Numerical experiments with accelerated conjugate gradient algorithm with Hessian / vector product - ACGHES - for unconstrained optimization

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In this Technical Report we document some numerical experiments with ACGHES - *accelerated conjugate gradient algorithm with Hessian / vector product* [1] for solving some problems from MINPACK2 Library.
ACGHES is a conjugate gradient algorithm in which the parameter β_k is computed by an approximation of the Hessian / vector product through finite difference as:

$$\beta_k = \frac{s_k^T \nabla^2 f(x_{k+1}) g_{k+1} - s_k^T g_{k+1}}{s_k^T \nabla^2 f(x_{k+1}) s_k}$$

The salient point with this formula for β_k computation is the presence of the Hessian. Observe that if the line search is exact we get the Daniel method [2].
For search direction computation, the algorithm uses a forward difference approximation to the Hessian / vector product in combination with a careful choice of the finite difference interval. Therefore, in an effort to use the Hessian in β_k we suggest a nonlinear conjugate gradient algorithm in which the Hessian / vector product $\nabla^2 f(x_{k+1}) s_k$ is approximated by finite differences:

$$\nabla^2 f(x_{k+1}) s_k = \frac{\nabla f(x_{k+1} + \delta s_k) - \nabla f(x_{k+1})}{\delta},$$

where

$$\delta = \frac{2\sqrt{\varepsilon_m}(1 + \|x_{k+1}\|)}{\|s_k\|},$$

and ε_m is epsilon machine. The computation of δ is implemented like in TN package [4] as:

$$\delta = \max\left\{\frac{\varphi}{\max\{10\varphi, \|s_k\|\}}, \frac{\varphi}{100}\right\}, \quad \varphi = 2\sqrt{\varepsilon_m}(1 + \|x_{k+1}\|\sqrt{n}).$$

The stopping criterion is $\|g_k\|_\infty \le 10^{-6}$, where $\|.\|_\infty$ is the maximum absolute component of a vector.

<u>1. Elastic - Plastic Torsion Problem</u>

Results obtained with ACGHES are presented in Table A1a

Table A1a. ACGHES results on elastic-plastic torsion problem.

n	#iter	#fg	CPU (sec)	fx
40000	2001	2097	30.74	-0.3458351472

Figure A1 presents the solution of the problem

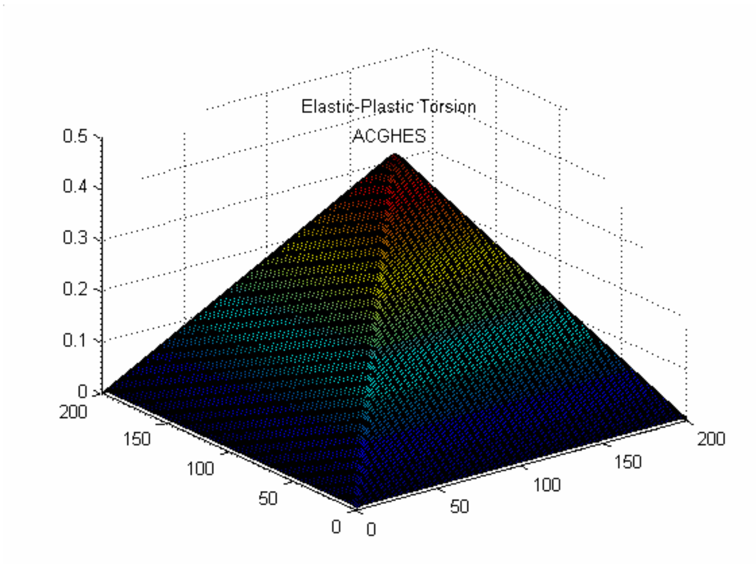

Fig. A1. Solution of elastic-plastic torsion problem. $nx = 200, ny = 200$. $c = 5$.
40000 variabile.

