

Global minimum finding in Morse potential optimization problems

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Morse potential function

$$V_M = \epsilon \sum_{i=1}^n \sum_{j>i}^n \left((e^{\rho_0(1-r_{ij}/r_0)} - 1)^2 - 1 \right)$$

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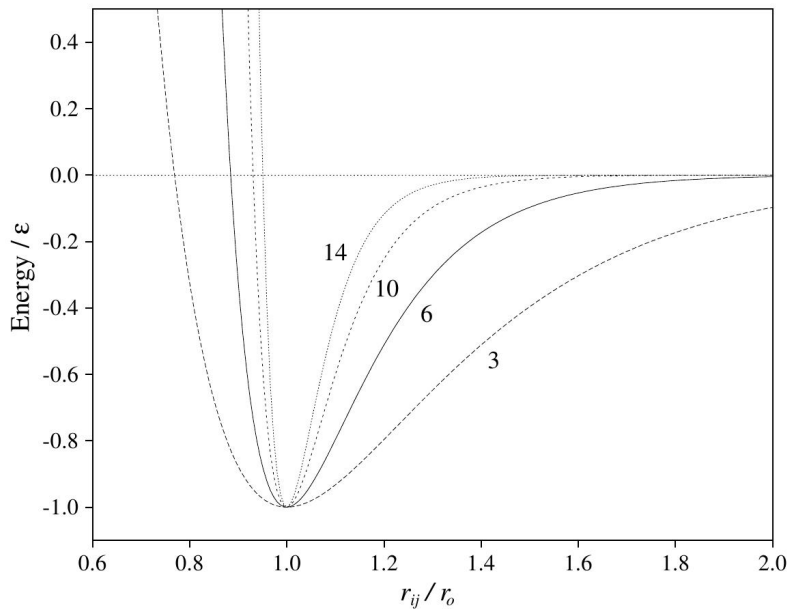
$$\epsilon = 1.0$$

$$r_0 = 1.0$$

Morse potential function

$$V_M = \sum_{i=1}^n \sum_{j>i}^n \left((e^{\rho_0(1-r_{ij})} - 1)^2 - 1 \right)$$

Morse potential function with various ρ value



The Cambridge Cluster Database

D. J. Wales, J. P. K. Doye, A. Dullweber, M. P. Hodges,
F. Y. Naumkin F. Calvo, J. Hernández-Rojas and T. F. Middleton

www-wales.ch.cam.ac.uk/CCD.html

Hefei National Laboratory for Physical Sciences at the Microscale
and School of Life Sciences, University of Science and Technology
of China

staff.ustc.edu.cn/~clj



Jorge Marques

Department of Chemistry Research in Computational Chemistry
and Molecular Modeling University of Coimbra, Portugal

apps.uc.pt/mypage/faculty/qtmarque/en/clusters



- Multi-Start

Global optimization methods

- Multi-Start
- Basin-Hopping (MSBH)

Global optimization methods

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- Basin-Hopping (MSBH)
- Big-Bang

Global optimization methods

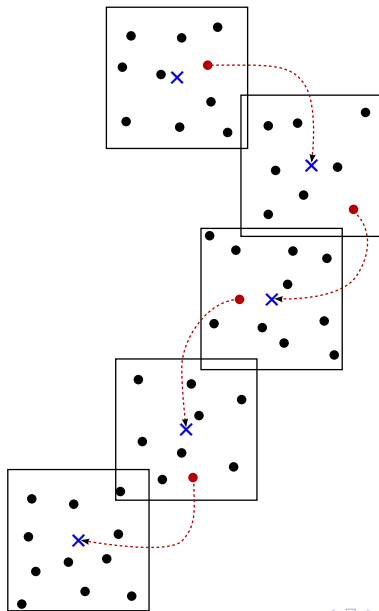
- Multi-Start
- Basin-Hopping (MSBH)
- Big-Bang
- “Forest”

