Performances of LBFGS-B for solving MINPACK-2 applications

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In this work I present the performances of LBFGS-B package [1, 2] for solving some applications from MINPACK-2 collection of Averick, Carter, Moré and Xue [3]. ($factr = 10^7$, $pgtol = 10^{-5}$)

1. Elastic-Plastic Problem

Experiment Nr. 1: $10^{-6} \le x \le 1$

```
Machine precision = 2.220D-16
 N =       40000    M =           5

At X0         0 variables are exactly at the bounds

At iterate    0    f= -3.33325D-01    |proj g|=  9.82649D-03
At iterate    1    f= -3.38196D-01    |proj g|=  4.86074D-03
At iterate    2    f= -3.40864D-01    |proj g|=  4.82202D-03
At iterate    3    f= -3.46289D-01    |proj g|=  4.62996D-03
At iterate    4    f= -3.49711D-01    |proj g|=  2.90606D-03
At iterate    5    f= -3.55068D-01    |proj g|=  4.06765D-03
At iterate    6    f= -3.57413D-01    |proj g|=  2.84401D-03
At iterate    7    f= -3.61722D-01    |proj g|=  3.89709D-03
At iterate    8    f= -3.65717D-01    |proj g|=  8.91855D-03
At iterate    9    f= -3.70032D-01    |proj g|=  4.27007D-03
At iterate   10    f= -3.71692D-01    |proj g|=  2.79878D-03
At iterate   11    f= -3.75148D-01    |proj g|=  2.15104D-03
At iterate   12    f= -3.77318D-01    |proj g|=  2.28291D-03
At iterate   13    f= -3.82112D-01    |proj g|=  3.08795D-03
At iterate   14    f= -3.84320D-01    |proj g|=  2.75195D-03
At iterate   15    f= -3.87384D-01    |proj g|=  2.64017D-03
At iterate   16    f= -3.89984D-01    |proj g|=  2.36031D-03
At iterate   17    f= -3.92149D-01    |proj g|=  2.57257D-03
At iterate   18    f= -3.94539D-01    |proj g|=  2.53056D-03
At iterate   19    f= -3.97136D-01    |proj g|=  2.73492D-03
At iterate   20    f= -3.98988D-01    |proj g|=  3.80687D-03
At iterate   21    f= -4.00893D-01    |proj g|=  2.34443D-03
At iterate   22    f= -4.02622D-01    |proj g|=  2.00092D-03
At iterate   23    f= -4.04278D-01    |proj g|=  1.91806D-03
At iterate   24    f= -4.05738D-01    |proj g|=  3.73180D-03
At iterate   25    f= -4.07884D-01    |proj g|=  2.48418D-03
At iterate   26    f= -4.09561D-01    |proj g|=  1.85810D-03
At iterate   27    f= -4.11012D-01    |proj g|=  2.21738D-03
At iterate   28    f= -4.12439D-01    |proj g|=  1.89261D-03
At iterate   29    f= -4.13809D-01    |proj g|=  1.57093D-03
At iterate   30    f= -4.15549D-01    |proj g|=  2.39053D-03
At iterate   31    f= -4.16855D-01    |proj g|=  1.65622D-03
```

```
At iterate   32    f= -4.17876D-01    |proj g|=  1.44566D-03
……................................
At iterate  156    f= -4.39239D-01    |proj g|=  1.73715D-05
At iterate  157    f= -4.39239D-01    |proj g|=  1.82151D-05
At iterate  158    f= -4.39240D-01    |proj g|=  5.08944D-05
At iterate  159    f= -4.39240D-01    |proj g|=  1.90596D-05
At iterate  160    f= -4.39241D-01    |proj g|=  1.63241D-05
At iterate  161    f= -4.39241D-01    |proj g|=  1.94863D-05
At iterate  162    f= -4.39242D-01    |proj g|=  7.58314D-05
At iterate  163    f= -4.39242D-01    |proj g|=  2.88157D-05
At iterate  164    f= -4.39243D-01    |proj g|=  1.25979D-05
At iterate  165    f= -4.39243D-01    |proj g|=  1.28531D-05
At iterate  166    f= -4.39243D-01    |proj g|=  1.93400D-05
At iterate  167    f= -4.39244D-01    |proj g|=  1.80818D-05
At iterate  168    f= -4.39244D-01    |proj g|=  1.14764D-05
At iterate  169    f= -4.39244D-01    |proj g|=  1.05279D-05
At iterate  170    f= -4.39244D-01    |proj g|=  1.16540D-05
At iterate  171    f= -4.39244D-01    |proj g|=  2.74846D-05
At iterate  172    f= -4.39244D-01    |proj g|=  1.02429D-05
At iterate  173    f= -4.39244D-01    |proj g|=  8.66268D-06

           •  * *
Tit   = total number of iterations
Tnf   = total number of function evaluations
Tnint = total number of segments explored during Cauchy searches
Skip  = number of BFGS updates skipped
Nact  = number of active bounds at final generalized Cauchy point
Projg = norm of the final projected gradient
F     = final function value
            * * *

   N   Tit  Tnf  Tnint  Skip  Nact     Projg        F
40000  173  184    177     0     0   8.663D-06  -4.392D-01
  F = -4.392444502129256E-001

CONVERGENCE: NORM OF PROJECTED GRADIENT <= PGTOL

 Cauchy                time 3.640E+00 seconds.
 Subspace minimization time 7.410E+00 seconds.
 Line search           time 6.030E+00 seconds.

 Total User time 1.895E+01 seconds.
```

Experiment Nr. 2: $10^{-6} \le x \le 0.1$

```
Machine precision = 2.220D-16
N =       40000    M =           5
The initial X is infeasible.  Restart with its projection.

At X0     25600 variables are exactly at the bounds

At iterate    0    f= -2.27362D-01    |proj g|=  9.82649D-03
At iterate    1    f= -2.31124D-01    |proj g|=  7.37423D-03
At iterate    2    f= -2.33410D-01    |proj g|=  3.67665D-03
At iterate    3    f= -2.36040D-01    |proj g|=  3.01381D-03
At iterate    4    f= -2.38705D-01    |proj g|=  3.15618D-03
At iterate    5    f= -2.41577D-01    |proj g|=  5.20763D-03
At iterate    6    f= -2.43579D-01    |proj g|=  3.21630D-03
At iterate    7    f= -2.45271D-01    |proj g|=  3.07742D-03
At iterate    8    f= -2.47397D-01    |proj g|=  5.79351D-03
At iterate    9    f= -2.49084D-01    |proj g|=  5.12010D-03
At iterate   10    f= -2.50305D-01    |proj g|=  2.74681D-03
At iterate   11    f= -2.51864D-01    |proj g|=  1.96521D-03
At iterate   12    f= -2.52848D-01    |proj g|=  4.43552D-03
At iterate   13    f= -2.53953D-01    |proj g|=  2.51711D-03
At iterate   14    f= -2.55098D-01    |proj g|=  1.85277D-03
At iterate   15    f= -2.55761D-01    |proj g|=  3.08173D-03
```

```
At iterate   16    f= -2.56404D-01    |proj g|=  1.53534D-03
At iterate   17    f= -2.57096D-01    |proj g|=  1.54249D-03
At iterate   18    f= -2.57569D-01    |proj g|=  1.86466D-03
At iterate   19    f= -2.58319D-01    |proj g|=  2.65115D-03
At iterate   20    f= -2.58983D-01    |proj g|=  2.10179D-03
……————
At iterate   99    f= -2.68610D-01    |proj g|=  4.82856D-05
At iterate  100    f= -2.68610D-01    |proj g|=  1.26268D-04
At iterate  101    f= -2.68610D-01    |proj g|=  4.27850D-05
At iterate  102    f= -2.68610D-01    |proj g|=  2.43769D-05
At iterate  103    f= -2.68611D-01    |proj g|=  4.15475D-05
At iterate  104    f= -2.68611D-01    |proj g|=  1.49247D-05
At iterate  105    f= -2.68611D-01    |proj g|=  3.29133D-05
At iterate  106    f= -2.68611D-01    |proj g|=  4.62609D-05
At iterate  107    f= -2.68612D-01    |proj g|=  2.00924D-05
At iterate  108    f= -2.68612D-01    |proj g|=  3.47262D-05
At iterate  109    f= -2.68613D-01    |proj g|=  7.18969D-05
At iterate  110    f= -2.68613D-01    |proj g|=  5.28461D-05
At iterate  111    f= -2.68613D-01    |proj g|=  4.58590D-05
At iterate  112    f= -2.68613D-01    |proj g|=  3.41303D-05
At iterate  113    f= -2.68613D-01    |proj g|=  1.62173D-05
At iterate  114    f= -2.68613D-01    |proj g|=  2.59606D-05
At iterate  115    f= -2.68614D-01    |proj g|=  1.93129D-05
At iterate  116    f= -2.68614D-01    |proj g|=  1.85860D-05
At iterate  117    f= -2.68614D-01    |proj g|=  5.97178D-06

           •  * *
Tit   = total number of iterations
Tnf   = total number of function evaluations
Tnint = total number of segments explored during Cauchy searches
Skip  = number of BFGS updates skipped
Nact  = number of active bounds at final generalized Cauchy point
Projg = norm of the final projected gradient
F     = final function value
           * * *

   N   Tit  Tnf  Tnint  Skip  Nact     Projg        F
40000  117  122   1774     0 13836   5.972D-06  -2.686D-01
  F = -2.686137174254426E-001

CONVERGENCE: NORM OF PROJECTED GRADIENT <= PGTOL

 Cauchy                time 1.710E+00 seconds.
 Subspace minimization time 3.820E+00 seconds.
 Line search           time 3.260E+00 seconds.

 Total User time 1.082E+01 seconds.
```

