Buckling and Pull-In Instability of Multi-Walled Carbon Nanotube Probes Near Graphite Sheets Using Power Series and Padé Approximants

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ABSTRACT
In this paper, integration of the power series method and the Padé approximants (PS-Padé) is utilized to study buckling and pull-in instability of multi-walled carbon nanotube (MWCNT) cantilevers in the vicinity of graphite sheets due to intermolecular forces. A hybrid nano-scale continuum model based on the Lennard–Jones potential is used to simulate the Van der Waals forces and evaluate the buckling of MWCNT. A closed form power series, based on the symbolic power series polynomials, is utilized to obtain a series solution for the governing boundary value differential equation of the nanotube. In order to handle the boundary conditions and increasing the accuracy of solution, the symbolic power series are transformed into Padé approximants. The governing differential equation is also solved numerically using the finite difference method. The PS-Padé results are compared with the numerical results and other methods reported in literature. The results obtained by using the PS-Padé approach correspond very well with the numerical results. Furthermore, the detachment length and the minimum gap between MWCNT and the graphite plane as important parameters of engineering designs are computed. It is found that for a fixed gap, the detachment length of a MWCNT can be increased with the increase of the radius, wall thickness and the effective Young modulus of the MWCNT.

Keywords - Cantilever, MWCNT, Padé, Pull-in instability, Symbolic power series.

I. Introduction
Multi-walled Carbon Nanotubes (MWCNTs) are types of nano-materials with outstanding mechanical properties. Nowadays, MWCNTs have attracted considerable attention because of their unique mechanical and chemical properties. These novel materials can be visualized in the form of nano-scale concentric cylinders rolled up by graphene sheets. There are numerous reports on the fabrication of single-walled carbon nanotubes (SWCNT) and MWCNT probes [1]-[3]. MWCNTs can be synthesized by different techniques, including laccase-mediator [4], situ oxidative polymerization method [5]-[7]. Single-walled and multi-walled carbon nanotubes have been utilized as electrochemical sensors [8], catalysts [9], [10], structures [11], and Atomic force microscopes (AFM) [12]. Electrically induced static and dynamic mechanical buckling and pull-in instability of MWCNT cantilevers have many applications, such as nanotube based electromechanical system (NEMS) switches [12]-[14].

Consider a typical MWCNT cantilever probe/switch suspended above a graphite surface with a small gap between them. When the size of the gap decreases to nanometers, the Van der Waals interaction buckles the MWCNT to the substrate. In a recent piece of work [15], the authors utilized a hybrid continuum model to consider the molecular force-induced buckling of the cantilever freestanding MWCNT probes/actuators suspended over graphite sheets. They carried out the governing equation of the deflection of MWCNT cantilever probes/actuators in the vicinity of thin and thick graphite layers. The governing equation of the hybrid distributed model leads to a fourth-order nonlinear, ordinary differential equation. Because of the nonlinearity of the governing equation of the distributed model, an exact solution does not yet exist.

Reference [15] used the Green’s function method with a simple second order polynomial as the shape function to obtain deflection and pull-in parameters of MWCNT cantilevers. They have also used the Adomian decomposition method (ADM) to obtain pull-in instability of MWCNT cantilevers. However, the accuracy of the results of the Green’s method and the Adomian decomposition method [15] for calculating deflection of MWCNT cantilevers near
the pull-in instability is not perfect. Reference [16] examined a monotone positive solution to obtain a resolution for the buckling of MWCNTs. The monotone solution is a comparatively accurate solution for low values of intermolecular forces, but it fails to evaluate the pull-in instability of MWCNT cantilevers.

The combination of any series solutions with the Padé approximants provides a powerful tool for increasing the accuracy of boundary value problems. Hence, the accuracy of the series methods can be enhanced by using Padé approximants.

In this study, in order to obtain an accurate analytical solution for pull-in instability of MWCNTs in the vicinity of graphite sheets, integration of symbolic power series with Padé approximants (PS-Padé) is used as a new approach to study the buckling and pull-in instability of MWCNT cantilever actuators. A fair comparison is made between the method presented and numerical results as well as between the Adomian decomposition method and monotone solution reported in literature.

