

Geachte promotor

De Tier 1 Evaluatiecommissie heeft uw aanvraag voor rekentijd grondig onderzocht en beslist u minimaal 4864 nodedagen toe te kennen op de Tier1 samen met 1 TB scratch space. U dient deze rekentijd te gebruiken gedurende de volgende 6 maanden met als einddatum 30/04/2015.

De bevindingen van de Commissie waren als volgt:

'The Tier 1 allocation board has decided to award 4864 node days to your Tier 1 application for 6 months ending on April 30, 2015 with 1 TB scratch space. As your application most probably contains an error in the calculation of the required number of node days, the board unfortunately is not certain about the exact resource requirement. The board therefore requires further clarification before this grant can take full effect.

The mandated persons have previous multi-year Tier 2 and Tier 1 experience. The CP2K code is well known to scale to very high core counts. The proposal states that excellent scaling is obtained up to 64 cores for a system of similar size. Due to the logarithmic scale of the illustration this is not completely clear. For this a table with parallel efficiencies would have been more precise (and more easy to read). (From the illustration, the board can only see that the parallel efficiency on 64 cores is better than 50% but it might easily be well over some 80%).

No attempt has been made to correlate information to the systems that will be studied in this proposal. It is unclear if we can expect scaling of up to 16 nodes, based on the scaling behavior for 256 H₂O molecules.

The proposal does not clearly state how many nodes will be used. The only mention is "several multi-node jobs simultaneously". Because of the HTC character of this proposal, the board suggests using single node jobs (if memory allows).

The resource estimation is based on delcatty results, which is similar to muk.

Finally, CP2K has good OpenMP, and hybrid MPI/OpenMP scaling behavior for different methods. The applicant is encouraged to explore this.'