Experiment Nr. 3: $10^{-6} \le x \le 0.01$

```
N =       40000    M =           5
The initial X is infeasible.  Restart with its projection.

At X0     38416 variables are exactly at the bounds

At iterate    0    f= -2.93004D-02    |proj g|=  9.82649D-03
At iterate    1    f= -3.38262D-02    |proj g|=  5.03413D-03
At iterate    2    f= -3.61834D-02    |proj g|=  4.00938D-03
At iterate    3    f= -3.79852D-02    |proj g|=  8.46520D-03
At iterate    4    f= -3.94163D-02    |proj g|=  5.33873D-03
At iterate    5    f= -3.99438D-02    |proj g|=  2.36317D-03
At iterate    6    f= -4.02979D-02    |proj g|=  3.11411D-03
At iterate    7    f= -4.10346D-02    |proj g|=  2.60864D-03
At iterate    8    f= -4.12592D-02    |proj g|=  6.73762D-03
At iterate    9    f= -4.14432D-02    |proj g|=  1.99280D-03
At iterate   10    f= -4.15623D-02    |proj g|=  1.12899D-03
At iterate   11    f= -4.17114D-02    |proj g|=  2.49742D-03
At iterate   12    f= -4.17233D-02    |proj g|=  4.65716D-03
```

```
At iterate   13    f= -4.18142D-02    |proj g|=  8.56937D-04
At iterate   14    f= -4.18381D-02    |proj g|=  3.91774D-04
At iterate   15    f= -4.18687D-02    |proj g|=  6.25324D-04
At iterate   16    f= -4.18750D-02    |proj g|=  1.54028D-03
At iterate   17    f= -4.18945D-02    |proj g|=  2.47027D-04
At iterate   18    f= -4.18989D-02    |proj g|=  1.97849D-04
At iterate   19    f= -4.19056D-02    |proj g|=  2.23240D-04
At iterate   20    f= -4.19078D-02    |proj g|=  3.22544D-04
……————
At iterate   34    f= -4.19135D-02    |proj g|=  4.40821D-05
At iterate   35    f= -4.19136D-02    |proj g|=  2.55498D-05
At iterate   36    f= -4.19136D-02    |proj g|=  3.00238D-05
At iterate   37    f= -4.19137D-02    |proj g|=  3.18071D-05
At iterate   38    f= -4.19137D-02    |proj g|=  2.15574D-05
At iterate   39    f= -4.19137D-02    |proj g|=  1.64028D-05
At iterate   40    f= -4.19137D-02    |proj g|=  1.91102D-05
At iterate   41    f= -4.19137D-02    |proj g|=  9.04357D-06

           •  * *
Tit   = total number of iterations
Tnf   = total number of function evaluations
Tnint = total number of segments explored during Cauchy searches
Skip  = number of BFGS updates skipped
Nact  = number of active bounds at final generalized Cauchy point
Projg = norm of the final projected gradient
F     = final function value
           * * *

   N   Tit  Tnf  Tnint  Skip  Nact     Projg        F
40000   41   45     62     0 30920   9.044D-06  -4.191D-02
  F = -4.191372337445779E-002

CONVERGENCE: NORM OF PROJECTED GRADIENT <= PGTOL

 Cauchy                time 1.700E-01 seconds.
 Subspace minimization time 6.500E-01 seconds.
 Line search           time 1.100E+00 seconds.

 Total User time 2.740E+00 seconds.
```

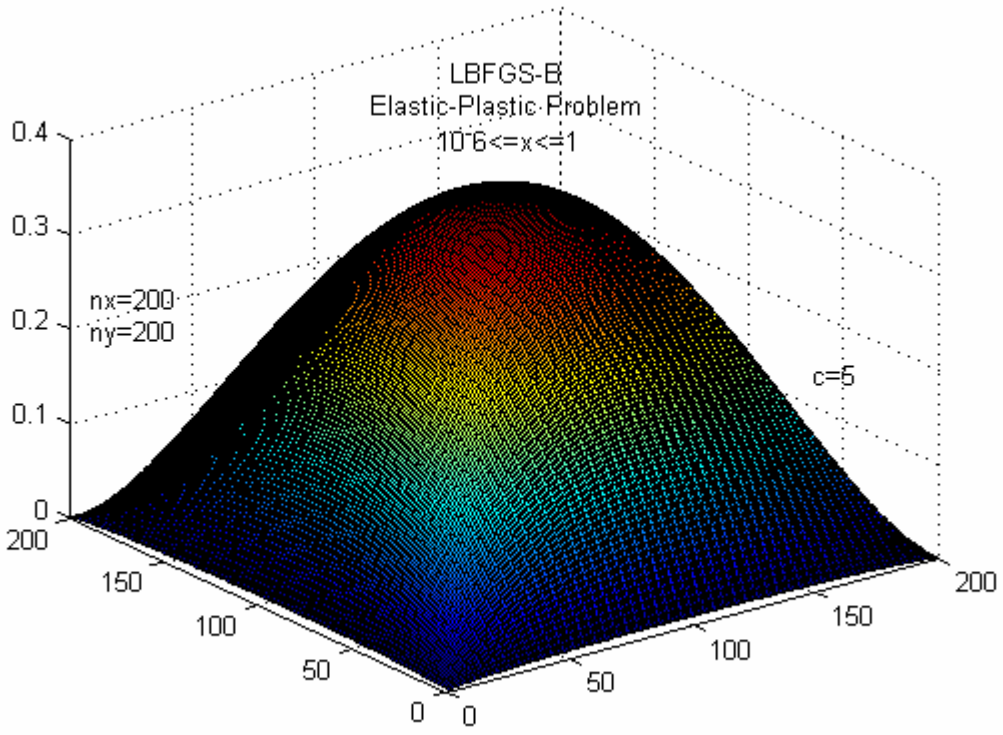

Fig. 1.1. Elastic-Plastic Problem.

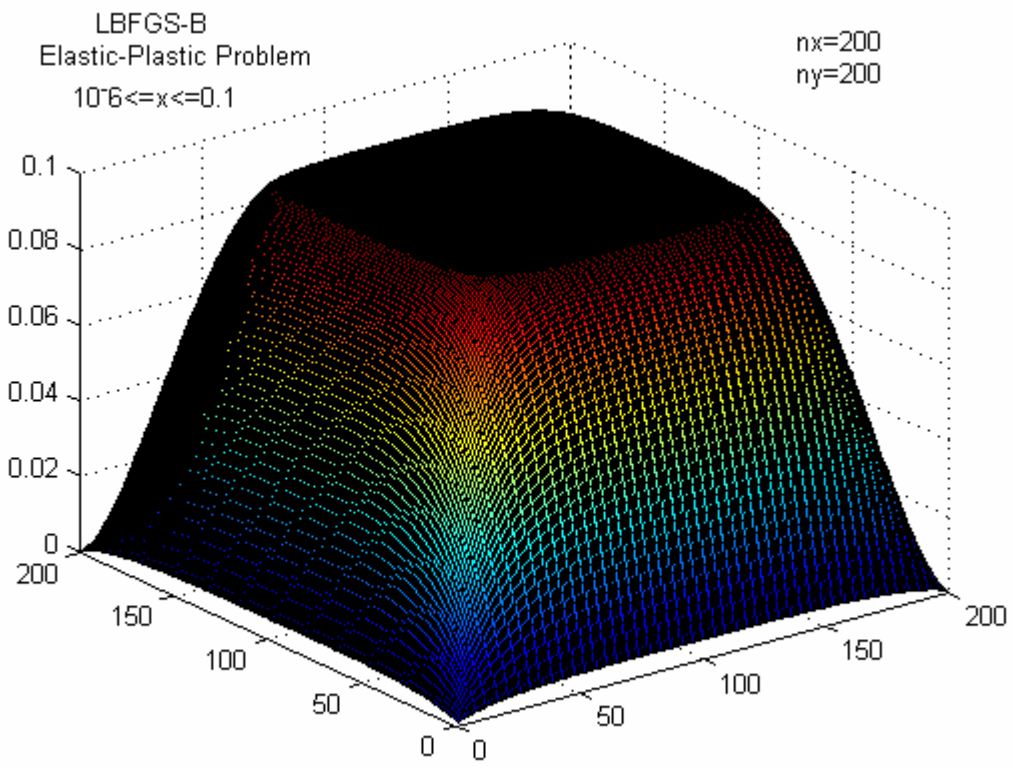

Fig. 1.2. Elastic-Plastic Problem.

