Optimal domain decomposition for 3D spherical mantle convection codes using minimal energy configurations of classical electrons

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To run a 3D spherical simulation with a reasonable resolution in an appropriate time, the code must work with more than one CPU in parallel. Typically a domain decomposition of the grid is applied, which is responsible for an optimal breakdown of the grid into p equal volumes, where p specifies the amount of domains and processors. An efficient domain decomposition minimizes the area between those sections, leading to a minimized overhead of data exchange between the processors. The resulting speedup of this method with the newly developed GAIA mantle convection code is presented in Figure 1 (right).

Halo-cells, or sometimes called ghost-cells, arise in domain decomposition as additional cells in each domain to build an overlapping zone where data is exchanged. These cells border each domain and are on the same position as their active cells on the neighboring domain. The ratio between the amount of halo-cells to grid cells is a first measure of efficiency for parallelization because it determines the amount of data transported from one domain to another.

One approach to decompose a sphere laterally is to distribute p points on the surface of a sphere so that the global potential energy becomes minimal. This is known as the Thomsom problem [Thomson, 1904]. After this step the domain affiliation for every cell is derived by its closest "Thomson" point. The resulting decomposition as shown in figure 1 leads to equal volumes which is important to balance the computational efforts for each CPU. Some p reproduce platonic solids; p=4 creates a tetrahedron, p=6 a cube and p=12 a dodecahedron. However, all p>1 show a certain symmetry [Wales and Ulker 2006].

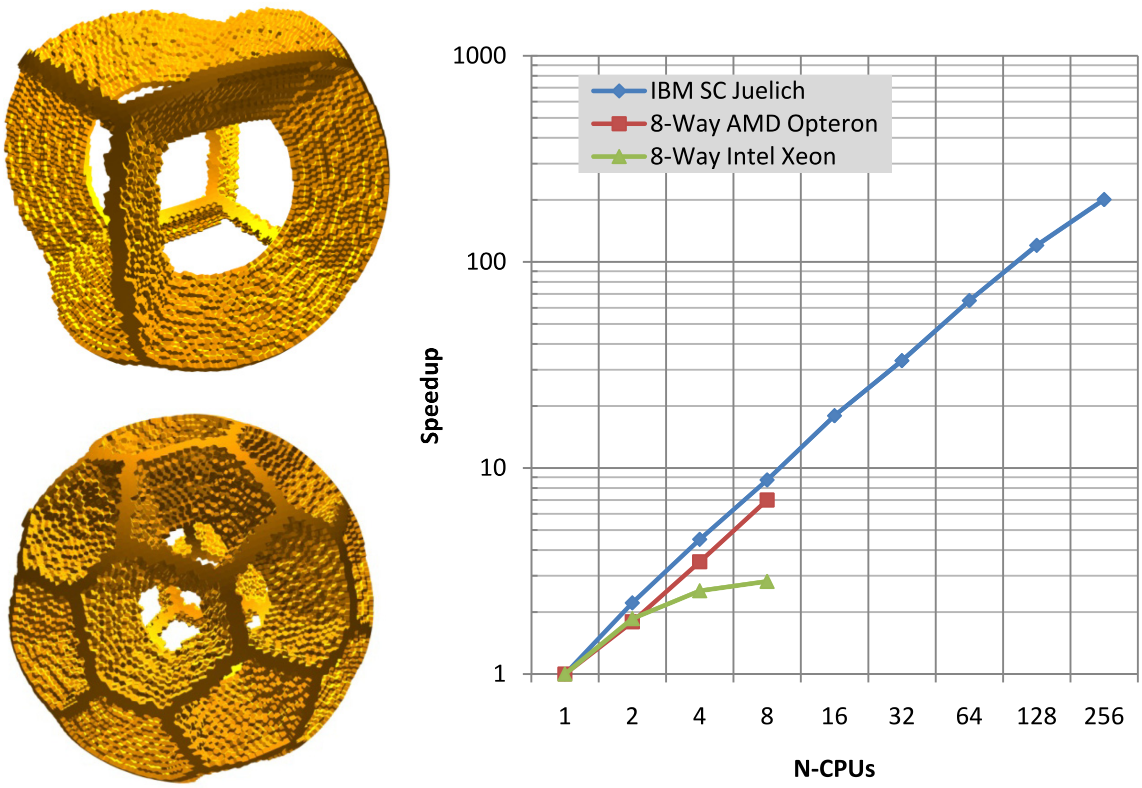

Figure 1: The resulting halo-cells after a domain decomposition of the spiral grid with a resolution of 0.55 and 24 shells. Left Top: Domain decomposition for six CPUs (equal to the cube); Left Bottom: 32 CPUs. Right: Code Speedup vs. CPUs.

Thomson, J. J. (1904), On the Structure of the Atom: an Investigation of the Stability and Periods of Oscillation of a number of Corpuscles arranged at equal intervals around the Circumference of a Circle; with Application of the Results to the Theory of Atomic Structure, *Philosophical Magazine Series 6, Volume 7, Number 39, pp. 237--265*
Wales, D. J. and S. Ulker (2006), Structure and Dynamics of Spherical Crystals Characterised for the Thomson Problem, Phys. Rev. B, 74, 212101