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FIELD OF RESEARCH

Many problems of theoretical chemistry can be ultimately reduced to the equivalent problems of either maximizing or minimizing a function or a functional. For complex functions and functionals deterministic search for critical points is often not the best way when the surfaces being explored have a rather large number of critical points. Of late, a number of soft-computing methods that can do the job better have come up. Notable among these are the Simulated Annealing method (SAM), evolutionary algorithms (EA^s) like Genetic Algorithms, Ant Colony Algorithms, Swarm-Intelligence driven algorithms and the Neural Network. My focus has been towards exploring these algorithms, especially the hybrids of them, to handle the following problems:

(1) Computing eigen-spectra of Hermitian matrices and to explore the various matrix partitioning schemes available, like the energy-dependent and the energy-independent wave operator formalism; to extract a small number of eigen-values and vectors for moderate size matrices.

(2) Finding local and global minima and maxima on complex potential energy surfaces of atomic and molecular clusters, spin-clusters etc.

(3) Finding 1^{st} and 2^{nd} order saddle points of the above-mentioned surfaces with a view to locating the transition structures.

(4) Thermal effects on cluster geometry and other properties, especially response properties.

(5) Constructing localized orbitals and optimizing basis functions.

(6) Development of methodologies to scope out the reaction pathways for some simple problems.

Presently, I have done some work towards the solution of the reactive scattering problem for three body systems using the wave packet evolution (in hyperspherical co-ordinates); parallelization of the code using MPI, OpenMP and mixed MPI-OpenMP parallelization.

Special emphasis has been given on the fine-tuning of relevant parameters of each algorithm and parallelization of the methods proposed, so that they become competitive with the existing computing schemes.

LIST OF PUBLICATIONS:

Serial Number	Year of Publication	Title	Name of the authors	Name of the Journal	Volume and Pages
1	2021	Dynamical calculations of O (3 P)+ OH (2 Π) reaction on the CHIPR potential energy surface using the fully coupled time-dependent wave-packet approach in hyperspherical coordinates	S Ghosh, **R Sharma**, S Adhikari, AJC Varandas	Physical Chemistry Chemical Physics	Vol: 23, Pg:21784-21796
2	2020	Structure elucidation and construction of isomerisation pathways in small to moderate-sized (6–27) MgO nanoclusters: an adaptive mutation simulated annealing based analysis with quantum chemical calculations	K Ghosh, **R Sharma**, P Chaudhury	Physical Chemistry Chemical Physics	Vol: 22, Pg: 9616-9629
3	2019	Fully coupled (J> 0) time-dependentwave-packet calculationsusing hyperspherical coordinates for the H+ O 2 reaction on the CHIPR potential energy surface	S Ghosh, **R Sharma**, S Adhikari, AJC Varandas	Physical Chemistry Chemical Physics	Vol: 21, Pg: 20166-20176
4	2018	3D time-dependent wave-packet approach in hyperspherical coordinates for the H+ O 2 reaction on the CHIPR and DMBE IV potential energy surfaces S Ghosh, R Sharma, S Adhikari, AJC Varandas Physical Chemistry Chemical Physics 20 (1), 478-488	S Ghosh, **R Sharma**, S Adhikari, AJC Varandas	Physical Chemistry Chemical Physics	Vol: 20, Pg: 478-488
5	2017	Beyond Born-Oppenheimer theory for ab initio constructed diabatic potential energy surfaces of singlet H3+ to study reaction dynamics using coupled 3D time-dependent wave-packet approach	Sandip Ghosh, Saikat Mukherjee, Bijit Mukherjee, Souvik Mandal, **Rahul Sharma**, Pinaki Chaudhury, Satrajit Adhikari	The Journal of Chemical Physics	Vol: 147, Pg: 074105
6	2017	Coupled 3D time-dependent quantum wave-packet study of the O+ OH reaction in hyperspherical coordinates on the CHIPR potential energy surface	S Ghosh, **R Sharma**, S Adhikari, AJC Varandas	Chemical Physics Letters	Vol: 675, Pg: 85-91
7	2015	Enhancing the branching ratios in the dissociation channels for O16O16O18 molecule by designing optimum laser pulses: A study using stochastic optimization	S Talukder, S Sen, BK Shandilya, **Rahul Sharma**, P Chaudhury, S Adhikari	The Journal of Chemical Physics	Vol:143 Pg: 144109
8	2015	Coupled 3D Time-dependent Wave-packet Approach	S Ghosh, T Sahoo,	The Journal of Physical Chemistry	Vol: 119, Pg: 12392-

