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E-man Part 4[#]: Tutorial on prospects of charged system search (CSS) algorithm in chemical sciences

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(Dedicated to Dr. P.V. Krishna Rao, our teacher and former professor of physical chemistry, Andhra University on his 75th birth anniversary)

ABSTRACT

CSS (*charged system search or Charge_Syst_Serch*) algorithm is another nature inspired multi-agent optimisation tool of this decade. It is applicable to variable selection in structure X (: activity, toxicity, property etc.) relationships (SXR), estimation of equilibrium constants of multiple chemical equilibria and rate constants of parallel/ consecutive kinetics profiles. The extensive application in engineering and advances in the algorithm brought CSS to the forefront of bandwagon of physics based swarm approaches viz. gravitational, big-bang_big-crunch, intelligent_water-drop etc. The Charge_Syst_Serch algorithm consists of calculation of the resultant force affecting each of a set of charged particles based on Coulomb and Gauss electrostatic interaction. Here, the magnitude of charge of a charged particle (CP) depends on fitness value of object function. Newton's law of mechanics directs the movement of CPs to refined positions in the search space. The iterative improvements of approximate (random) solutions converge to true optimum. CSS algorithm converged to Pareto optimal solution of non-convex functions and it finds application in parametric models. Incorporation of magnetic forces, chaos and correction for fence crossing during refinement improved efficacy of CSS. The binary hybridization of CSS with another E-man module viz. ant colony optimisation (ACO), particle swarm optimization (PSO), Big-Bang_Big-crunch (BB_BC) is the development with a right perspective of deriving synergistic benefits of both worlds. This combination at the same time diminishes the short comings of individual component algorithms. The concept of fields of forces, again from Physics, mimicking ACO, PSO and CSS is another landmark to probe deep into core mathematics for future prospects. These multi-agent search/optimization tools designed for multi objective multi-dimensional-non-linear-convex functions with constraints/ discontinuities are implementable on parallel software and hardware architectures.

Keywords: Charged System, Multi-object-functions, E-man, Nature mimicking, SXR, Chemical equilibria, Chemical kinetics, Electrostatics, Magnetic force, hybrid E-man.

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