



Acquisition Services Management (ASM) Division  
Subcontracts, ASM-SUB  
P.O. Box 1663, Mail Stop D447  
Los Alamos, New Mexico 87545  
505-665-3814 / Fax 505-665-9022  
E-mail: dknox@lanl.gov

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**Subject: Question and Answer Set 8  
Trinity and NERSC-8 Computing Platforms Project  
LA-UR-13-26915**

Greetings:

Interested parties are advised of the following questions or concerns that have been submitted to the Trinity and NERSC-8 Project team and to the accompanying Project responses below. Each of these questions refer to the miniDFT benchmark:

**Question/Issue 1**

Is 10,000 MPI ranks per k-point (~40 MPI ranks per node) a strict requirement? It might be more optimal to run fewer MPI ranks per k-point in the MPI+X Optimized version.

**Project Response 1**

The MiniDFT run rules for Capability Improvement do not require 10k MPI ranks per k-point. This requirement was removed from the MiniDFT README on June 4, but was not propagated to the web page until Sept 3.

**Question/Issue 2**

Are there a minimum number of k-points that must be used? If so, what is it?

**Project Response 2**

A minimum of two k-points must be used for the Capability Improvement.

**Question/Issue 3**

Are there any criteria for selecting nk1, nk2, and nk3? Are they generally the same or not?

**Project Response 3**

There are no criteria for selecting nk1, nk2, and nk3. These are independent parameters.

**Question/Issue 4**

For the KPOINTS parameter, can we use the "automatic" option?

**Project Response 4**

The KPOINTS automatic option is recommended as the simplest way to generate the k-point list.

**Darren Knox**



Acquisition Services Management  
Los Alamos National Security, LLC  
Los Alamos National Laboratory