

# Numerical experiments with accelerated hybrid conjugate gradient algorithm with modified secant condition

## - AHYBRIDM -

### for unconstrained optimization

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In this Technical Report we document some numerical experiments with *AHYBRIDM - accelerated hybrid conjugate gradient algorithm with modified secant condition* [1,2] for solving some problems from MINPACK2 Library.

In AHYBRIDM the parameter  $\beta_k$  is computed as a convex combination of  $\beta_k^{HS}$  (Hestenes-Stiefel) and  $\beta_k^{DY}$  (Dai-Yuan) formulae, i.e.  $\beta_k^C = (1-\theta_k)\beta_k^{HS} + \theta_k\beta_k^{DY}$ . The parameter  $\theta_k$  in the convex combination is computed in such a way so that the direction corresponding to the conjugate gradient algorithm to be the Newton direction and the pair  $(s_k, y_k)$  to satisfy the modified secant condition given by Zhang *et al.* [3] and Zhang and Xu [4], where  $s_k = x_{k+1} - x_k$  and  $y_k = g_{k+1} - g_k$ . The algorithm uses the standard Wolfe line search conditions. Numerical comparisons with conjugate gradient algorithms show that this hybrid computational scheme outperforms a variant of the hybrid conjugate gradient algorithm given by Andrei [5], in which the pair  $(s_k, y_k)$  satisfies the secant condition  $\nabla^2 f(x_{k+1})s_k = y_k$ , as well as the Hestenes-Stiefel, the Dai-Yuan conjugate gradient algorithms, and the hybrid conjugate gradient algorithms of Dai and Yuan.

The search direction  $d_{k+1}$  is computed as

$$d_{k+1} = -g_{k+1} + (1-\theta_k) \frac{y_k^T g_{k+1}}{y_k^T s_k} s_k + \theta_k \frac{g_{k+1}^T g_{k+1}}{y_k^T s_k} s_k,$$

where

$$\theta_k = \frac{\left( \frac{\delta \eta_k}{s_k^T s_k} - 1 \right) s_k^T g_{k+1} - \frac{y_k^T g_{k+1}}{y_k^T s_k} \delta \eta_k}{g_k^T g_{k+1} + \frac{g_k^T g_{k+1}}{y_k^T s_k} \delta \eta_k},$$

and  $\delta \geq 0$  is a scalar parameter.

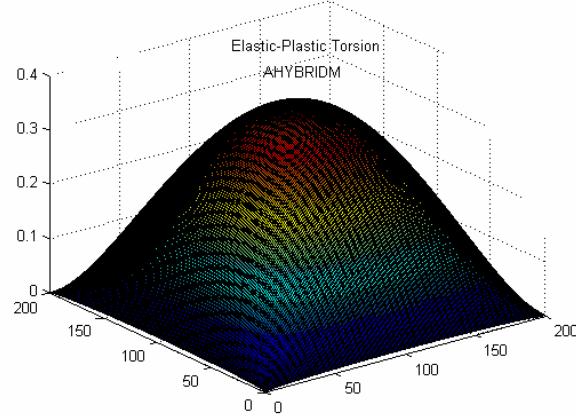
#### 1. Elastic - Plastic Torsion Problem

