On ninth order, explicit Numerov type methods with constant coefficients.

Ch. Tsitouras and T. E. Simos

Mathematics Subject Classification (2010). Primary 65L05; Secondary 65L06.

Keywords. Initial Value Problem, Second Order, Order conditions, Phase-Lag, Quadruple precision, Mathematica.

SUPPLEMENTARY

Appendix A. Algorithm in Mathematica

The following Mathematica Package returns the coefficients of the nine (effectively) stages, ninth order method, with respect to free parameters c_3, c_4, c_5, a_{94}, $a_{10,6}$ and $a_{10,9}$. Thirty three digits of accuracy are returned, since we are interested in use at quadruple precision.

```
BeginPackage["numerov‘"];
Clear["numerov‘*"]
Numerov9::usage = " Numerov9[x1,x2,x3,x4,x5,x6] \
for effectively 9-stages 9-order explicit Numerov"
Begin["‘Private‘"];
Clear["numerov‘Private‘*"];

Numerov9[cc3_?NumericQ, cc4_?NumericQ, cc5_?NumericQ, aa106_?NumericQ,
   aa94_?NumericQ, aa109_?NumericQ] :=
 Module[{c3, c4, c5, a106, a94, a109, b, b1, b2, b4, b6, b7, c, a,
   a31, a32, a41, a42, a43, a51, a52, a53, a54, a61, a62, a63, a64,
   a65, a71, a72, a73, a74, a75, a76, a81, a82, a83, a84, a85, a86,
   a87, a91, a92, a93, a95, a96, a97, a98, a101, a102, a103, a104,
   a105, a107, a108, e, so, s, p, pl, v},
  c3 = Rationalize[cc3, 10^-33];
  c4 = Rationalize[cc4, 10^-33]; c5 = Rationalize[cc5, 10^-33];
  a106 = Rationalize[aa106, 10^-33]; a94 = Rationalize[aa94, 10^-33];
  a109 = Rationalize[aa109, 10^-33];
  b = {b1, b2, 0, b4, b4, b6, b6, b7, b7, b1};
```

```
  c = {-1, 0, c3, c4, -c4, -c5, c5, c3, -c3, 1};
  a = {{0, 0, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0, 0,
     0}, {a31, a32, 0, 0, 0, 0, 0, 0, 0, 0}, {a41, a42, a43, 0, 0, 0,
     0, 0, 0, 0}, {a51, a52, a53, a54, 0, 0, 0, 0, 0, 0}, {a61, a62,
     a63, a64, a65, 0, 0, 0, 0, 0}, {a71, a72, a73, a74, a75, a76, 0,
     0, 0, 0}, {a81, a82, a83, a84, a85, a86, a87, 0, 0, 0}, {a91,
     a92, a93, a94, a95, a96, a97, a98, 0, 0}, {a101, a102, a103,
     a104, a105, a106, a107, a108, a109, 0}};
  e = {1, 1, 1, 1, 1, 1, 1, 1, 1, 1};
  so = Solve[{-1 + b.e, -(1/12) + b.c^2/2, -(1/360) +
       b.c^4/24, -(1/20160) + b.c^6/720, -(1/1814400) +
       b.c^8/40320} == {0, 0, 0, 0, 0}, {b1, b2, b4, b6, b7}];
  b = Simplify[b /. so[[1]]];
  so = Solve[ Join[(a.e - 1/2*(c^2 + c))[[3 ;; 10]],
                   (a.c - 1/6*(c^3 - c))[[3 ;; 10]],
                   (a.c^2 - 1/12*(c^4 + c))[[4 ;; 10]]] == Array[0 &, 23],
    {a31, a32, a41, a42, a51, a52, a61, a62, a71, a72, a81, a82, a43, a53,
                         a63, a73, a83, a91, a92, a93, a101, a102, a103}];
  a = Expand[a /. so[[1]]];
  so = Solve[{-(b.c/120) - b.a.c/6 - b.a.a.c, -(1/20160) - b.c/720 -
       b.a.c/24 - 1/2 b.a.a.c + b.a.a.a.e, -(1/5040) - b.c/180 +
       1/6 b.a.c^2 + b.a.(c a.c), -(1/3360) + b.c^2/120 +
       1/6 b.(c a.c) + b.(c a.a.c), -(b.c/1008) + 1/24 b.a.c^2 +
       1/2 b.a.(c a.c) - b.a.(c a.a.e),
      b.c^2/720 + 1/24 b.(c a.c) + 1/2 b.(c a.a.c) - b.(c a.a.a.e),
      b.c^2/180 - 1/6 b.(c a.c^2) - b.(c a.(c a.c)),
      b.c^2/240 + 1/12 b.(c a.c) - 1/120 b.(c a.e) -
       1/6 b.(a.c a.e) + 1/2 b.(c a.a.c) - b.(a.e a.a.c),
      1/17280 + b.a.(a.e a.a.e), 47/181440 + b.(c a.(c a.a.e)),
      -(373/1814400) + b.(a.e a.a.a.e), 799/907200 + b.(a.e a.(c a.c)),
      1/16200 + 1/36 b.(c^3 a.c^3), 31/181440 + b.(c a.a.a.c),
      -(1/1814400) + b.a.a.a.a.e} == Array[0 &, 15],
      {a54, a65, a76, a74, a87, a75, a86, a96, a108,
                  a107, a104, a105, a64, a85, a84}];
  a = Expand[a /. so[[1]]];
  so = Solve[{-(1/1814400) + 1/2 b.a.a.a.c^2 == 0,
     13/907200 + b.a.a.(c a.c) == 0}, {a95, a97}];
  a95 = Simplify[so[[1, 1, 2]]];
  a97 = Simplify[so[[1, 2, 2]]];
  so = Solve[-(71/907200) + b.a.(c a.a.c) == 0, a98];
  a98 = Expand[so[[1, 1, 2]]]; a = Rationalize[N[a, 35],10^-33];
  b = Rationalize[N[b, 35],10^-33]; c = Rationalize[N[c, 35],10^-33];
  Return[{a, b, c}]]
End[];
EndPackage[];
```

