Analysis of efficiency of software packages for solving anomalous diffusion problems

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❖ Description

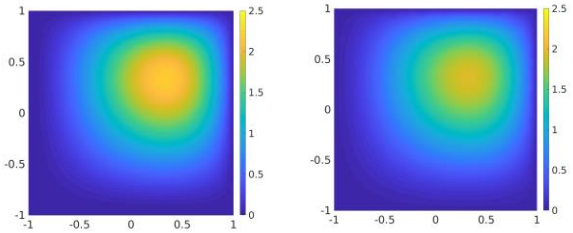
Anomalous diffusion examines processes in which the brownian movement hypothesis is violated. It can be found in many physical processes – supercon-ductivity, protein diffusion within cells, diffusion through porous media, supercold atoms, ion channels in the plasma membrane, moisture distribution in cement. Anomalous diffusion can also be found in many biological systems, like DNA sequences and heartbeat intervals.

❖ Use of HPC infrastructure

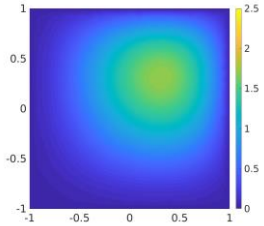
The Avitohol supercomputer was used to obtain the simulation results. It is located in the HPC center of IICT-BAS [1] and it is maintained by the National Center for High-Performance and Distributed Computing (NCHDC), subject to the National Roadmap for Research Infrastructures (NRRI) [2]. The results were obtained by using up to 1 HP Cluster Platform SL250S GEN8 servers, each with 2 Intel Xeon E2650 v2 CPUs and 2 Intel Xeon Phi 7120P coprocessors.

❖ Analysed packages and results

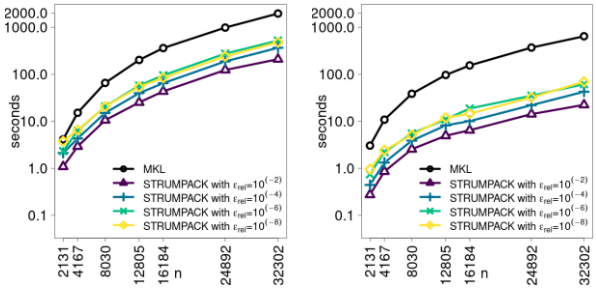
Solving this problem is a computationally expensive problem, which requires large computational resources. There are many methods and software packages for solving the systems of linear algebraic equations, that the problem is reduced to. We examined several software packages for effectively solving large scale problems of this type. Intel's Math Kernel Library (MKL) is the standard High Performance library provided by Intel for their architecture. STRUCtured Matrices Package (STRUMPACK) is a software package that uses Hierarchically Semi-separable compression to lower the computational complexity and allows for faster solving of the problem. On Figure 1 we have shown the solution for a model square problem (a,b,c) and a comparison of the examined solvers.



(a) *t = 0* (b) *t = 0,05*



(c) *t = 0,1*



(d) Sequential (e) Parallel with 16 cores

Figure 1: Solving a problem in a square fomain (up). Comparison of computational methods (down).

1. http://www.iict.bas.bg/avitohol/
2. http://nchdc.acad.bg