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Generation of skeletal mechanism by means of projected entropy participation indices SAMUEL PAOLUCCI, University of Notre Dame, MAURO VALORANI, PIETRO PAOLO CIOTTOLI, RICCARDO MALPICA GALASSI, La Sapienza University of Rome — When the dynamics of reactive systems develop very-slow and very-fast time scales separated by a range of active time scales, with gaps in the fast/active and slow/active time scales, then it is possible to achieve multi-scale adaptive model reduction along-with the integration of the ODEs using the G-Scheme. The scheme assumes that the dynamics is decomposed into active, slow, fast, and invariant subspaces. We derive expressions that establish a direct link between time scales and entropy production by using estimates provided by the G-Scheme. To calculate the contribution to entropy production, we resort to a standard model of a constant pressure, adiabatic, batch reactor, where the mixture temperature of the reactants is initially set above the auto-ignition temperature. Numerical experiments show that the contribution to entropy production of the fast subspace is of the same magnitude as the error threshold chosen for the identification of the decomposition of the tangent space, and the contribution of the slow subspace is generally much smaller than that of the active subspace. The information on entropy production associated with reactions within each subspace is used to define an entropy participation index that is subsequently utilized for model reduction.

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