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COMPUTING GROWTH RATE UNDER INTERVAL UNCERTAINTY: THE DETERMINISTIC TRANSPORT CODE S_N

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Abstract

The paper presents numerical computations of deterministic S_N transport for the multigroup energy and linear discontinuous spatial discretization on tetrahedral meshes for anisotropic scattering of Legendre order L. We use the Power method to describe this phenomenon and in particular, implemented interval results for the Rayliegh Quotient iteration for the spectral radius. As an extension, we computed the solution for the system of second order ordinary differential equation using the Euler-Chevbyshev matrix square root method whereby, the result obtained from Power method respectively, the Rayleigh Quotation iteration, becomes free of charge as useful tools. The technique can be interpreted as an acceleration problem for the described phenomenon.

Keywords: Deterministic transport S_N ATTILA, anisotropic scattering of Legendre order L, power method, interval arithmetic, nuclear science, Euler-Chevbyshev matrix square root method.

1.0 Introduction

The paper presents applications of the well known Power method [1] for the determination of growth rate of a system. Included in the presentation is the multigroup in energy, and linear discontinuous finite element spatial discretization of the S_N equations on tetrahedral meshes [2]. The S_N transport code is facilitated by the Krylov subspace iteration. ATTILA [3] is being known to be a three – dimensional discrete ordinate (S_N) code which has the capacity to solve the discrete equations on a tetrahedral mesh by employing the linear discontinuous (LD) finite-element spatial differencing scheme. The LD scheme would yield the angular flux within each tetrahedron as a function which is linear for the four unknowns in each tetrahedron where, the angular flux is permitted to discontinue at the boundaries.

With a well simplified approach to the presentation, firstly, consider dynamic or discrete system listing the current values of its parameters $(x_1, x_2, \ldots x_n)$. Now, in the continous time, their dynamics may be represented as

$$x_i = f(x_1, x_2, \ldots x_n) \tag{1.1}$$

Quite interestingly, such system as Equation (1.1) may be transformed to an equivalent system.

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$$f(x_1, x_2, \ldots x_n) = c + \sum_{j=1}^{n} a_{ij} x_j \tag{1.2}$$

Using a shift operator $x_i \to x_i - v_j$, one obtains an equivalent system of Equation (1.2) in the form

$$f_i(x_1, x_2, \ldots x_n) = c + \sum_{j=1}^{n} a_{ij} x_j \tag{1.3}$$

The equation of state for problem be written as

$$x_i = \sum_{j=1}^{n} a_{ij} x_j \qquad \text{(dynamic continuous system),} \tag{1.4}$$

and,

$$x_i\,(t+1) = \sum_{j=1}^{n} a_{ij} x(t) \qquad \text{(dynamic discrete system)} \tag{1.5}$$

Continuous dynamical system usually represented an idealization, useful for algorithm analysis and design. computing solution to system of Equations (1.4) and (1.5) uses the approach of eigenvalues and eigenvectors for analyses of growth rates of a system.

These growth rates are patterned in the form of uncertainties. Computing these growth rates will certainly by measured based on the knowledge of spectral radius. Determination of growth rate under interval uncertainty is NP-hard [4]. Computing growth rate λ under uncertainty usually results in excess widths. Our main goal is to narrow this excess width created by interval in the range [λ,λ] as much as possible. This leads to the deep knowledge of Perron vectors of an interval matrix and we shall give more of these properties later in the work.

The k-eigenvalue problem principally focuses attempts to determine if these is self-sustaining time-independent chain reaction is neutron transport calculations-that is, criticality situation. The smallest eigenvalue on the other hand, represents the effective number of neutrons created and the magnetic signifies if these is self sustaining reaction where, eigenvector connotes the asymptotic power distribution.

The remaining sections in the paper is arranged as follows: Section two discusses the formulation of discrete S_N equation on tetrahedral meshes with boundary conditions given angular quadrature set with **N** specified nodes and weights formulated on **anisotropic scattering of Legendre order L** in the sense of [3,5]. In section three, the concept of interval operations of vectors and matrices are highlighted. Section 4 gives numerical illustration based on Perron vector.

2.0 The Deterministic S_N Codes

We follow the line of presentation of [2] by adopting the CGS units, a review of deterministic S_N code for the multigroup in energy transport is presented in this section. Our aim is to bring to focus the numerical approximation to the requested results.