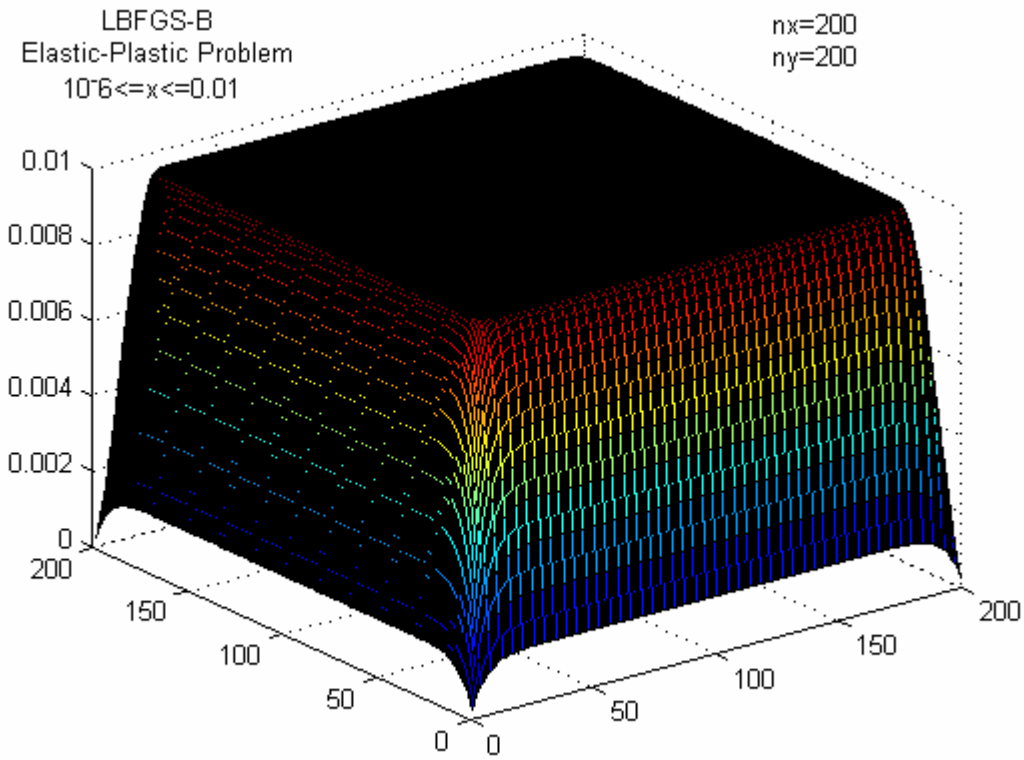

Fig. 1.3. Elastic-Plastic Problem. $10^{-6} \le x \le 0.01$

2. Pressure Distribution in a Journal Bearing

Experiment Nr. 1: $-1 \le x \le +1$

```
Machine precision = 2.220D-16
N =       40000    M =           5

At X0         0 variables are exactly at the bounds
At iterate    0    f=  2.87025D+01    |proj g|=  3.30830D-01

At iterate    1    f=  2.16670D+01    |proj g|=  1.19752D-01
At iterate    2    f=  2.00492D+01    |proj g|=  1.33400D-01
At iterate    3    f=  1.89632D+01    |proj g|=  1.40080D-01
At iterate    4    f=  1.79474D+01    |proj g|=  1.12639D-01
At iterate    5    f=  1.67409D+01    |proj g|=  9.70343D-02
At iterate    6    f=  1.59323D+01    |proj g|=  9.10611D-02
At iterate    7    f=  1.54774D+01    |proj g|=  7.75786D-02
At iterate    8    f=  1.48672D+01    |proj g|=  5.19757D-02
At iterate    9    f=  1.43256D+01    |proj g|=  1.25968D-01
At iterate   10    f=  1.37210D+01    |proj g|=  5.71891D-02
At iterate   11    f=  1.31526D+01    |proj g|=  5.87379D-02
….............
At iterate  616    f= -2.82891D-01    |proj g|=  3.70931D-05
At iterate  617    f= -2.82891D-01    |proj g|=  6.17672D-05
At iterate  618    f= -2.82891D-01    |proj g|=  4.20657D-05
At iterate  619    f= -2.82891D-01    |proj g|=  2.85228D-05
At iterate  620    f= -2.82891D-01    |proj g|=  3.21102D-05
At iterate  621    f= -2.82891D-01    |proj g|=  9.43134D-05
At iterate  622    f= -2.82891D-01    |proj g|=  2.89228D-05
At iterate  623    f= -2.82891D-01    |proj g|=  9.68184D-06
```

- * *

```
Tit   = total number of iterations
Tnf   = total number of function evaluations
Tnint = total number of segments explored during Cauchy searches
Skip  = number of BFGS updates skipped
Nact  = number of active bounds at final generalized Cauchy point
Projg = norm of the final projected gradient
F     = final function value
           * * *

   N   Tit   Tnf  Tnint  Skip  Nact     Projg        F
40000  623   648    623     0     0   9.682D-06  -2.829D-01
  F = -2.828912681338695E-001

CONVERGENCE: NORM OF PROJECTED GRADIENT <= PGTOL

 Cauchy                time 1.346E+01 seconds.
 Subspace minimization time 2.642E+01 seconds.
 Line search           time 1.979E+01 seconds.

 Total User time 7.047E+01 seconds.
```

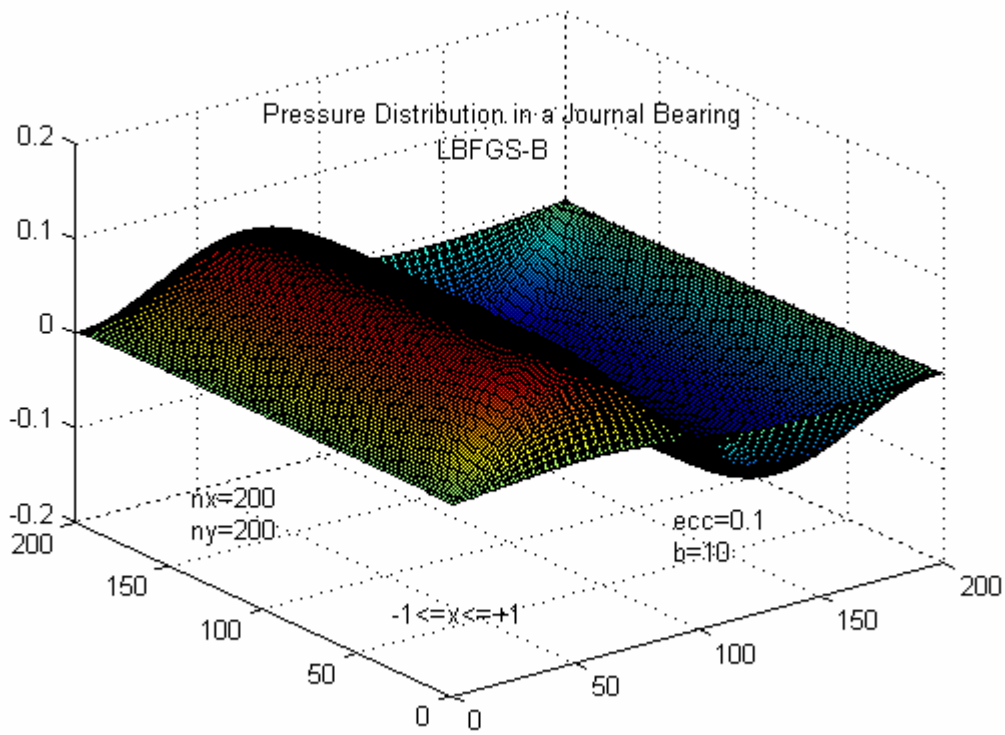

Fig. 2.1. Pressure Distribution ina Journal Bearing. $-1 \le x \le +1$

Experiment Nr. 2: $10^{-6} \le x \le 1$

```
Machine precision = 2.220D-16
 N =       40000    M =           5
 The initial X is infeasible.  Restart with its projection.

At X0     20000 variables are exactly at the bounds
At iterate    0    f=  2.87025D+01    |proj g|=  3.30830D-01
At iterate    1    f=  2.16677D+01    |proj g|=  1.19752D-01
At iterate    2    f=  2.00506D+01    |proj g|=  1.33393D-01
```

```
At iterate    3    f=  1.89650D+01    |proj g|=  1.40073D-01
At iterate    4    f=  1.79496D+01    |proj g|=  1.12631D-01
At iterate    5    f=  1.67440D+01    |proj g|=  9.20318D-02
At iterate    6    f=  1.59359D+01    |proj g|=  9.10444D-02
At iterate    7    f=  1.54816D+01    |proj g|=  7.75643D-02
At iterate    8    f=  1.48720D+01    |proj g|=  5.19654D-02
At iterate    9    f=  1.43393D+01    |proj g|=  9.07854D-02
At iterate   10    f=  1.37153D+01    |proj g|=  5.57832D-02
At iterate   11    f=  1.31736D+01    |proj g|=  1.04764D-01
At iterate   12    f=  1.26640D+01    |proj g|=  9.45456D-02
At iterate   13    f=  1.23025D+01    |proj g|=  7.04888D-02
At iterate   14    f=  1.17311D+01    |proj g|=  5.54567D-02
At iterate   15    f=  1.12638D+01    |proj g|=  1.26673D-01
At iterate   16    f=  1.07572D+01    |proj g|=  7.69293D-02
At iterate   17    f=  1.03425D+01    |proj g|=  5.86258D-02
At iterate   18    f=  9.74770D+00    |proj g|=  5.64800D-02
At iterate   19    f=  9.47532D+00    |proj g|=  2.16729D-01
At iterate   20    f=  9.02413D+00    |proj g|=  5.89166D-02
At iterate   21    f=  8.74062D+00    |proj g|=  6.80307D-02
….............
At iterate 2409    f= -1.80570D-01    |proj g|=  2.10845D-05
At iterate 2410    f= -1.80571D-01    |proj g|=  5.52482D-05
At iterate 2411    f= -1.80572D-01    |proj g|=  1.98768D-05
At iterate 2412    f= -1.80572D-01    |proj g|=  7.75128D-05
At iterate 2413    f= -1.80573D-01    |proj g|=  3.17516D-05
At iterate 2414    f= -1.80573D-01    |proj g|=  9.03660D-05
At iterate 2415    f= -1.80574D-01    |proj g|=  1.35152D-05
At iterate 2416    f= -1.80574D-01    |proj g|=  3.41623D-05
At iterate 2417    f= -1.80574D-01    |proj g|=  2.68234D-05
At iterate 2418    f= -1.80575D-01    |proj g|=  4.11197D-05
At iterate 2419    f= -1.80576D-01    |proj g|=  7.44779D-06

           •  * *
Tit   = total number of iterations
Tnf   = total number of function evaluations
Tnint = total number of segments explored during Cauchy searches
Skip  = number of BFGS updates skipped
Nact  = number of active bounds at final generalized Cauchy point
Projg = norm of the final projected gradient
F     = final function value
           * * *

   N   Tit  Tnf  Tnint  Skip  Nact     Projg        F
40000 2419 2429  25995     0 12862   7.448D-06  -1.806D-01
  F = -1.805755151835819E-001

CONVERGENCE: NORM OF PROJECTED GRADIENT <= PGTOL

 Cauchy                time 5.330E+01 seconds.
 Subspace minimization time 9.517E+01 seconds.
 Line search           time 8.091E+01 seconds.

 Total User time 2.621E+02 seconds.
```

