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MUTILS - a set of efficient modeling tools for multi-core CPUs implemented in MEX

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The need for computational performance is common in scientific applications, and in particular in numerical simulations, where high resolution models require efficient processing of large amounts of data. Especially in the context of geological problems the need to increase the model resolution to resolve physical and geometrical complexities seems to have no limits. Alas, the performance of new generations of CPUs does not improve any longer by simply increasing clock speeds. Current industrial trends are to increase the number of computational cores. As a result, parallel implementations are required in order to fully utilize the potential of new processors, and to study more complex models.

We target simulations on small to medium scale shared memory computers: laptops and desktop PCs with $\sim$8 CPU cores and up to tens of GB of memory to high-end servers with $\sim$50 CPU cores and hundereds of GB of memory. In this setting MATLAB is often the environment of choice for scientists that want to implement their own models with little effort. It is a useful general purpose mathematical software package, but due to its versatility some of its functionality is not as efficient as it could be. In particular, the challanges of modern multi-core architectures are not fully addressed.

We have developed MILAMIN 2 - an efficient FEM modeling environment written in native MATLAB. Amongst others, MILAMIN provides functions to define model geometry, generate and convert structured and unstructured meshes (also through interfaces to external mesh generators), compute element and system matrices, apply boundary conditions, solve the system of linear equations, address non-linear and transient problems, and perform post-processing. MILAMIN strives to combine the ease of code development and the computational efficiency. Where possible, the code is optimized and/or parallelized within the MATLAB framework. Native MATLAB is augmented with the MUTILS library - a set of MEX functions that implement the computationally intensive, performance critical parts of the code, which we have identified to be bottlenecks. Here, we discuss the functionality and performance of the MUTILS library. Currently, it includes:

1. time and memory efficient assembly of sparse matrices for FEM simulations
2. parallel sparse matrix - vector product with optimizations speficic to symmetric matrices and multiple degrees of freedom per node
3. parallel point in triangle location and point in tetrahedron location for unstructured, adaptive 2D and 3D meshes (useful for 'marker in cell' type of methods)
4. parallel FEM interpolation for 2D and 3D meshes of elements of different types and orders, and for different number of degrees of freedom per node
5. a stand-alone, MEX implementation of the Conjugate Gradients iterative solver
6. interface to METIS graph partitioning and a fast implementation of RCM reordering