

4D01: ON-DEMAND GENERATION OF REDUCED MECHANISMS BASED ON HIERARCHICALLY EXTENDED INTRINSIC LOW-DIMENSIONAL MANIFOLDS IN GENERALIZED COORDINATES.

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In your new hierarchical concept for the extension of the ILDMs into the domain of slow chemistry a one dimensional ILDM is found using a criterion of minimal distance to the line connecting the pure mixing state. This criterion seems somewhat ad hoc. Can the quality of the one-dimensional ILDM in the slow chemistry region be improved when the next step in the hierarchy is available?

Reply by Karin König

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The concept of hierarchical extension consists of both the use of the ILDM-hierarchy and additional constraints, which allow connecting the ILDM boundary with the mixing point. The criterion for a hierarchically extended m-dimensional ILDM is first that it is a subset of a higher-dimensional ILDM. Then, to reduce the dimension to its desired value, an additional constraint is applied, namely the condition that the extended ILDM is the set of points of the higher dimensional manifold, which form an m-dimensional manifold with the property that it minimizes the distance towards the mixing point. This criterion mimics the effect of diffusion processes, which, in composition space, evolve manifolds toward minimal surfaces. It is therefore a quite natural choice for reaction/diffusion systems. The algorithm works for higher dimensions, too. Therefore the quality can be improved when the next step in the hierarchy is available.