II. Mathematical Model

Fig. 1 shows a physical schematic of a typical MWCNT cantilever near a surface consisting of graphene layers, with interlayer distance \( d \). The length of MWCNT is \( L \), the mean radius value is \( R_w \), the number of walls of nanotube is \( N_w \), and the gap between MWCNT and the graphite surface is \( D \).

Based on continuum mechanics, a MWCNT is modeled by concentric cylindrical tubes. \( E \) is the Young’s modulus of MWCNT which typically is in the range of 0.9 to 1.2 TPa, and the cross-sectional moment of inertia \( I \) is equal to \( \pi (R_w^4 - R_i^4)/4 \) [15]. By neglecting the effect of large displacement (finite kinematics) for \( LD/\alpha > 10 \) and applying the Euler theory [20], the governing equation of a MWCNT cantilever can be written as the following boundary value ordinary differential equation [15]:

\[
E_{\text{eff}} I \frac{d^4 u}{dx^4} = q_{\text{int}}(D - U) \tag{1-a}
\]

subject to the following geometrical boundary conditions at fixed end:

\[
U(0) = \frac{du}{dx}(0) = 0 \tag{1-b}
\]

and, natural boundary conditions at free end, as follows:

\[
\frac{d^2 u}{dx^2}(L) = \frac{d^3 u}{dx^3}(L) = 0 \tag{1-c}
\]

where \( X \) is the position along MWCNT measured from the bending side, \( U \) is the deflection of MWCNT cantilever and \( q_{\text{int}} \) is the intermolecular force per unit length of MWCNT. According to the work of [15], \( q_{\text{int}} \) can be represented as:

\[
q_{\text{int}} = 4C_6\sigma^2\pi^2NN_wR_w \frac{d}{d(D-U+Nd/2)} \tag{2}
\]

In (2), \( \sigma \approx 38\text{nm}^2 \) [22] is the graphene surface density and \( C_6 = 15.2 \text{ eV Å}^6 \) is the attractive constants for the carbon-carbon interaction [23]. By substituting (2) in (1) and using the following substitutions:

\[
x = \frac{X}{L}, \quad u = \frac{U}{D} \left( \frac{n}{4} \right) \tag{3-a}
\]

and:

\[
f_n = \begin{cases} 
C_6\sigma^2\pi^2NN_wR_wL^4 \frac{d}{D_{\text{eff}}I(D-U+Nd/2)} & (n = 4) \\
4C_6\sigma^2\pi^2NN_wR_wL^4 \frac{d}{D_{\text{eff}}I(D+Nd/2)} & (n = 5)
\end{cases} \tag{3-b}
\]

the dimensionless form of (1) can be obtained as follows:

\[
\frac{d^4 u}{dx^4} = f_n \left( 1 - u(x) \right)^n \tag{4-a}
\]

\[
u(0) = u'(0), \quad \text{at} \quad x = 0, \tag{4-b}
\]

\[
u''(1) = u''(1) = 0, \quad \text{at} \quad x = 1 \tag{4-c}
\]

In the following text, \( n = 4 \) and \( n = 5 \) correspond to the large number and small number of graphene layers, accordingly. In the equations, prime denotes differentiation with respect to non-dimensional length of \( x \).

III. Analytical Solution

Equation (4-a) subject to (4-b) and (4-c) can be solved using a symbolic power series enhanced with Padé approximants. The basic idea of the symbolic power series method and Padé approximants are explained in the works of [17], [18] and also [24, 25].