Results obtained with AHYBRIDM are presented in Table A1a

**Table A1a.** AHYBRIDM results on elastic-plastic torsion problem.

n	#iter	#fg	CPU (sec)	fx
40000	241	269	6.02	-0.4392678188

Figure A1 presents the solution of the problem



**Fig. A1.** Solution of elastic-plastic torsion problem.  $nx = 200, ny = 200 . c = 5.$   
40000 variable.

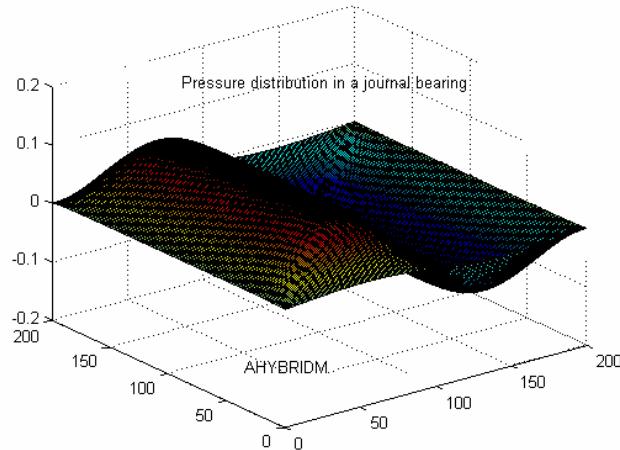
## 2) Pressure distribution in a journal bearing

Results obtained with AHYBRIDM are presented in Table A2a

**Table A2a.** AHYBRIDM results on pressure distribution in a journal bearing problem.

n	#iter	#fg	CPU (sec)	fx
40000	634	669	15.77	-0.2828929487

Figure A2 presents the solution of the problem



**Fig. A2.** Solution of pressure distribution in a journal bearing problem.  
40000 variable.

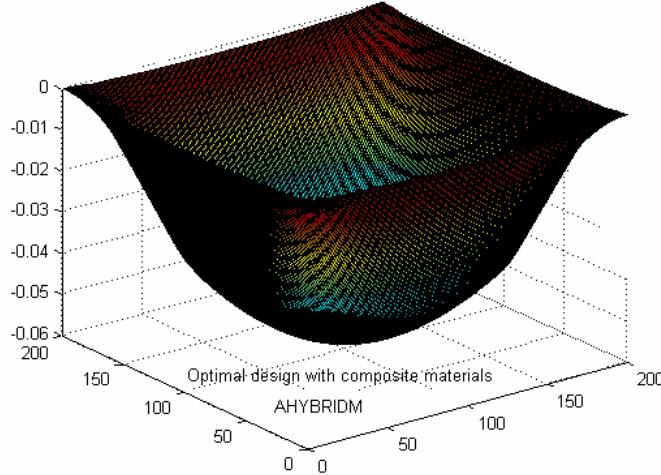
### 3) Optimal design with composite materials

Results obtained with AHYBRIDM are presented in Table A3a

**Table A3a.** AHYBRIDM results on optimal design with composite materials problem.

n	#iter	#fg	CPU (sec)	fx
40000	1003	1033	42.95	-0.011381289

Figure A3 presents the solution of the problem.



**Fig. A3.** Solution of optimal design with composite materials problem.  $n = 40000$ .

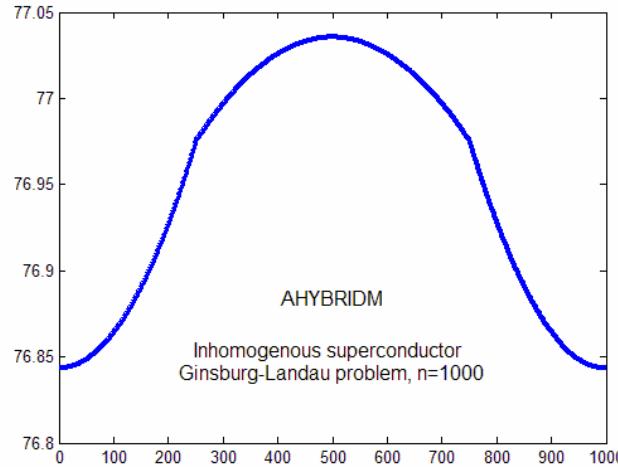
### 4) Inhomogenous Superconductors Ginzburg-Landau (1-dimensional)

Results obtained with AHYBRIDM are presented in Table A4a

**Table A4a.** AHYBRIDM results on Ginzburg-Landau (1-dimensional) problem.

n	#iter	#fg	CPU (sec)	fx
1000	100001	195816	15.96	-8456.19197519

Figure A4 illustrates the solution of the problem corresponding to 1000 discretization points.



