

## Some Samples of Rationale about Resource Estimates

Here are some notes and samples of rationale about resource requests which are required during application.

### Rationale for Requesting more than 80,000 points (in Japanese: 80,000点を超えて希望する理由)

#### General Notes

- If there are multiple research subjects in a single application, please estimate CPU points for each subject.
- Please specify name of software, jobtype, and number of nodes/CPU cores/GPUs in the estimates.

#### Example 1

(1) Structural Analysis of Associated/Dissociated states of XXX and YYY

The system consists of XXX, YYY, and solvent water molecules and the total number of atoms in this system is ~150,000. We are planning to run XXX ns MD simulations for each of associated and dissociated state. N nodes of jobtype=small will be used for each of MD simulation. AAA-version will be employed as the MD-engine. We once ran MD simulation of ZZZ system, which system size is comparable to the XXX+YYY system, with AAA-version using N jobtype=small nodes on RCCS. H hours were necessary to run 1 ns in this calculation. Therefore, we request  $2$  (# of states) \* XXX (ns) \* N (# of nodes) H (hours/ns) \* 45 (points/node hour) = ZZZ points.

(2) Association Free Energy of XXX-YYY

Using structures obtained in 1 as the initial structures, we are planning to calculate association free energy of XXX-YYY with umbrella sampling method. To obtain enough accurate estimate of free energy, W umbrella windows and XXX ns MD simulations for each window is expected to be necessary. We will use N nodes of jobtype=small as the former topic. Therefore, we request  $W$  (# of windows) \* XXX (ns) \* N (nodes) \* H (hours/ns) \* 45 (points/node hour) = YYY points for this topic.

Adding UUU (small value) points for other minor analyses to the above values, we request ZZZZZZ CPU points in total.

#### Example 2

We will examine all substitution patterns of A, B, and C positions of ligand YYY in complex XXX. A, B, and C positions have Na, Nb, and Nc substitution patterns, respectively. Substituted complex is then optimized using BBB-version with the XXX/YYY level of theory. For the promising substitutes for the catalyst of ZZZ reaction, we will further investigate their structures and properties by using VVVV level of theory.

It takes H hours for XXX/YYY optimization of the intact XXX complex using N cores of our in-house computer (CPU model: \*\*\* \*\*\*\*). R hours were required for VVVV level calculation using N cores of the same machine. Although performance of our in-house computer is slightly worse than RCCS ones, some of larger substituents will require more CPU times than the intact ones and some trial and error steps will be required for the structural optimization. We thus consider that CPU times required by N-cores of our in-house machine and jobtype=core node are comparable. For more accurate VVVVV calculations, we will try for up to ten candidates.

Therefore, we request  $N_a * N_b * N_c$  (# of combinations) \* N (cores) \* H (hours) \* 1 (points/core hour) + 10 (# of candidates) \* N (cores) \* R (hours) \* 1 (point/core hour) = ZZZZZZ points.

### Rationale for Requesting Disk Space (/home or /save) more than Standard Size (in Japanese: [長期保存ファイル(ホームディレクトリ)を標準値を超えて希望する理由])

#### General Notes

- Please use /save region for the long-term storage of large data.
- Please note that /save region is not the target of backuping.

#### Examples

- Size of single trajectory of XXX is SSS GB. We need NNNN of trajectories for the later analysis. Including small margin (20%) for file manipulation, we request /save space of  $1.2$  (margin factor) \* SSS (GB) \* NNNN (# of trajectories).
- Size of the dataset required for the calculation is XXXXX GB. We are planning to use N distinct datasets simultaneously for the smoother progress of the research project. Taking other minor analysis data into account, we request XXXXX \* N GB (minimal data size) + standard size (500 GB) on the /save region.