2) Pressure distribution in a journal bearing
Results obtained with ACGHES are presented in Table A2a

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

n	#iter	#fg	CPU (sec)	fx
40000	631	666	23.37	-0.2828924854

Figure A2 presents the solution of the problem

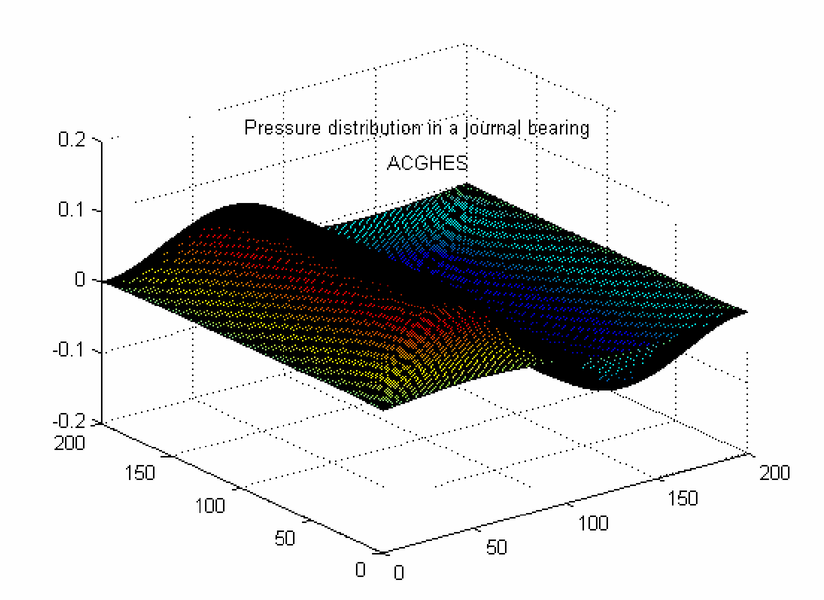

Fig. A2. Solution of pressure distribution in a journal bearing problem.
40000 variabile.

3) Optimal design with composite materials

Results obtained with ACGHES are presented in Table A3a

Table A3a. ACGHES results on optimal design with composite materials problem.

n	#iter	#fg	CPU (sec)	fx
40000	1017	1052	60.64	-0.011381289

Figure A3 presents the solution of the problem.

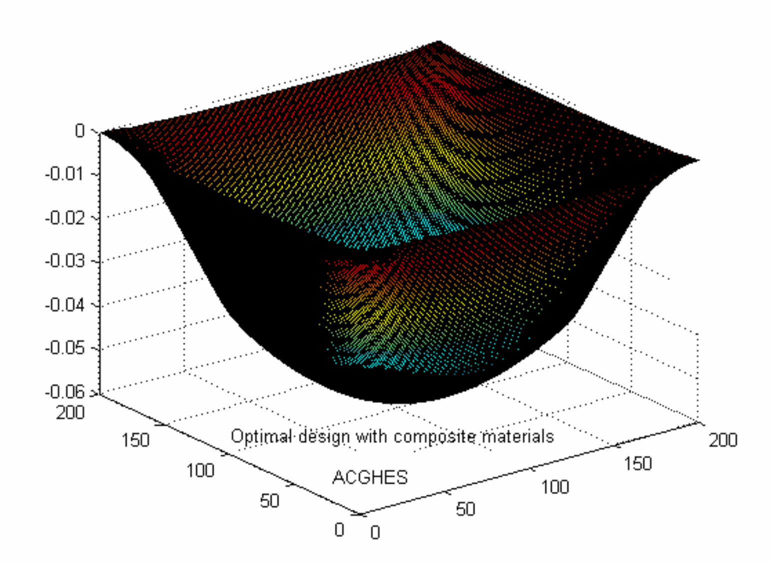

Fig. A3. Solution of optimal design with composite materials problem. $n = 40000$.

