Finding the solutions to non-linear equations using the Interval/Newton Generalized Bisection Method

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Abstract

The Interval-Newton Generalized-Bisection method (IN/GB) was used to determine the three solutions for the Peng-Robinson (PR) equation of State (EOS). At a temperature (T) of $298.15\ K$and pressure (P) of $63.0 * 10^5\ Pa$, the computed molar volumes are $v_1 = 0.000194931$, $v_2 = 0.0000996359$ and $v_3 = 0.0000722323\ \frac{m^3}{mol}$. This is an important application of the IN/GB because the PR EOS is the preferred equation in the petroleum industry to modelling single and multicomponent mixtures at conditions from medium to high pressures (*i. e.* ~1-100 bar). The IN/GB finds the three specific volumes and it uses the molar volume domain (*i. e.* not initial guesses) as the single input. These volumes (largest and smallest) correspond to the vapor and liquid phases that are present in separation processes.

Keywords: process modeling, interval arithmetic, interval newton, generalized-bisection, cubic equation of state

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Literature Review

The objective of this paper is to discuss the implementation of the Interval Newton/Generalized Bisection (IN/GB) method to determine the roots of a single-variable problem $f(x) = 0$ in a domain where it has three solutions using only the independent variable domain as input (*i.e.* not individual initial guesses).

The IN/GB method uses intervals instead of real numbers. Mathematical intervals are used rather than numbers in interval mathematics. Interval arithmetic provides rules for traditional operations: sum, subtraction, multiplication and division. The results are summarized in a set of rules that determine range of the resulting interval (Kearfott, 2023; Stradi *et al*. 2004)

The IN/GB method solves nonlinear problems of the form $f(x) = 0$. For continuous functions, the IN/GB method finds all the roots of a problem with mathematical certainty. There is a mathematical guarantee that all solutions are found. Consequently, if no solution is found then there is no solution in the domain of the search. The method is discussed in the literature over different applications and has been the subject of previous research (Kearfott, 2023; Stradi, 2013; Stradi & Haven, 2013; Moore, *et al*. (2009); Stradi *et al*. 2004; Sengupta, 1981; Moore, 1966)

The IN/GB method needs an interval-arithmetic programming environment which in turn requires programming in F77, C, or C++ with significant time invested in validations (Kearfott & Novoa, 1990). In this paper the INTerval LABoratory program (Rump, 1999) is used to handle the basic interval arithmetic and reduce the code writing overhead. The IN/GB method is computationally intensive and generally requires long computation times. In a cloud environment the processing time varies according to the available computational capacity (Stradi, 2020). There are applications of interval arithmetic to other problems such as that of Fan *et al*. (2025) that used intervals to assess risk in maritime operations. Zhang *et al*. (2024) developed an affine arithmetic algorithm for calculating short-circuit current intervals in distribution networks with distributed power sources while considering power fluctuations. Rossi *et al*. (2024) proposed the use of interval arithmetic for the verification of results generated from open-loop neural networks utilized in autonomous driving.

The real-value Newton-Raphson (NR) method is used to find the roots of non-linear equations while requiring an initial guess. It is a local method, and it is preferred due to its quadratic convergence in which the search procedure is repeated to determine each solution. The IN/GB method uses interval operations, and it only needs the domain of the variable to execute a search to find the solutions, this is done without additional reinitialization or initial guesses. Other papers have discussed interval arithmetic to determine the initial interval for the real-value NR method (Saskia *et al*., 2024).

The computational process has four steps. First, the domain is substituted into the function $f(x)$ and the result gives the image of the domain of x through $f(x)$ (*i.e.* the hull). Second, if zero is contained by the image, then the process continues, there is a root in the domain. Otherwise, it stops because there are not any solutions in the selected domain (Ichida & Fujii, 1979; Kearfott, 2023).

Third, if the image of the domain is completely contained by the original domain, then there is only one solution, and it can be determined with the real-valued Newton-Raphson (NR) method (Neumaier, 1990). The latter converges rapidly to the solution in the domain.

