Removing the Fat from Sausages

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All quantum chemical calculations – whether using Hartree-Fock theory, DFT or coupled-cluster theory – require electron repulsion integrals between basis function products. In most calculations, the basis functions are contracted gaussians centred on nuclei [1] and the products are therefore sums of collinear gaussians. In some cases, these sums involve dozens of gaussians and the electron repulsion integrals are therefore computationally expensive [2].

However, we propose that these gaussian sums can often be replaced by much shorter sums without significantly affecting the energy or other properties. To construct the shorter sums, we use a potential-modelling theory [3] that was derived many years ago but that has not been applied in this way previously. We find that it is sometimes possible to reduce the number of gaussians by an order of magnitude, and the integral cost by two orders of magnitude, and this can significantly accelerate the speeds of Hartree-Fock and DFT calculations [4].

A selection of numerical results will be presented.

References

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