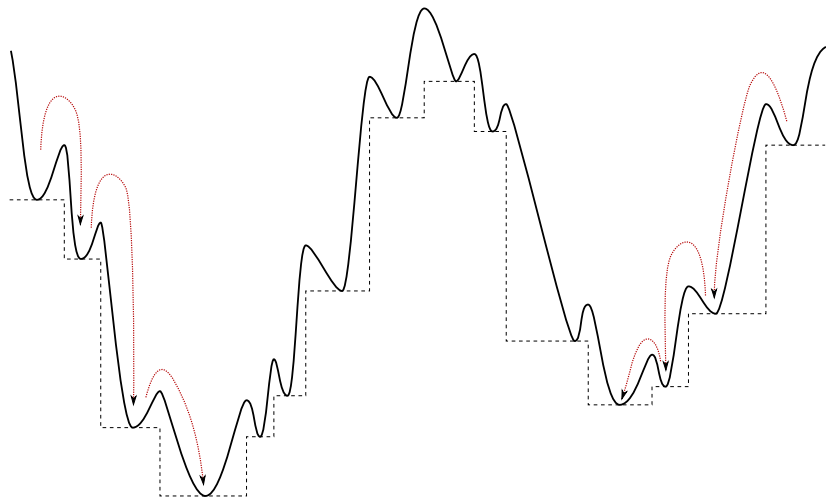
Global optimization methods

- Multi-Start
- Basin-Hopping (MSBH)
- Big-Bang
- “Forest”
- Dynamic lattice searching method

Global optimization methods

- Multi-Start
- Basin-Hopping (MSBH)
- Big-Bang
- “Forest”
- Dynamic lattice searching method
- Genetic algorithms





- Conjugate gradient method

Local minimization methods

- Conjugate gradient method
- L-BFGS method

Local minimization methods

- Conjugate gradient method
- L-BFGS method
- Cauchy's method

Local minimization methods

- Conjugate gradient method
- L-BFGS method
- Cauchy's method
- Powell's method

- C/C++ language
(GCC/MinGW, Clang, ICC compilers)
- Linux, Mac OS X, Windows platform
- OpenMP, MPI, CUDA parallel programming technologies
- Interactive/batch mode

n - number of atoms

n	UK (CCD)	ISDCT
20	-97.417393	-97.41739307417
80	-690.577890	-690.5778902004155952
147	-1531.498857	-1531.498857189995761

Computational experiments. MSBH

n - number of atoms

n	CN	ISDCT
150	-1570.956895	-1570.956894507743300
155	-1639.571558	-1639.571558368015758
160	-1705.794373	-1705.794372516992553
165	-1774.727689	-1774.727688598778741
170	-1842.786500	-1842.786499541551848
175	-1911.754684	-1911.754684452901074
180	-1979.907966	-1979.907965818779076
185	-2048.617785	-2048.617785496087890
190	-2119.104888	-2119.104888297832076
195	-2189.107474	-2189.107474368099702
200	-2260.148943	-2260.148943425931975

Computational experiments. MSBH

n - number of atoms

n	CN	ISDCT
205	-2329.258501	-2329.258501195624831
210	-2400.884161	-2400.884161410538582
215	-2473.351504	-2473.226631779617037
220	-2544.094288	-2543.330357862101664
225	-2616.672973	-2616.672972732320432
230	-2691.174648	-2691.174648208746930
235	-2767.215086	-2767.215085893439664
240	-2839.054430	-2839.099924748702961

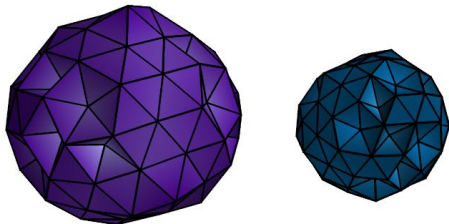
CN	-2839.054430
PT	-2839.099925
ISDCT	-2839.099924748702961

Computational experiments. MSBH

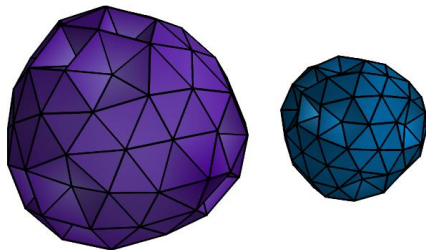
n - number of atoms

n	ISDCT
241	-2852.824892760237617
242	-2866.778881119791095
243	-2882.570361710750603
244	-2897.072046039199449
245	-2910.707949590559110
246	-2924.392845202200078
247	-2940.026081163837716
248	-2955.679013676632167
249	-2971.203337277484479
250	-2985.771711418945870