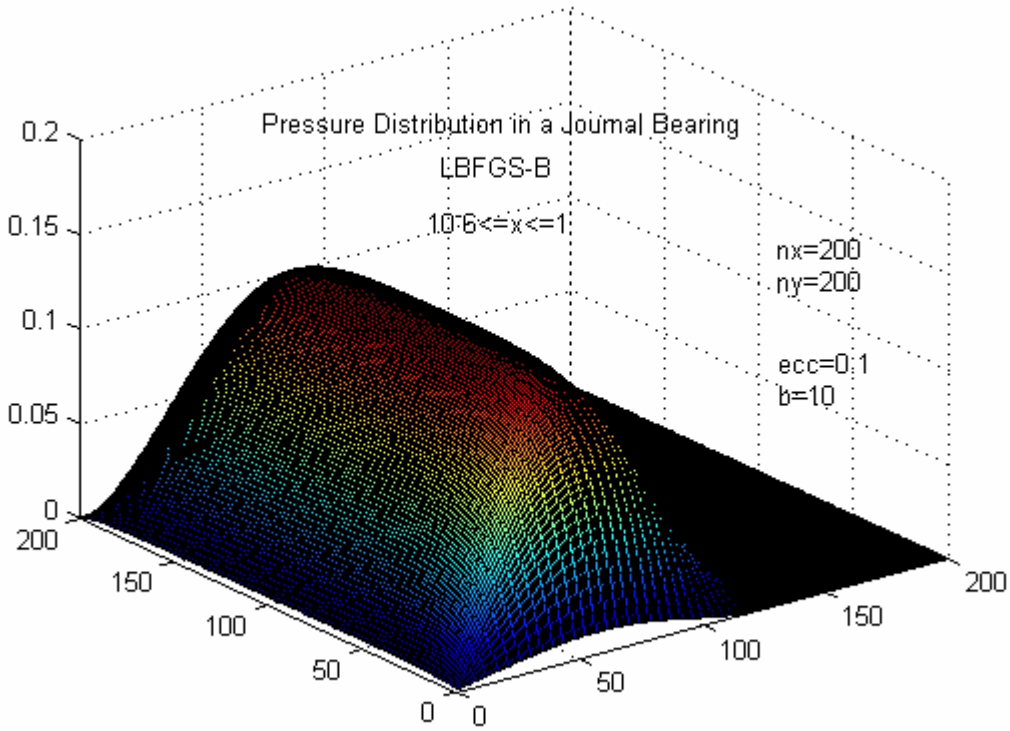

Fig. 2.2. Pressure Distribution ina Journal Bearing. $10^{-6} \le x \le 1$

Experiment Nr. 3: $-1 \le x \le 10^{-6}$

```
Machine precision = 2.220D-16
 N =       40000    M =           5
 The initial X is infeasible.  Restart with its projection.

At X0     20000 variables are exactly at the bounds
At iterate    0    f= -3.97933D-06    |proj g|=  3.11032D-04
At iterate    1    f= -9.73192D-04    |proj g|=  3.10060D-04
At iterate    2    f= -6.24320D-02    |proj g|=  3.15244D-02
At iterate    3    f= -9.13205D-02    |proj g|=  1.45127D-02
At iterate    4    f= -1.05779D-01    |proj g|=  9.46613D-03
At iterate    5    f= -1.10980D-01    |proj g|=  6.21533D-03
At iterate    6    f= -1.14641D-01    |proj g|=  4.60089D-03
At iterate    7    f= -1.17137D-01    |proj g|=  4.73985D-03
At iterate    8    f= -1.22605D-01    |proj g|=  4.51284D-03
At iterate    9    f= -1.24835D-01    |proj g|=  1.05051D-02
At iterate   10    f= -1.27961D-01    |proj g|=  4.18540D-03
At iterate   11    f= -1.30008D-01    |proj g|=  3.99618D-03
At iterate   12    f= -1.31304D-01    |proj g|=  3.65453D-03
At iterate   13    f= -1.33633D-01    |proj g|=  5.75883D-03
At iterate   14    f= -1.35576D-01    |proj g|=  1.13337D-02
At iterate   15    f= -1.37485D-01    |proj g|=  3.14584D-03
At iterate   16    f= -1.39455D-01    |proj g|=  3.36157D-03
At iterate   17    f= -1.40905D-01    |proj g|=  7.34938D-03
At iterate   18    f= -1.42100D-01    |proj g|=  1.67447D-02
At iterate   19    f= -1.43867D-01    |proj g|=  2.71058D-03
At iterate   20    f= -1.44721D-01    |proj g|=  4.27122D-03
At iterate   21    f= -1.46054D-01    |proj g|=  6.95359D-03
At iterate   22    f= -1.46675D-01    |proj g|=  3.60654D-03
At iterate   23    f= -1.47223D-01    |proj g|=  2.13190D-03
At iterate   24    f= -1.48858D-01    |proj g|=  3.71210D-03
At iterate   25    f= -1.49042D-01    |proj g|=  1.46912D-02
At iterate   26    f= -1.49830D-01    |proj g|=  2.70297D-03
At iterate   27    f= -1.50788D-01    |proj g|=  1.76059D-03
```

```
At iterate   28    f= -1.51772D-01    |proj g|=  2.63119D-03
At iterate   29    f= -1.52553D-01    |proj g|=  2.14523D-02
At iterate   30    f= -1.53614D-01    |proj g|=  2.44727D-03
At iterate   31    f= -1.53856D-01    |proj g|=  1.60108D-03
At iterate   32    f= -1.55001D-01    |proj g|=  2.43294D-03
….........
At iterate  364    f= -1.80598D-01    |proj g|=  1.80598D-05
At iterate  365    f= -1.80598D-01    |proj g|=  4.58971D-05
At iterate  366    f= -1.80598D-01    |proj g|=  1.66346D-05
At iterate  367    f= -1.80598D-01    |proj g|=  5.11086D-05
At iterate  368    f= -1.80599D-01    |proj g|=  6.05280D-05
At iterate  369    f= -1.80599D-01    |proj g|=  1.16807D-04
At iterate  370    f= -1.80599D-01    |proj g|=  6.12205D-05
At iterate  371    f= -1.80599D-01    |proj g|=  1.88634D-05
At iterate  372    f= -1.80599D-01    |proj g|=  1.24717D-05
At iterate  373    f= -1.80599D-01    |proj g|=  2.19302D-05
At iterate  374    f= -1.80599D-01    |proj g|=  5.60128D-05
At iterate  375    f= -1.80599D-01    |proj g|=  1.55732D-05
At iterate  376    f= -1.80599D-01    |proj g|=  2.74537D-05
At iterate  377    f= -1.80599D-01    |proj g|=  7.20121D-06

           •  * *
Tit   = total number of iterations
Tnf   = total number of function evaluations
Tnint = total number of segments explored during Cauchy searches
Skip  = number of BFGS updates skipped
Nact  = number of active bounds at final generalized Cauchy point
Projg = norm of the final projected gradient
F     = final function value
           * * *

   N   Tit  Tnf  Tnint  Skip  Nact     Projg        F
40000  377  391    796     0 12904   7.201D-06  -1.806D-01
  F = -1.805987908176998E-001

CONVERGENCE: NORM OF PROJECTED GRADIENT <= PGTOL

 Cauchy                time 6.720E+00 seconds.
 Subspace minimization time 1.403E+01 seconds.
 Line search           time 1.167E+01 seconds.

 Total User time 3.839E+01 seconds.
```