K-eigenvalue problem tends to determine whether there is self-sustaining time-independent chain reaction in neutron transport calculations (critically problem). The k-eigenvalue problem, smallest eigenvalue defines the only effective number of neutrons created whose magnitude specifies if there is self-sustaining reaction [5].

On the other hand, eigenvector always signifies the asymptotic power distribution in the chain reaction in the isotropic S_N transport deterministic code.

Considering an angular quadrature set with N-specified nodes and weights $\{\Omega_m, \omega_m\}$ with anisotropic scattering of Legendre order L, the steady state S_N transport equation [2] for the energy group g = 1,2,…*G* in three domains $r \in \partial V$ is written in the form:

$$\left(\Omega_m \nabla + \sigma_{l,g}(r)\right)\psi_{g,m}(r) = \sum_{g'=1}^{G}\sum_{l=0}^{L}\sigma_{l,g'\to g}(r)\sum_{n=-l}^{l}Y_{\ln}(\Omega_m)\phi^{n}_{l,g'}(r) + \tfrac{1}{k}\chi_g(r)\sum_{g'=l}^{G}\nu\sigma_{f,g'}(r)\phi^{0}_{0,g'}(r) \tag{2.1}$$

Where, $m = 1,2,\ldots,N$, $Y_{\ln}(\hat{\Omega})$ are the spherical harmonics function.

Then, the scalar flux moments are

$$\psi'_{l,g}(r) = \sum_{m=l}^{N}\omega_m Y_{\ln}(\hat{\Omega}_m)\psi_{g,m}(r)\ , \tag{2.2}$$

The boundary conditions specified at the surface r_b with outward unit normal $\hat{n}$ are

$$\psi_{m'}(r_b) = \Gamma(\hat{\Omega}_m),\ for\ (\hat{\Omega}_m.\hat{n}) < 0 \tag{2.3}$$

Where, the reflected image of $\hat{\Omega}_m$ is denoted by

$$\hat{\Omega}_{m'} = \hat{\Omega}_m - 2\hat{n}(\hat{\Omega}_m.\hat{n}) \tag{2.4}$$

The discrete finite element meshes on tetrahedral is now reviewed for discussion. Given energy group g, the angular flux is expanded in a set of four independent linear basis function L_j on a tetrahedron T_s (with cell index s) in the form:

$$\psi'_{g,m,s}(r) = \sum_{j=l}^{4}\psi_{g,m,j,s}L_j(r) \tag{2.5}$$

To evaluate the weak transport equation for every quadrature angle m, and for each of the functions $L_j, i = 1,2,\ldots,4$ on cell T_s, we have

$$\begin{aligned}&\int_{\partial T_s}(\hat{\Omega}_m.\hat{n})\psi^{b}_{g.m}L_i ds - \int_{T_s}\psi_{g,m,s}(r)dV + \sigma_{l,g,s}(r)L_i\\ &= \sum_{g'}^{G}\sum_{l=0}^{L}\sigma_{l,g'\to g,s}Y_{\ln}(\hat{\Omega}_m)\int_{T_s}\phi^{n}_{l,g'}(r)L_i dV + \frac{1}{k}\chi_{g,s}\sum_{g'=l}^{G}\nu\sigma_{f,g',s}\int_{T_s}\phi^{0}_{0,g'}(r)L_i dV\end{aligned} \tag{2.6}$$

Method of Equation (2.6) consists of four equations for the four unknown $\psi_{m,j,k}$ on each cell s in each angle $\hat{\Omega}_m$.

We give the boundary fluxes appearing in the first term on the left side of Equation (2.6) for a cell *k* with face *j* and outward normal $\hat{n}_j$ by the equation

$$(\hat{\Omega}_m.\hat{n}_j)\psi^{b}_{g,m} = \begin{cases}(\hat{\Omega}_m.\hat{n}_j)\psi_{g,m,i(j),s}\ , & \hat{\Omega}_m.\hat{n}_j > 0, \hat{n}_j \in V\\ (\hat{\Omega}_m.\hat{n}_j)\psi_{g,m,i(j),l}\ , & \hat{\Omega}_m.\hat{n}_j < 0, \hat{n}_j \backslash \in V\ \ \partial V\\ (\hat{\Omega}.\hat{n}_j)\Gamma(\hat{\Omega}_m)\ , & \hat{\Omega}_m.\hat{n}_j < 0, \hat{n}_j\ on \in \partial V\end{cases} \tag{2.7}$$