Fourth, If the image of the domain is not completely contained, then the intersection of the original domain and the image domain is taken. If the intersection interval is smaller in size than the original interval, then it is sent to a queue to be analyzed as the process moves forward, forming a stack of intervals. If the intersection does not generate a smaller interval than the original then the original interval is bisected, and the new intervals join the stack and are used as search domains in later calculations. If there is no intersection, then there is no solution in the original interval.

The process is repeated until all intervals in the stack are processed. This procedure will render all the solutions in the independent variable domain within the specified tolerance.

Methodology

The IN/GB method makes use of the INTLAB (INTerval LABoratory) environment (Rump, 1999) that provides interval arithmetic operations. The IN/GB method was programmed and used to solve an equation of state (EOS) for the molar volumes of heterogenous phases (liquid and vapor) in equilibrium for carbon dioxide. This is a computation routinely performed in the petroleum industry to model separation processes such as distillation.

At a given temperature and pressure, an equation of state (EOS) allows for the determination of the molar volume of a substance or mixture. Cubic EOS under saturation conditions (where both liquid and vapor coexist) have three solutions: one corresponds to vapor (largest), another corresponds to liquid (smallest), and the intermediate solution has no physical interpretation.

The Peng-Robinson EOS (Eq. 1) is used to determine the molar volumes of both vapor and liquid phases of carbon dioxide (Peng & Robinson, 1977; Smith *et al.*, 2017).

$$P = \frac{RT}{v-b} + \frac{a}{(v-\varepsilon b)(v-\sigma b)} \quad (1)$$

The form $f(x) = 0$ in which the EOS is utilized for the IN/GB method is the following:

$$f(v) = \frac{RT}{v-b} + \frac{a}{(v-\varepsilon b)(v-\sigma b)} - P = 0$$

The parameters for the EOS are the following:

Parameter	Value	Units
R	8.314	$\frac{J}{mol.K}$
P	$63.0 * 10^5$	Pa
T	298.15	K
ε	$1-\sqrt{2}$	$dimensionless$

σ	$1+\sqrt{2}$	$dimensionless$
a	0.402036	$\frac{Pa.m^6}{mol^2}$
b	$2.66646 * 10^{-5}$	$\frac{m^3}{mol}$

Table 1. Parameters used in the Peng-Robinson equation of state

The domain of the search and initial middle point are the following:

Domain limit	Value	Units
$v_{min} = 1.9 * b$	0.0000506628	$\frac{m^3}{mol}$
$v_{max} = 9.0 * b$	0.000239982	$\frac{m^3}{mol}$
$v_{mid} = 9.0 * b$	0.145322	$\frac{m^3}{mol}$

Table 2. Domain of search for the volume solution of the Peng-Robinson equation of state

The general procedure for the *n*-dimensional problem computes the image of the original interval through Equation 2, where x is the variable (that in our case is the molar volume v) where the Gauss Seidel method is used (Hansen, 1992; Kearfott, 1996):

$$X(i+1) = \frac{-f\big(X0_{mid}(i)\big) - \sum_{\substack{k=1 \\ k \neq i}}^{n} J(i,k) * \big(X0(k) - x0_{mid}(k)\big)}{J(i,i)} + x0_{mid}(i) \quad (2)$$

$$X_N(i) = X(i+1) \cap X0(i) \quad (3)$$

where

$X(i+1)$ is the $(i+1)$ estimation of the solution for the interval variable $X(i)$.
$x0_{mid}(i)$ is the value of the midpoint of the initial interval $X0(i)$.
$X0(k)$ is the initial interval for the variable $X(k)$.
$f(x0_{mid}(i))$ is the function evaluated at the midpoint of the interval variable $X(i)$.
$J(i,k)$ is the interval number that occupies the *i-th* row and *k-th* column position of the interval Jacobian matrix evaluated at the initial interval conditions $X0$.

$X_N(i)$ is the intersection of the computed interval $X(i+1)$ and $X0(i)$, the result becomes the initial interval for the next iteration. The process continues until the solution is computed to a specified tolerance.