**Fig. A4.** Solution of Ginzburg-Landau (1-dimensional) problem.  $n = 1000$ .

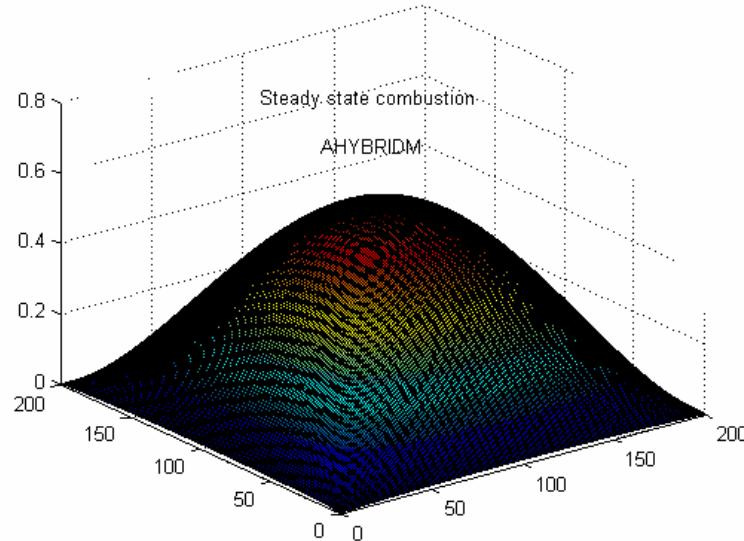
## 5) Steady State Combustion

Results obtained with AHYBRIDM are presented in Table A5a

**Table A5a.** AHYBRIDM results on steady state combustion problem.

n	#iter	#fg	CPU (sec)	fx
40000	299	333	19.19	-5.61144849

Figure A5 illustrates the solution of the problem.



**Fig. A5.** Solution of steady state combustion problem.  $n = 40000$ .

## 6) Molecular conformation (Jones Clusters)

Results obtained with AHYBRIDM are presented in Table A6a

**Table A6a.** AHYBRIDM results on molecular conformation problem.

n	#iter	#fg	CPU (sec)	fx
3000	1846	4827	229.99	-6626.746943

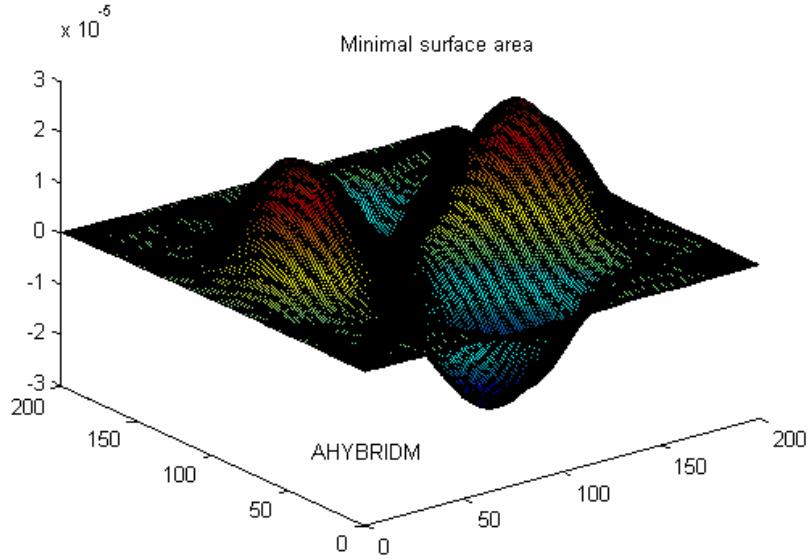
## 7) Minimal Surface Area

Results obtained with AHYBRIDM are presented in Table A7a

**Table A7a.** AHYBRIDM results on minimal surface area problem.

n	#iter	#fg	CPU (sec)	fx
40000	282	306	10.99	1.00

Figure A7 illustrates the solution of minimal surface area problem



**Fig. A7.** Solution of the minimal surface area problem.  $n = 40000$ .

Table A8 presents a comparison between AHYBRIDM and TN [8] for solving these applications.