To obtain the Power iteration method from Equation (2.7), the discretized S_N equations in the form of operator was initiated in [2] and is given by

$$L\psi = MSD\psi + \tfrac{1}{k} MFD\psi \qquad (2.8)$$

In Equation (2.7) L is the transport operator, S is the scattering operator, and F is the fission operator, while the operators M and D denote respectively, the moment to discrete and discrete to moment operators. Their aim is to convert a vector of scalar flux moments to angular fluxes and vice versa.

By arrangement of equation (2.8) and multiplying both sides by D, we obtain in [2] that

$$\varphi^{l=1} = \tfrac{1}{k_l} D(L-MSD)^{-1} F\phi^1, \quad \left(where\ \phi^l = D\psi^l, |= 0,1,\ldots\right) \qquad (2.9)$$

In other words, there are a total n-meshes and G energy groups in a reactor core neutron transport equations obtained from method of Equation (2.9). In the fundamental mode, k_0 represents the multiplicative factor k_{eff} and ϕ_0 are the scalar fluxes. Therefore, the set of higher eigenpairs is $\{k_i, \phi_i, i \geq 1\}$.

Method of Equation (2.9) is a Fixed Source Problem (FSP) and it belongs to the family of Implicitly Restarted Arnoldi Method (IRAM). The drawback of using IRAM efficiently on FSP with strong up scatter is its high computational complexity across time in high dimension [6,7].

We use the basic tools of the power method and Rayleigh Quotient iteration in the sense of [8] for obtaining solution to Equation (2.9) implemented in the interval version of Moore's arithmetic [8], e.g.,. The algorithm for the Power method in real floating point arithmetic is given below.

Algorithm

Define $y^{(0)} \in R^n$ and ε - order of accuracy.

For $k = 0,1,\ldots,$ compute

$w^{(k+1)} = Ay^{(k)}$

(1) $y^{(k+1)} = Aw^{(k+1)}$

(2) $\eta^{(k+1)} = \dfrac{\left\|y^{(k+1)}\right\|_2}{\left\|w^{(k+1)}\right\|_2}$

(3) If converged, $\eta = \eta^{(k+1)}$, quit, end

In real floating point arithmetic operations, the perturbation error to the computation is that for a given $\left(A + \Delta A^{(k)}\right)v^{(k)} = \lambda^{((k))} v^{(k)}, and\ \Delta A^{(k)} = -\dfrac{r^{(k)}\left[v^{(k)}\right]^T}{\left\|v^{(k)}\right\|_2^2}$, where

$r^{(k)} = Av^{(k)} - \lambda^{(k)} v^{(k)}$.

It follows that

$$\left|\lambda^{(k)} - \lambda_1\right| = \frac{\left\|\Delta A^{(k)}\right\|_2}{q(\lambda_1)} = \frac{\left\|r^{(k)}\right\|_2}{\left\|v^{(k)}\right\|_2} q(\lambda_1)^{-1} \quad , \qquad (2.10)$$

for $q(\lambda_1)=\dfrac{\left|\left[h^{(k)}\right]^T v^{(k)}\right|}{\left\|h^{(k)}\right\|_2\left\|v^{(k)}\right\|_2}$ (2.11)

The $h^{(k)}$ is a multiple of $\left(A^T\right)^k h^{(0)}$

3.0 The Interval Matrix Operation On Power Method

We hereby signify with the following notations:

An interval matrix $A=\left[\underline{A},\overline{A}\right]$ is a matrix whose entries are expressed in terms of uncertainty with the following:

$A_c=\frac{1}{2}\left(\underline{A}+\overline{A}\right), \Delta=\frac{1}{2}\left(\overline{A}-\underline{A}\right)$ (3.1)

If $=\left[\underline{b},\overline{b}\right]$ is an interval vector, then $b_c=\frac{1}{2}\left[\underline{b}+\overline{b}\right], \delta=\frac{1}{2}\left[\overline{b}-\underline{b}\right]$

Thus interval matrix and interval vector respectively can be expressed in the form of midpoint – radius interval thus:

$[A]=\left[A_c-\Delta, A_c+\Delta\right], while, [b]=\left[b,-\delta, b_c+\delta\right].$

Interval arithmetic obeys the four operators of (+,-,/,*) for real numbers. For further details interested readers are referred to [9-13].