The equations 2-3 reduce to the following for one dimension (Eqs. 4-5):

$$X_1 = x0_{mid} + \frac{-f(x0_{mid})}{f'(X0)} \qquad (4)$$

$$X_N = X_1 \cap X0 \qquad (5)$$

where
$f'(X_0)$ *is the firstorder derivative evaluated at the initial interval* $X0$
X_N *is the interval number intersection used in the succeeding computations*

Results and Discussion

The search starts with the following molar volume interval:

Initial molar volume interval:

$$X0 = [1.9b, 9b]$$

the specific numerical values are:

$$X0 = [0.0000506628, 0.000239982]$$

The function evaluation of the initial interval contains zero, and consequently the computations may proceed:

$$f(X0) = [-8.28936 * 10^7, 9.12221 * 10^7]$$

The initial middle point is:

$$x0_{mid} = 0.145322$$

The function evaluation of the mid-point is determined using interval arithmetic:

$$-f(x0_{mid}) = 3.12356 * 10^5$$

In a multivariate problem the Jacobian matrix would be computed next, however in a problem with one variable, the first order derivative is the only derivative needed:

$$f'(X0) = [-0.429136 * 10^{13}, 1.02678 * 10^{13}\ ]$$

The derivative contains zero and consequently generates two disjoint sets to consider in the computations:

$$\frac{-f(x0_{mid})}{f'(X0)} =$$

$$[-\infty, -0.304211 * 10^{-7}] \cup [0.727873 * 10^{-7}, \infty]$$

$$X_1 - x0_{mid} =$$
$$[-\infty, -0.304211 * 10^{-7}] \cup [0.727873 * 10^{-7}, \infty]$$

$$X_1 = [-\infty, -0.304211 * 10^{-7}] \cup [0.727873 * 10^{-7}, \infty] + x0_{mid}$$

The intersection of each of the intervals generated with the original interval generates two new domains of search:

$$X_1 = [-\infty, 0.000145292] \cup [0.000145395, \infty]$$

The intersection of original interval and its image through the IN/GB is computed:

$$X_N = X_1 \cap X_0$$

$$X_N = \begin{cases} [-\infty, 0.000145292] \cap [0.0000506628, 0.000239982] \\ [0.000145395, \infty] \cap [0.0000506628, 0.000239982] \end{cases}$$

These are the two new domains of search:

$$X_N = \begin{cases} [0.0000506628, 0.000145292] \\ [0.000145395, 0.000239982] \end{cases}$$

The difference between the upper and lower limit for each interval is larger than the tolerance (*i. e.* $1*10^{-8}$), and consequently the intervals are halved. The process will restart with theese new intervals until the specified tolerance is reached.

The resulting intervals from bisection are the following:

$$X_N = \begin{cases} [0.0000506628, 0.0000979774], [0.0000979774, 0.000145292] \\ [0.000145395, 0.000192689], [0.000192689, \quad 0.000239982] \end{cases}$$

The computational overhead is evidently growing, and the procedure is automated to deal with an increasing queue of intervals to test.

The following intervals generate three the solutions of the problem. These are taken from the stack generated by the IN/GB method. The other intervals in the stack are eventually discarded.

Interval 1 from the interval stack:

$$X0 = [0.000192689, 0.000239982]$$

$$x0_{mid} = 0.000216334$$

$$f(X0) = [-3.2898 * 10^6, 2.8607 * 10^6]$$

$$X_1 = x0_{mid} + \frac{-f(x0_{mid})}{f'(X0)} \quad (3)$$

$$-f(x0_{mid}) = 2.07471 * 10^5$$

$$f'(X0) = [-5.36017 * 10^{10}, 4.38620 * 10^{10}\ ]$$

The ratio of the function and its derivative generate two disjoint sets:

$$\frac{-f(x0_{mid})}{f'(X0)} =$$

$$[-\infty, -0.387060 * 10^{-5}] \cup [0.473008 * 10^{-5}, \infty]$$

$$X_1 - x0_{mid} =$$

$$[-\infty, -0.387060 * 10^{-5}] \cup [0.473008 * 10^{-5}, \infty]$$

The image of the initial interval through the IN/GB method is the following:

$$X_1 = [-\infty, 0.000212464] \cup [0.000221065, \infty]$$

$$X_N = X_1 \cap X_0$$

$$X_N = \begin{cases} [-\infty, 0.000212464] \cap [0.000192688, 0.000239982] \\ [0.000221065, \infty] \cap [0.000192688, 0.000239982] \end{cases}$$

$$X_N = \begin{cases} [0.000192688, 0.000212464] \\ [0.000221065, 0.000239982] \end{cases}$$