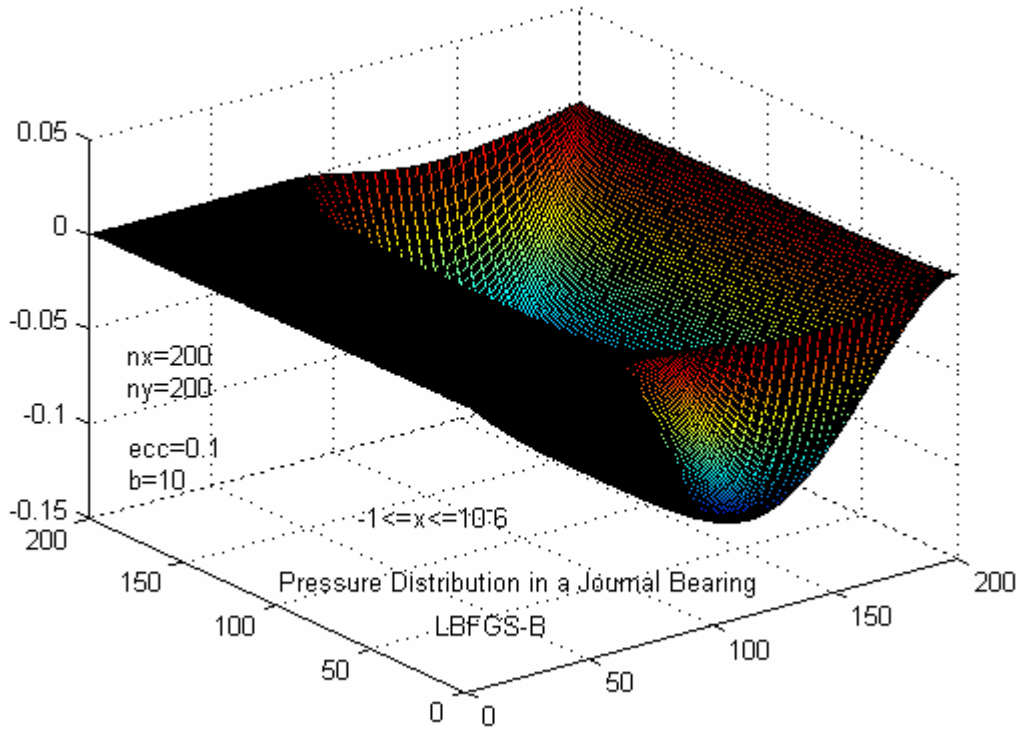

Fig. 2.3. Pressure Distribution ina Journal Bearing. $-1 \le x \le 10^{-6}$

3. Optimal Desing with Composite Materials

Experiment Nr. 1: $-1 \le x \le 0$

```
Machine precision = 2.220D-16
 N =       40000    M =           5

At X0         0 variables are exactly at the bounds
At iterate    0    f=  4.82823D-02    |proj g|=  9.82649D-03
At iterate    1    f=  4.66238D-02    |proj g|=  4.88456D-03
At iterate    2    f=  4.56882D-02    |proj g|=  4.90187D-03
At iterate    3    f=  4.39773D-02    |proj g|=  5.52349D-03
At iterate    4    f=  4.32905D-02    |proj g|=  3.13796D-03
At iterate    5    f=  4.22220D-02    |proj g|=  4.63934D-03
At iterate    6    f=  4.13522D-02    |proj g|=  3.82642D-03
At iterate    7    f=  3.99627D-02    |proj g|=  4.23901D-03
At iterate    8    f=  3.92792D-02    |proj g|=  3.13650D-03
At iterate    9    f=  3.81062D-02    |proj g|=  2.99023D-03
At iterate   10    f=  3.72445D-02    |proj g|=  3.01842D-03
At iterate   11    f=  3.61042D-02    |proj g|=  2.81188D-03
At iterate   12    f=  3.48983D-02    |proj g|=  4.91329D-03
At iterate   13    f=  3.38869D-02    |proj g|=  2.87298D-03
At iterate   14    f=  3.34806D-02    |proj g|=  2.71800D-03
At iterate   15    f=  3.24715D-02    |proj g|=  2.73637D-03
At iterate   16    f=  3.11311D-02    |proj g|=  5.11471D-03
At iterate   17    f=  3.00815D-02    |proj g|=  3.16049D-03
At iterate   18    f=  2.92143D-02    |proj g|=  3.14879D-03
At iterate   19    f=  2.83559D-02    |proj g|=  3.18600D-03
At iterate   20    f=  2.73905D-02    |proj g|=  2.90856D-03
At iterate   21    f=  2.69292D-02    |proj g|=  2.66652D-03
At iterate   22    f=  2.64199D-02    |proj g|=  2.43973D-03
At iterate   23    f=  2.51593D-02    |proj g|=  6.96560D-03
At iterate   24    f=  2.47170D-02    |proj g|=  3.29839D-03
```

```
At iterate   25    f=  2.41365D-02    |proj g|=  2.68768D-03
At iterate   26    f=  2.33309D-02    |proj g|=  3.28573D-03
…........
At iterate  639    f= -1.13799D-02    |proj g|=  6.07895D-05
At iterate  640    f= -1.13799D-02    |proj g|=  4.83012D-05
At iterate  641    f= -1.13799D-02    |proj g|=  1.66293D-05
At iterate  642    f= -1.13799D-02    |proj g|=  1.03480D-05
At iterate  643    f= -1.13799D-02    |proj g|=  1.83425D-05
At iterate  644    f= -1.13799D-02    |proj g|=  5.23743D-05
At iterate  645    f= -1.13800D-02    |proj g|=  1.89723D-05
At iterate  646    f= -1.13800D-02    |proj g|=  8.66926D-06

           •  * *
Tit   = total number of iterations
Tnf   = total number of function evaluations
Tnint = total number of segments explored during Cauchy searches
Skip  = number of BFGS updates skipped
Nact  = number of active bounds at final generalized Cauchy point
Projg = norm of the final projected gradient
F     = final function value
           * * *

   N   Tit   Tnf  Tnint  Skip  Nact     Projg        F
40000  646   649    744     0     0   8.669D-06  -1.138D-02
  F = -1.137996459564602E-002

CONVERGENCE: NORM OF PROJECTED GRADIENT <= PGTOL

 Cauchy                time 1.486E+01 seconds.
 Subspace minimization time 2.666E+01 seconds.
 Line search           time 2.790E+01 seconds.

 Total User time 7.943E+01 seconds.
```

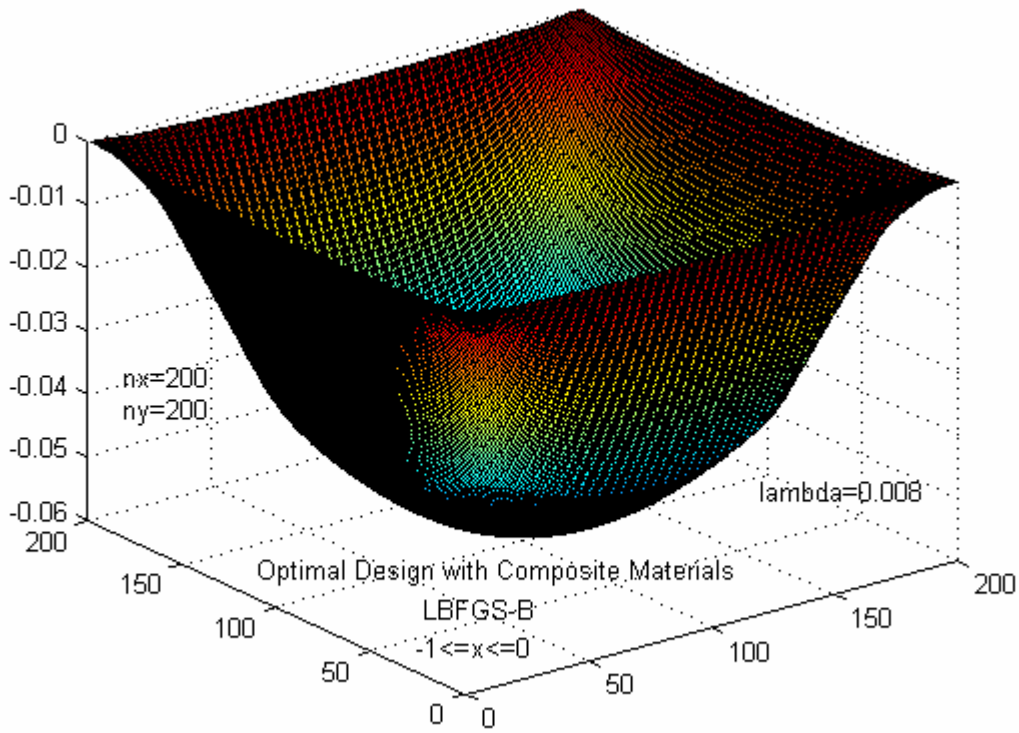

Fig. 3.1. Optimal Design with Composite Materials. $-1 \le x \le 0$

Experiment Nr. 2: $-0.02 \le x \le 0$

```
Machine precision = 2.220D-16
 N =       40000    M =           5
 The initial X is infeasible.  Restart with its projection.

At X0     20736 variables are exactly at the bounds
At iterate    0    f= -4.88812D-03    |proj g|=  2.69795D-03
At iterate    1    f= -5.08789D-03    |proj g|=  2.37948D-03
At iterate    2    f= -5.24016D-03    |proj g|=  1.48651D-03
At iterate    3    f= -5.41576D-03    |proj g|=  1.59695D-03
At iterate    4    f= -5.58032D-03    |proj g|=  2.60112D-03
At iterate    5    f= -5.72189D-03    |proj g|=  2.53849D-03
At iterate    6    f= -5.86335D-03    |proj g|=  2.64678D-03
At iterate    7    f= -5.99509D-03    |proj g|=  2.77682D-03
At iterate    8    f= -6.12105D-03    |proj g|=  1.71936D-03
At iterate    9    f= -6.22718D-03    |proj g|=  1.77257D-03
At iterate   10    f= -6.32450D-03    |proj g|=  1.05248D-03
At iterate   11    f= -6.42948D-03    |proj g|=  1.65236D-03
At iterate   12    f= -6.51209D-03    |proj g|=  2.46103D-03
At iterate   13    f= -6.59822D-03    |proj g|=  1.08416D-03
At iterate   14    f= -6.67922D-03    |proj g|=  2.50626D-03
At iterate   15    f= -6.75374D-03    |proj g|=  1.12242D-03
At iterate   16    f= -6.83220D-03    |proj g|=  3.79547D-03
….....................
At iterate  115    f= -8.17826D-03    |proj g|=  6.53614D-05
At iterate  116    f= -8.17841D-03    |proj g|=  2.19371D-05
At iterate  117    f= -8.17849D-03    |proj g|=  1.58066D-05
At iterate  118    f= -8.17887D-03    |proj g|=  1.00071D-04
At iterate  119    f= -8.17930D-03    |proj g|=  1.97769D-05
At iterate  120    f= -8.17942D-03    |proj g|=  1.71485D-05
At iterate  121    f= -8.17952D-03    |proj g|=  1.93031D-05
At iterate  122    f= -8.17955D-03    |proj g|=  1.18019D-05
At iterate  123    f= -8.17999D-03    |proj g|=  2.41765D-05
At iterate  124    f= -8.18006D-03    |proj g|=  9.83187D-06

           •  * *
Tit   = total number of iterations
Tnf   = total number of function evaluations
Tnint = total number of segments explored during Cauchy searches
Skip  = number of BFGS updates skipped
Nact  = number of active bounds at final generalized Cauchy point
Projg = norm of the final projected gradient
F     = final function value
           * * *

   N   Tit  Tnf  Tnint  Skip  Nact     Projg        F
40000  124  127    734     0  7420   9.832D-06  -8.180D-03
  F = -8.180057940062857E-003

CONVERGENCE: NORM OF PROJECTED GRADIENT <= PGTOL

 Cauchy                time 3.440E+00 seconds.
 Subspace minimization time 3.620E+00 seconds.
 Line search           time 5.040E+00 seconds.

 Total User time 1.378E+01 seconds.
```

