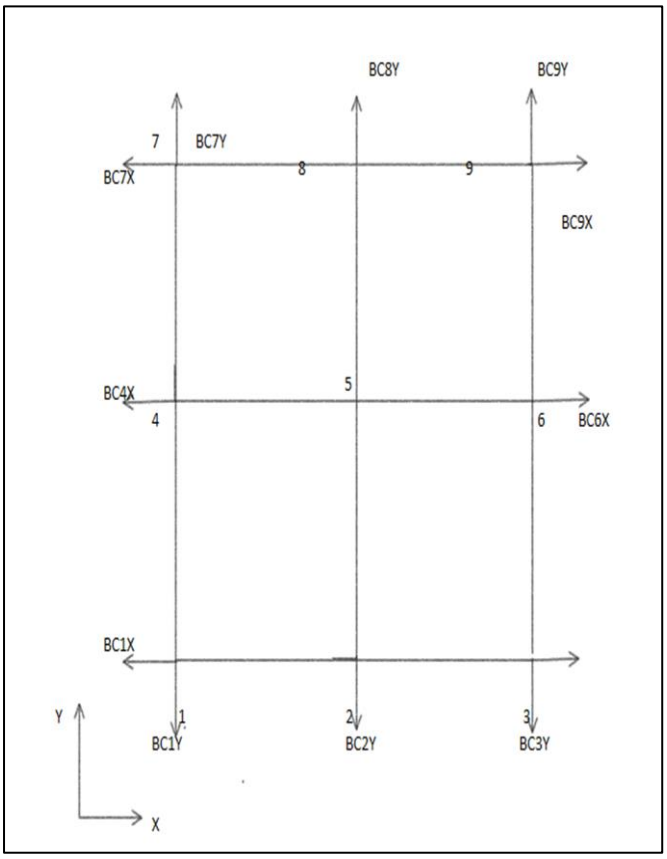

Fig. 1 - 2D square of 9 equidistant free nodes and 9 Dirichlet boundary conditions.

Mathews [5] classically solved the system resulting from 9 linear algebraic equations using Gaussian elimination method in a more efficient scheme by extending the tridiagonal algorithm to the more sophisticated penta-diagonal algorithm for his arbitrary chosen BC vector,

b = [100,20,20,80,0,0,260,180,180] T . . . . . (5)

and arrived at the solution vector:

U=[55,7143,43,2143,27,1429,79,6429,70,0000,45,3571,112 ,357,111,786,84,2857]T .. . . (6)

Now the BC vector for the proposed statistical solution corresponding to equation 5 is simply rewritten,

[100/4, 20/4, 20/4, 20/4, 80/4, 0, 0.260 / 4, 180/4, 180/4] T ... . . . (7)

The calculated transfer matrix D = E-I can be multiplied by the vector BC (b) from the equation. 7, we obtain,

U=[55,7132187 43,2126846 27,1417885 79,6412506 69,9978638 45,3555412112,856079 111,784111 84,2846451]T . . . . ..(8)

If we compare the numerical results of the proposed statistical solution (Eq 8)) with that of Mathews(Eq 6), we find a striking precision

Case B

The solutions for quantum particles in a one-dimensional infinite potential well, quantum particles in a two-dimensional infinite potential well, and quantum particles in a three-dimensional box follow from the theory explained in section 2.

These solutions are explained in detail in references 7,8,9 respectively. So there is no point repeating them.

Case C

Somewhat surprisingly, the Bmatrix chains initially introduced to solve the time-dependent PDE are able to evaluate bounded single, double and triple integration with high accuracy [3,4].

For a simple integration ($I=\int y\,dx$) on a line discretized by 7 free nodes equidistant at distance h from each other, the limited statistical integration formula (Is) is given by [4],

Is=6 h2/77 (6*4 +11* 9 + 14* 16+15* 25 +14* 36 + 11*49 + 6*64)

On the other hand, to evaluate the limited double integral ($I=\int\int W\,dx\,dy$) on the 9 free nodes of rectangular figure 1, we can show that the statistical weights are: (1,2,1,2, 3, 2,1,2,1)/15 which is sufficiently precise.

IV. CONCLUSION

The classical finite difference method for solving time-dependent partial differential equations has become quite tedious and requires the use of off-the-shelf algorithms such as those in MATLAB.

We propose an alternative revolutionary statistical technique using Bmatrix chains, which are a product of the Cairo techniques.

The proposed method is valid for both classical macroscopic physics such as the heat diffusion equation and modern microscopic quantum mechanics such as Schrödinger's PDE.

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NB: In the previous calculations, the author used his own double precision algorithm as explained in reference 10,11.

No ready-made algorithms such as Python or MATLAB are needed.

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