**Table A8.** Comparison between AHYBRIDM and TN packages.

#problem	n	AHYBRIDM			TN		
		#iter	#fg	CPU(sec)	#iter	#fg	CPU(sec)
1	40000	241	269	6.02	13	307	<b>5.60</b>
2	40000	634	669	15.77	33	798	<b>14.47</b>
3	40000	1003	1033	<b>42.95</b>	54	1744	49.95
4	1000	100001	195816	15.96	340	6134	<b>1.20</b>
5	40000	299	333	19.19	27	477	<b>18.21</b>
6	3000	1846	4827	229.99	1403	37395	1417.63
7	40000	282	306	10.99	16	317	<b>8.20</b>

Table A9 presents a comparison between AHYBRIDM and LBFGS [6,7] for solving these applications.

**Table A9.** Comparison between AHYBRIDM and LBFGS packages.

#problem	n	AHYBRIDM			LBFGS		
		#iter	#fg	CPU(sec)	#iter	#fg	CPU(sec)
1	40000	241	269	<b>6.02</b>	346	755	6.40
2	40000	634	669	15.77	856	914	<b>15.29</b>
3	40000	1003	1033	42.95	656	4214	<b>19.85</b>
4	1000	100001	195816	15.96	1908	2001	<b>0.43</b>
5	40000	299	333	19.19	503	1301	<b>19.0</b>
6	3000	1846	4827	229.99	1551	5241	<b>56.21</b>
7	40000	282	306	10.99	428	441	<b>10.24</b>

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### Results of AHYBRIDM on Applications from MINPACK2.

Conjugate Gradient Algorithm AHYBRIDM, Neculai Andrei  
Accelerated - AHYBRIDM: convex combination of HS,DY:  
from Newton direction with modified secant condition  
Powell restart. September 23, 2008

1 AHYBRIDM Algorithm. Function **Elastic-Plastic Torsion Problem**  
stoptest= 1

n	iter	irs	fgcnt	lscnt	time(c)	fxnew	gnorm
40000	241	0	269	27	602	- .4392678188056E+00	.3175759862606E-04
TOTAL	241	0	269	27	6.02 (seconds)	proc=	.00%
Total # iter for DY= 108 i.e. 44.81							
Total # iter for HS= 133 i.e. 55.19							
Total # iter for CC= 0 i.e. .00							

Conjugate Gradient Algorithm AHYBRIDM, Neculai Andrei  
Accelerated - AHYBRIDM: convex combination of HS,DY:  
from Newton direction with modified secant condition  
Powell restart. September 23, 2008

1 AHYBRIDM Algorithm. Function **Pressure Distribution Problem**  
stoptest= 1

n	iter	irs	fgcnt	lscnt	time(c)	fxnew	gnorm
40000	634	0	669	34	1577	- .2828929487236E+00	.2262124595661E-04
TOTAL	634	0	669	34	15.77 (seconds)	proc=	.00%
Total # iter for DY= 290 i.e. 45.74							
Total # iter for HS= 344 i.e. 54.26							
Total # iter for CC= 0 i.e. .00							

Conjugate Gradient Algorithm AHYBRIDM, Neculai Andrei  
Accelerated - AHYBRIDM: convex combination of HS,DY:  
from Newton direction with modified secant condition  
Powell restart. September 23, 2008