First we define the following terms.

Definition 3.1. A Real number $\lambda\in R$ is an eigenvalue of $[A]=\left[A_c-\Delta, A_c+\Delta\right]$ if and only if the interval matrix $\left[\left(A_c-\lambda I\right)-\Delta,\left(A_c-\lambda I\right)+\Delta\right]$ is singular.

To decide which eigenvalue is real or complex for the interval matrix A, we use the following technique due to [12,13].

$(i)\, if\ \max\left(\left|\left(A_c-\lambda I\right)^{-1}\right|\Delta\right)_{ij}\geq 1$, then λ is a real eigenvalue of $A;(ii)\, if\ \rho\left(\left|\left(A_c-\lambda I\right)^{-1}\right|\Delta\right)\leq$, then λ is not a real eigenvalue of *A*.

Definition 3.2 A vector $O\notin x\in R''$ is a real eigenvector of *A* if and only it satisfies [13] assertion $T_z A_{zz} x x^T T_z \leq T_z x x^T A_{-zz}^T T_z$, $z=sign\, x$.

Where the matrices are respectively well defined. It holds that if $\lambda\in R$ and $0\notin x\in R''$, then (λ,x) is a real eigenpair of $A=\left[A_c-\Delta, A_c+\Delta\right]\leq\Delta|x|$, then (λ,x) where $x\neq 0$ is a real eigenpair of *A* if and only if

$\max\limits_{x_i\neq 0}\dfrac{\left(\left(T_z A_c T_z-\Delta\right)|x|\right)_i}{|x_i|}\leq\lambda\leq\min\limits_{x_j\neq 0}\dfrac{\left(\left(T_z A_c T_z+\Delta\right)|x|\right)_j}{|x_j|}$, where $z=sign\ x$. (3.2)

For the symmetric matrix case and for each $i\in\{1,2,\ldots,n\}$ the set $\{\lambda,(A):A\in \mathrm{A}, A\, symmetric\}$ is a compact interval, denoted as $\left[\underline{\lambda'(A),\lambda_i(A)}\right]$. To compute an external eigenvalues for the matrix $A=\left[A_c-\Delta, A_c+\Delta\right]$, we have a representation in the form:

$\overline{\lambda}_i(A) = \max_{\|x\|_2=1}\left(x^T A_c x + |x|^T \Delta |x|\right) = \max_{x\in Y_n} \lambda_1(A_{-zz}),\ \underline{\lambda}_i(A) = \min_{\|x\|_2=1}\left(x^T A_c x - |x|^T \Delta |x|\right) = \min_{x\in Y_n} \lambda_1(A_{zz})$(3.3)

The matrix $A_{yz} = A_c - T_y \Delta T_z$ is well defined so that

$$\left[\underline{\lambda}_i(A), \overline{\lambda}_i\right] \subseteq \left[\underline{\lambda}_i(A_c) - \rho(\Delta), \underline{\lambda}_i(A_c) + \rho(\Delta)\right], (i = 1,2,\ldots,n) \quad (3.4)$$

Therefore, for each eigenvalue $\lambda_i(A)\, of\ A \in \mathrm{A}$, there follows [13] the inequality relation:

$$\lambda_n(A_c) - \rho(\Delta) \le \lambda_i(A) \le \lambda_i(A_c) + \rho(\Delta) \quad (3.5)$$

The implication of these is that we then introduce a generalized eigenvalue problem $Ax = \lambda Bx$ where A is Hermittian and B Hermittian positive definite for which holds

$$B^{-\frac{1}{2}} A B^{-\frac{1}{2}}\left(B^{\frac{1}{2}} x\right) = \lambda\left(B^{\frac{1}{2}} x\right) \quad (3.6)$$

Equation 3.6 is the standard Hermittian eigenvalue problem and areas of applications include but not limited to second order ordinary differential equation

$$\frac{d^2 y}{dt^2} + Ay = O, y(0) = y_0, y^l(0) = y_0^l \quad (3.7)$$

With solution in the form:

$$y(t) = \cos\left(\sqrt{A}t\right)y_0 + \left(\sqrt{A}\right)^{-1} \sin\left(\sqrt{A}t\right)y_0^l \quad (3.8)$$

Where, $\sqrt{A}$ is the square root of A [14]. To compute the square root of A, we adopted the matrix square root iteration formula in the form of the Euler Chebbyshev iteration [15] given in the algorithm below.
Algorithm 3.1: Euler-Chevbyshev method.

