Computational Experience with TN and LBFGS

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TN (Nash)

```
  Truncated Newton Method

  Application T1.  January 9, 2009
  TN algorithm.   Elastic-Plastic Torsion Problem
  ----------------------------------------------------------------
  Number of variables:                        N  40000
  Severity of the Linesearch:               ETA   .2500000000000E+00
  Desired accuracy for the solution:       XTOL   .3162277660168E-07
  Accuracy of computed function values: ACCRCY   .1000000000000E-14
  Maximum number of INNER iterations per step: 20000
  ----------------------------------------------------------------

    N   NITER    NEFV     CPU       F-value

40000      13     307     570   -.4392678E+00

  Truncated Newton Method

  Application T2.  January 9, 2009
  TN algorithm.   Pressure Distribution Problem
  ----------------------------------------------------------------
  Number of variables:                        N  40000
  Severity of the Linesearch:               ETA   .2500000000000E+00
  Desired accuracy for the solution:       XTOL   .3162277660168E-07
  Accuracy of computed function values: ACCRCY   .1000000000000E-14
  Maximum number of INNER iterations per step: 20000
  ----------------------------------------------------------------

    N   NITER    NEFV     CPU       F-value

40000      33     798    1496   -.2828929E+00


  Truncated Newton Method

  Application T3.  January 9, 2009
  TN algorithm.   Optimal design with composite materials
  ----------------------------------------------------------------
  Number of variables:                        N  40000
  Severity of the Linesearch:               ETA   .2500000000000E+00
  Desired accuracy for the solution:       XTOL   .3162277660168E-07
  Accuracy of computed function values: ACCRCY   .1000000000000E-14
  Maximum number of INNER iterations per step: 20000
  ----------------------------------------------------------------

    N   NITER    NEFV     CPU       F-value

40000      54    1744    5092   -.1138130E-01
```

```
Truncated Newton Method

Application T4.  January 9, 2009
TN algorithm.   Ginzburg-Landau 1D Problem
-----------------------------------------------------------------
Number of variables:                        N   1000
Severity of the Linesearch:               ETA   .2500000000000E+00
Desired accuracy for the solution:       XTOL   .3162277660168E-07
Accuracy of computed function values: ACCRCY   .1000000000000E-14
Maximum number of INNER iterations per step:   500
-----------------------------------------------------------------

   N   NITER    NEFV     CPU       F-value

 1000     382    9350     166   -.8456192E+04


Truncated Newton Method

Application T5.  January 9, 2009
TN algorithm.   Steady State Combustion Problem
-----------------------------------------------------------------
Number of variables:                        N  40000
Severity of the Linesearch:               ETA   .2500000000000E+00
Desired accuracy for the solution:       XTOL   .3162277660168E-07
Accuracy of computed function values: ACCRCY   .1000000000000E-14
Maximum number of INNER iterations per step: 20000
-----------------------------------------------------------------

   N   NITER    NEFV     CPU       F-value

40000      27     477    1845   -.5611449E+01



Truncated Newton Method

Application T6.  January 9, 2009
TN algorithm.   Jones Cluster Problem (Molecular Conformation)
-----------------------------------------------------------------
Number of variables:                        N   3000
Severity of the Linesearch:               ETA   .2500000000000E+00
Desired accuracy for the solution:       XTOL   .3162277660168E-07
Accuracy of computed function values: ACCRCY   .1000000000000E-14
Maximum number of INNER iterations per step:  1500
-----------------------------------------------------------------

   N   NITER    NEFV     CPU       F-value

 3000    1403   37395  141766   -.6576856E+04



Truncated Newton Method

Application T7.  January 9, 2009
TN algorithm.   Minimal Surface Area Problem
-----------------------------------------------------------------
```

```
Number of variables:                          N  40000
Severity of the Linesearch:                 ETA   .2500000000000E+00
Desired accuracy for the solution:         XTOL   .3162277660168E-07
Accuracy of computed function values: ACCRCY   .1000000000000E-14
Maximum number of INNER iterations per step: 20000
-----------------------------------------------------------------

   N    NITER    NEFV     CPU       F-value

 40000      22     349     922    .1000000E+01
```

