
Fugaku Commercial Software

VASP

User's Guide

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1 . Preface

Purpose of this document

This document describes how to use VASP, which is maintained by the RIKEN Center for Computational Science (R-CCS) on the supercomputer "Fugaku".

- For general information on how to use Fugaku, please refer to the manuals in the Fugaku Portal
- Please refer to the VASP manual for general VASP usage

Prerequisite

The user shall have executed procedures such as the conclusion of a license agreement for VASP in accordance with the "Flow to Start Using" and shall have received a notice of completion for the software usage environment.

2. Executing VASP Solver

The following is the directory of a sample job script that executes a VASP solver. Please modify it as appropriate for your work environment. This job is submitted to the computation node.

```
/vol0004/apps/isv/VASP6/sample_script
```

2.1. Setting module command

- module command
Used to set environment variables.
- module use
Specifies where *modulefile* is stored. Do not change.
- module load *modulefile*
Sets environment variables defined in *modulefile*.

```
module load VASP6  
is specified, the latest version installed on Fugaku is used.
```

Important: Environment variables set by the module load command may include runtime parameters. When specifying runtime parameters, be sure to specify them after the module load command.

To use a specific version, change the *modulefile*.

Example: Using 6.4.1 version

```
module load VASP6/6.4.1
```

➤ module avail

Displays a list of available *modulefiles*.

```
module use /vol0004/apps/isv/VASP6/modulefiles  
module avail VASP6
```

➤ module show *modulefile*

Displays what is set by the module command.

Example: Show what is set when VASP6 is specified

```
module use /vol0004/apps/isv/VASP6/modulefiles  
module show VASP6
```

3. Change in the environment of VASP

When environmental changes are made to VASP, the details and date of the changes will be posted on the Fugaku Portal. Please check the details of the changes and take action if necessary. The following is a list of expected changes, their impact on users, and how to deal with them.

- **VASP Version Upgrade**

If you use the latest version specified with VASP6 in module load, the software version executed after the change date will be changed to the newly latest version. If you want to keep using the currently using version, add the product version to the module load specification.

- **VASP specific version removal**

If the version to be deleted is specified in module load, the software will not be available after the change date. Please change the module load settings to switch to another available version.

4. Support

Please contact the Fugaku support (<https://fugaku.zendesk.com/hc/en-us/requests/new>) for Fugaku-specific content. For general information on VASP, please visit VASP forum (<https://www.vasp.at/>).