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

Results obtained with ACGHES are presented in Table A4a

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

n	#iter	#fg	CPU (sec)	fx
1000	300001	368942	46.48	-0.845619E+4

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

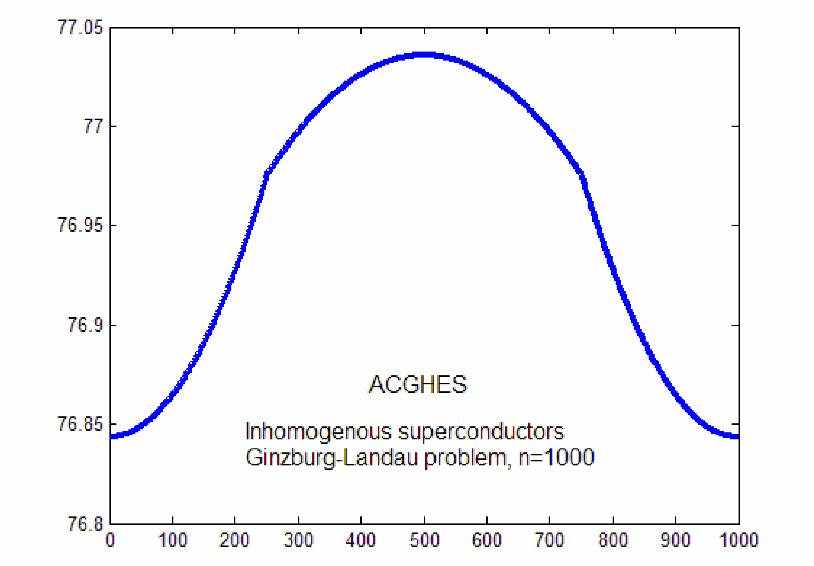

Fig. A4. Solution of Ginzburg-Landau (1-dimensional) problem. $n = 1000$.

5) Steady State Combustion

Results obtained with ACGHES are presented in Table A5a

Table A5a. ACGHES results on steady state combustion problem.

n	#iter	#fg	CPU (sec)	fx
40000	299	333	28.13	-5.611448493

Figure A5 illustrates the solution of the problem.

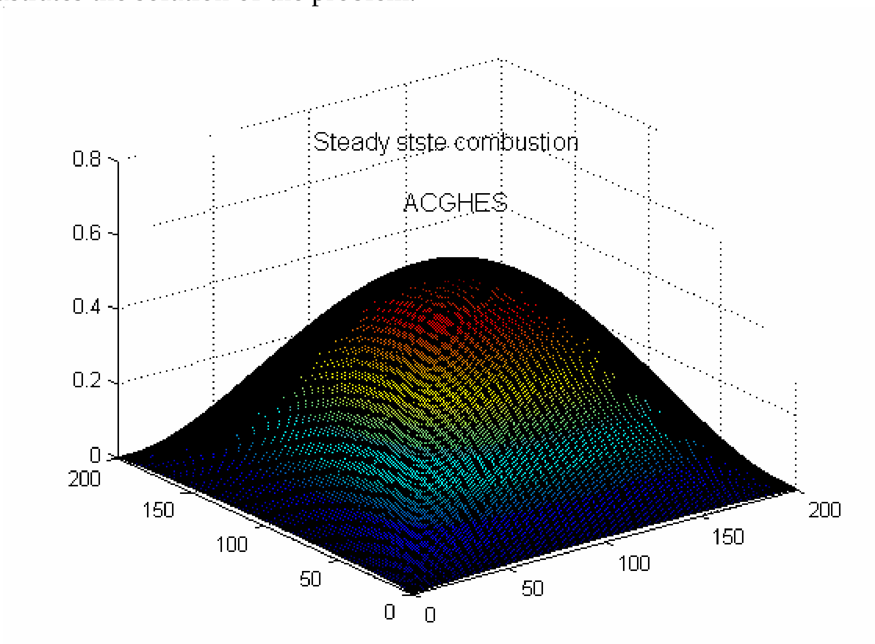

Fig. A5. Solution of steady state combustion problem. $n = 40000$.

6) Molecular conformation (Jones Clusters)

Results obtained with ACGHES are presented in Table A6a

Table A6a. ACGHES results on molecular conformation problem.

n	#iter	#fg	CPU (sec)	fx
3000	6001	6002	209.69	-4494.653725

7) Minimal Surface Area

Results obtained with ACGHES are presented in Table A7a

Table A7a. ACGHES results on minimal surface area problem.