Given a matrix $A \in R^{nxn}$, whose real eigenvalues are not on R^-, it is required to compute $X_k \to A^{\frac{1}{2}}\ as\ k \to \infty$.

(1) Define $C = \frac{A}{\|A\|}, R_0 = I, S_0 = C,$

(2) $R_{k+1} = R_k\left(\frac{3}{8}I + \frac{3}{4}S_k\left(I - \frac{1}{6}S_k\right)\right),$

(3) $S_{k+1} = S_k\left(\frac{3}{8}I + \frac{3}{4}S_k\left(I - \frac{1}{6}S_k\right)\right)^{-2},$

(4) $X_k = \sqrt{\|A\|}R_k$

4.0 Numerical Example

Example 1

We set $A = \begin{bmatrix} -4 & 14 & 0 \\ -5 & 13 & 0 \\ -1 & 0 & 2 \end{bmatrix}$ in the second order differential equation (3.7) where we introduce some kind of uncertainty

$[-\varepsilon, \varepsilon]$ into the coefficients of the matrix with $\varepsilon = 2\%$ tolerance. The initial starting vector is $x^{(0)} = (1,1,1)^T$
The actual values for the eigenvalues of *A* are $\lambda_1 = 2.000.\ \lambda_2 = 3.000,\ and\ \lambda_3 = 6.000$.

Thus the spectral radius is 6.000.

To demonstrate our methods in interval arithmetic operations, for the Power method and Rayleigh quotient applied on the problem 1, we construct the following Table for the compound results.

Table 1: Showing interval results for Power method and Rayleigh quotient iteration

Iterations ***k***	**Results for Interval Vectors**	**Interval Spectral Radius** $\lambda_i(x)$	**Interval results for Rayleigh Quotient Iteration** $(\lambda_i x)$
0	$(1,1,1)^T$		
1	$\begin{bmatrix}\begin{bmatrix}1 \quad , \quad 1 \\ 0.798792750, 0.0801192838 \\ 0.094567403, 0.105367792\end{bmatrix}\end{bmatrix}$	[9.94, 10.06]	[6.273333333,6.393333333]
2	$\begin{bmatrix}0.999999999, 0.999999995 \\ 0.748252691, 0.753389062 \\ -0.1187830454, -0.103764776\end{bmatrix}$	[7,145231297,7.23880708]	[6.836215531,7.3838728205]
3	$\begin{bmatrix}0.999999997, 1.000000000 \\ 0.728656412, 0.733545288 \\ -0.197138620, -0.178489153\end{bmatrix}$	[6.442948285,6.580439372]	[6.42102567,6.568626195]
4	$\begin{bmatrix}0.999999997, 0.999999994 \\ 0.719854181, 0.724866184 \\ -0.230920402, -.0210891553\end{bmatrix}$	[6.170559429,6.300735136]	[6.050462767,6.178658220]
5	$\begin{bmatrix}0.999999999, 0.999999999 \\ 0.715641032, 0.720823436 \\ -0.236622869, -0.225220483\end{bmatrix}$	[6.04817987,6.178406093]	[5.991058372,6.1219998693]
6	$\begin{bmatrix}0.999999994, 0.999999996 \\ 0.713563051, 0.718885849 \\ -0.254211898, -0.232057957\end{bmatrix}$	[5.989594089,6.121440167]	[5.961491889,6.094494923]
7	$\begin{bmatrix}0.999999994, 0.999999999 \\ 0.711998456, 0.717483926 \\ -0.259829797, -0.23698721\end{bmatrix}$	[5.946230396,6.080873129]	[5.590087646,6.074489927]

In the Boltzman equation [6] to which the Power method is highly effective, the source iteration may become extremely slow if the problem medium is scattering dominant, i.e., if the scattering ratio $\left(\frac{\rho_2}{\rho_1} \to 1\right)$.