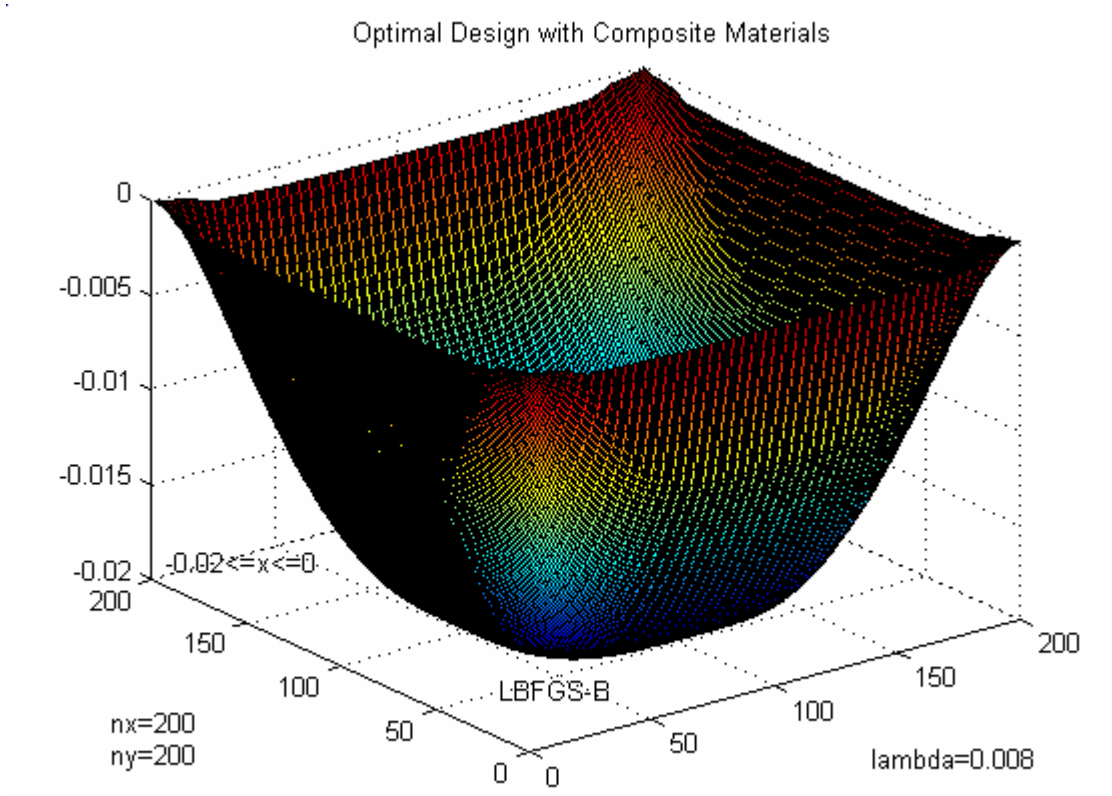

Fig. 3.2. Optimal Design with Composite Materials. $-0.02 \le x \le 0$

4. Inhomogeneous superconductors. 1-D Ginzburg-Landau Problem

Experiment Nr. 1: $0 \le x \le 10^8$

```
Machine precision = 2.220D-16
 N =        1000    M =           5

At X0         0 variables are exactly at the bounds
At iterate    0    f= -1.6618577793520E-04  |proj g|=  1.1096874798623E-04
At iterate    1    f= -1.66196D-04    |proj g|=  1.79319D-02
At iterate    2    f= -1.66204D-04    |proj g|=  2.45482D-02
At iterate    3    f= -1.66210D-04    |proj g|=  1.66307D-02
At iterate    4    f= -1.66219D-04    |proj g|=  1.57647D-02
At iterate    5    f= -1.66226D-04    |proj g|=  1.34935D-02
At iterate    6    f= -1.66233D-04    |proj g|=  2.86339D-02
At iterate    7    f= -1.66244D-04    |proj g|=  1.26278D-02
At iterate    8    f= -1.66250D-04    |proj g|=  1.25049D-02
At iterate    9    f= -1.66258D-04    |proj g|=  1.20620D-02
At iterate   10    f= -1.66266D-04    |proj g|=  1.76618D-02
At iterate   11    f= -1.66276D-04    |proj g|=  1.19937D-02
At iterate   12    f= -1.66283D-04    |proj g|=  1.13946D-02
At iterate   13    f= -1.66291D-04    |proj g|=  1.07480D-02
At iterate   14    f= -1.66297D-04    |proj g|=  1.63524D-02
At iterate   15    f= -1.66306D-04    |proj g|=  1.09565D-02
….............
At iterate34886    f= -8.45619D+03    |proj g|=  6.61242D-04
At iterate34887    f= -8.45619D+03    |proj g|=  9.20667D-04
At iterate34888    f= -8.45619D+03    |proj g|=  4.90336D-04
At iterate34889    f= -8.45619D+03    |proj g|=  5.64717D-04
At iterate34890    f= -8.45619D+03    |proj g|=  6.24048D-04
At iterate34891    f= -8.45619D+03    |proj g|=  1.67050D-03
```

```
At iterate34892    f= -8.45619D+03    |proj g|=  6.66551D-04
At iterate34893    f= -8.45619D+03    |proj g|=  6.08047D-04
At iterate34894    f= -8.45619D+03    |proj g|=  7.99222D-04
At iterate34895    f= -8.45619D+03    |proj g|=  2.33060D-03

           •  * *
Tit   = total number of iterations
Tnf   = total number of function evaluations
Tnint = total number of segments explored during Cauchy searches
Skip  = number of BFGS updates skipped
Nact  = number of active bounds at final generalized Cauchy point
Projg = norm of the final projected gradient
F     = final function value
           * * *

   N   Tit   Tnf   Tnint  Skip  Nact     Projg        F
 1000 34895 36076  34895     0     0   2.331D-03  -8.456D+03
  F =   -8456.191964914546000

CONVERGENCE: REL_REDUCTION_OF_F <= FACTR*EPSMCH

 Cauchy                time 1.486E+01 seconds.
 Subspace minimization time 2.416E+01 seconds.
 Line search           time 1.165E+01 seconds.

 Total User time 6.300E+01 seconds.
```

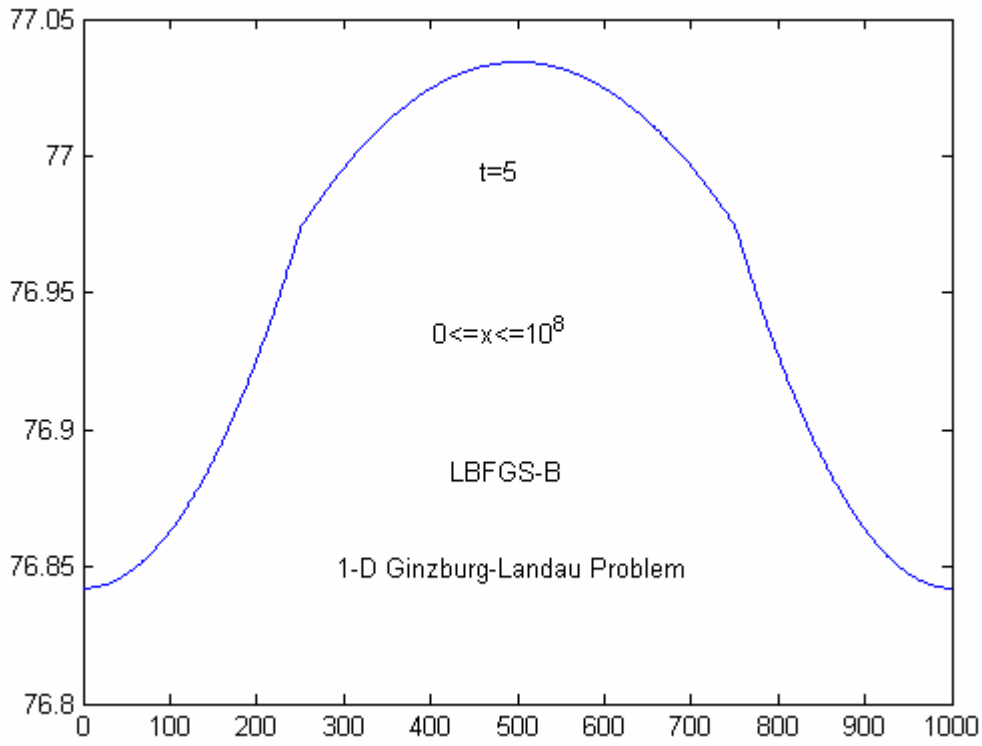

Fig. 4.1. 1-D Ginzburg-Landau Problem. $0 \le x \le 10^8$

Experiment Nr. 2: $0 \le x \le 10$

```
Machine precision = 2.220D-16
 N =        1000    M =           5

At X0         0 variables are exactly at the bounds
At iterate    0    f= -1.6618577793520E-04    |proj g|=  1.1096874798623E-
04
At iterate    1    f= -1.66196D-04    |proj g|=  1.79319D-02
At iterate    2    f= -1.66204D-04    |proj g|=  2.45482D-02
At iterate    3    f= -1.66210D-04    |proj g|=  1.66307D-02
At iterate    4    f= -1.66219D-04    |proj g|=  1.57647D-02
At iterate    5    f= -1.66226D-04    |proj g|=  1.34935D-02
At iterate    6    f= -1.66233D-04    |proj g|=  2.86339D-02
At iterate    7    f= -1.66244D-04    |proj g|=  1.26278D-02
At iterate    8    f= -1.66250D-04    |proj g|=  1.25049D-02
At iterate    9    f= -1.66258D-04    |proj g|=  1.20620D-02
At iterate   10    f= -1.66266D-04    |proj g|=  1.76618D-02
At iterate   11    f= -1.66276D-04    |proj g|=  1.19937D-02
At iterate   12    f= -1.66283D-04    |proj g|=  1.13946D-02
…............
At iterate10270    f= -2.82708D+02    |proj g|=  7.49079D-04
At iterate10271    f= -2.82708D+02    |proj g|=  8.64891D-04
At iterate10272    f= -2.82708D+02    |proj g|=  1.17714D-03
At iterate10273    f= -2.82708D+02    |proj g|=  7.93226D-04
At iterate10274    f= -2.82708D+02    |proj g|=  2.56088D-03
At iterate10275    f= -2.82708D+02    |proj g|=  6.33951D-04
At iterate10276    f= -2.82708D+02    |proj g|=  7.06845D-04
At iterate10277    f= -2.82708D+02    |proj g|=  1.20232D-03
At iterate10278    f= -2.82708D+02    |proj g|=  3.52335D-03

           *  * *
Tit   = total number of iterations
Tnf   = total number of function evaluations
Tnint = total number of segments explored during Cauchy searches
Skip  = number of BFGS updates skipped
Nact  = number of active bounds at final generalized Cauchy point
Projg = norm of the final projected gradient
F     = final function value
           * * *


   N   Tit   Tnf   Tnint  Skip  Nact     Projg        F
 1000 10278 10643  11438     0   391   3.523D-03  -2.827D+02
  F =    -282.707702750158900

CONVERGENCE: REL_REDUCTION_OF_F <= FACTR*EPSMCH

 Cauchy                time 4.300E+00 seconds.
 Subspace minimization time 6.770E+00 seconds.
 Line search           time 3.720E+00 seconds.

 Total User time 1.747E+01 seconds.
```

