Molecular Formation Problem

The Leonard- Jones Clusters (Molecular Conformation) Problem
21 Conjugate Gradient Algorithms

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In this work I present the results of 21 conjugate gradient algorithms for solving the Lennard-Jones cluster problem. This problem arises in the study of low-energy states of proteins and in the study of cluster statics, where $ndim = 3$, $natoms = 1000$.

All conjugate gradient algorithms are implemented in the same manner (CGALL.FOR) using the same stopping criteria:

$$\|g_k\|_\infty \le \varepsilon_g \quad \text{or} \quad |\alpha_k g_k^T d_k| \le \varepsilon_f |f(x_{k+1})|,$$

where $\varepsilon_f = 10^{-10}$ and $\varepsilon_g = 10^{-6}$.

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   CG with angle restart.   November 8, 2006

     1    CG-HS Algorithm:Lennard-Jones potential                Function
          Hestenes and Stiefel.  stoptest= 6

    n   iter   irs  fgcnt lscnt   time(c)        fxnew              gnorm
-------------------------------------------------------------------------------
 3000   2557     0   3171   608     24782 -.6631497390299E+04  .1267453136553E-01
-------------------------------------------------------------------------------
TOTAL   2557     0   3171   608    247.82 (seconds)    proc=    .00%

   CG with angle restart.   November 8, 2006

     2    CG-FR Algorithm:Lennard-Jones potential                Function
          Fletcher and Reeves.  stoptest= 6

    n   iter   irs  fgcnt lscnt   time(c)        fxnew              gnorm
-------------------------------------------------------------------------------
 3000   5501     0   6974  1473     54461 -.5401987751176E+04  .5550106770570E+03
-------------------------------------------------------------------------------
TOTAL   5501     0   6974  1473    544.61 (seconds)    proc=    .00%

   CG with angle restart.   November 8, 2006

     3    CG-PRP Algorithm:Lennard-Jones potential                Function
          Polak-Ribiere and Polyak.  stoptest= 6

    n   iter   irs  fgcnt lscnt   time(c)        fxnew              gnorm
-------------------------------------------------------------------------------
 3000   2008     0   2776   763     21644 -.6619382688012E+04  .3091295541058E-01
-------------------------------------------------------------------------------
TOTAL   2008     0   2776   763    216.44 (seconds)    proc=    .00%

   CG with angle restart.   November 8, 2006

     4    CG-PRP+ Algorithm:Lennard-Jones potential                Function
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          Polak-Ribiere and Polyak plus.  stoptest= 6

    n   iter   irs  fgcnt lscnt   time(c)        fxnew              gnorm
-------------------------------------------------------------------------------
 3000   2399     0   3282   877     25594 -.6608459148448E+04  .1497131284373E-01
-------------------------------------------------------------------------------
TOTAL   2399     0   3282   877    255.94 (seconds)    proc=    .00%

   CG with angle restart.   November 8, 2006

     5    CG-CD Algorithm:Lennard-Jones potential                Function
          Conjugate Descent - Fletcher. stoptest= 6

    n   iter   irs  fgcnt lscnt   time(c)        fxnew              gnorm
-------------------------------------------------------------------------------
 3000   4070    15   4641   570     36334 -.6639534084590E+04  .1892329169536E+01
-------------------------------------------------------------------------------
TOTAL   4070    15   4641   570    363.34 (seconds)    proc=    .37%

   CG with angle restart.   November 8, 2006

     6    CG-LS Algorithm:Lennard-Jones potential                Function
          Liu and Storey.  stoptest= 6

    n   iter   irs  fgcnt lscnt   time(c)        fxnew              gnorm
-------------------------------------------------------------------------------
 3000   1540     0   2072   527     16162 -.6601686106922E+04  .2083038898103E-01
-------------------------------------------------------------------------------
TOTAL   1540     0   2072   527    161.62 (seconds)    proc=    .00%

   CG with angle restart.   November 8, 2006

     7    CG-DY Algorithm:Lennard-Jones potential                Function
          Dai and Yuan.  stoptest= 6

    n   iter   irs  fgcnt lscnt   time(c)        fxnew              gnorm
-------------------------------------------------------------------------------
 3000   5501     0   5516    15     43344 -.5322950720681E+04  .6022083737179E+03
-------------------------------------------------------------------------------
TOTAL   5501     0   5516    15    433.44 (seconds)    proc=    .00%

   CG with angle restart.   November 8, 2006

     8    CG-DL Algorithm:Lennard-Jones potential                Function
          Dai and Liao (t=1).  stoptest= 6

    n   iter   irs  fgcnt lscnt   time(c)        fxnew              gnorm
-------------------------------------------------------------------------------
 3000   1944     0   2366   416     18502 -.6642551795698E+04  .1651407170156E-01
-------------------------------------------------------------------------------
TOTAL   1944     0   2366   416    185.02 (seconds)    proc=    .00%

