Discrete Exterior Calculus for large scale problems

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Finite difference time domain (FDTD) method, and finite integration technique (FIT), are classical approaches for solving wave propagation problems. We apply discrete exterior calculus (DEC) to generalize these finite difference schemes. Advantage of DEC is its general notation of metric-independent differential operator called **discrete exterior derivative**. Independently of the chosen dimension and finite element meshing, the discrete exterior derivative realizes Stokes' theorem exactly. Wave problems include calculation on primal and dual meshes. Relations between primal and dual values are determined by metric-dependent operator called **discrete Hodge star**. This become diagonal matrix by choosing orthogonal duality, i.e., corresponding primal and dual elements are orthogonal with respect to the metric tensor.

Efficiency of the numerical scheme depends on quality of meshing. For large tasks we employ structured simplicial grids, which produce more isotropic properties than cubic tiling. With these grids, we can nearly eliminate the numerical dispersion, which is the most significant cause of error in traditional finite difference schemes. This is done without additional computational cost by estimating curvature of the fields of single frequency solution. We can adapt the numerical scheme with changing material parameters by grid refinement. In addition, our mesh generation tool allows adaptation of curved surfaces and 4-dimensional space-time meshing, which allows modeling of moving/transforming cavities.

Our largest tasks with the Maxwell equations reach up to billions of unknowns. Implementation employs message passing interface (MPI) and domain decomposition method leading to almost perfect scalability, i.e., task size scales proportionally with number of computing cores.