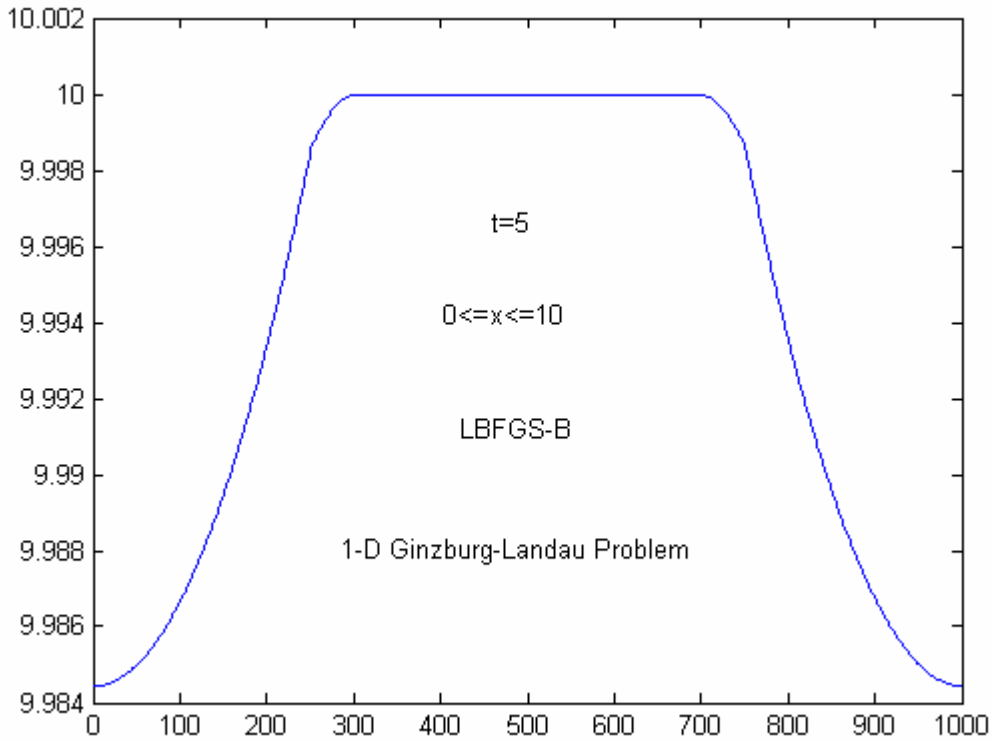

Fig. 4.2. 1-D Ginzburg-Landau Problem. $0 \le x \le 10$

5. Steady State Combustion

Experiment Nr. 1: $0 \le x \le 1$

```
Machine precision = 2.220D-16
 N =       40000    M =           5

At X0         0 variables are exactly at the bounds
At iterate    0    f= -4.26758D+00    |proj g|=  5.87788D-02
At iterate    1    f= -4.40500D+00    |proj g|=  9.50250D-02
At iterate    2    f= -4.68262D+00    |proj g|=  6.60953D-02
At iterate    3    f= -4.74680D+00    |proj g|=  2.92183D-02
At iterate    4    f= -4.80580D+00    |proj g|=  2.32778D-02
At iterate    5    f= -4.91010D+00    |proj g|=  3.03746D-02
At iterate    6    f= -4.94694D+00    |proj g|=  2.85772D-02
At iterate    7    f= -4.97365D+00    |proj g|=  1.53144D-02
At iterate    8    f= -5.00602D+00    |proj g|=  1.37152D-02
At iterate    9    f= -5.03370D+00    |proj g|=  1.05649D-02
At iterate   10    f= -5.11502D+00    |proj g|=  2.48048D-02
At iterate   11    f= -5.12824D+00    |proj g|=  1.43081D-02
At iterate   12    f= -5.14838D+00    |proj g|=  1.25899D-02
At iterate   13    f= -5.16890D+00    |proj g|=  2.35558D-02
At iterate   14    f= -5.18856D+00    |proj g|=  8.61632D-03
At iterate   15    f= -5.21288D+00    |proj g|=  9.30991D-03
At iterate   16    f= -5.23252D+00    |proj g|=  5.50135D-03
At iterate   17    f= -5.27064D+00    |proj g|=  1.28027D-02
At iterate   18    f= -5.27861D+00    |proj g|=  1.18342D-02
….........
At iterate  344    f= -5.61144D+00    |proj g|=  2.97090D-05
At iterate  345    f= -5.61144D+00    |proj g|=  1.54610D-05
At iterate  346    f= -5.61144D+00    |proj g|=  1.71500D-05
At iterate  347    f= -5.61144D+00    |proj g|=  2.93417D-05
At iterate  348    f= -5.61144D+00    |proj g|=  2.17386D-05
At iterate  349    f= -5.61144D+00    |proj g|=  1.98620D-05
```

```
At iterate  350    f= -5.61144D+00    |proj g|=  6.01255D-05
At iterate  351    f= -5.61144D+00    |proj g|=  1.43655D-05
At iterate  352    f= -5.61144D+00    |proj g|=  1.30056D-05
At iterate  353    f= -5.61145D+00    |proj g|=  1.28157D-05
At iterate  354    f= -5.61145D+00    |proj g|=  5.22733D-05
At iterate  355    f= -5.61145D+00    |proj g|=  2.18559D-05
At iterate  356    f= -5.61145D+00    |proj g|=  1.05479D-05
At iterate  357    f= -5.61145D+00    |proj g|=  1.52356D-05
At iterate  358    f= -5.61145D+00    |proj g|=  2.10509D-05
At iterate  359    f= -5.61145D+00    |proj g|=  3.21010D-05
At iterate  360    f= -5.61145D+00    |proj g|=  9.92642D-06

           •  * *
Tit   = total number of iterations
Tnf   = total number of function evaluations
Tnint = total number of segments explored during Cauchy searches
Skip  = number of BFGS updates skipped
Nact  = number of active bounds at final generalized Cauchy point
Projg = norm of the final projected gradient
F     = final function value
           * * *

   N   Tit   Tnf  Tnint  Skip  Nact     Projg        F
40000  360   372    424     0     0   9.926D-06  -5.611D+00
  F =      -5.611445877814369

CONVERGENCE: NORM OF PROJECTED GRADIENT <= PGTOL

 Cauchy                time 8.520E+00 seconds.
 Subspace minimization time 1.474E+01 seconds.
 Line search           time 2.562E+01 seconds.

 Total User time 5.482E+01 seconds.
```

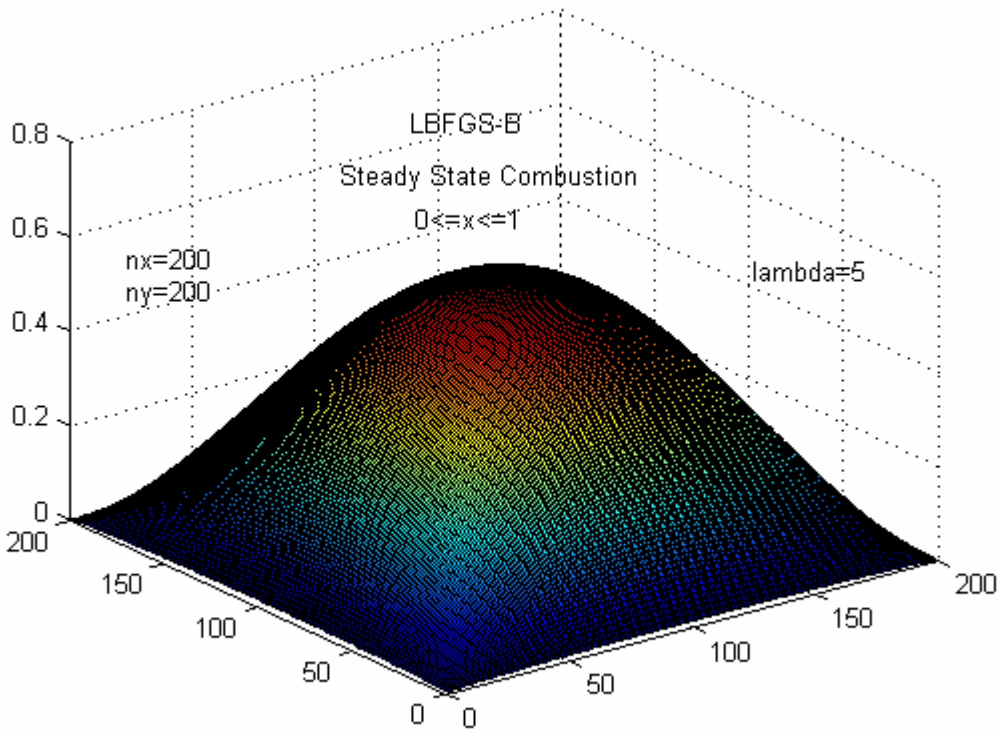

Fig. 5.1. Steady State Combustion. $0 \le x \le 1$

Experiment Nr. 2: $0 \le x \le 0.2$

```
Machine precision = 2.220D-16
 N =       40000    M =           5
 The initial X is infeasible.  Restart with its projection.

At X0     31684 variables are exactly at the bounds
At iterate    0    f= -3.83389D+00    |proj g|=  5.87788D-02
At iterate    1    f= -4.01601D+00    |proj g|=  9.50250D-02
At iterate    2    f= -4.27550D+00    |proj g|=  8.50861D-02
At iterate    3    f= -4.34251D+00    |proj g|=  2.41235D-02
At iterate    4    f= -4.40558D+00    |proj g|=  2.70233D-02
At iterate    5    f= -4.51818D+00    |proj g|=  5.65976D-02
At iterate    6    f= -4.56518D+00    |proj g|=  3.33560D-02
At iterate    7    f= -4.59443D+00    |proj g|=  1.30425D-02
At iterate    8    f= -4.64212D+00    |proj g|=  1.81070D-02
At iterate    9    f= -4.68917D+00    |proj g|=  1.38621D-02
At iterate   10    f= -4.75068D+00    |proj g|=  2.29109D-02
At iterate   11    f= -4.80623D+00    |proj g|=  1.32098D-02
At iterate   12    f= -4.86801D+00    |proj g|=  3.11987D-02
At iterate   13    f= -4.95068D+00    |proj g|=  1.04294D-02
At iterate   14    f= -4.96128D+00    |proj g|=  1.29259D-02
….............
At iterate  178    f= -5.44131D+00    |proj g|=  2.95050D-05
At iterate  179    f= -5.44131D+00    |proj g|=  1.34321D-05
At iterate  180    f= -5.44131D+00    |proj g|=  1.13158D-05
At iterate  181    f= -5.44131D+00    |proj g|=  6.05288D-05
At iterate  182    f= -5.44131D+00    |proj g|=  2.11816D-05
At iterate  183    f= -5.44131D+00    |proj g|=  1.04274D-05
At iterate  184    f= -5.44131D+00    |proj g|=  1.24765D-05
At iterate  185    f= -5.44131D+00    |proj g|=  7.77967D-06

           •  * *
Tit   = total number of iterations
Tnf   = total number of function evaluations
Tnint = total number of segments explored during Cauchy searches
Skip  = number of BFGS updates skipped
Nact  = number of active bounds at final generalized Cauchy point
Projg = norm of the final projected gradient
F     = final function value
           * * *

   N   Tit  Tnf  Tnint  Skip  Nact     Projg        F
40000  185  196   1012     0  7960   7.780D-06  -5.441D+00
  F =      -5.441311513692021

CONVERGENCE: NORM OF PROJECTED GRADIENT <= PGTOL

 Cauchy                time 3.330E+00 seconds.
 Subspace minimization time 6.290E+00 seconds.
 Line search           time 1.504E+01 seconds.

 Total User time 2.768E+01 seconds.
```