LBFGS (Nocedal)

```
   L-BFGS Algorithm.   Elastic-Plastic Torsion Problem
Number of BFGS updates M= 3 January 9, 2009

      n     iter   fgcnt     time          fxnew                gnorm2
-------------------------------------------------------------------------------------
  40000      381     399      673   -.4392674132720E+00    .4971116500015E-04

   L-BFGS Algorithm.   Elastic-Plastic Torsion Problem
Number of BFGS updates M= 5 January 9, 2009

      n     iter   fgcnt     time          fxnew                gnorm2
-------------------------------------------------------------------------------------
  40000      346     755      653   -.4392677559075E+00    .5381376897767E-04

   L-BFGS Algorithm.   Elastic-Plastic Torsion Problem
Number of BFGS updates M= 7 January 9, 2009

      n     iter   fgcnt     time          fxnew                gnorm2
-------------------------------------------------------------------------------------
  40000      342    1106      692   -.4392678005491E+00    .3995535751961E-04

   L-BFGS Algorithm.   Elastic-Plastic Torsion Problem
Number of BFGS updates M= 9 January 9, 2009

      n     iter   fgcnt     time          fxnew                gnorm2
-------------------------------------------------------------------------------------
  40000      316    1431      685   -.4392678108470E+00    .5425504709693E-04
-------------------------------------------------------------------------------------


   L-BFGS Algorithm.   Pressure Distribution Problem
Number of BFGS updates M= 3 January 8, 2009

      n     iter   fgcnt     time          fxnew                gnorm2
-------------------------------------------------------------------------------------
  40000      856     914     1551   -.2828929058887E+00    .2996880109306E-04

   L-BFGS Algorithm.   Pressure Distribution Problem
Number of BFGS updates M= 5 January 8, 2009

      n     iter   fgcnt     time          fxnew                gnorm2
-------------------------------------------------------------------------------------
  40000      814    1759     1564   -.2828929295173E+00    .3015639731448E-04
   L-BFGS Algorithm.   Pressure Distribution Problem
Number of BFGS updates M= 7 January 8, 2009

      n     iter   fgcnt     time          fxnew                gnorm2
-------------------------------------------------------------------------------------
  40000      799    2579     1651   -.2828929416860E+00    .2517069133647E-04

   L-BFGS Algorithm.   Pressure Distribution Problem
Number of BFGS updates M= 9 January 8, 2009

      n     iter   fgcnt     time          fxnew                gnorm2
-------------------------------------------------------------------------------------
  40000      773    3373     1713   -.2828929346610E+00    .3556990170108E-04
-------------------------------------------------------------------------------------
```

L-BFGS Algorithm. **Optimal Design with Composite Materials**
Number of BFGS updates M= 3 January 8, 2009

n	iter	fgcnt	time	fxnew	gnorm2
40000	1809	1838	4761	-.1138122865547E-01	.2023777688460E-04

L-BFGS Algorithm. Optimal Design with Composite Materials
Number of BFGS updates M= 5 January 8, 2009

n	iter	fgcnt	time	fxnew	gnorm2
40000	859	2704	2380	-.1138128573610E-01	.2660425854793E-04

L-BFGS Algorithm. Optimal Design with Composite Materials
Number of BFGS updates M= 7 January 8, 2009

n	iter	fgcnt	time	fxnew	gnorm2
40000	843	3553	2472	-.1138128632483E-01	.3063106124306E-04

L-BFGS Algorithm. Optimal Design with Composite Materials
Number of BFGS updates M= 9 January 8, 2009

n	iter	fgcnt	time	fxnew	gnorm2
40000	**656**	**4214**	**2023**	**-.1138129442545E-01**	**.3241232447072E-04**