The procedure continues with bisection until the process signal that the interval generated is fully contained by the original domain of that iteration.

The interval from the IN/GB method is

$$X0 = [0.000194603, 0.000196518]$$

The image generated is

$$X_1 = [0.0000194670, 0.000195074]$$

Since the original interval $(x0)$ contains its image (x_1) $(x_1 \subset x_0)$ then the real valued NR method is implemented to finish the computations:

$Initial\ point\ and\ function\ values\ for\ the\ real-valued\ NR\ method$:

$$x_1 = x_0 + \frac{-f(x_0)}{f'(x_0)}$$

$$x_0 = 0.000194872$$

$$-f(x_0) = -539.124852$$

$$f'(x_0) = -9.17739 * 10^9$$

$$x_1 = 0.000194931$$

when the image by the IN/GB method is fully contained by the original interval, the use of NR method converges to the single root within the interval, this is graphically depicted in Figure 1.

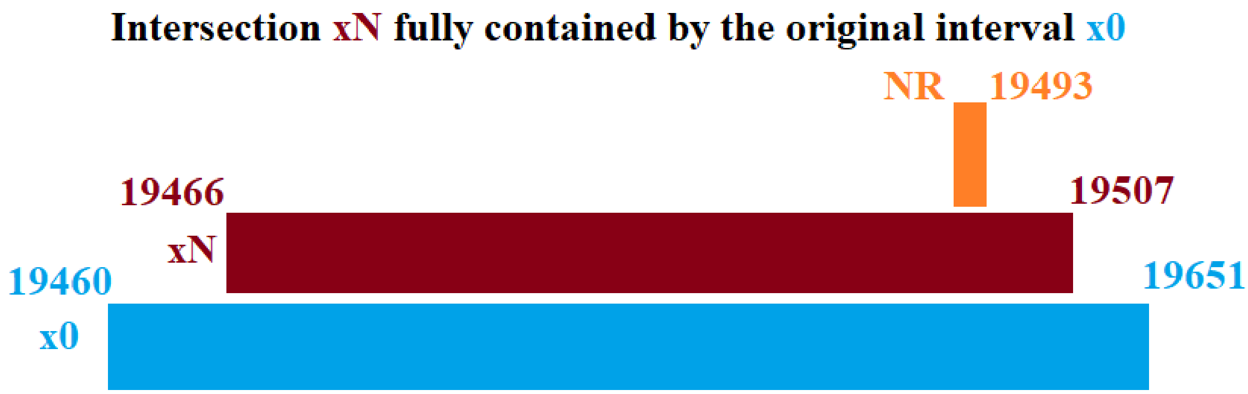

Figure 1. (First root) Intersection is fully contained in original interval. (The first five non-zero digits are shown, the rest are omitted for clarity)

The initial point for the real-valued NR method is the middle point of the intersection interval, the Newton-Raphson method iterates two times to reach the solution:

The procedure continues with two iterations to achieve the final solution with the specified tolerance (*i. e.* $1*10^{-8}$).

