README 1.2

What's Virtual Fugaku?

Virtual Fugaku is a software stack for high performance computing, which is available as a Singularity container containing various pre-built software packages based on Spack.
It currently targets for Amazon Graviton 3E on which RHEL 8.10 is running.
You can freely download the container from the Sylabs Cloud Library and use it for your work.
In addition, we are planning to make Virtual Fugaku available for other machines and in some other ways such as Spack's feature of build caches.

Software Packages

Virtual Fugaku 1.2 includes the following packages along with their many dependencies:

- AutoDock-Vina 1.2.3 (autodock-vina)
- CP2K 2024.1 (cp2k)
- CPMD 4.3 (cpmd)
- DARSHAN 3.4.5 (darshan-runtime)
- Fire Dynamics Simulator 6.8.0 (fds)
- FFmpeg 5.1.4 (ffmpeg)
- FrontISTR 5.3 (frontistr)
- GENESIS 2.1.3 (genesis)
- GNU Scientific Library (GSL) 2.7.1 (gsl)
- Gnuplot 6.0.0 (gnuplot)
- GrADS 2.2.3 (grads)
- GROMACS 2024.2 (gromacs)
- Julia 1.10.2 (julia)
- LAMMPS 20230802.3 (lammps)
- Metis 5.1.0 (metis)
- Open Babel 3.1.1 (openbabel)
- OpenFoam 2312 (openfoam)
- OpenMX 3.9 (openmx)
- Paraview 5.12.1 (paraview)
- Parmetis 4.0.3 (parmetis)
- PETSC 3.21.2 (petsc)
- Persistence of Vision Raytracer 3.7.0.8 (povray)
- Atomic Simulation Environment 3.21.1 (py-ase)
- Matplotlib (py-matplotlib)
- MPI for Python (py-mpi4py)
- netCDF4 1.6.5 (py-netcdf4)
- NumPy (py-numpy)
- pandas (py-pandas)
- scikit-learn (py-scikit-learn)

- SciPy (py-scipy)
- TensorFlow 2.14.1 (py-tensorflow)
- TOML 0.10.2 (py-toml)
- PyTorch 2.1.1 (py-torch)
- Xarray 2023.7.0 (py-xarray)
- Quantume Espresso 7.3.1 (quantum-espresso)
- SALMON 2.0.0 (salmon-tddft)
- SCALE 5.4.4 (scale)
- Terminal Multiplexer 3.4 (tmux)
- Weather Research and Forecasting 4.5.1 (wrf)

These packages are selected from those that are most frequently used on the supercomputer Fugaku. They are built with GCC 14.1.0 and EA*-enabled OpenMPI 4.1.6.
* Elastic Fabric Adapter