n	#iter	#fg	CPU (sec)	fx
40000	281	308	16.13	1

Figure A7 illustrates the solution of minimal surface area problem

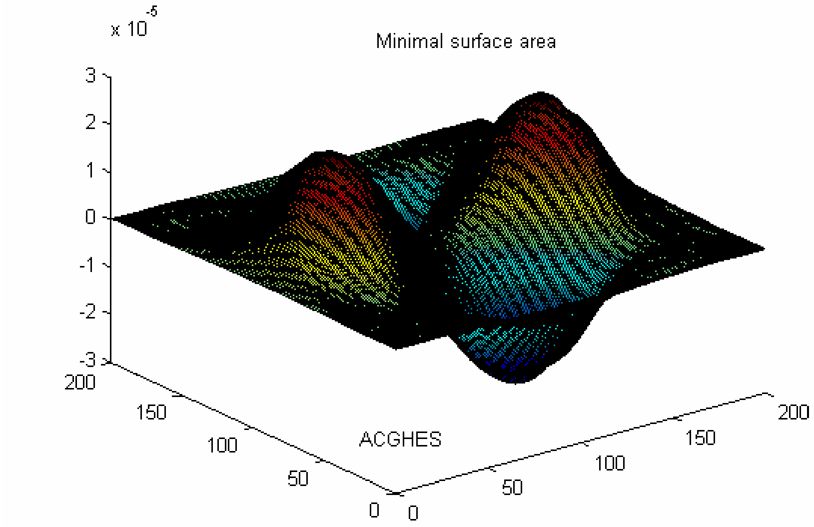

Fig. A7. Solution of the minimal surface area problem. $n = 40000$.

Table A8 presents a comparison between ACGHES and TN [4] for solving these applications.

Table A8. Comparison between ACGHES and TN packages.

		ACGHES			TN		
#problem	n	#iter	#fg	CPU(sec)	#iter	#fg	CPU(sec)
1	40000	2001#	2097	30.31	13	307	**5.60**
2	40000	631	666	**23.34**	33	798	**14.47**
3	40000	1017	1052	**60.64**	54	1744	49.95
4	1000	>2000‡	>2000	46.48	340	6134	**1.20**
5	40000	299	333	**28.13**	27	477	**18.21**
6	3000	6001†	6002	**209.69**	1403	37395	1417.63
7	40000	281	308	**16.13**	16	317	**8.20**

Even that we increase the maximum number of iterations, ACGHES is unable to get an accurate solution. In this case $\|g_{2001}\| = 0.070189$

‡ ACGHES package needs more than 300000 iterations to get a solution with $\|g_{300001}\| = 0.00446311$

† The problem is difficult. ACGHES need more than 6000 iterations. In this case ACGHES did not get a solution. The infinite norm of the gradient is: $\|g_{6001}\|_\infty = 0.11077117e+03$

Even that ACGHES uses the same strategy for Hessian / vector product as that used in TN package we see that ACGHES achieves a slight numerical improvement over TN.
Table A9 shows a comparison between ACGHES and LBFGS [3] for solving these applications.

Table A9. Comparison between ACGHES and LBFGS packages.

		ACGHES			LBFGS		
#problem	n	#iter	#fg	CPU(sec)	#iter	#fg	CPU(sec)
1	40000	2001#	2097	30.31	346	755	**6.40**
2	40000	631	666	23.34	856	914	**15.29**
3	40000	1017	1052	60.64	656	4214	**19.85**
4	1000	>2000‡	>2000	46.48	1908	2001	**0.43**
5	40000	299	333	28.13	503	1301	**19.0**
6	3000	6001†	6002	209.69	1551	5241	**56.21**
7	40000	281	308	16.13	428	441	**10.24**

References

[1] **Andrei, N.,** *Accelerated conjugate gradient algorithm with finite difference Hessian / vector product approximation for unconstrained optimization*. ICI Technical Report, March 4, 2008.

[2] **Daniel, J.W.,** *The conjugate gradient method for linear and nonlinear operator equations.* SIAM J. Numer. Anal., 4 (1967), pp.10-26.

[3] **Liu, D., Nocedal, J.,** *On the limited memory BFGS method for large scale optimization*, Mathematical Programming B 45 (1989) 503-528.

[4] **Nash, S.G.,** *Preconditioning of truncated-Newton methods.* SIAM J. on Scientific and Statistical Computing, 6 (1985), pp.599-616.

September 22, 2008