The solution provides the **first of the three volumes**:

$$x_1 = 0.000194931$$
$$f(x_1) = -3.725290 * 10^{-9}$$

The error measurement is computed as follows:

$$e = \sqrt{(x_1 - x_0)^2} \qquad (5)$$

The numerical value of the error is:

$$e = 1.177206 * 10^{-11}$$

The procedure continues to determine the **second root** just as was done previously:

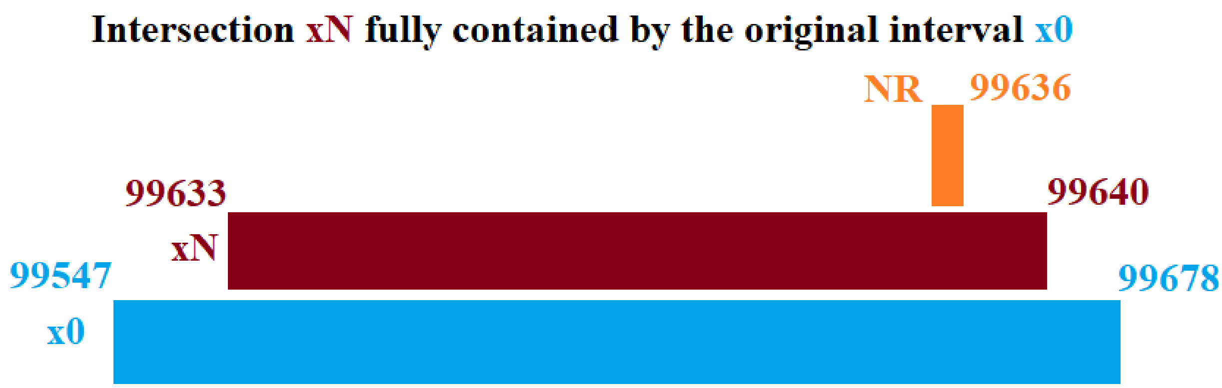

Figure 2. (Second root) Intersection is fully contained in original interval

This is the interval from the NR method

$$X0 = [0.0000995470, 0.0000996780]$$

The image generated is

$$X_1 = [0.0000996330, 0.0000996397]$$

Since the original interval (x_0) contains its image (x_1) $(x_1 \subset x_0)$ then the real valued NR method is implemented to finish the computations:

The **second solution** is found with a single iteration of the real-valued NR:

$$x_1 = 0.0000996359$$
$$f(x_1) = -1.71848 * 10^{-5}$$

$$e = 4.66449 * 10^{-10}$$

The process continues to determine the **third root**:

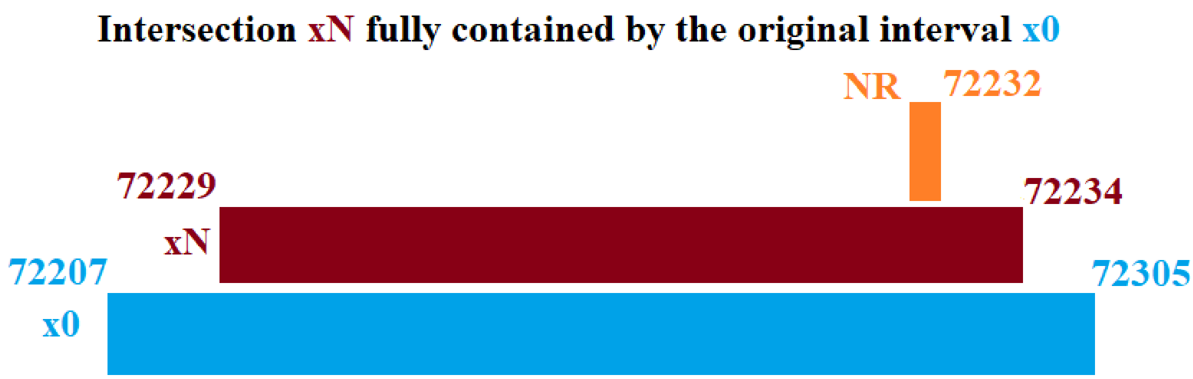

Figure 3. (Third root) Intersection is fully contained in original interval

This is the interval from the IN/GB method

$$X0 = [0.0000722074, 0.0000723050]$$

The image generated is

$$X_1 = [0.0000722294, 0.0000722345]$$

Since the original interval ($x0$) contains its image (x_N) ($x_1 \subset x_0$) then the real valued NR method is implemented to finish the computations:

The **third** solution is found with a single iteration of the real-valued NR:

$$x_1 = 0.0000722323$$
$$f(x_1) = 4.888549 * 10^{-4}$$

$$e = 3.120807 * 10^{-10}$$

The solutions found by the IN/GB are summarized on Table 3.