L-BFGS Algorithm. **Ginzburg-Landau (1-dimensional)**
Number of BFGS updates M= 3 January 8, 2009

n	iter	fgcnt	time	fxnew	gnorm2
1000	1908	2001	48	-.1718319208564E-03	.1444624844288E-01

L-BFGS Algorithm. **Steady State Combustion - Bratu**
Number of BFGS updates M= 3 January 9, 2009

n	iter	fgcnt	time	fxnew	gnorm2
40000	740	776	2731	-.5611447434734E+01	.4290597251963E-04

L-BFGS Algorithm. Steady State Combustion - Bratu
Number of BFGS updates M= 5 January 9, 2009

n	iter	fgcnt	time	fxnew	gnorm2
40000	**503**	**1301**	**1920**	**-.5611448490517E+01**	**.4437990070301E-04**

L-BFGS Algorithm. Steady State Combustion - Bratu
Number of BFGS updates M= 7 January 9, 2009

n	iter	fgcnt	time	fxnew	gnorm2
40000	522	1842	2062	-.5611448497617E+01	.4405870194056E-04

L-BFGS Algorithm. Steady State Combustion - Bratu
Number of BFGS updates M= 9 January 9, 2009

n	iter	fgcnt	time	fxnew	gnorm2
40000	501	2357	2040	-.5611448480843E+01	.4610522697016E-04

L-BFGS Algorithm. **Jones Clusters (Molecular Conformation)**
Number of BFGS updates M= 3 January 9, 2009

```
      n     iter   fgcnt     time          fxnew                gnorm2
-------------------------------------------------------------------------------------
   3000     1930    2001     6967   -.6613534243165E+04    .4571920141689E+00

    L-BFGS Algorithm.   Jones Clusters (Molecular Conformation)
 Number of BFGS updates M= 5 January 9, 2009

      n     iter   fgcnt     time          fxnew                gnorm2
-------------------------------------------------------------------------------------
   3000     1551    3623     5625   -.6602132026911E+04    .3827556039252E-03

    L-BFGS Algorithm.   Jones Clusters (Molecular Conformation)
 Number of BFGS updates M= 7 January 9, 2009

      n     iter   fgcnt     time          fxnew                gnorm2
-------------------------------------------------------------------------------------
   3000     1551    5241     5620   -.6610370139041E+04    .4268140295915E-03

    L-BFGS Algorithm.   Jones Clusters (Molecular Conformation)
 Number of BFGS updates M= 9 January 9, 2009

      n     iter   fgcnt     time          fxnew                gnorm2
-------------------------------------------------------------------------------------
   3000     1048    6338     3816   -.6626189460436E+04    .3834472015488E-03
-------------------------------------------------------------------------------------


    L-BFGS Algorithm.    Minimal surface area problem
 Number of BFGS updates M= 3 January 9, 2009

      n     iter   fgcnt     time          fxnew                gnorm2
-------------------------------------------------------------------------------------
  40000      428     441     1036    .1421353295447E+01    .3052936828957E-04

    L-BFGS Algorithm.    Minimal surface area problem
 Number of BFGS updates M= 5 January 9, 2009

      n     iter   fgcnt     time          fxnew                gnorm2
-------------------------------------------------------------------------------------
  40000      448     898     1138    .1421353240881E+01    .2955888848323E-04

    L-BFGS Algorithm.    Minimal surface area problem
 Number of BFGS updates M= 7 January 9, 2009

      n     iter   fgcnt     time          fxnew                gnorm2
-------------------------------------------------------------------------------------
  40000      467    1372     1252    .1421353240739E+01    .2818708529408E-04

    L-BFGS Algorithm.    Minimal surface area problem
 Number of BFGS updates M= 9 January 9, 2009

      n     iter   fgcnt     time          fxnew                gnorm2
-------------------------------------------------------------------------------------
  40000      439    1822     1255    .1421353228094E+01    .3039593999088E-04
-------------------------------------------------------------------------------------
```

January 9, 2009