1 AHYBRIDM Algorithm. Function **Optimal Design with Composite Materials**  
stoptest= 1

n	iter	irs	fgcnt	lscnt	time(c)	fxnew	gnorm
40000	1003	1	1033	29	4295	- .1138128968418E-01	.3945613304656E-04
TOTAL	1003	1	1033	29	42.95 (seconds)	proc=	.10%
Total # iter for DY= 213 i.e. 21.24							
Total # iter for HS= 599 i.e. 59.72							
Total # iter for CC= 191 i.e. 19.04							

Conjugate Gradient Algorithm AHYBRIDM, Neculai Andrei  
Accelerated - AHYBRIDM: convex combination of HS,DY:  
from Newton direction with modified secant condition  
Powell restart. September 23, 2008

1 AHYBRIDM Algorithm. Function **Ginzburg-Landau (1-dimensional)**  
stoptest= 1

n	iter	irs	fgcnt	lscnt	time(c)	fxnew	gnorm
---	------	-----	-------	-------	---------	-------	-------

```
-----
1000 100001 ***** 195816 4398      1596 -.8456191975196E+04 .1529281676142E-02
-----
TOTAL 100001 ***** 195816 4398      15.96 (seconds)    proc= 185.75%
```

Total # iter for DY= 3840 i.e. 3.84  
Total # iter for HS= 95556 i.e. 95.56  
Total # iter for CC= 604 i.e. .60

Conjugate Gradient Algorithm AHYBRIDM, Neculai Andrei  
Accelerated - AHYBRIDM: convex combination of HS,DY:  
from Newton direction with modified secant condition  
Powell restart. September 23, 2008

1 AHYBRIDM Algorithm. Function **Steady State Combustion**  
stoptest= 1

n	iter	irs	fgcnt	lscnt	time(c)	fxnew	gnorm
40000	299	0	333	33	1919	-.5611448493607E+01	.2374287969378E-04
TOTAL	299	0	333	33	19.19 (seconds)	proc=	.00%

Total # iter for DY= 33 i.e. 11.04  
Total # iter for HS= 238 i.e. 79.60  
Total # iter for CC= 28 i.e. 9.36

Conjugate Gradient Algorithm AHYBRIDM, Neculai Andrei  
Accelerated - AHYBRIDM: convex combination of HS,DY:  
from Newton direction with modified secant condition  
Powell restart. September 23, 2008

1 AHYBRIDM Algorithm. Function **Jones Clusters (Molecular Conformation)**  
stoptest= 1

n	iter	irs	fgcnt	lscnt	time(c)	fxnew	gnorm
3000	1846	48	4827	262	22999	-.6626746943257E+04	.8821996097925E-05
TOTAL	1846	48	4827	262	229.99 (seconds)	proc=	2.60%

Total # iter for DY= 312 i.e. 16.90  
Total # iter for HS= 1172 i.e. 63.49  
Total # iter for CC= 362 i.e. 19.61

Conjugate Gradient Algorithm AHYBRIDM, Neculai Andrei  
Accelerated - AHYBRIDM: convex combination of HS,DY:  
from Newton direction with modified secant condition  
Powell restart. September 23, 2008

1 AHYBRIDM Algorithm. Function **Minimal Surface Area**  
stoptest= 1

n	iter	irs	fgcnt	lscnt	time(c)	fxnew	gnorm
40000	282	2	306	23	1099	.1000000005398E+01	.3825667056994E-04
TOTAL	282	2	306	23	10.99 (seconds)	proc=	.71%

Total # iter for DY= 47 i.e. 16.67  
Total # iter for HS= 214 i.e. 75.89  
Total # iter for CC= 21 i.e. 7.45

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### Results of LBFGS [6,7] on Applications from MINPACK2.