Search domain $[v_{min}$ =1.9 b, v_{max} =9.0 b] $\left(\frac{m^3}{mol}\right)$	Iterations real-valued NR method	Solution molar volume v $\left(\frac{m^3}{mol}\right)$	Root value $(f(v) = 0)$	Error e $\sqrt{(x_1 - x_0)^2}$
[0.0000506628, 0.000239982]	2	0.000194931	$-3.72529 * 10^{-9}$	$1.17721 * 10^{-11}$
	1	0.0000996358	$-1.71849 * 10^{-5}$	$4.66449 * 10^{-10}$
	1	0.0000722322	$4..88855 * 10^{-4}$	$3.12081 * 10^{-10}$

Table 3. Roots for the Peng-Robinson EOS utilizing the IN/GB method

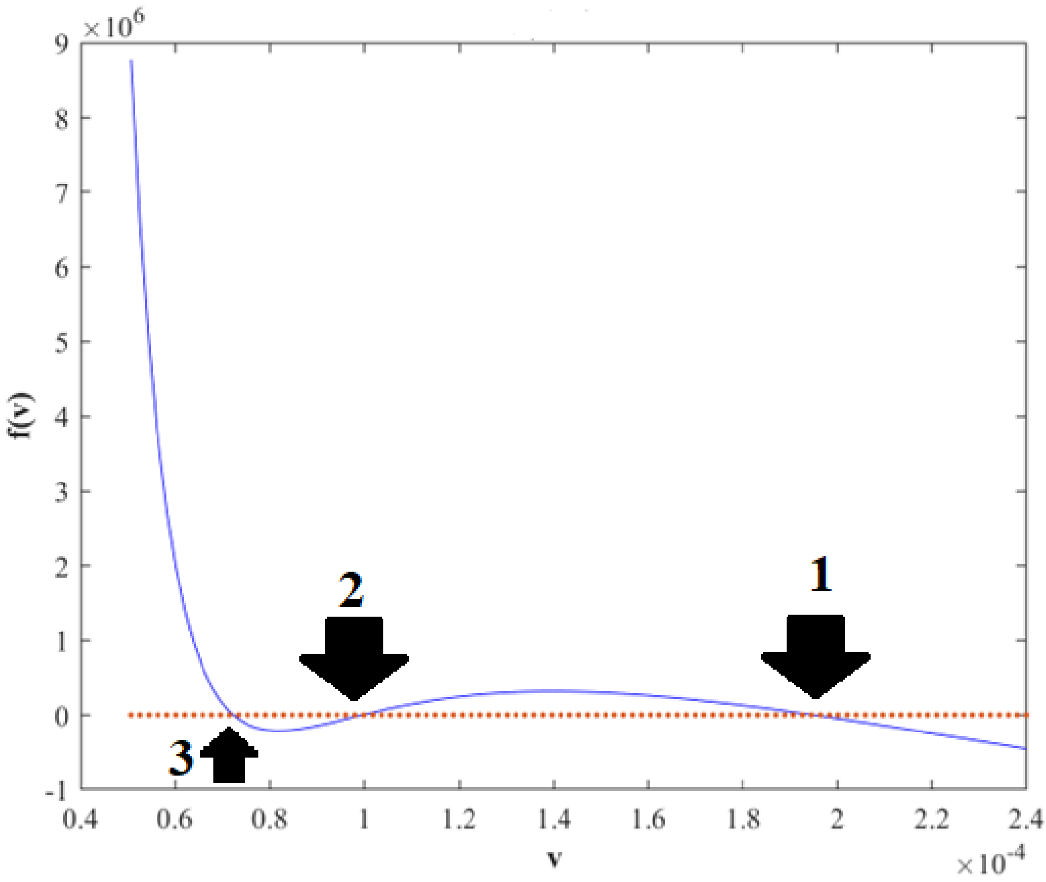

Figure 1. Function and its roots determined by the IN/GB method (The arrows indicate the locations of the roots)

The domain of search is subdivided into smaller segments until these segments are thinner than the specified tolerance or the real-valued NR method is called. The interval size evolution with root computation is shown in Figure 2.