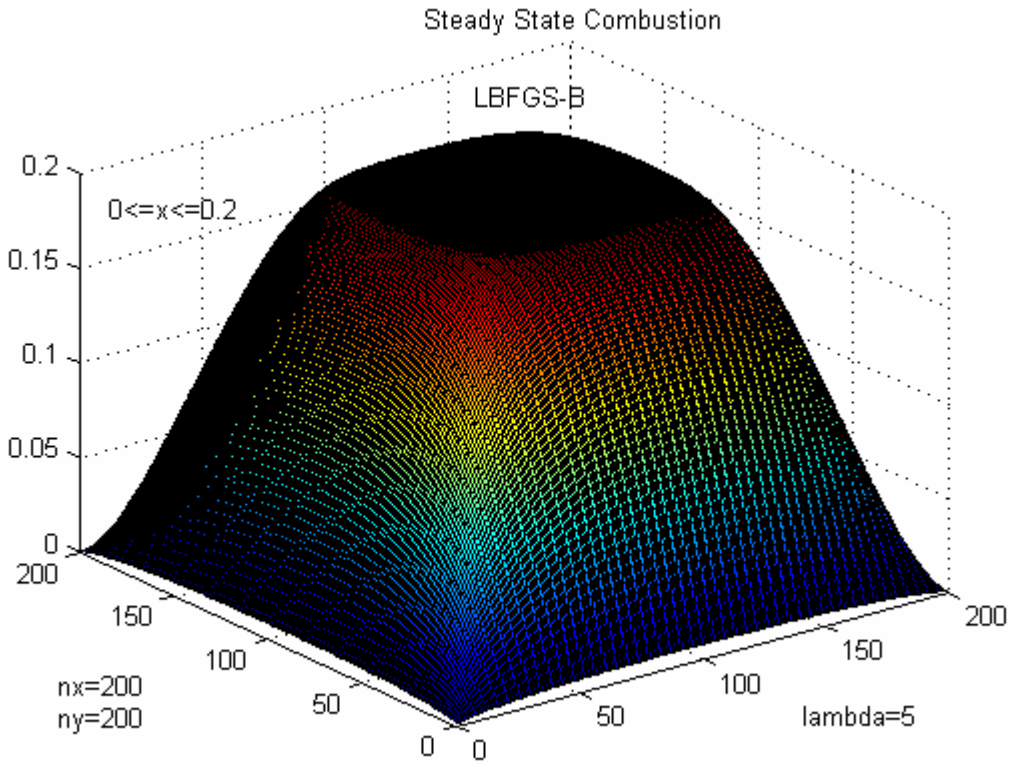

Fig. 5.2. Steady State Combustion. $0 \le x \le 0.2$

Experiment Nr. 3: $0 \le x \le 0.1$

```
Machine precision = 2.220D-16
 N =       40000    M =           5
 The initial X is infeasible.  Restart with its projection.

At X0     38416 variables are exactly at the bounds
At iterate    0    f= -3.78610D+00    |proj g|=  5.87788D-02
At iterate    1    f= -4.09758D+00    |proj g|=  7.57875D-02
At iterate    2    f= -4.46457D+00    |proj g|=  4.66471D-02
At iterate    3    f= -4.60982D+00    |proj g|=  4.46340D-02
At iterate    4    f= -4.70843D+00    |proj g|=  6.07989D-02
At iterate    5    f= -4.81890D+00    |proj g|=  3.45638D-02
At iterate    6    f= -4.89484D+00    |proj g|=  6.20360D-02
At iterate    7    f= -4.95995D+00    |proj g|=  4.00912D-02
At iterate    8    f= -4.99446D+00    |proj g|=  1.78662D-02
At iterate    9    f= -5.04156D+00    |proj g|=  2.01486D-02
At iterate   10    f= -5.06078D+00    |proj g|=  5.95964D-02
At iterate   11    f= -5.08468D+00    |proj g|=  2.52394D-02
At iterate   12    f= -5.10119D+00    |proj g|=  2.00788D-02
At iterate   13    f= -5.11335D+00    |proj g|=  1.77597D-02
….............
At iterate  118    f= -5.28523D+00    |proj g|=  4.18481D-05
At iterate  119    f= -5.28524D+00    |proj g|=  1.33515D-04
At iterate  120    f= -5.28524D+00    |proj g|=  1.11211D-04
At iterate  121    f= -5.28524D+00    |proj g|=  3.83484D-05
At iterate  122    f= -5.28524D+00    |proj g|=  2.47000D-05
At iterate  123    f= -5.28524D+00    |proj g|=  4.59851D-05
At iterate  124    f= -5.28524D+00    |proj g|=  2.52612D-05
At iterate  125    f= -5.28524D+00    |proj g|=  6.08641D-05
At iterate  126    f= -5.28524D+00    |proj g|=  3.23468D-05
At iterate  127    f= -5.28524D+00    |proj g|=  2.49857D-05
At iterate  128    f= -5.28524D+00    |proj g|=  9.77874D-06

           •   * *
Tit   = total number of iterations
```

```
Tnf   = total number of function evaluations
Tnint = total number of segments explored during Cauchy searches
Skip  = number of BFGS updates skipped
Nact  = number of active bounds at final generalized Cauchy point
Projg = norm of the final projected gradient
F     = final function value
           * * *

   N   Tit   Tnf  Tnint  Skip  Nact     Projg        F
40000  128   130    909     0 14796   9.779D-06  -5.285D+00
  F =      -5.285237708934600

CONVERGENCE: NORM OF PROJECTED GRADIENT <= PGTOL

 Cauchy                time 2.260E+00 seconds.
 Subspace minimization time 3.680E+00 seconds.
 Line search           time 1.070E+01 seconds.

 Total User time 1.829E+01 seconds.
```

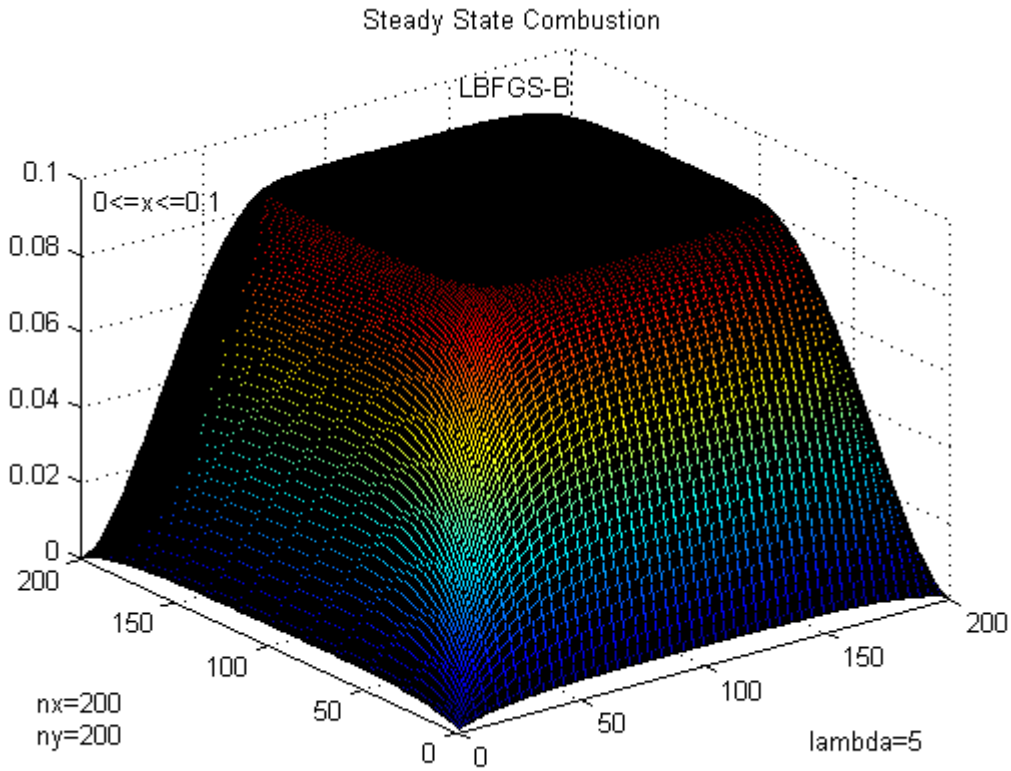

Fig. 5.3. Steady State Combustion. $0 \le x \le 0.1$

References

[1] **R. H. Byrd, P. Lu, J. Nocedal and C. Zhu,** "A limited memory algorithm for bound constrained optimization", SIAM J. Scientific Computing 16 (1995), no. 5, pp. 1190—1208.

[2] **C. Zhu, R.H. Byrd, P. Lu, J. Nocedal,** "L-BFGS-B: FORTRAN Subroutines for Large Scale Bound Constrained Optimization" Tech. Report, NAM-11, EECS Department, Northwestern University, 1994.

[3] **B.M. Averick, R.G. Carter, J.J. Moré, G-L Xue**, "The MINPACK-2 test problem collection". Preprint MCS-P153-0692, Mathematics and Computer Science Division, Argonne NationalLaboratory, 9700 South Cass Avenue, Argonne, Illinois, 60439, USA, June 1992.

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