L-BFGS Algorithm. **Elastic-Plastic Torsion Problem**  
 Number of BFGS updates M= 3 February 9, 2007

n	iter	fgcnt	time	fxnew	gnorm2
<hr/>					
40000	381	399	660	-.4392674132720E+00	.4971116500015E-04
<hr/>					
L-BFGS Algorithm. <b>Elastic-Plastic Torsion Problem</b>					
Number of BFGS updates M= 5 February 9, 2007					
n	iter	fgcnt	time	fxnew	gnorm2
<hr/>					
40000	346	755	640	-.4392677559075E+00	.5381376897767E-04
<hr/>					
L-BFGS Algorithm. <b>Elastic-Plastic Torsion Problem</b>					
Number of BFGS updates M= 7 February 9, 2007					
n	iter	fgcnt	time	fxnew	gnorm2
<hr/>					
40000	342	1106	674	-.4392678005491E+00	.3995535751961E-04
<hr/>					
L-BFGS Algorithm. <b>Elastic-Plastic Torsion Problem</b>					
Number of BFGS updates M= 9 February 9, 2007					
n	iter	fgcnt	time	fxnew	gnorm2
<hr/>					
40000	316	1431	674	-.4392678108470E+00	.5425504709693E-04
<hr/>					

L-BFGS Algorithm. **Pressure Distribution Problem**  
 Number of BFGS updates M= 3 February 8, 2007

n	iter	fgcnt	time	fxnew	gnorm2
<hr/>					
40000	856	914	1529	-.2828929058887E+00	.2996880109306E-04
<hr/>					
L-BFGS Algorithm. <b>Pressure Distribution Problem</b>					
Number of BFGS updates M= 5 February 8, 2007					
n	iter	fgcnt	time	fxnew	gnorm2
<hr/>					
40000	814	1759	1539	-.2828929295173E+00	.3015639731448E-04
<hr/>					
L-BFGS Algorithm. <b>Pressure Distribution Problem</b>					
Number of BFGS updates M= 7 February 8, 2007					
n	iter	fgcnt	time	fxnew	gnorm2
<hr/>					
40000	799	2579	1623	-.2828929416860E+00	.2517069133647E-04
<hr/>					
L-BFGS Algorithm. <b>Pressure Distribution Problem</b>					
Number of BFGS updates M= 9 February 8, 2007					
n	iter	fgcnt	time	fxnew	gnorm2
<hr/>					
40000	773	3373	1678	-.2828929346610E+00	.3556990170108E-04
<hr/>					

L-BFGS Algorithm. **Optimal Design with Composite Materials**  
 Number of BFGS updates M= 3 February 8, 2007

n	iter	fgcnt	time	fxnew	gnorm2
<hr/>					
40000	1809	1838	4708	-.1138122865547E-01	.2023777688460E-04
<hr/>					
L-BFGS Algorithm. <b>Optimal Design with Composite Materials</b>					
Number of BFGS updates M= 5 February 8, 2007					
n	iter	fgcnt	time	fxnew	gnorm2
<hr/>					
40000	859	2704	2342	-.1138128573610E-01	.2660425854793E-04
<hr/>					
L-BFGS Algorithm. <b>Optimal Design with Composite Materials</b>					
Number of BFGS updates M= 7 February 8, 2007					

n	iter	fgcnt	time	fxnew	gnorm2
40000	843	3553	2429	-.1138128632483E-01	.3063106124306E-04
L-BFGS Algorithm. Optimal Design with Composite Materials					
Number of BFGS updates M= 9 February 8, 2007					
40000	656	4214	1985	-.1138129442545E-01	.3241232447072E-04

L-BFGS Algorithm. **Ginzburg-Landau (1-dimensional)**  
Number of BFGS updates M= 3 February 9, 2007

n	iter	fgcnt	time	fxnew	gnorm2
1000	1908	2001	43	-.1718319208564E-03	.1444624844288E-01
L-BFGS Algorithm. Ginzburg-Landau (1-dimensional)					
Number of BFGS updates M= 3 February 9, 2007					
2000	1881	2001	68	-.1675274151520E-03	.1366505584700E-01