III.1 Symbolic Power Series Method

Based on the symbolic power series method, the fourth-order differential equation of (4-a) can be written as a system of four first order differential equation, as follows:
\[
\frac{du_1(x)}{dx} = u_2(x) \\
\frac{du_2(x)}{dx} = u_3(x) \\
\frac{du_3(x)}{dx} = u_4(x) \\
\frac{du_4(x)}{dx} = \frac{f_n}{(1-u_i(x))^{n}}
\]

subject to the following boundary conditions:
\[
\begin{align*}
  u_1(0) &= 0, & u_2(0) &= 0, \\
  u_1(0) &= P, & u_3(0) &= Q \\
  u_4(1) &= 0, & u_4(0) &= 0.
\end{align*}
\]

Here, \(P\) and \(Q\) are constants which later will be computed from the boundary conditions, (4-c) or (7). Based on the method of symbolic power series introduced by [17], [18], the solution procedure is started as follows:

\[
\begin{align*}
  u_1(x) &= 0 + e_1 \\
  u_2(x) &= 0 + e_2 \\
  u_3(x) &= P + e_3 \\
  u_4(x) &= f_n + e_4
\end{align*}
\]

Substituting (8) in (5) and neglecting higher order terms yields:
\[
\begin{align*}
  e_1 &= 0, \\
  e_2 &= P, \\
  e_3 &= Q, \\
  e_4 &= f_n = 0.
\end{align*}
\]

Solving (9) for \(e_1\) to \(e_4\) and substituting the obtained values into (8) and considering a higher term gives the first approximation of the solution as:
\[
\begin{align*}
  u_1(x) &= 0 + e_1x \\
  u_2(x) &= Px + e_2x^2 \\
  u_3(x) &= P + Qx + e_3x^2 \\
  u_4(x) &= f_n + e_4x^2
\end{align*}
\]

Again, substituting (10) in (5) and neglecting higher order terms yields:
\[
\begin{align*}
  P - 2e_1 &= 0, \\
  Q - 2e_2 &= 0, \\
  2e_3 &= f_n, \\
  2e_4 &= 0.
\end{align*}
\]

Substituting the new values of \(e_1\) to \(e_4\) into (10) and considering a higher term results in:
\[
\begin{align*}
  u_1(x) &= \frac{P}{2}x^2 + e_1x^3 \\
  u_2(x) &= \frac{Q}{2}x^2 + Px + e_2x^3, \\
  u_3(x) &= \frac{f}{2}x^2 + Qx + P + e_3x^3 \\
  u_4(x) &= f_n + e_4x^3
\end{align*}
\]

By substituting \(e_j\) to \(e_4\) in (5) and repeating this procedure, the following power series for \(u_1\) is obtained after eight iterations:
\[
\begin{align*}
  u_1(x) &= \frac{f_n}{1-u_1(x)} \\
  u_2(x) &= \frac{Q}{2}x^2 + P + e_2x^3, \\
  u_3(x) &= \frac{f}{2}x^2 + Qx + P + e_3x^3 \\
  u_4(x) &= f_n + e_4x^3
\end{align*}
\]

By substituting (10) in (5) and neglecting higher order terms yields:
\[
\begin{align*}
  e_1 &= 0, \\
  e_2 &= P, \\
  e_3 &= Q, \\
  e_4 &= f_n = 0.
\end{align*}
\]

Solving (9) for \(e_1\) to \(e_4\) and substituting the obtained values into (8) and considering a higher term gives the first approximation of the solution as:
\[
\begin{align*}
  u_1(x) &= 0 + e_1x \\
  u_2(x) &= Px + e_2x^2 \\
  u_3(x) &= P + Qx + e_3x^2 \\
  u_4(x) &= f_n + e_4x^2
\end{align*}
\]

Again, substituting (10) in (5) and neglecting higher order terms yields:
\[
\begin{align*}
  P - 2e_1 &= 0, \\
  Q - 2e_2 &= 0, \\
  2e_3 &= f_n, \\
  2e_4 &= 0.
\end{align*}
\]

Substituting the new values of \(e_1\) to \(e_4\) into (10) and considering a higher term results in:

\[
\begin{align*}
  u_1(x) &= \frac{P}{2}x^2 + e_1x^3 \\
  u_2(x) &= \frac{Q}{2}x^2 + Px + e_2x^3, \\
  u_3(x) &= \frac{f}{2}x^2 + Qx + P + e_3x^3 \\
  u_4(x) &= f_n + e_4x^3
\end{align*}
\]