   CG with angle restart.   November 8, 2006

     9    CG-DL+ Algorithm:Lennard-Jones potential                Function
          Dai and Liao plus (t=1).  stoptest= 6

    n   iter   irs  fgcnt lscnt   time(c)        fxnew              gnorm
-------------------------------------------------------------------------------
 3000   1234     0   1508   271     11790 -.6603546674709E+04  .1589662020591E-01
-------------------------------------------------------------------------------
TOTAL   1234     0   1508   271    117.90 (seconds)    proc=    .00%

   CG with angle restart.   November 8, 2006

    10    CG-SDC Algorithm:Lennard-Jones potential                Function
          Andrei: beta=gtg/yts-delta*gtg*stg/(yts**2).  stoptest= 6

    n   iter   irs  fgcnt lscnt   time(c)        fxnew              gnorm
-------------------------------------------------------------------------------
 3000    934     1   1075   139      8417 -.6606489613292E+04  .1613187109870E-01
-------------------------------------------------------------------------------
TOTAL    934     1   1075   139     84.17 (seconds)    proc=    .11%

   CG with angle restart.   November 8, 2006

    11    CG-hDY Algorithm:Lennard-Jones potential                Function
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          Hybrid Dai and Yuan. max(c*DY,min(HS,DY)). stoptest= 6

    n   iter   irs  fgcnt lscnt   time(c)        fxnew              gnorm
-------------------------------------------------------------------------------
 3000   1778     0   2130   348     16661 -.6610244818980E+04  .2103146439446E-01
-------------------------------------------------------------------------------
TOTAL   1778     0   2130   348    166.61 (seconds)    proc=    .00%

   CG with angle restart.   November 8, 2006

    12    CG-hDYz Algorithm:Lennard-Jones potential                Function
          Hybrid Dai and Yuan. max(0,min(HS,DY)). stoptest= 6

    n   iter   irs  fgcnt lscnt   time(c)        fxnew              gnorm
-------------------------------------------------------------------------------
 3000    773     0    891   116      6977 -.6593170961895E+04  .1743331188875E-01
-------------------------------------------------------------------------------
TOTAL    773     0    891   116     69.77 (seconds)    proc=    .00%

   CG with angle restart.   November 8, 2006

    13    CG-GN Algorithm:Lennard-Jones potential                 Function
          Gilbert and Nocedal.  stoptest= 6

    n   iter   irs  fgcnt lscnt   time(c)        fxnew              gnorm
-------------------------------------------------------------------------------
 3000   2675     0   3645   963     28425 -.6639744036805E+04  .1595261008294E-01
-------------------------------------------------------------------------------
TOTAL   2675     0   3645   963    284.25 (seconds)    proc=    .00%

   CG with angle restart.   November 8, 2006

    14    CG-HuS Algorithm:Lennard-Jones potential                 Function
          Hu and Storey. max(0,min(PRP,FR)). stoptest= 6

    n   iter   irs  fgcnt lscnt   time(c)        fxnew              gnorm
-------------------------------------------------------------------------------
 3000   1224     0   1649   424     12864 -.6601108405756E+04  .1688851454275E-01
-------------------------------------------------------------------------------
TOTAL   1224     0   1649   424    128.64 (seconds)    proc=    .00%

   CG with angle restart.   November 8, 2006

    15    CG-TaS Algorithm:Lennard-Jones potential                 Function
          Touat-Ahmed and Storey. (PRP <= FR). stoptest= 6

    n   iter   irs  fgcnt lscnt   time(c)        fxnew              gnorm
-------------------------------------------------------------------------------
 3000   1590     0   2183   589     17023 -.6628820304737E+04  .1787149977166E-01
-------------------------------------------------------------------------------
TOTAL   1590     0   2183   589    170.23 (seconds)    proc=    .00%

   CG with angle restart.   November 8, 2006

    16    CG-LS&CD Algorithm:Lennard-Jones potential                Function
          Hybrid Liu&Storey-Conjugate Descent. max(0,min(LS,CD)) stoptest= 6

    n   iter   irs  fgcnt lscnt   time(c)        fxnew              gnorm
-------------------------------------------------------------------------------
 3000   1573     0   2060   485     16080 -.6611082968690E+04  .1450462636336E-01
-------------------------------------------------------------------------------
TOTAL   1573     0   2060   485    160.80 (seconds)    proc=    .00%

   CG with angle restart.   November 8, 2006

    17    CG-BM Algorithm:Lennard-Jones potential                 Function
          Birgin and Martinez (scaled Perry). Theta spectral. stoptest= 6

    n   iter   irs  fgcnt lscnt   time(c)        fxnew              gnorm
-------------------------------------------------------------------------------
 3000   1413     0   1675   261     13105 -.6601279362720E+04  .1272924474585E-01
-------------------------------------------------------------------------------
TOTAL   1413     0   1675   261    131.05 (seconds)    proc=    .00%