In particular, the Rayleigh quotient iteration was implemented and is given by the equation

$$\lambda = r(x) = \frac{x^T A x}{x^T x},$$

which has been found to be a minimization of the least squares problem

$$\min_{\lambda} \|(A - \lambda I)\|_2 .$$

Further details can be found in [8].

Table 2: Computed Results for Euler-Chevbyshev Algorithm 3.1

Iteration k	R_k	S_k	X_k
1	$\begin{pmatrix} 0.0628 & 1.6856 & 0.3750 \\ -0.030 & 1.6541 & 0.3750 \\ 0.2434 & 0.4234 & 0.6106 \end{pmatrix}$	$\begin{pmatrix} 0.8919 & 0.1513 & 0 \\ -0.0540 & 1.0757 & 0 \\ -0.1889 & 0.2267 & 0.8920 \end{pmatrix}$	$\begin{pmatrix} 2.4523 & 0 & 0 \\ 0 & 2.4523 & 0 \\ 0 & 0 & 2.4523 \end{pmatrix}$
2	$\begin{pmatrix} -0.0233 & 1.7988 & 0.3542 \\ -0.1698 & 1.7543 & 0.3542 \\ 0.1587 & 0.5300 & 0.5768 \end{pmatrix}$	$\begin{pmatrix} 0.0000 & 0.0000 & 0 \\ -0.0000 & 1.0000 & 0 \\ -0.0005 & 0.0006 & 0.9998 \end{pmatrix}$	$\begin{pmatrix} 0.1540 & 4.1333 & 0.9196 \\ -0.2282 & 4.0564 & 0.9196 \\ 0.5968 & 0.0383 & 1.4974 \end{pmatrix}$
3	$\begin{pmatrix} -0.0234 & 1.7989 & 0.3542 \\ -0.1699 & 1.7544 & 0.3542 \\ 0.1586 & 0.5302 & 0.5767 \end{pmatrix}$	$\begin{pmatrix} 0.0000 & 0.0000 & 0 \\ -0.0000 & 1.0000 & 0 \\ -0.0000 & 0.0000 & 1.0000 \end{pmatrix}$	$\begin{pmatrix} -0.0571 & 4.4110 & 0.8686 \\ -0.4164 & 4.3020 & 0.8686 \\ 0.3892 & 1.2998 & 1.4143 \end{pmatrix}$
4	$\begin{pmatrix} -0.0234 & 1.7989 & 0.3542 \\ -0.1699 & 1.7544 & 0.3542 \\ 0.1586 & 0.5302 & 0.5767 \end{pmatrix}$	$\begin{pmatrix} 0.0000 & 0.0000 & 0 \\ -0.0000 & 1.0000 & 0 \\ 0 & 0 & 1.0000 \end{pmatrix}$	$\begin{pmatrix} -0.0574 & 4.4113 & 0.8685 \\ -0.4166 & 4.3023 & 0.8685 \\ 0.3889 & 1.3002 & 1.4142 \end{pmatrix}$

In Table 2, column 4 names X_k, is the result for the matrix square root while column 3, named S_k is the inverse matrix square root computed by the Euler-Chevbyshev algorithm. Convergence to the approximate solution was achieved at the third iteration. In the implementation of Euler-Chevbyshev algorithm, we obtain result for the estimate for the matrix norm $\|A\|$ from the results computed by the Rayleigh Quotient iteration free of charge which are freely applicable in providing result for the system of second order ordinary differential equation given in Equation (3.8).

5.0 Conclusion

The paper presented methods for computing the deterministic S_N transport codes for tetrahedral meshes in line with [1]. After transforming the problem into the equivalent eigenvalue problem, we use the interval arithmetic computation to execute the Rayleigh Quotient iterations and the Power method which form the reason for the studies when expressed, the data entries of the coefficients matrix under interval uncertainty. As a gain in the computation, the calculated result obtained by the Power method as a bye product was implemented in the Euler-Chevbyshev algorithm for computing square root of a matrix with positive eigenvalues. This can be further used without additional calculation in the solution to a second order ordinary differential equation, a concept being interpreted as an acceleration solving techniques.

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