By substituting (10) in (5) and neglecting higher order terms yields:
\[
\begin{align*}
  e_1 &= 0, \\
  e_2 &= P, \\
  e_3 &= Q, \\
  e_4 &= f_n = 0.
\end{align*}
\]

Solving (9) for \(e_1\) to \(e_4\) and substituting the obtained values into (8) and considering a higher term gives the first approximation of the solution as:
\[
\begin{align*}
  u_1(x) &= 0 + e_1x \\
  u_2(x) &= Px + e_2x^2 \\
  u_3(x) &= P + Qx + e_3x^2 \\
  u_4(x) &= f_n + e_4x^2
\end{align*}
\]

Again, substituting (10) in (5) and neglecting higher order terms yields:
\[
\begin{align*}
  P - 2e_1 &= 0, \\
  Q - 2e_2 &= 0, \\
  2e_3 &= f_n, \\
  2e_4 &= 0.
\end{align*}
\]

Substituting the new values of \(e_1\) to \(e_4\) into (10) and considering a higher term results in:
The relative error is computed from:

\[
\text{Error} = \frac{|u_{\text{Analytical}} - u_{\text{Numerical}}|}{u_{\text{Numerical}}} \quad (23)
\]

where, \(u_{\text{Analytical}}\) and \(u_{\text{Numerical}}\) are the MWCNT cantilever tip deflection, computed from the analytical method (i.e. PS or PS-Padé) and the tip deflection computed using numerical method, respectively. The Error represents the relative error.

### Table 1

The Evaluated Tip Deflection of a Typical MWCNT Cantilever Using Different Terms of PS Method for \(f_e=0.5\)

<table>
<thead>
<tr>
<th>Series Size</th>
<th>Tip Deflection PS, (n=4)</th>
<th>Error (n=4)</th>
<th>Tip Deflection PS, (n=5)</th>
<th>Error (n=5)</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>0.06250</td>
<td>1.903E-01</td>
<td>0.06250</td>
<td>2.491E-01</td>
</tr>
<tr>
<td>5</td>
<td>0.06250</td>
<td>1.903E-01</td>
<td>0.06250</td>
<td>2.491E-01</td>
</tr>
<tr>
<td>6</td>
<td>0.06250</td>
<td>1.903E-01</td>
<td>0.06250</td>
<td>2.491E-01</td>
</tr>
<tr>
<td>7</td>
<td>0.07215</td>
<td>6.525E-02</td>
<td>0.07516</td>
<td>9.700E-02</td>
</tr>
<tr>
<td>8</td>
<td>0.08228</td>
<td>6.592E-02</td>
<td>0.09350</td>
<td>1.233E-01</td>
</tr>
<tr>
<td>9</td>
<td>0.07396</td>
<td>4.190E-02</td>
<td>0.07737</td>
<td>7.046E-02</td>
</tr>
<tr>
<td>10</td>
<td>0.07946</td>
<td>2.945E-02</td>
<td>0.08842</td>
<td>6.228E-02</td>
</tr>
<tr>
<td>11</td>
<td>0.07564</td>
<td>2.015E-02</td>
<td>0.07983</td>
<td>4.087E-02</td>
</tr>
<tr>
<td>12</td>
<td>0.07833</td>
<td>1.476E-02</td>
<td>0.08613</td>
<td>3.707E-02</td>
</tr>
<tr>
<td>13</td>
<td>0.07646</td>
<td>9.511E-03</td>
<td>0.08137</td>
<td>2.236E-02</td>
</tr>
<tr>
<td>14</td>
<td>0.07722</td>
<td>6.816E-03</td>
<td>0.08475</td>
<td>1.826E-02</td>
</tr>
<tr>
<td>15</td>
<td>0.07684</td>
<td>4.494E-03</td>
<td>0.08223</td>
<td>1.211E-02</td>
</tr>
<tr>
<td>16</td>
<td>0.07743</td>
<td>3.087E-03</td>
<td>0.08400</td>
<td>9.263E-03</td>
</tr>
<tr>
<td>Numerical</td>
<td>0.077192</td>
<td>0.083233676</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### Table 2