Inserting the values for the free parameters mentioned in the main text we may produce a ninth order method with minimized principal truncation error, i.e. the corresponding coefficients of the 10th order.

```
In[1]:=Numerov9[-4/9, -1/12, -5/7, -1/7, 11/7, 1/5]
```

```
Out[1]= {{{0, 0, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0, 0, 0},
    {-130/2187, -140/2187, 0, 0, 0, 0, 0, 0, 0, 0},
    {-121/82944, -2981/331776, -341/12288, 0, 0, 0, 0, 0, 0, 0},
    {36337590879052/25604198389403023,  237493461816790/14228756859045911,
    356507807858085/12720168546017594, -41228276539304/41295275850476333,
    0, 0, 0, 0, 0, 0},
    {-1149056066217543/30734474519634232, 202919103952276029/35304906986166887,
    8065973767341360/9981891002272517, -19221426218069682 5/42396977924109749,
    -4830739539325571 0/35200019170324741, 0, 0, 0, 0, 0},
    {-503025452795934/21044094574408427, 37912402622404981/9046487610676402,
    1090370115731537/29312832618740557, -12800841651197886/5347473178831361,
    -72216809641053730/37427522093182653, 16942860117131/988224741182196,
     0, 0, 0, 0},
     {1204223593680585/30297031116359276, -123024260775828871/24911411889431988,
     584914982150403/11907823594053710, 47017869633294986/18701348572530987,
    77402911380345653/31688595042010811, -2118275137915627/80185700995213633,
    -8070751723468829/39525422089933558, 0, 0, 0},
    {-2480625196966811/79986097620672763, -3427002259639544/4394049852802029,
    -36376112444372887/77130325262935213, 11/7,
    -7188253499514651/33438637318138757, 545435165201609/15491504931107479,
    10600629156165181/34806735078576264, -2323518310234004/25068419959969283, 0, 0},
    {3116320709932343 4/35458563299485315, -116671946587398527 5/7218621502059453,
    -91724484536340507/13980653079398810, 197453036658114100 1/19422494188479671,
    252764117971794085 9/37306315952388780, -1/7,
    -11930584526645439/11327867780174561, -1882740483675215/16904304514513714,
    1/5, 0}};

   {96757/20820800, -325837/168000, 0, 290635776/231045815,
   290635776/231045815, 9817456103/105762984000, 9817456103/105762984000,
   537286851/4697929600, 537286851/4697929600, 96757/20820800};

   {-1, 0, -4/9, -1/12, 1/12, 5/7, -5/7, -4/9, 4/9, 1}}
```