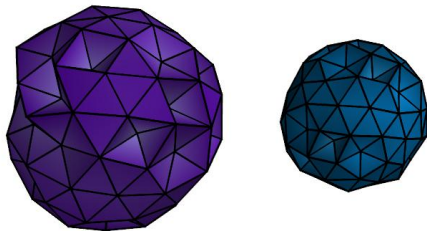
150 atoms cluster; CN, ISDCT



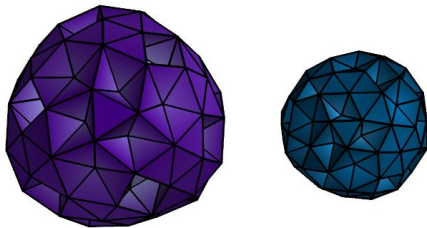
155 atoms cluster; CN, ISDCT



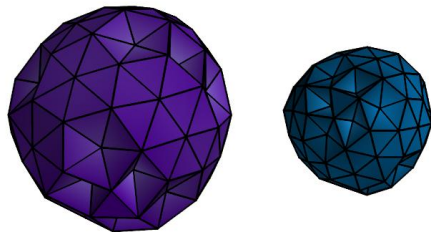
160 atoms cluster; CN, ISDCT



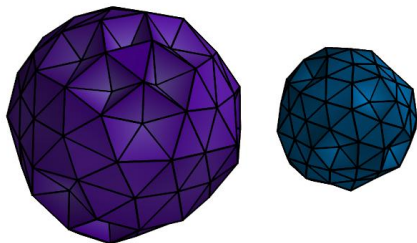
165 atoms cluster; CN, ISDCT



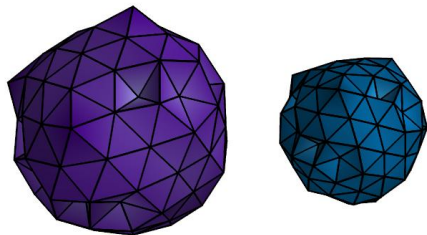
170 atoms cluster; CN, ISDCT



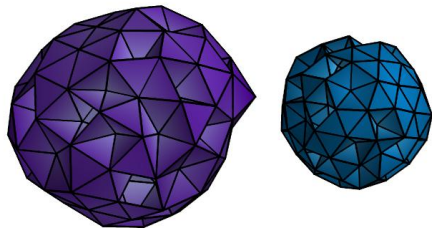
175 atoms cluster; CN, ISDCT



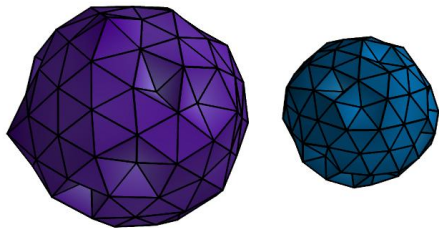
180 atoms cluster; CN, ISDCT



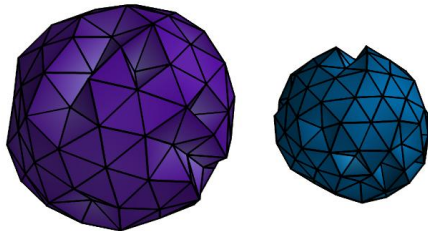
185 atoms cluster; CN, ISDCT



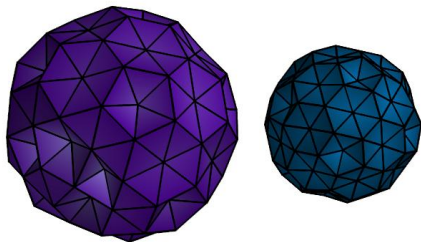
195 atoms cluster; CN, ISDCT



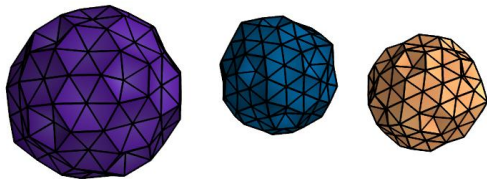