The Evaluated Tip Deflection of a Typical MWCNT Cantilever Using Different Terms of PS-Padé for \(f_e=0.5\)

<table>
<thead>
<tr>
<th>Padé Size</th>
<th>Tip Deflection PS-Padé, (n=4)</th>
<th>Error (n=4)</th>
<th>Tip Deflection PS-Padé, (n=5)</th>
<th>Error (n=5)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(12,2)</td>
<td>0.07368</td>
<td>4.544E-02</td>
<td>0.07405</td>
<td>1.103E-01</td>
</tr>
<tr>
<td>(3,3)</td>
<td>0.07525</td>
<td>2.519E-02</td>
<td>0.08009</td>
<td>3.777E-02</td>
</tr>
<tr>
<td>(4,4)</td>
<td>0.07724</td>
<td>5.716E-04</td>
<td>0.08344</td>
<td>2.449E-03</td>
</tr>
<tr>
<td>(5,5)</td>
<td>0.07710</td>
<td>1.148E-03</td>
<td>0.08353</td>
<td>3.504E-03</td>
</tr>
<tr>
<td>(6,6)</td>
<td>0.07719</td>
<td>1.795E-05</td>
<td>0.08323</td>
<td>3.415E-05</td>
</tr>
<tr>
<td>(7,7)</td>
<td>0.07719</td>
<td>2.054E-06</td>
<td>0.08323</td>
<td>4.200E-06</td>
</tr>
<tr>
<td>(8,8)</td>
<td>0.07719</td>
<td>9.067E-07</td>
<td>0.08324</td>
<td>2.537E-05</td>
</tr>
<tr>
<td>(9,9)</td>
<td>0.07719</td>
<td>1.460E-08</td>
<td>0.08325</td>
<td>5.240E-08</td>
</tr>
<tr>
<td>Numerical</td>
<td>0.0771924</td>
<td>0.0832336</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The results in Table 2 show the relative error between analytical and numerical results is less than 0.0034% by selecting PS-Padé size of \([6,6]\). It is worth noticing that the Padé approximants with size \([6,6]\) are obtained from 15 terms of power series (i.e. \(O(x^{16})\)). Comparing this error with the same series size of the PS method (i.e. 15 terms and relative error of 1.2%), shows the PS-Padé method could compute deflection of MWCNT cantilever with more accuracy than the PS method. The results of PS-Padé with size of \([6,6]\) with 0.0034% error are very similar to the numerical results. Therefore, the Padé size of \([6,6]\) is selected, for convenience.

### IV. Results and Discussion

In order to verify the convergence of Padé approximants, deflection of a typical nanotube-actuator, which is used in the work of [15], is computed analytically using the symbolic power series method. Then the power series are converted to Padé approximants. The solution results are compared with the numerical results as well as the monotone method [16], the Green’s method and Adomian decomposition method [15]. Numerical results are obtained using the finite difference method based on collocation points and Newton’s method [27], [28]. A highly accurate solution with a relative tolerance of \(10^{-8}\) is achieved. Table 1 and Table 2 compare MWCNT cantilever tip deflection \((u_{tip})\), computed using different terms of symbolic power series and different sizes of Padé approximants, respectively. These tables ensure the convergence and accuracy of the power series and Padé approximants. Table 2 reveals that higher accuracy can be obtained by evaluating more terms of the Padé approximants.
numerically simulated and the results are compared with the results of the PS-Padé method. The results show that for $f_n$ greater than critical value of intermolecular force ($f^*$), a numerical solution does not exist and the MWCNT collapses on to the sheets. The pull-in value of MWCNT-graphite attraction and the MWCNT pull-in tip deflection can also be evaluated using the PS-Padé technique by setting $d\varphi(1)/df_n \rightarrow \infty$ in the solution.

The relationship between $f_n$ and $u_{tip}$ are presented in Figs. 2 and 3 for large and small numbers of graphene layers. Fig. 3 depicts the non-dimensional tip deflection of MWCNT which it increases from zero to pull-in instability as $f_n$ raises from zero to $f^*$. Table 3 compares the obtained values of $f^*$ using different methods for large and small numbers of graphene layers. When intermolecular attraction exceeds the critical value of $f^*$, no solution exists and the instability occurs.