L-BFGS Algorithm. **Steady State Combustion - Bratu**  
Number of BFGS updates M= 3 February 8, 2007

n	iter	fgcnt	time	fxnew	gnorm2
40000	740	776	2712	-.5611447434734E+01	.4290597251963E-04
L-BFGS Algorithm. Steady State Combustion - Bratu					
Number of BFGS updates M= 5 February 8, 2007					
40000	503	1301	1900	-.5611448490517E+01	.4437990070301E-04
L-BFGS Algorithm. Steady State Combustion - Bratu					
Number of BFGS updates M= 7 February 8, 2007					
40000	522	1842	2035	-.5611448497617E+01	.4405870194056E-04
L-BFGS Algorithm. Steady State Combustion - Bratu					
Number of BFGS updates M= 9 February 8, 2007					
40000	501	2357	2017	-.5611448480843E+01	.4610522697016E-04

L-BFGS Algorithm. **Jones Clusters (Molecular Conformation)**  
Number of BFGS updates M= 3 February 8, 2007

n	iter	fgcnt	time	fxnew	gnorm2
3000	1930	2001	6961	-.6613534243165E+04	.4571920141689E+00
L-BFGS Algorithm. Jones Clusters (Molecular Conformation)					
Number of BFGS updates M= 5 February 8, 2007					
3000	1551	3623	5626	-.6602132026911E+04	.3827556039252E-03
L-BFGS Algorithm. Jones Clusters (Molecular Conformation)					
Number of BFGS updates M= 7 February 8, 2007					

n	iter	fgcnt	time	fxnew	gnorm2
3000	1551	5241	5621	-.6610370139041E+04	.4268140295915E-03
L-BFGS Algorithm. Jones Clusters (Molecular Conformation)					
Number of BFGS updates M= 9 February 8, 2007					
n	iter	fgcnt	time	fxnew	gnorm2
3000	1048	6338	3816	-.6626189460436E+04	.3834472015488E-03

L-BFGS Algorithm. <b>Minimal surface area problem</b>					
Number of BFGS updates M= 3 February 8, 2007					
n	iter	fgcnt	time	fxnew	gnorm2
40000	428	441	1024	.1421353295447E+01	.3052936828957E-04
L-BFGS Algorithm. Minimal surface area problem					
Number of BFGS updates M= 5 February 8, 2007					
n	iter	fgcnt	time	fxnew	gnorm2
40000	448	898	1114	.1421353240881E+01	.2955888848323E-04
L-BFGS Algorithm. Minimal surface area problem					
Number of BFGS updates M= 7 February 8, 2007					
n	iter	fgcnt	time	fxnew	gnorm2
40000	467	1372	1228	.1421353240739E+01	.2818708529408E-04
L-BFGS Algorithm. Minimal surface area problem					
Number of BFGS updates M= 9 February 8, 2007					
n	iter	fgcnt	time	fxnew	gnorm2
40000	439	1822	1227	.1421353228094E+01	.3039593999088E-04

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### **Results of TN [8] on Applications from MINPACK2.**

Truncated Newton Method  
 Application L1. March 16, 2007  
 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	560	-.4392678E+00

Truncated Newton Method  
 Application T2. March 16, 2007  
 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 1447 -.2828929E+00

Truncated Newton Method  
Application T3. March 16, 2007  
TN algorithm. **Optimal Design with composite materials** 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 54 1744 4995 -.1138130E-01

Truncated Newton Method  
Application T4. March 16, 2007  
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 340 6134 120 -.8456192E+04

Truncated Newton Method  
Application T5. March 16, 2007  
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 1821 -.5611449E+01

Truncated Newton Method  
Application T6. March 16, 2007  
TN algorithm. **Jones Clusters (Molecular Conformation)** Problem  
-----  
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 141763 -.6576856E+04

Truncated Newton Method  
Application T7. March 20, 2007  
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 16 317 820 .1000000E+01

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