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Comparison of algorithms for numerical optimization of chemical reaction rate coefficients in plasma simulation SANG-YOUNG CHUNG, DEUK-CHUL KWON, Plasma Technology Research Center, National Fusion Research Institute — For a reliable plasma simulation accurate rate coefficients for chemical reactions are important. The set of the rate coefficients should include essential reactions like appearing and disappearing of main species. However, some of them are hard to achieve from literature survey, experiments or calculations. Then, researchers have been estimated the missing rate coefficients and looked for proper rate coefficients until the simulation results agree with experiments. These searching process can be done by researchers with trial and error method, but can be done by numerical optimization method with less human efforts. In this study rate coefficients were numerically optimized with several algorithms including steepest descent, Newton, modified Newton and Broyden-Fletcher-Goldfarb-Shanno algorithms. A spatially averaged global code were used to simulate plasma while numerical optimizations. The accuracy and efficiency of algorithms were compared with each other. The methods to determine initial starting point of the optimization were also discussed.

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