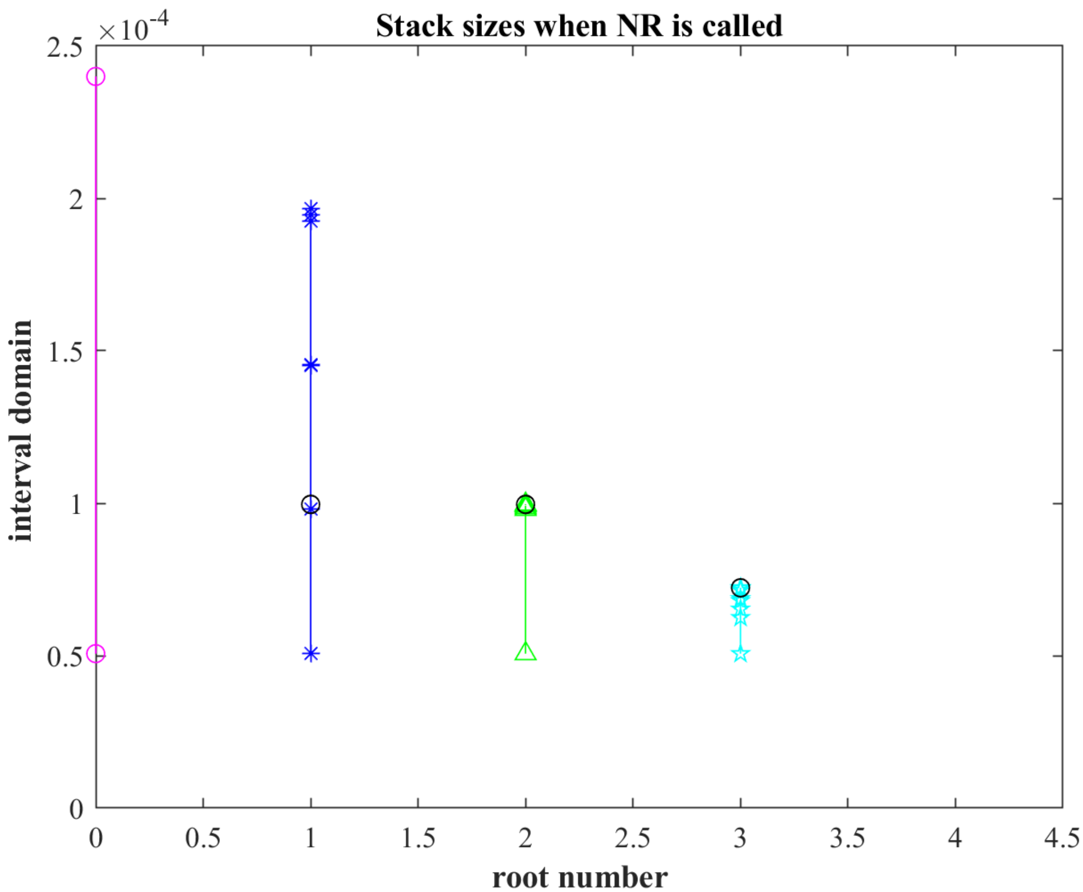

Figure 2. Interval domains for roots 1-3 when the real-valued NR process is called. [the black circle indicates the domain that was used to determine corresponding root]

Conclusions

1. The three molar volumes for the Peng-Robinson were determined by the IN/GB method. The values are (v=) 0.000194931, 0.0000996358, and 0.0000722322 $\left(\frac{m^3}{mol}\right)$.

2. The process proceeds by means of the Interval Newton (IN) method that generates an interval image that has to have smaller dimensions. Bisection is applied when the original interval does not become.

3. An implementation of the IN/GB methods using INTLAB provides the interval arithmetic necessary to solve increasingly complex problems with a smaller programming overhead.

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