Table 3

<table>
<thead>
<tr>
<th>Model</th>
<th>$f^*$ (n=4)</th>
<th>Error (n=4)</th>
<th>$f^*$ (n=5)</th>
<th>Error (n=5)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Numerical</td>
<td>0.939</td>
<td>-</td>
<td>0.769</td>
<td>-</td>
</tr>
<tr>
<td>Monotone Solution</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Green’s Function</td>
<td>1.025</td>
<td>9.2</td>
<td>0.841</td>
<td>9.4</td>
</tr>
<tr>
<td>Adomian method</td>
<td>0.814</td>
<td>13.3</td>
<td>0.661</td>
<td>14</td>
</tr>
<tr>
<td>PS 15 terms of series</td>
<td>0.810</td>
<td>13.7</td>
<td>0.670</td>
<td>12.9</td>
</tr>
<tr>
<td>PS Padé (6,6)</td>
<td>0.939</td>
<td>0</td>
<td>0.769</td>
<td>0</td>
</tr>
</tbody>
</table>

The results in Figs. 2 and 3 and Table 3 reveal that the PS-Padé method is more accurate than other methods in comparison with the numerical results. The centerline deflection of a typical MWCNT under intermolecular force for a large number of graphene layers and a small number of graphene layers are shown in Fig. 4 and Fig. 5, respectively.

These figures compare the PS-Padé results with the numerical results as well as with Green’s function method and the Adomian method [15]. The obtained PS-Padé solution at the onset of pull-in
instability for the large number of graphene layers (i.e. \( n=4 \)) is as follows:

\[
(24)
\]

The PS-Padé solution at the onset of instability for the small number of graphene layers is:

\[
(25)
\]

When the gap between the plane and the suspended nanotube is small enough, the nanotube may collapse on to the graphite sheets without applying voltage due to the intermolecular attractions. The stable length is an important parameter for design of nano-switches or AFM probes and some other engineering applications [12]-[14]. By substituting the obtained value of \( f^{\prime \prime}_0 \) at the onset of instability in definition of \( f^{\prime}_0 \) (i.e. (3-b)), then solving for corresponding minimum gap \( (D_{\text{min}}) \) and detachment length \( (L_{\text{max}}) \) of freestanding MWCNT, the following relations are obtained:

\[
L_{\text{max}} = \begin{cases} 
0.939 \varepsilon E R_0 D & \text{form } = 4 \\
0.192 \varepsilon E R_0 (D + N d/2)^{\frac{3}{2}} & \text{form } = 5 
\end{cases}
\]

\[
D_{\text{max}} = \begin{cases} 
1.065 C_{\sigma} \sigma^{2} \pi N d L^2 & \text{for } n = 4 \\
5.201 C_{\sigma} \sigma^{2} \pi N d L^2 & \text{for } n = 5
\end{cases}
\]

Equation (26) shows the detachment length of a MWCNT would increase with an increase of the radius, wall thickness or effective Young modulus of the MWCNT.

V. Conclusions

A mathematical model based on a nano-scale continuum model and the Lennard–Jones potential is used to study buckling of MWCNT cantilevers near the graphite sheets. The governing equation leads to a fourth-order ordinary differential equation. Then, integration of the Adomian decomposition method and the Padé approximants is used as a new accurate technique to obtain a solution for buckling of MWCNT cantilevers. The ADM-Padé solution is compared with the numerical method, Green’s function, the Adomian solution and a symbolic power series in figures and tables. Comparison between the Adomian results and ADM-Padé results show that Padé approximants enhanced the convergence of Adomian decomposition polynomials to handling the governing boundary value problem near the pull-in area. Finally, by using the ADM-Padé technique, the critical value of Van der Waals attraction \( (f^{\prime \prime}_0) \) and detachment length of MWCNT as basic parameters for design and selecting components of nano-electro mechanical systems has been determined.

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