ADF Performance Plan Summary

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The ADF Performance Plan investigated load imbalance and identified potential to improve the performance by up to a factor of two for an important feature in the main computation, for which a Proof of Concept has been suggested. This would have a significant impact on runtimes for users of this feature in the code.

For a particular calculation (medium-sized molecule with hybrid exchange-correlation functional), the division of work was found to be unequal and not provided frequently enough to the workers. POP experts suggested implementing a work stealing algorithm to improve both aspects by allowing cores to take work from others when they are running low. A POP Audit had already found the application to have good Communication Efficiency with little to improve in that regard.

ADF is a computational chemistry application which uses density functional theory calculations to predict the structure and reactivity of molecules. It is developed by Amsterdam based company Software for Chemistry & Materials (SCM).

"I can honestly say your analysis gave us a new insight into performance of one of the newer features available in ADF. What is more important, it clearly showed us the limitations of the current implementation and pointed us to the ways to improve it."

– Alexei Yakovlev, Software developer SCM.

A full technical report can be found at ***https://pop-coe.eu/sites/default/files/pop_files/pop-pp-adf.pdf***

For more information, contact: POP team
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