   CG with angle restart.   November 8, 2006

    18    CG-BM+ Algorithm:Lennard-Jones potential                 Function
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          Birgin and Martinez plus (scaled Perry). Theta spectral. stoptest= 6

    n   iter   irs  fgcnt lscnt   time(c)        fxnew              gnorm
-------------------------------------------------------------------------------
 3000   1694     0   1967   272     15398 -.6642659205875E+04  .1580313944848E-01
-------------------------------------------------------------------------------
TOTAL   1694     0   1967   272    153.98 (seconds)    proc=    .00%

   CG with angle restart.   November 8, 2006

    19    CG-sPRP Algorithm:Lennard-Jones potential                 Function
          Scaled Polak-Ribiere and Polyak. Theta spectral. stoptest= 6

    n   iter   irs  fgcnt lscnt   time(c)        fxnew              gnorm
-------------------------------------------------------------------------------
 3000   2907     0   4007  1088     31242 -.6630306464234E+04  .2306653554131E-01
-------------------------------------------------------------------------------
TOTAL   2907     0   4007  1088    312.42 (seconds)    proc=    .00%

   CG with angle restart.   November 8, 2006

    20    CG-sFR Algorithm:Lennard-Jones potential                 Function
          Scaled Fletcher and Revees. Theta spectral. stoptest= 6

    n   iter   irs  fgcnt lscnt   time(c)        fxnew              gnorm
-------------------------------------------------------------------------------
 3000   5501     0   7320  1819     57118 -.5392548839340E+04  .5344695488089E+03
-------------------------------------------------------------------------------
TOTAL   5501     0   7320  1819    571.18 (seconds)    proc=    .00%

   CG with angle restart.   November 8, 2006

    21    CG-sFR Algorithm:Lennard-Jones potential                 Function
          Andrei: beta = ytg/yts-ytg*stg/(yts**2). Theta spectral. stoptest= 6

    n   iter   irs  fgcnt lscnt   time(c)        fxnew              gnorm
-------------------------------------------------------------------------------
 3000   1835     0   2073   234     16236 -.6653650580426E+04  .1775567519005E-01
-------------------------------------------------------------------------------
TOTAL   1835     0   2073   234    162.36 (seconds)    proc=    .00%
```

Important Remarks:

1) For the conjugate gradient method with sufficient descent comdition (betatype = 10) the parameter β is computed as:

$$\beta_k^a = \frac{1}{y_k^T s_k}\left(g_{k+1} - \delta_k \frac{\|g_{k+1}\|^2}{y_k^T s_k} s_k \right)^T g_{k+1} ,$$

where

$$\delta_k = \frac{y_k^T g_{k+1}}{\|g_{k+1}\|^2} .$$

2) For the conjugate gradient method with sufficient descent comdition (betatype = 21) the parameter β is computed as:

$$\beta_k^A = \frac{1}{y_k^T s_k}\left(y_{k+1} - \frac{g_{k+1}^T y_k}{y_k^T s_k} s_k \right)^T g_{k+1} .$$

3) Sinoptic Table: $n = ndim \times natoms$.

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-------------------------------------------------------
       n    iter    fgcnt   time(c)          fx
    3000    2557     3171   24782   -.6631497390299E+04   1
    3000    5501     6974   54461   -.5401987751176E+04   2
```

3000	2008	2776	21644	-.6619382688012E+04	3	
3000	2399	3282	25594	-.6608459148448E+04	4	
3000	4070	4641	36334	-.6639534084590E+04	5	
3000	1540	2072	16162	-.6601686106922E+04	6	
3000	5501	5516	43344	-.5322950720681E+04	7	
3000	1944	2366	18502	-.6642551795698E+04	8	
3000	1234	1508	11790	-.6603546674709E+04	9	
3000	934	1075	8417	-.6606489613292E+04	10	
3000	1778	2130	16661	-.6610244818980E+04	11	
3000	773	891	**6977**	-.6593170961895E+04	12	
3000	2675	3645	28425	-.6639744036805E+04	13	
3000	1224	1649	12864	-.6601108405756E+04	14	
3000	1590	2183	17023	-.6628820304737E+04	15	
3000	1573	2060	16080	-.6611082968690E+04	16	
3000	1413	1675	13105	-.6601279362720E+04	17	
3000	1694	1967	15398	-.6642659205875E+04	18	
3000	2907	4007	31242	-.6630306464234E+04	19	
3000	5501	7320	57118	-.5392548839340E+04	20	
3000	1835	2073	16236	**-.6653650580426E+04**	21	the best objective

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