200 atoms cluster; CN, ISDCT



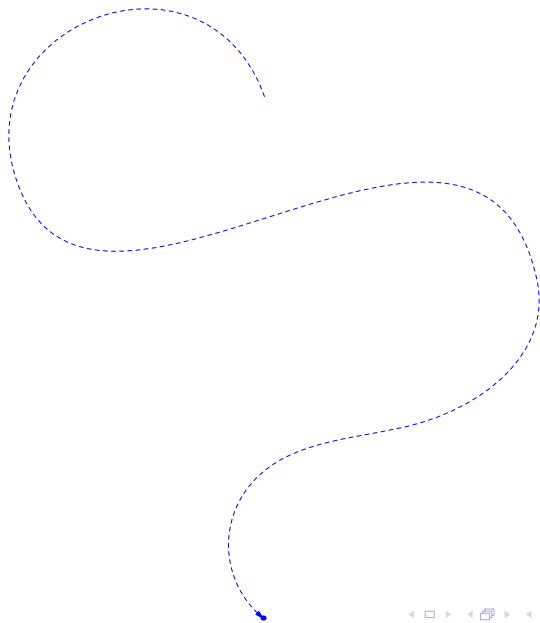
230 atoms cluster; CN, ISDCT



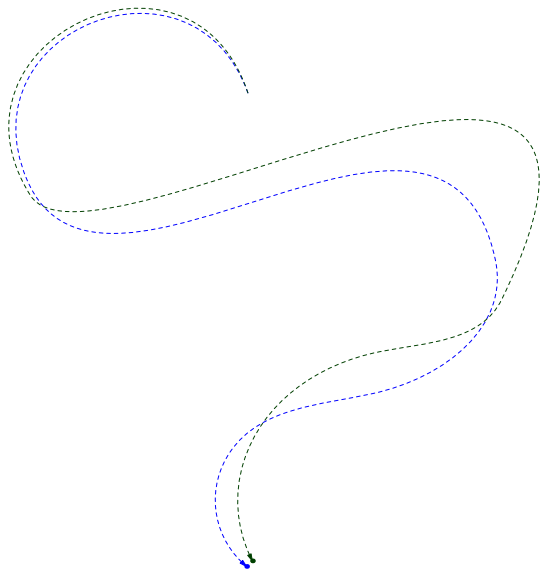
240 atoms cluster; CN, ISDCT, PT



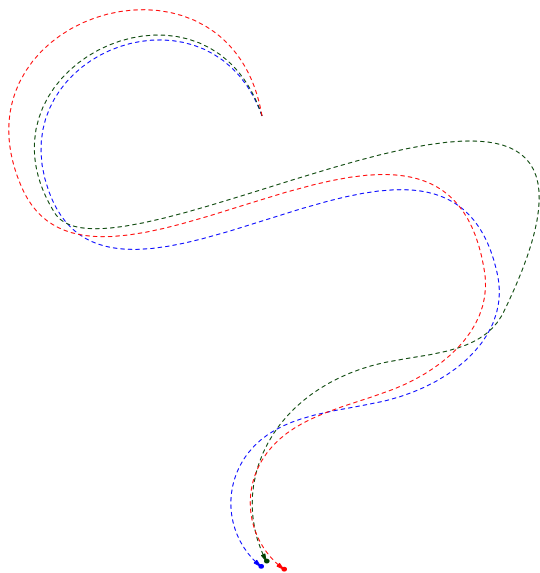
Local methods test



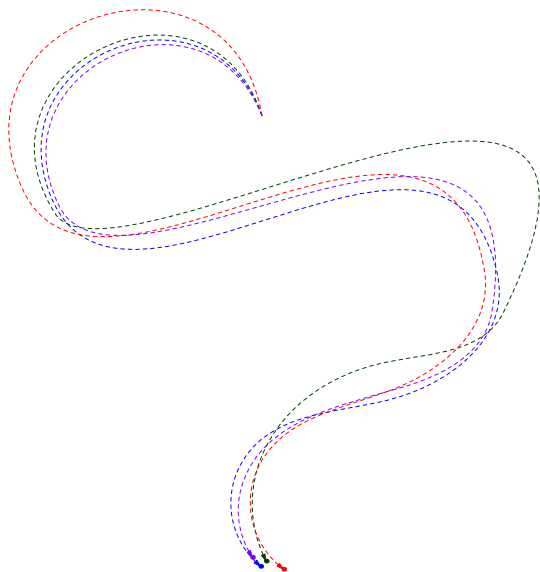
Local methods test



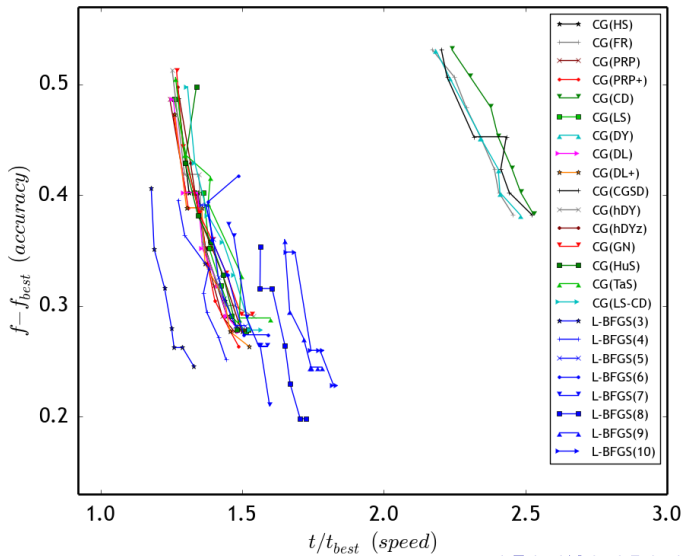
Local methods test



Local methods test



Local methods test



- Such problems can be “solved”
- Such problems **should** be investigated more deeply and intensely
- Multi-method technology – good choice for many complex problems
- Methods (local and global) selection and their parameters settings – crucial issue for optimization program performance and results obtaining

