From muffin tins to robots – 7 decades of DFT

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Arguably, (Kohn-Sham) DFT had its roots in Slater's 1951 paper on local electron gas exchange, as an approximation to Hartree-Fock theory (I don't think Slater would have called it DFT…) , that provided the basis for the Xα method which was introduced into chemistry with the Xα-Scattered Wave method that used a so-called muffin-tin potential providing spherical solutions solved on radial grids. I will trace some of the history of DFT through the 1960s and 70s, showing how Xα -SW opened doors and attracted chemists, particularly for transition-metal systems, into the 80s when techniques from quantum chemistry, notably Gaussian basis sets, took the forefront along with ever-improving exchange-correlation functionals. I'll then fast-forward to today with the advent of artificial intelligence and machine learning. Example applications will be drawn from our own work, with apologies to the myriad others whose work is surely even more exemplary.