Appendix B. Mathematica Implementation

Here we implement a simplified Mathematica program for illustrating the usage of our new methods. We particularly embed the coefficients of the new high phase-lag order method (NEW9p).

```
NumerovSol[fcn_, x0_, xe_, ystart0_, ystart1_, n_] :=
           Module[{a, b, c, h, x, m, y, f, f0, f1},
a={{0,0,0,0,0,0,0,0,0,0},
{0,0,0,0,0,0,0,0,0,0},
{1/16,5/16,0,0,0,0,0,0,0,0},
{583391411644877/9801735844870202,7290530044141359/18052269610174832,
-109928853873626/11870182062528097,0,0,0,0,0,0,0},
{-1264609201132142/33286410731333461,-1091818303013521/5910345749949432,
32815143590726245/78584957833693987,-10032620616920844/31653683222600797,
0,0,0,0,0,0},
{6646327897215827/55966054002628338,3324572561143889/6298743678722111,
7503052548888415/37249375033135477,-4557755600894453/24752971591968361,
-2515007079640954/23219589725085715,0,0,0,0,0},
{-3408086000138927/28663758530853786,-26178851268544425/43062258404047892,
```

```
61673268177814162/39369956391724003,-59044933381840649/47553056586104932,
23221672689470467/90509474011570183,647108498818917/18860535609750067,0,0,0,0},
{-44346756472929/5119234490495267,5328983116107436/33035858464446179,
8702060533181845/36713474431621477,-5033532648172153/28008542208144491,
4666933835398849/30150513821099534,348597142952732/46932039494276745,
46674738918537/1651619100332158O,0,0,0},
{1193279287963711/41967429555307147,4671783491314937/30053470147530539,
-2260681119587372/4566121347779735,27674766720428048/67297682600973051,
-7740796239815592/38196359713646827,-922122327377857/37557990510639504,
-173214146477З/84704827201632566,124345124858245/56074051861605146,0,0},
{36475060426729740/35840680803401177,392600106283128311/41653159902804031,
-815656348398310516/25410290542467199,1221908240851986475/44369558619959733,
552959632147255706/18829491455327673,-14805591149675947/12633273312913248,
-1346449973729988573/89362779606041204,-5161996081162918/34777002286245501,
-128840458892089198/7213060827691083,0}};
b={179964412582644/45681110021827271,14768373688604307/36678493441550362,0,
-13741041996703464/18080472338434339,-13741041996703464/18080472338434339,
11950337026591352/34150086035078823,11950337026591352/34150086035078823,
22376134858147551/31748376559360495,22376134858147551/31748376559360495,
179964412582644/45681110021827271};
c={-1,0,1/2,24296874801485189/42166633847925649,
-24296874801485189/42166633847925649,2/3,-2/3,1/2,-1/2,1};
```

```
   h = N[(xe - x0)/n, 33];
   x = x0 + Range[0, n]*h;
   m = Length[ystart0];
   y = Array[Array[0 &, m] &, n + 1];
   y[[1]] = ystart0;
   y[[2]] = ystart1;
   f = Array[Array[0 &, m] &, 10];
   f[[2]] = fcn[x[[1]], y[[1]]];
   Do[ f0 = f[[2]];
       f1 = fcn[x[[k]], y[[k]]];
        f = Array[Array[0 &, m] &, 10];
        f[[1]] = f0; f[[2]] = f1;
       Do[f[[o]] = fcn[x[[k]] + c[[o]]*h,
                       (1 + c[[o]])*y[[k]]
                       - c[[o]]*y[[k - 1]] +  h^2*a[[o]].f]
       , {o, 3, 10}];
    y[[k + 1]] = N[2*y[[k]] - y[[k - 1]] + h^2*b.f, 33];
    y[[k + 1]] = Rationalize[y[[k + 1]], 10^-33]
    ,{k, 2, n}];
   Return[{x, y}]];
```

