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Robust ResNets for Chemically Reacting Flows

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Abstract : Chemically reacting flows are common in engineering applications such as hypersonic flow, combustion, explosions, manufacturing process, and environmental assessments. The number of reactions in combustion simulations can exceed 100, making a large number of flow and combustion problems beyond the capabilities of current supercomputers. Motivated by this, deep neural networks (DNNs) will be introduced with the goal of eventually replacing the existing chemistry software packages with DNNs. The DNNs used in this paper are motivated by the Residual Neural Network (ResNet) architecture. In the continuum limit, ResNets become an optimization problem constrained by an ODE. Such a feature allows the use of ODE control techniques to enhance the DNNs. In this work, DNNs are constructed, which update the species un at the n^{th} timestep to u^{n+1} at the $n+1^{th}$ timestep. Parallel DNNs are trained for each species, taking in u^n as input and outputting one component of u^{n+1}. These DNNs are applied to multiple species and reactions common in chemically reacting flows such as H_2-O_2 reactions. Experimental results show that the DNNs are able to accurately replicate the dynamics in various situations and in the presence of errors.

Keywords : chemical reacting flows, computational fluid dynamics, ODEs, residual neural networks, ResNets
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