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Molecular Dynamics based lattice gas automata ALEXANDER WAGNER, REZA PARSA, Department of Physics, North Dakota State University — We present a lattice gas (LG) model derived from an underlying Molecular Dynamics (MD) simulation. In principle any MD simulation will result in a corresponding MDLG model. The question is then for which cases can we derive LG collision operators that only depend on the current state of the LG system. We show that for systems that approximate an ideal gas we can recover the standard lattice Boltzmann algorithm to good approximation. We conclude with an outlook for extending this approach to derive coarse grained lattice gas models for fluctuating dynamics and non-ideal systems.

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