In the input we give

```
fcn     : Function f(x,y)
x0      : Starting point
xe      : End-point
ystart0 : vector y(x0)
ystart1 : vector y(x0+h)
n       : number of steps in [x0,xe]
```

and get as output

```
x : The grid
y : y(x)
```

Then we may apply the Module to the semi-linear system. First we define the function using lists, in the following way

```
In[1]:=fcn[x_, y_] := {{-199, -198}, {99, 98}}.{y[[1]], y[[2]]}
                      + {(y[[1]] + y[[2]])^2 + Sin[10 x]^2 -  1,
                      (y[[1]] + 2 y[[2]])^2 + 1/10^6*Cos[x]^2 - 1/10^6};
```

and then run the problem using 5500 steps by typing:

```
In[2]:=sol = NumerovSol[fcn, 0, 10, {2, -1}, {2 Cos[10/550]
       - 1/1000*Sin[1/550], -Cos[10/550] + 1/1000*Sin[1/550]}, 5500];
```

Thus we may get the corresponding lower rightmost entry in Table - 7 of the main article.

```
In[3]:=-Log10[Max[Max[Abs[2 Cos[10 sol[[1]]] - 1/1000*Sin[sol[[1]]] -
     sol[[2]][[All, 1]]]], Max[Abs[-Cos[10*sol[[1]]]
     + 1/1000*Sin[sol[[1]]] - sol[[2]][[All, 2]]]]]]
Out[3]=20.8328619544
```

which is rounded to 20.8 for the presentation.

We finally remark that lists are used even for the scalar cases, e.g. for producing the lower leftmost rounded entry for the Table - 4 of the main article we may type,

```
In[4]:=fcn[x_, y_] := {-100*y[[1]]};
In[5]:=sol = NumerovSol[fcn, 0, 10*Pi, {1}, {Cos[10*10*Pi/4000]}, 4000];
In[6]:=-Log10[Max[Abs[Cos[10*sol[[1]]] - sol[[2]][[All, 1]]]]]
Out[6]=16.0998062917
```

Ch. Tsitouras
TEI of Sterea Hellas,
Dept. of Automation Engineering (Head),
GR34400, Psahna Campus, Greece.
e-mail: tsitouras@teiste.gr

T. E. Simos

1. Department of Mathematics, College of Sciences, King Saud University,
   P. O. Box 2455, Riyadh 11451, Saudi Arabia.
2. Group Leader, Group of Modern Computational Methods,
   Ural Federal University, 620002, 19 Mira Street, Ekaterinburg, Russian Fed.
3. Department of Automation Engineering, TEI of Sterea Hellas,
   GR 34400, Psachna Campus, Greece.
4. Section of Mathematics, Department of Civil Engineering,
   Democritus University of Thrace, Xanthi, Greece.

Postal Address: 10 Konitsis Street, GR-175 64 Athens, Greece.
e-mail: tsimos.conf@gmail.com
URL: http://theodoresimos.org/