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76401. *Cleaner Air Through Parallelized Simulations of Novel Mathematical Models of Gas-Surface Interactions.*

A new particle based theory of thermophoresis is used to model gas-surface interactions from Random Billiard Dynamical Systems (RBDS). This particular RBDS model has been expanded from the typical single-particle model to accommodate high density particle simulations that are necessary for more complex interactions to model thermophoretic effects. Due to the high number of simple calculations required at each time step of simulation, the model is ideal for parallelizing. A parallel algorithm is introduced that models gas particles in a 3 dimensional simulation. The main objective for this work is to improve the model for thermophoresis being used for pollution control applications. Some results are presented that demonstrate the agreement of theory with experimental result. In addition, the runtime speedup from the serial to the parallel algorithm is shown. Finally, future developments are discussed. (Received September 19, 2016)