		inHyperspherical Coordinates: the D++ H2 Reaction on the Triple-sheeted DMBE Potential Energy Surface	S Adhikari, **Rahul Sharma**, AJC Varandas	A	12403
9	2015	Low-temperature D+ + H2 reaction: A time-dependent coupled wave-packet study in hyperspherical coordinates	Tapas Sahoo, Sandip Ghosh, Satrajit Adhikari, **Rahul Sharma,** António J. C. Varandas	The Journal of Chemical Physics	Vol: 142 Pg: 024304
10	2014	Coupled 3D Time-Dependent Wave-Packet Approach in Hyperspherical Coordinates: Application to the Adiabatic Singlet-State (11A′) D++ H2 Reaction	T Sahoo, S Ghosh, S Adhikari, **Rahul Sharma,** AJC Varandas	The Journal of Physical Chemistry A	Vol:118 Pg:4837-4850
11	2014	A generalized recipe to construct elementary or multi-step reaction paths via a stochastic formulation: Application to the conformational change in noble gas clusters	S Talukder, S Sen, **Rahul Sharma,** SK Banik, P Chaudhury	Chemical Physics	Vol:43 Pg:5-11
12	2014	A new adaptive mutation simulated annealing algorithm: application to the study of pure and mixed Pt–Pd clusters	SK Biring, **Rahul Sharma,** P Chaudhury	Journal of Mathematical Chemistry	Vol:52 Pg:368-397
13	2013	Structural and Infra Red Spectroscopic Aspects of Ion-Water Clusters: A Study Based on a Combined Stochastic and Quantum Chemical Approach	SK Biring, **Rahul Sharma,** R Misra, P Chaudhury	Journal of Cluster Science	Vol: 24 Pg: 1-23
14	2012	A constrained variational approach to the designing of low transport band gap materials: A multiobjective random mutation hill climbing method	K Sarkar, **Rahul Sharma,** SP Bhattacharyya	International Journal of Quantum Chemistry	Vol: 112 Pg: 1547-1558
15	2011	A "classical" trajectory driven nuclear dynamics by a parallelized quantum-classical approach to a realistic model Hamiltonian of benzene radical cation	S Sardar, AK Paul, **Rahul Sharma,** S Adhikari	International Journal of Quantum Chemistry	Vol: 111 Pg: 2741-2759
16	2011	Solving symmetric eigenvalue problem via genetic algorithms: Serial versus parallel implementation	S Nandy, **Rahul Sharma,** SP Bhattacharyya	Applied Soft Computing	Vol: 11 Pg: 3946-3961
17	2011	A Density-Genetic Algorithm Method for Computing Electronic Structures of Doped and Undoped Polythiophene Oligomers: A Modified Su–Schrieffer–Heeger Hamiltonian-Based Study	**Rahul Sharma,** S Nandy, P Chaudhury, SP Bhattacharyya	Materials and Manufacturing Processes	Vol: 26 Pg: 354-362
18	2010	Blending determinism with	K Sarkar,	Journal of Chemical	Vol: 6

		evolutionary computing: Applications to the calculation of the molecular electronic structure of polythiophene	**Rahul Sharma,** SP Bhattacharyya	Theory and Computation	Pg: 718-726
19	2010	Exploring NLO response of 9, 10-donor-acceptor substituted Bichromophoric Anthracene Derivatives	R Misra, **Rahul Sharma,** SP Bhattacharyya	Journal of Computational Methods in Science and Engineering	Vol: 10 Pg: 149-164
20	2009	On optimal designing of low frequency polychromatic fields for facile photo-dissociation of model diatomic molecules	S Ghosh, K Maji, **Rahul Sharma,** SP Bhattacharyya	Journal of Chemical Sciences	Vol: 121 Pg: 757-766
21	2009	A search for lowest energy structures of ZnS quantum dots: Genetic algorithm tight-binding study	S Pal, **Rahul Sharma,** B Goswami, P Sarkar, SP Bhattacharyya	The Journal of Chemical Physics	Vol: 130 Pg: 214703
22	2009	The multistate multimode vibronic dynamics of benzene radical cation with a realistic model Hamiltonian using a parallelized algorithm of the quantumclassical approach	S Sardar, AK Paul, **Rahul Sharma,** S Adhikari	The Journal of Chemical Physics	Vol: 130 Pg: 144302
23	2009	Computation of molecular electronic structure by genetic algorithm	**Rahul Sharma,** R Saha, S Nandy, SP Bhattacharyya, P Chaudhury	Materials and Manufacturing Processes	Vol: 24 Pg: 155-161
24	2009	Theoretical prediction of ring structures for ZnS quantum dots	S Pal, **Rahul Sharma,** B Goswami, P Sarkar	Chemical Physics Letters	Vol: 467 Pg: 365-368
25	2008	On Solving Energy-Dependent Partitioned Real Symmetric Matrix Eigenvalue Problem by a Parallel Genetic Algorithm	**Rahul Sharma,** S Nandy, SP Bhattacharyya	Journal of Theoretical and Computational Chemistry	Vol: 7 Pg: 1103-1120
26	2008	A density-matrix-based simulated annealing (SA) technique for locating minimum energy structures on the neutral polythiophene potential energy surface	S Nandy, P Chaudhury, **Rahul Sharma,** SP Bhattacharyya	Journal of Theoretical and Computational Chemistry	Vol: 7 Pg: 977-987
27	2007	Target excitation in 2-D quantum dots by optimized chirped pulses	M Ghosh, **Rahul Sharma,** SP Bhattacharyya	Chemical Physics Letters	Vol: 449 Pg: 165-170
28	2007	Direct search for wave operator by A Genetic Algorithm (GA): Route to few eigenvalues of a Hamiltonian	**Rahul Sharma,** SP Bhattacharyya	Proceedings of IEEE Congress on Evolutionary Computation, 2007. CEC 2007	Vol: Pg: 3812-3817
29	2007	Instability and pattern formation in reaction-diffusion systems: A higher order analysis	SS Riaz, **Rahul Sharma,** SP Bhattacharyya, DS Ray	The Journal of Chemical Physics	Vol: 127 Pg: 064503
30	2006	On solving energy-dependent	**Rahul Sharma,**	Pramana	Vol: 66

		partitioned eigenvalue problem by genetic algorithm: The case of real symmetric Hamiltonian matrices	S Nandy, SP Bhattacharyya		Pg: 1125-1130